



Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 12:22 PM JST

PDB ID : 6IXH
EMDB ID : EMD-9747
Title : Type VI secretion system membrane core complex
Authors : Yin, M.; Yan, Z.
Deposited on : 2018-12-10
Resolution : 4.00 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.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

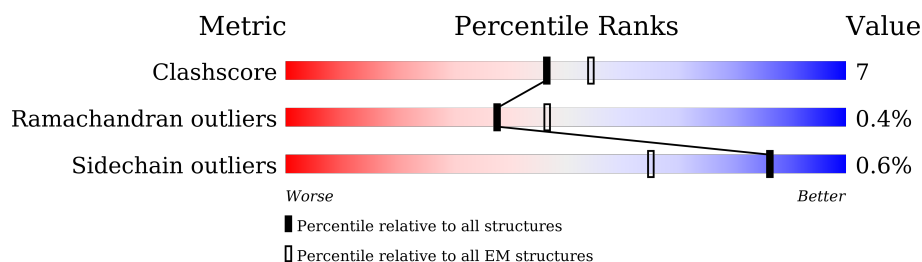
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

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





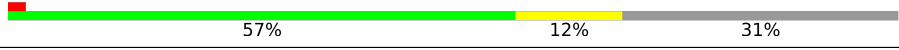



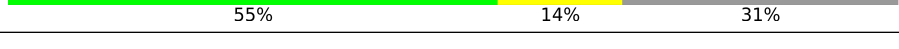
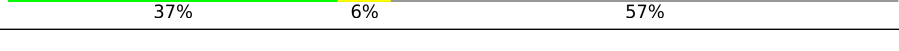
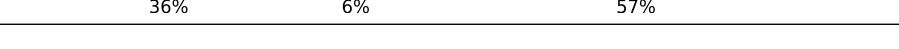
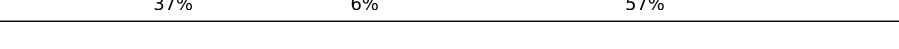







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 ≥ 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	178	
1	B	178	
1	C	178	
1	D	178	
1	E	178	
1	F	178	
1	G	178	
1	H	178	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	178	
1	J	178	
1	K	178	
1	L	178	
1	M	178	
1	N	178	
1	O	178	
2	P	1129	
2	Q	1129	
2	R	1129	
2	S	1129	
2	T	1129	
2	U	1129	
2	V	1129	
2	W	1129	
2	X	1129	
2	Y	1129	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 52280 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 Type VI Secretion System TssJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	135	Total	C	N	O	S	0	0
			1020	646	178	194	2		
1	B	135	Total	C	N	O	S	0	0
			1020	646	178	194	2		
1	C	135	Total	C	N	O	S	0	0
			1020	646	178	194	2		
1	D	135	Total	C	N	O	S	0	0
			1020	646	178	194	2		
1	E	135	Total	C	N	O	S	0	0
			1020	646	178	194	2		
1	F	133	Total	C	N	O	S	0	0
			1006	639	174	191	2		
1	G	133	Total	C	N	O	S	0	0
			1006	639	174	191	2		
1	H	133	Total	C	N	O	S	0	0
			1006	639	174	191	2		
1	I	133	Total	C	N	O	S	0	0
			1006	639	174	191	2		
1	J	133	Total	C	N	O	S	0	0
			1006	639	174	191	2		
1	K	123	Total	C	N	O	S	0	0
			924	589	159	174	2		
1	L	123	Total	C	N	O	S	0	0
			924	589	159	174	2		
1	M	123	Total	C	N	O	S	0	0
			924	589	159	174	2		
1	N	123	Total	C	N	O	S	0	0
			924	589	159	174	2		
1	O	123	Total	C	N	O	S	0	0
			924	589	159	174	2		

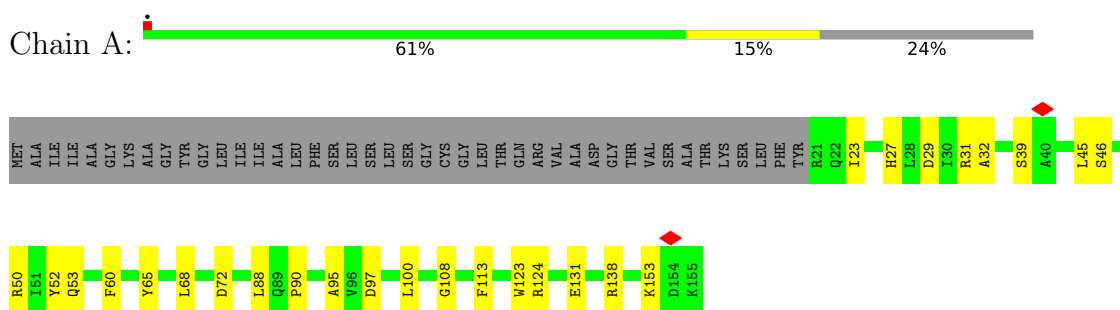
- Molecule 2 is a protein called Type VI Secretion System TssM.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	485	Total	C	N	O	S	0	0
			3771	2385	660	709	17		
2	Q	485	Total	C	N	O	S	0	0
			3771	2385	660	709	17		
2	R	485	Total	C	N	O	S	0	0
			3771	2385	660	709	17		
2	S	485	Total	C	N	O	S	0	0
			3771	2385	660	709	17		
2	T	485	Total	C	N	O	S	0	0
			3771	2385	660	709	17		
2	U	481	Total	C	N	O	S	0	0
			3735	2364	652	702	17		
2	V	481	Total	C	N	O	S	0	0
			3735	2364	652	702	17		
2	W	481	Total	C	N	O	S	0	0
			3735	2364	652	702	17		
2	X	481	Total	C	N	O	S	0	0
			3735	2364	652	702	17		
2	Y	481	Total	C	N	O	S	0	0
			3735	2364	652	702	17		

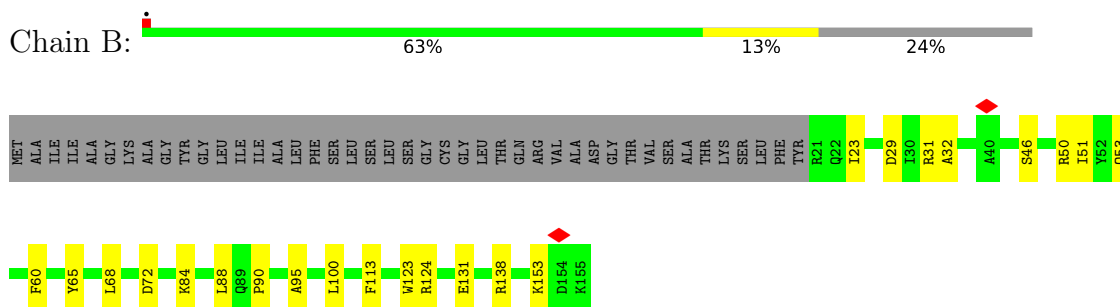
3 Residue-property plots

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.

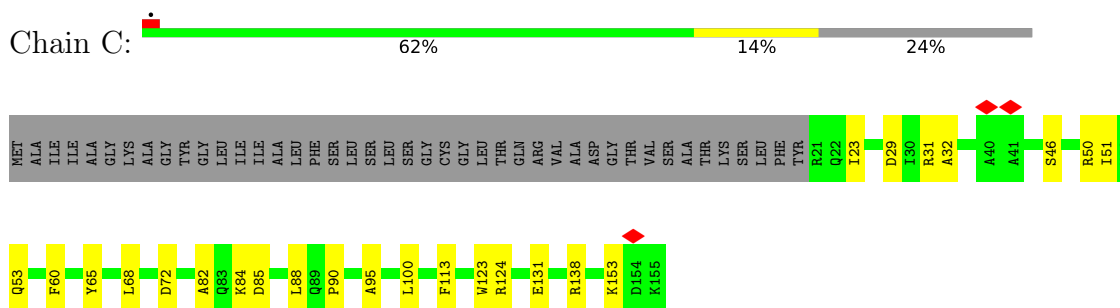
- Molecule 1: Type VI Secretion System TssJ



- Molecule 1: Type VI Secretion System TssJ

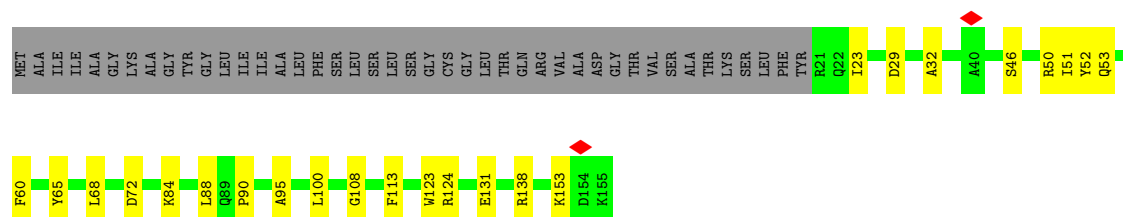


- Molecule 1: Type VI Secretion System TssJ

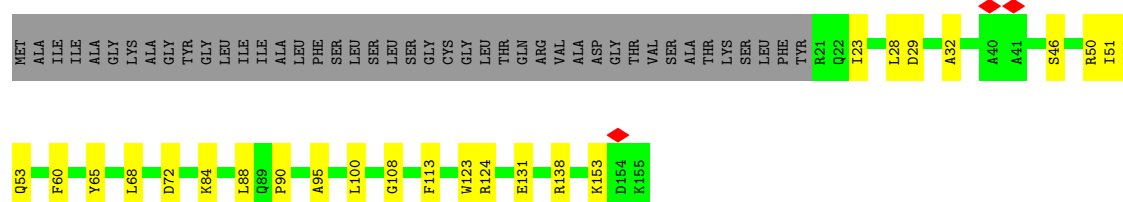


- Molecule 1: Type VI Secretion System TssJ

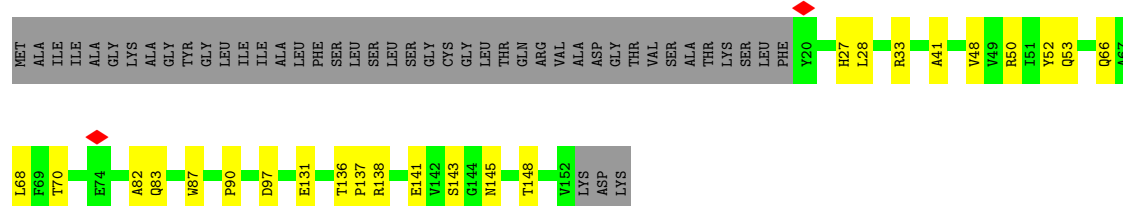




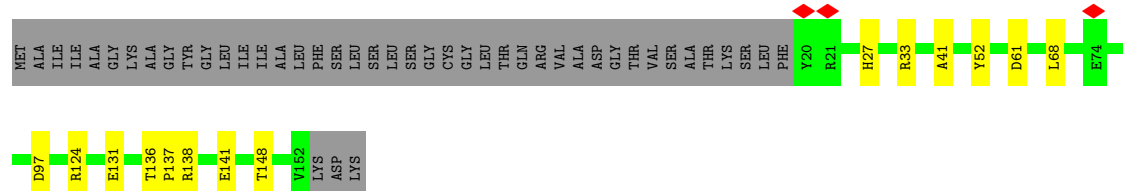
• Molecule 1: Type VI Secretion System TssJ



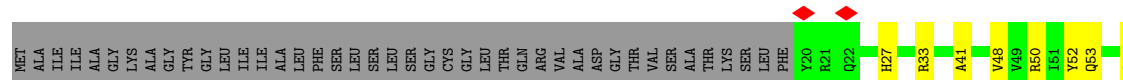
• Molecule 1: Type VI Secretion System TssJ



• Molecule 1: Type VI Secretion System TssJ

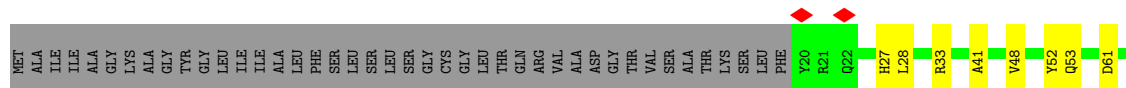


• Molecule 1: Type VI Secretion System TssJ

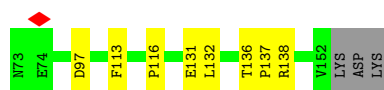




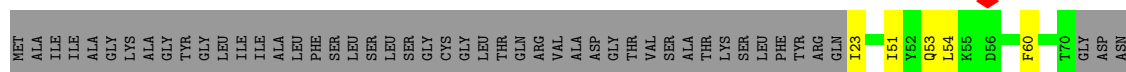
• Molecule 1: Type VI Secretion System TssJ



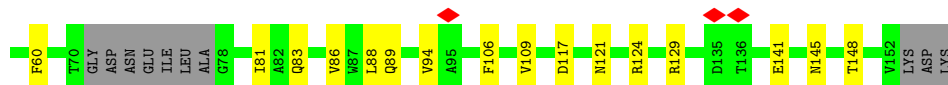
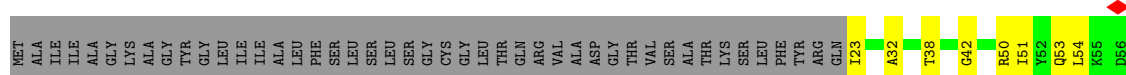
• Molecule 1: Type VI Secretion System TssJ



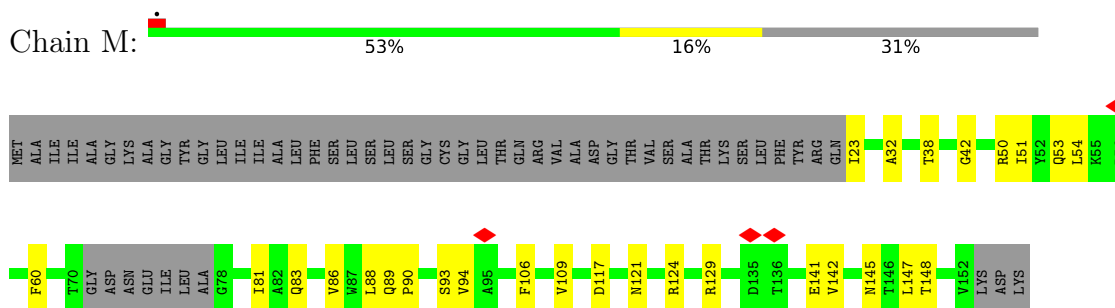
• Molecule 1: Type VI Secretion System TssJ



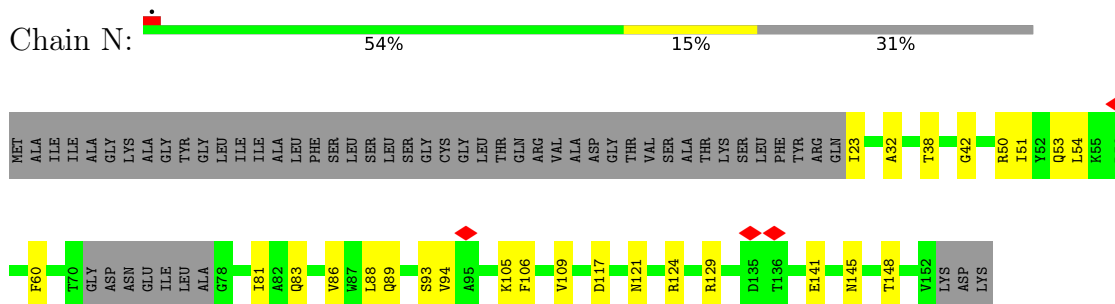
• Molecule 1: Type VI Secretion System TssJ



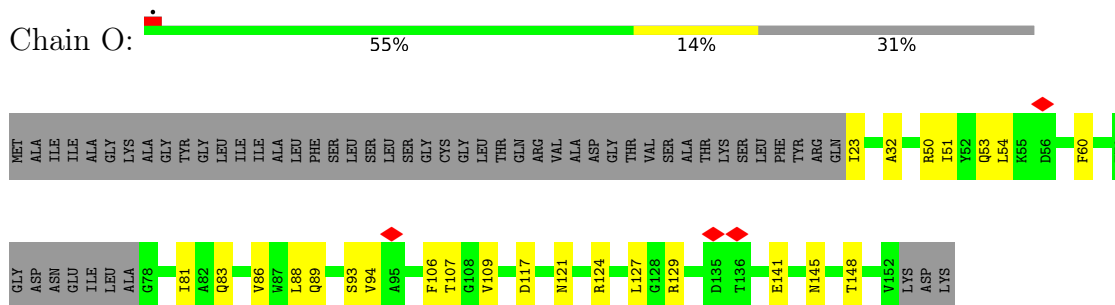
• Molecule 1: Type VI Secretion System TssJ



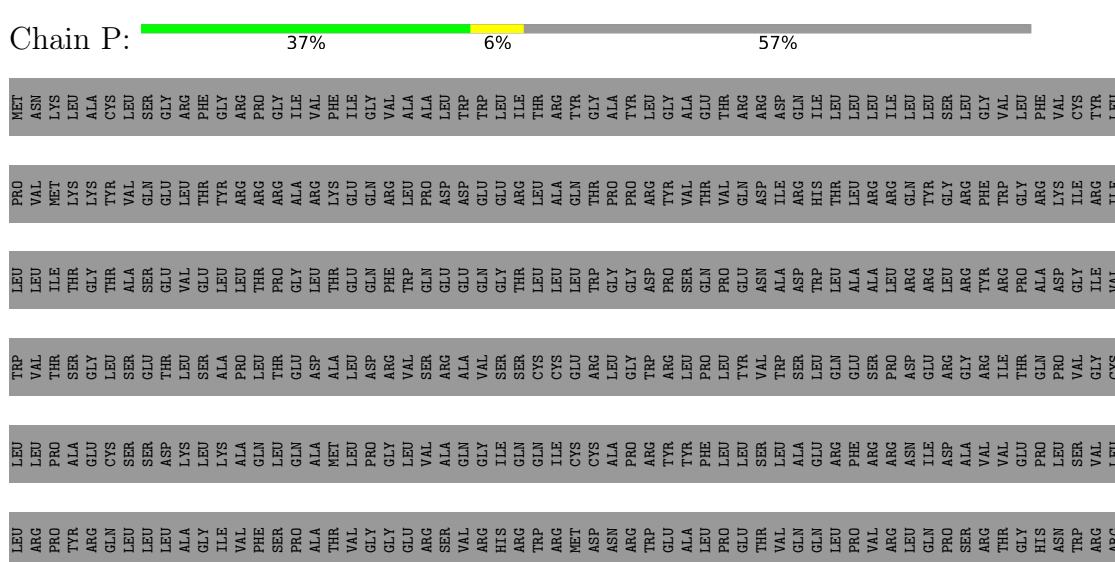
- Molecule 1: Type VI Secretion System TssJ



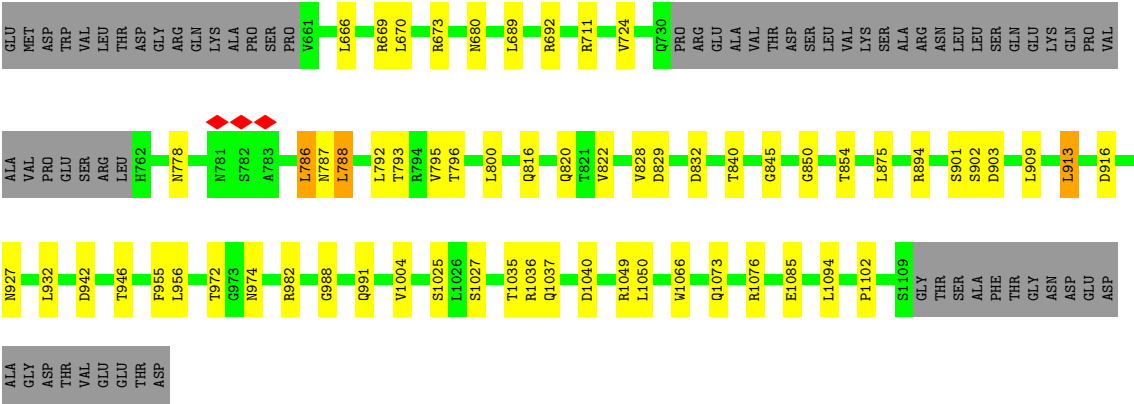
- Molecule 1: Type VI Secretion System TssJ



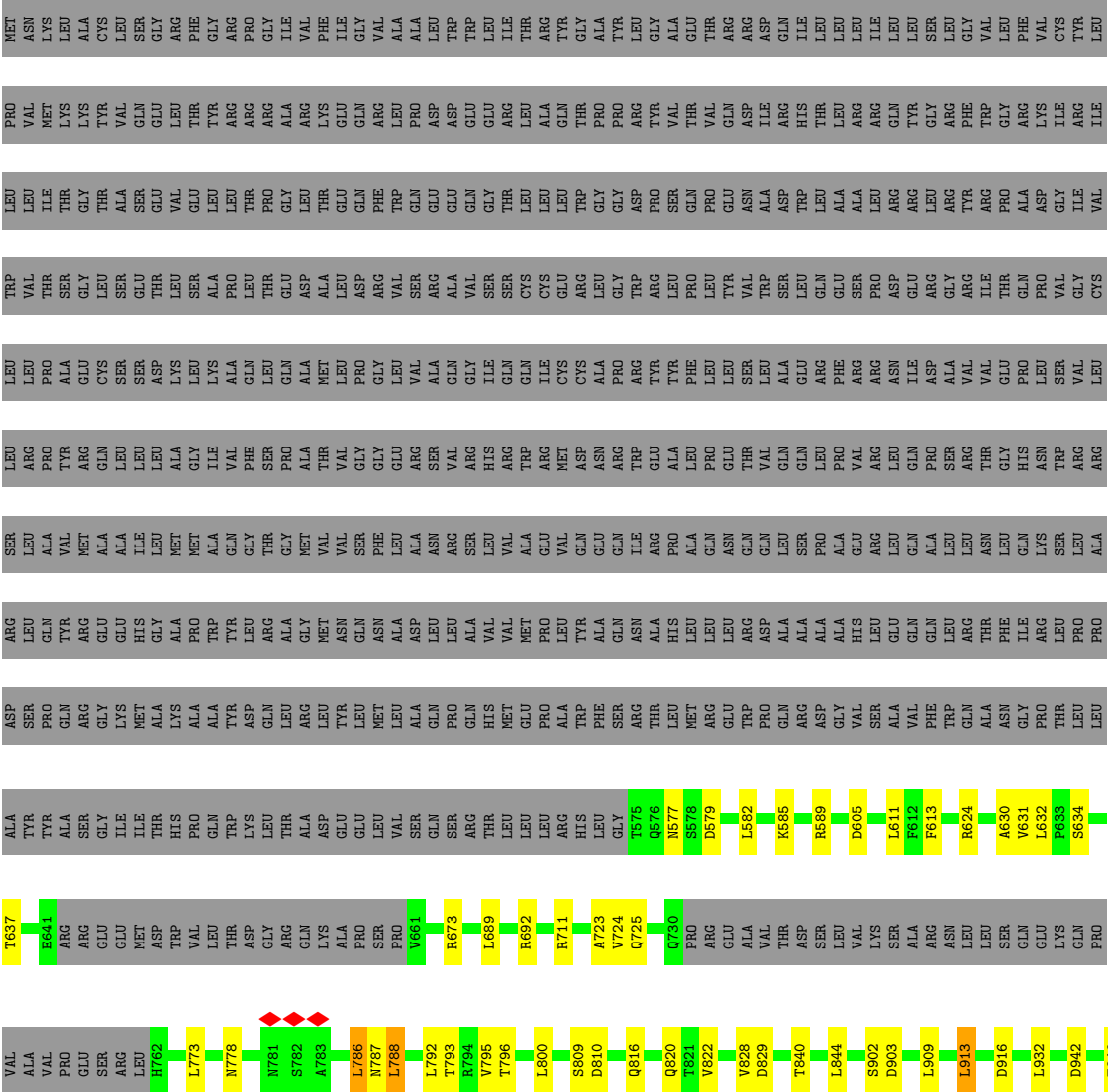
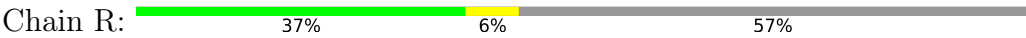
- Molecule 2: Type VI Secretion System TssM







• Molecule 2: Type VI Secretion System TssM



- Molecule 2: Type VI Secretion System TssM

[illegible]



[illegible]

L823	Q824	A841	L844	G852	Q853	T854	V855	F856	V857	R858	L868	R878	W879	R880	V884	W887	K898	D903	A904	Y912	L913	N914	N927	R947	Q948	A954	F955	A958	G973	E980	M990	Q991	D997	A1017	D1018	T1019	E1020	A1021	F1022	G1023										
THR	ASP	SER	LEU	VAL	LYS	SER	ALA	ARG	ASN	LEU	SER	GLN	GLY	PRO	VAL	VAL	GLU	SER	ARG	LEU	H762	L773	D777	N778	Q779	D784	M785	L786	L792	T793	R794	R801	I805	S808	P811	Q812	A813	M814	M815	Q816	L817	L818	A819	Q820	T821	V822				
ARG	GLU	GLU	MET	ASP	TRP	VAL	LEU	THR	THR	ASP	GLY	ARG	GLN	LYS	ALA	PRO	SER	SER	PRO	V661	R667	Q668	R669	L670	R673	Y674	F675	F678	R692	S698	D699	V700	T701	E702	M707	A708	D709	V710	R711	L715	V716	N720	A723	G726	Q730	PRO	ARG	GLU	ALA	VAL

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	44069	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.225	Depositor
Minimum map value	-0.138	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (\AA)	448.80002, 448.80002, 448.80002	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.32, 1.32, 1.32	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	0.36	0/1037	0.54	0/1412
1	B	0.36	0/1037	0.55	0/1412
1	C	0.36	0/1037	0.54	0/1412
1	D	0.37	0/1037	0.55	0/1412
1	E	0.37	0/1037	0.55	0/1412
1	F	0.47	0/1024	0.54	0/1397
1	G	0.46	0/1024	0.54	0/1397
1	H	0.47	0/1024	0.53	0/1397
1	I	0.46	0/1024	0.55	0/1397
1	J	0.47	0/1024	0.52	0/1397
1	K	0.31	0/940	0.53	0/1282
1	L	0.31	0/940	0.52	0/1282
1	M	0.31	0/940	0.52	0/1282
1	N	0.31	0/940	0.52	0/1282
1	O	0.31	0/940	0.52	0/1282
2	P	0.57	0/3850	0.65	1/5245 (0.0%)
2	Q	0.57	0/3850	0.65	1/5245 (0.0%)
2	R	0.58	0/3850	0.65	1/5245 (0.0%)
2	S	0.57	0/3850	0.65	1/5245 (0.0%)
2	T	0.57	0/3850	0.64	1/5245 (0.0%)
2	U	0.42	0/3814	0.65	0/5197
2	V	0.41	0/3814	0.64	0/5197
2	W	0.42	0/3814	0.64	0/5197
2	X	0.42	0/3814	0.65	0/5197
2	Y	0.41	0/3814	0.64	1/5197 (0.0%)
All	All	0.47	0/53325	0.62	6/72665 (0.0%)

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.

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
-----	-------	---------------------	---------------------

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
2	P	0	3
2	Q	0	2
2	R	0	3
2	S	0	2
2	T	0	2
2	U	0	4
2	V	0	2
2	W	0	4
2	X	0	3
2	Y	0	3
All	All	0	33

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	689	LEU	CA-CB-CG	5.87	128.80	115.30
2	Q	689	LEU	CA-CB-CG	5.76	128.55	115.30
2	P	689	LEU	CA-CB-CG	5.70	128.40	115.30
2	R	689	LEU	CA-CB-CG	5.67	128.34	115.30
2	T	689	LEU	CA-CB-CG	5.55	128.07	115.30
2	Y	948	GLY	N-CA-C	5.12	125.90	113.10

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	23	ILE	Peptide
1	B	23	ILE	Peptide
1	C	23	ILE	Peptide
1	D	23	ILE	Peptide
1	E	23	ILE	Peptide
2	P	630	ALA	Peptide
2	P	786	LEU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	P	788	LEU	Peptide
2	Q	786	LEU	Peptide
2	Q	788	LEU	Peptide
2	R	630	ALA	Peptide
2	R	786	LEU	Peptide
2	R	788	LEU	Peptide
2	S	786	LEU	Peptide
2	S	788	LEU	Peptide
2	T	786	LEU	Peptide
2	T	788	LEU	Peptide
2	U	710	VAL	Peptide
2	U	785	MET	Peptide
2	U	824	GLN	Peptide
2	U	947	ARG	Peptide
2	V	785	MET	Peptide
2	V	947	ARG	Peptide
2	W	710	VAL	Peptide
2	W	785	MET	Peptide
2	W	824	GLN	Peptide
2	W	947	ARG	Peptide
2	X	785	MET	Peptide
2	X	824	GLN	Peptide
2	X	947	ARG	Peptide
2	Y	710	VAL	Peptide
2	Y	785	MET	Peptide
2	Y	947	ARG	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	1020	0	1013	16	0
1	B	1020	0	1013	14	0
1	C	1020	0	1013	18	0
1	D	1020	0	1013	15	0
1	E	1020	0	1013	16	0
1	F	1006	0	992	15	0
1	G	1006	0	992	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1006	0	992	13	0
1	I	1006	0	992	14	0
1	J	1006	0	992	11	0
1	K	924	0	915	14	0
1	L	924	0	915	14	0
1	M	924	0	915	17	0
1	N	924	0	915	16	0
1	O	924	0	915	15	0
2	P	3771	0	3713	40	0
2	Q	3771	0	3713	41	0
2	R	3771	0	3713	41	0
2	S	3771	0	3713	38	0
2	T	3771	0	3713	40	0
2	U	3735	0	3671	58	0
2	V	3735	0	3671	63	0
2	W	3735	0	3671	58	0
2	X	3735	0	3671	56	0
2	Y	3735	0	3671	64	0
All	All	52280	0	51520	676	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 7.

All (676) 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:95:ALA:HB1	1:G:33:ARG:HH21	1.63	0.64
1:A:95:ALA:HB1	1:F:33:ARG:HH21	1.63	0.64
1:C:95:ALA:HB1	1:H:33:ARG:HH21	1.63	0.64
2:T:822:VAL:HG22	2:T:828:VAL:HG21	1.81	0.62
1:E:95:ALA:HB1	1:J:33:ARG:HH21	1.64	0.62
2:X:711:ARG:O	2:X:711:ARG:NH1	2.33	0.62
2:V:613:PHE:HB3	2:V:692:ARG:HH21	1.64	0.62
2:Y:613:PHE:HB3	2:Y:692:ARG:HH21	1.64	0.62
2:U:613:PHE:HB3	2:U:692:ARG:HH21	1.65	0.61
2:W:613:PHE:HB3	2:W:692:ARG:HH21	1.64	0.61
2:X:613:PHE:HB3	2:X:692:ARG:HH21	1.64	0.61
1:D:95:ALA:HB1	1:I:33:ARG:HH21	1.65	0.61
1:M:50:ARG:HD3	1:M:83:GLN:HE21	1.65	0.61
1:O:50:ARG:HD3	1:O:83:GLN:HE21	1.66	0.61
1:L:50:ARG:HD3	1:L:83:GLN:HE21	1.65	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:801:ARG:HB3	2:W:818:LEU:HD11	1.82	0.60
2:U:711:ARG:O	2:U:711:ARG:NH1	2.35	0.60
1:C:50:ARG:NH1	1:C:72:ASP:OD2	2.34	0.60
1:E:50:ARG:NH1	1:E:72:ASP:OD2	2.35	0.60
2:S:822:VAL:HG22	2:S:828:VAL:HG21	1.83	0.60
2:Y:814:MET:HA	2:Y:817:LEU:HB2	1.84	0.59
2:U:801:ARG:HB3	2:U:818:LEU:HD11	1.83	0.59
2:R:822:VAL:HG22	2:R:828:VAL:HG21	1.84	0.59
1:D:50:ARG:NH1	1:D:72:ASP:OD2	2.35	0.59
1:N:50:ARG:HD3	1:N:83:GLN:HE21	1.68	0.59
2:P:916:ASP:N	2:P:916:ASP:OD2	2.35	0.58
1:G:131:GLU:O	1:G:138:ARG:NH1	2.37	0.58
1:A:50:ARG:NH1	1:A:72:ASP:OD2	2.36	0.58
1:N:53:GLN:HB2	1:N:81:ILE:HB	1.86	0.58
1:F:131:GLU:O	1:F:138:ARG:NH1	2.37	0.58
2:P:903:ASP:OD1	2:P:1049:ARG:NH2	2.36	0.58
1:N:23:ILE:O	1:N:129:ARG:NH2	2.37	0.58
2:P:822:VAL:HG22	2:P:828:VAL:HG21	1.84	0.58
2:Y:801:ARG:HB3	2:Y:818:LEU:HD11	1.84	0.58
2:R:903:ASP:OD1	2:R:1049:ARG:NH2	2.36	0.58
1:I:131:GLU:O	1:I:138:ARG:NH1	2.36	0.57
2:S:903:ASP:OD1	2:S:1049:ARG:NH2	2.37	0.57
1:B:50:ARG:NH1	1:B:72:ASP:OD2	2.36	0.57
1:J:131:GLU:O	1:J:138:ARG:NH1	2.37	0.57
1:L:23:ILE:O	1:L:129:ARG:NH2	2.37	0.57
1:O:23:ILE:O	1:O:129:ARG:NH2	2.38	0.57
1:G:27:HIS:ND1	1:G:97:ASP:OD1	2.38	0.57
2:P:786:LEU:HB3	2:P:840:THR:HG22	1.87	0.57
1:F:27:HIS:ND1	1:F:97:ASP:OD1	2.38	0.57
2:U:1077:MET:O	2:U:1079:ASN:ND2	2.38	0.57
1:K:23:ILE:O	1:K:129:ARG:NH2	2.37	0.57
2:R:786:LEU:HB3	2:R:840:THR:HG22	1.86	0.57
1:H:131:GLU:O	1:H:138:ARG:NH1	2.37	0.56
1:M:23:ILE:O	1:M:129:ARG:NH2	2.38	0.56
2:V:808:SER:OG	2:V:814:MET:SD	2.63	0.56
2:X:1077:MET:O	2:X:1079:ASN:ND2	2.38	0.56
2:S:999:GLN:HE22	2:S:1014:THR:HG22	1.68	0.56
2:V:1077:MET:O	2:V:1079:ASN:ND2	2.38	0.56
2:P:902:SER:OG	2:P:903:ASP:N	2.39	0.56
2:T:786:LEU:HB3	2:T:840:THR:HG22	1.88	0.56
2:W:946:THR:HG22	2:W:949:LEU:H	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:808:SER:OG	2:X:814:MET:SD	2.64	0.56
2:R:1029:VAL:HG22	2:R:1035:THR:HG22	1.88	0.56
2:W:716:VAL:O	2:W:720:ASN:N	2.37	0.56
1:M:121:ASN:HD21	1:M:124:ARG:HH21	1.54	0.56
2:W:808:SER:OG	2:W:814:MET:SD	2.64	0.56
2:V:1030:SER:OG	2:V:1076:ARG:NH2	2.39	0.55
2:W:1030:SER:OG	2:W:1076:ARG:NH2	2.39	0.55
2:Y:1077:MET:O	2:Y:1079:ASN:ND2	2.39	0.55
2:Y:816:GLN:O	2:Y:820:GLN:N	2.38	0.55
2:P:999:GLN:HE22	2:P:1014:THR:HG22	1.71	0.55
2:V:716:VAL:O	2:V:720:ASN:N	2.38	0.55
1:L:53:GLN:HB2	1:L:81:ILE:HB	1.88	0.55
2:W:1077:MET:O	2:W:1079:ASN:ND2	2.39	0.55
2:S:786:LEU:HB3	2:S:840:THR:HG22	1.88	0.55
2:U:808:SER:OG	2:U:814:MET:SD	2.64	0.55
2:T:680:ASN:HD21	2:Y:711:ARG:HB3	1.70	0.55
2:Q:903:ASP:OD1	2:Q:1049:ARG:NH2	2.38	0.55
2:V:784:ASP:HB3	2:V:786:LEU:HD23	1.89	0.55
2:S:1029:VAL:HG22	2:S:1035:THR:HB	1.90	0.54
1:N:51:ILE:HG23	1:N:109:VAL:HG22	1.90	0.54
1:K:53:GLN:HB2	1:K:81:ILE:HB	1.89	0.54
2:W:615:ASP:OD1	2:W:615:ASP:N	2.39	0.54
2:X:1030:SER:OG	2:X:1076:ARG:NH2	2.40	0.54
1:E:50:ARG:NH2	2:Y:1035:THR:O	2.40	0.54
2:U:716:VAL:O	2:U:720:ASN:N	2.38	0.54
1:H:27:HIS:ND1	1:H:97:ASP:OD1	2.41	0.54
2:Q:786:LEU:HB3	2:Q:840:THR:HG22	1.89	0.54
2:V:898:LYS:O	2:V:1097:ARG:NH1	2.41	0.54
2:Q:680:ASN:HD21	2:V:711:ARG:HB3	1.73	0.54
2:T:942:ASP:O	2:T:946:THR:OG1	2.25	0.54
1:B:50:ARG:NH2	2:V:1035:THR:O	2.41	0.54
2:S:955:PHE:HA	2:S:1102:PRO:HG2	1.88	0.54
2:W:816:GLN:O	2:W:820:GLN:N	2.41	0.54
2:T:1035:THR:O	2:T:1035:THR:OG1	2.26	0.54
2:Y:716:VAL:O	2:Y:720:ASN:N	2.37	0.54
1:O:51:ILE:HG23	1:O:109:VAL:HG22	1.90	0.54
2:R:988:GLY:HA3	2:R:1076:ARG:HH21	1.73	0.54
2:S:916:ASP:OD1	2:S:916:ASP:N	2.40	0.53
2:R:942:ASP:O	2:R:946:THR:OG1	2.26	0.53
2:X:716:VAL:O	2:X:720:ASN:N	2.38	0.53
2:Y:854:THR:HA	2:Y:858:ARG:HB2	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:ARG:NH2	2:X:1035:THR:O	2.40	0.53
1:K:121:ASN:HD21	1:K:124:ARG:HH21	1.55	0.53
2:U:854:THR:HA	2:U:858:ARG:HB2	1.89	0.53
2:Y:808:SER:OG	2:Y:814:MET:SD	2.66	0.53
2:Y:1030:SER:OG	2:Y:1076:ARG:NH2	2.41	0.53
1:M:51:ILE:HG23	1:M:109:VAL:HG22	1.90	0.53
2:T:631:VAL:HA	2:T:634:SER:HB3	1.91	0.53
2:S:988:GLY:HA3	2:S:1076:ARG:HH21	1.73	0.53
2:P:955:PHE:HA	2:P:1102:PRO:HG2	1.91	0.53
2:R:955:PHE:HA	2:R:1102:PRO:HG2	1.89	0.53
2:T:901:SER:O	2:T:1049:ARG:NH2	2.41	0.53
1:O:53:GLN:HB2	1:O:81:ILE:HB	1.91	0.53
2:Q:942:ASP:O	2:Q:946:THR:OG1	2.26	0.53
2:S:942:ASP:O	2:S:946:THR:OG1	2.26	0.53
2:V:716:VAL:HA	2:V:719:MET:HB2	1.91	0.53
1:A:50:ARG:NH2	2:U:1035:THR:O	2.42	0.53
1:L:51:ILE:HG23	1:L:109:VAL:HG22	1.91	0.53
1:L:54:LEU:HB3	1:L:106:PHE:HB2	1.89	0.53
2:P:988:GLY:HA3	2:P:1076:ARG:HH21	1.74	0.53
2:Y:841:ALA:HB2	2:Y:856:PHE:HD2	1.74	0.53
1:L:121:ASN:HD21	1:L:124:ARG:HH21	1.57	0.52
2:V:946:THR:HG22	2:V:949:LEU:H	1.73	0.52
2:X:816:GLN:O	2:X:820:GLN:N	2.42	0.52
2:X:854:THR:HA	2:X:858:ARG:HB2	1.90	0.52
1:K:54:LEU:HB3	1:K:106:PHE:HB2	1.91	0.52
2:Y:898:LYS:O	2:Y:1097:ARG:NH1	2.42	0.52
1:M:53:GLN:HB2	1:M:81:ILE:HB	1.91	0.52
2:T:579:ASP:H	2:T:582:LEU:HD13	1.75	0.52
2:W:898:LYS:O	2:W:1097:ARG:NH1	2.43	0.52
1:K:51:ILE:HG23	1:K:109:VAL:HG22	1.92	0.52
2:U:898:LYS:O	2:U:1097:ARG:NH1	2.42	0.52
2:Y:723:ALA:HA	2:Y:773:LEU:HD11	1.92	0.52
1:L:60:PHE:O	1:L:124:ARG:NH1	2.43	0.52
2:U:946:THR:HG22	2:U:949:LEU:H	1.74	0.52
2:U:816:GLN:O	2:U:820:GLN:N	2.41	0.52
1:M:54:LEU:HB3	1:M:106:PHE:HB2	1.91	0.52
1:N:60:PHE:O	1:N:124:ARG:NH1	2.43	0.52
1:N:121:ASN:HD21	1:N:124:ARG:HH21	1.57	0.52
1:O:60:PHE:O	1:O:124:ARG:NH1	2.43	0.52
2:Q:613:PHE:HB3	2:Q:692:ARG:HH21	1.74	0.52
1:A:131:GLU:HB3	1:A:138:ARG:HH12	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:54:LEU:HB3	1:O:106:PHE:HB2	1.92	0.52
2:S:972:THR:OG1	2:S:974:ASN:OD1	2.28	0.51
2:T:988:GLY:HA3	2:T:1076:ARG:HH21	1.75	0.51
2:W:699:ASP:HA	2:W:702:GLU:HB3	1.92	0.51
2:P:1084:THR:OG1	2:P:1085:GLU:N	2.43	0.51
2:R:778:ASN:HA	2:R:787:ASN:HD21	1.75	0.51
2:R:972:THR:OG1	2:R:974:ASN:OD1	2.28	0.51
2:W:723:ALA:HA	2:W:773:LEU:HD11	1.92	0.51
2:X:898:LYS:O	2:X:1097:ARG:NH1	2.43	0.51
1:C:131:GLU:HB3	1:C:138:ARG:HH12	1.75	0.51
1:K:60:PHE:O	1:K:124:ARG:NH1	2.44	0.51
2:U:699:ASP:HA	2:U:702:GLU:HB3	1.92	0.51
1:M:60:PHE:O	1:M:124:ARG:NH1	2.44	0.51
1:B:131:GLU:HB3	1:B:138:ARG:HH12	1.75	0.51
2:Q:988:GLY:HA3	2:Q:1076:ARG:HH21	1.75	0.51
2:Q:585:LYS:HB3	2:Q:589:ARG:HH21	1.75	0.51
2:Q:822:VAL:HG22	2:Q:828:VAL:HG21	1.91	0.51
2:U:903:ASP:HB3	2:U:1045:TRP:HD1	1.76	0.51
2:X:639:ILE:HD11	2:X:667:ARG:HG3	1.93	0.51
2:P:972:THR:OG1	2:P:974:ASN:OD1	2.29	0.51
2:Q:850:GLY:O	2:Q:854:THR:OG1	2.25	0.51
2:T:585:LYS:HB3	2:T:589:ARG:HH21	1.75	0.51
2:V:726:GLY:O	2:V:762:HIS:NE2	2.36	0.51
2:P:577:ASN:OD1	2:P:577:ASN:N	2.45	0.50
2:T:577:ASN:OD1	2:T:577:ASN:N	2.44	0.50
2:T:955:PHE:HA	2:T:1102:PRO:HG2	1.93	0.50
2:T:972:THR:OG1	2:T:974:ASN:OD1	2.30	0.50
2:T:999:GLN:HE22	2:T:1014:THR:HG22	1.76	0.50
2:Y:579:ASP:OD2	2:Y:669:ARG:NH1	2.43	0.50
2:U:726:GLY:O	2:U:762:HIS:NE2	2.36	0.50
1:D:131:GLU:HB3	1:D:138:ARG:HH12	1.75	0.50
2:S:901:SER:OG	2:T:1083:ARG:NH1	2.45	0.50
2:U:579:ASP:OD2	2:U:669:ARG:NH1	2.44	0.50
1:J:27:HIS:ND1	1:J:97:ASP:OD1	2.44	0.50
2:S:585:LYS:HB3	2:S:589:ARG:HH21	1.75	0.50
2:V:723:ALA:HA	2:V:773:LEU:HD11	1.94	0.50
2:P:793:THR:HA	2:P:796:THR:HG22	1.93	0.50
2:S:902:SER:OG	2:S:903:ASP:N	2.44	0.50
2:T:829:ASP:OD1	2:T:829:ASP:N	2.45	0.50
2:T:991:GLN:HB2	2:T:1004:VAL:HG12	1.92	0.50
2:U:954:ALA:O	2:U:958:ALA:N	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:639:ILE:HD11	2:Y:667:ARG:HG3	1.94	0.50
1:C:50:ARG:NH2	2:W:1035:THR:O	2.43	0.50
1:O:121:ASN:HD21	1:O:124:ARG:HH21	1.58	0.50
2:Q:901:SER:OG	2:R:1083:ARG:NH1	2.45	0.50
2:S:809:SER:OG	2:S:810:ASP:OD2	2.30	0.50
2:U:723:ALA:HA	2:U:773:LEU:HD11	1.92	0.50
2:W:1030:SER:HB3	2:W:1033:ALA:H	1.76	0.50
1:E:131:GLU:HB3	1:E:138:ARG:HH12	1.77	0.50
2:S:579:ASP:H	2:S:582:LEU:HD13	1.76	0.50
2:W:726:GLY:O	2:W:762:HIS:NE2	2.36	0.50
2:W:841:ALA:HB2	2:W:856:PHE:HD2	1.77	0.50
2:X:723:ALA:HA	2:X:773:LEU:HD11	1.93	0.50
1:A:46:SER:HB2	1:A:90:PRO:HD3	1.94	0.49
2:T:902:SER:OG	2:T:903:ASP:N	2.45	0.49
1:C:85:ASP:OD1	1:C:85:ASP:N	2.44	0.49
1:N:141:GLU:O	1:N:148:THR:OG1	2.28	0.49
2:Q:577:ASN:N	2:Q:577:ASN:OD1	2.45	0.49
2:Q:955:PHE:HA	2:Q:1102:PRO:HG2	1.93	0.49
2:R:579:ASP:H	2:R:582:LEU:HD13	1.76	0.49
2:V:954:ALA:O	2:V:958:ALA:N	2.45	0.49
1:D:46:SER:HB2	1:D:90:PRO:HD3	1.94	0.49
1:I:27:HIS:ND1	1:I:97:ASP:OD1	2.46	0.49
2:P:778:ASN:HA	2:P:787:ASN:HD21	1.76	0.49
2:S:577:ASN:N	2:S:577:ASN:OD1	2.44	0.49
2:X:699:ASP:HA	2:X:702:GLU:HB3	1.94	0.49
2:U:1030:SER:OG	2:U:1076:ARG:NH2	2.45	0.49
2:R:577:ASN:OD1	2:R:577:ASN:N	2.44	0.49
2:R:909:LEU:HG	2:R:913:LEU:HD21	1.93	0.49
2:T:778:ASN:HA	2:T:787:ASN:HD21	1.76	0.49
2:U:841:ALA:HB2	2:U:856:PHE:HD2	1.77	0.49
2:W:997:ASP:OD1	2:W:1023:GLY:N	2.46	0.49
2:X:1029:VAL:HG22	2:X:1035:THR:HG22	1.93	0.49
2:P:1085:GLU:O	2:T:894:ARG:NH1	2.46	0.49
2:Q:894:ARG:NH1	2:R:1085:GLU:O	2.43	0.49
2:Q:1027:SER:HA	2:Q:1037:GLN:HA	1.95	0.49
2:S:792:LEU:HA	2:S:795:VAL:HG12	1.94	0.49
2:Y:1064:SER:HB2	2:Y:1066:TRP:HZ3	1.77	0.49
2:W:814:MET:HA	2:W:817:LEU:HB2	1.94	0.49
1:K:141:GLU:O	1:K:148:THR:OG1	2.28	0.49
2:Q:792:LEU:HA	2:Q:795:VAL:HG12	1.94	0.49
2:V:816:GLN:O	2:V:820:GLN:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:903:ASP:HB3	2:V:1045:TRP:HD1	1.78	0.49
2:W:880:ARG:HA	2:W:884:VAL:HB	1.94	0.49
2:R:792:LEU:HA	2:R:795:VAL:HG12	1.94	0.49
2:T:793:THR:HA	2:T:796:THR:HG22	1.95	0.49
2:V:854:THR:HA	2:V:858:ARG:HB2	1.94	0.49
1:C:46:SER:HB2	1:C:90:PRO:HD3	1.94	0.49
1:N:86:VAL:HG11	1:N:94:VAL:HG11	1.95	0.49
2:S:1027:SER:HA	2:S:1037:GLN:HA	1.95	0.49
2:V:699:ASP:HA	2:V:702:GLU:HB3	1.95	0.49
2:W:878:ARG:NH2	2:W:927:ASN:OD1	2.39	0.49
2:X:954:ALA:O	2:X:958:ALA:N	2.45	0.49
1:B:32:ALA:HB2	1:B:88:LEU:HD21	1.95	0.48
2:S:778:ASN:HA	2:S:787:ASN:HD21	1.77	0.48
2:S:991:GLN:HB2	2:S:1004:VAL:HG12	1.95	0.48
2:W:801:ARG:NH1	2:W:829:ASP:OD2	2.45	0.48
2:X:1030:SER:HB3	2:X:1033:ALA:H	1.78	0.48
2:U:880:ARG:NE	2:U:1103:GLU:OE2	2.43	0.48
2:V:841:ALA:HB2	2:V:856:PHE:HD2	1.77	0.48
2:X:903:ASP:HB3	2:X:1045:TRP:HD1	1.78	0.48
1:E:32:ALA:HB2	1:E:88:LEU:HD21	1.94	0.48
1:G:61:ASP:O	1:G:124:ARG:NH2	2.45	0.48
1:O:86:VAL:HG11	1:O:94:VAL:HG11	1.95	0.48
2:Q:778:ASN:HA	2:Q:787:ASN:HD21	1.78	0.48
2:Q:793:THR:HA	2:Q:796:THR:HG22	1.95	0.48
2:Q:972:THR:OG1	2:Q:974:ASN:OD1	2.31	0.48
2:Y:726:GLY:O	2:Y:762:HIS:NE2	2.38	0.48
1:C:53:GLN:HE22	1:C:100:LEU:HA	1.77	0.48
2:P:991:GLN:HB2	2:P:1004:VAL:HG12	1.96	0.48
2:Y:954:ALA:O	2:Y:958:ALA:N	2.46	0.48
1:C:51:ILE:HB	1:C:84:LYS:HB3	1.96	0.48
2:S:909:LEU:HG	2:S:913:LEU:HD21	1.95	0.48
2:V:880:ARG:HA	2:V:884:VAL:HB	1.95	0.48
2:U:639:ILE:HD11	2:U:667:ARG:HG3	1.95	0.48
2:W:639:ILE:HD11	2:W:667:ARG:HG3	1.94	0.48
2:X:579:ASP:OD2	2:X:669:ARG:NH1	2.46	0.48
1:A:32:ALA:HB2	1:A:88:LEU:HD21	1.95	0.48
1:H:72:ASP:OD1	1:H:72:ASP:N	2.46	0.48
1:I:72:ASP:N	1:I:72:ASP:OD1	2.47	0.48
2:P:579:ASP:H	2:P:582:LEU:HD13	1.79	0.48
2:U:784:ASP:HB3	2:U:786:LEU:HD23	1.96	0.48
2:V:1030:SER:HB3	2:V:1033:ALA:H	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:841:ALA:HB2	2:X:856:PHE:HD2	1.78	0.48
2:U:814:MET:HA	2:U:817:LEU:HB2	1.95	0.48
2:Y:784:ASP:HB3	2:Y:786:LEU:HD23	1.96	0.48
1:L:86:VAL:HG11	1:L:94:VAL:HG11	1.96	0.47
1:M:32:ALA:HB2	1:M:88:LEU:HD12	1.96	0.47
2:V:814:MET:HA	2:V:817:LEU:HB2	1.95	0.47
2:W:854:THR:HA	2:W:858:ARG:HB2	1.95	0.47
2:X:878:ARG:NH2	2:X:927:ASN:OD1	2.39	0.47
1:D:60:PHE:O	1:D:124:ARG:NH1	2.47	0.47
1:L:141:GLU:O	1:L:148:THR:OG1	2.31	0.47
1:M:86:VAL:HG11	1:M:94:VAL:HG11	1.95	0.47
2:X:880:ARG:HA	2:X:884:VAL:HB	1.95	0.47
2:X:980:GLU:OE1	2:X:1083:ARG:NH2	2.47	0.47
1:O:141:GLU:O	1:O:148:THR:OG1	2.30	0.47
2:T:1027:SER:HA	2:T:1037:GLN:HA	1.96	0.47
2:Q:991:GLN:HB2	2:Q:1004:VAL:HG12	1.95	0.47
2:X:784:ASP:HB3	2:X:786:LEU:HD23	1.96	0.47
2:Y:698:SER:OG	2:Y:699:ASP:N	2.47	0.47
2:W:954:ALA:O	2:W:958:ALA:N	2.46	0.47
2:X:871:ALA:O	2:X:875:LEU:N	2.47	0.47
2:Y:852:GLY:HA2	2:Y:855:VAL:HG12	1.97	0.47
1:E:46:SER:HB2	1:E:90:PRO:HD3	1.96	0.47
2:P:585:LYS:HB3	2:P:589:ARG:HH21	1.80	0.47
2:P:1027:SER:HA	2:P:1037:GLN:HA	1.97	0.47
2:Q:909:LEU:HG	2:Q:913:LEU:HD21	1.95	0.47
2:S:607:ASP:OD1	2:Y:778:ASN:ND2	2.47	0.47
1:C:32:ALA:HB2	1:C:88:LEU:HD21	1.97	0.47
1:D:32:ALA:HB2	1:D:88:LEU:HD21	1.96	0.47
1:E:51:ILE:HB	1:E:84:LYS:HB3	1.97	0.47
1:M:141:GLU:O	1:M:148:THR:OG1	2.30	0.47
2:P:586:MET:HG3	2:P:670:LEU:HD21	1.96	0.47
2:Q:816:GLN:O	2:Q:820:GLN:N	2.47	0.47
2:R:613:PHE:HB3	2:R:692:ARG:HH21	1.78	0.47
2:U:980:GLU:OE1	2:U:1083:ARG:NH2	2.48	0.47
2:V:901:SER:HA	2:V:1049:ARG:HH22	1.80	0.47
2:V:985:THR:OG1	2:V:986:ALA:N	2.47	0.47
2:X:726:GLY:O	2:X:762:HIS:NE2	2.36	0.47
2:Y:699:ASP:HA	2:Y:702:GLU:HB3	1.97	0.47
2:Y:805:ILE:HG12	2:Y:815:MET:HA	1.97	0.47
2:Y:878:ARG:NH2	2:Y:927:ASN:OD1	2.39	0.47
2:Y:980:GLU:OE1	2:Y:1083:ARG:NH2	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:GLN:HE22	1:E:100:LEU:HA	1.80	0.47
2:P:601:ASP:OD1	2:P:601:ASP:N	2.43	0.47
2:U:887:TRP:HE3	2:U:912:TYR:HD2	1.63	0.47
2:W:784:ASP:HB3	2:W:786:LEU:HD23	1.96	0.47
2:Y:887:TRP:HE3	2:Y:912:TYR:HD2	1.63	0.47
1:B:46:SER:HB2	1:B:90:PRO:HD3	1.96	0.47
2:P:607:ASP:OD2	2:V:778:ASN:ND2	2.47	0.47
2:P:792:LEU:HA	2:P:795:VAL:HG12	1.97	0.47
2:R:793:THR:HA	2:R:796:THR:HG22	1.96	0.47
2:V:1028:TRP:HB3	2:V:1078:LEU:HD21	1.96	0.47
2:Y:880:ARG:HA	2:Y:884:VAL:HB	1.97	0.47
2:P:850:GLY:O	2:P:854:THR:OG1	2.27	0.46
2:R:724:VAL:HG13	2:R:725:GLN:HG3	1.97	0.46
2:S:1084:THR:OG1	2:S:1085:GLU:N	2.48	0.46
2:T:909:LEU:HG	2:T:913:LEU:HD21	1.96	0.46
2:U:1028:TRP:HB3	2:U:1078:LEU:HD21	1.96	0.46
2:X:711:ARG:HH12	2:X:717:ALA:HB2	1.80	0.46
1:E:60:PHE:O	1:E:124:ARG:NH1	2.48	0.46
1:J:46:SER:O	1:J:46:SER:OG	2.33	0.46
2:U:698:SER:OG	2:U:699:ASP:N	2.48	0.46
2:U:880:ARG:HA	2:U:884:VAL:HB	1.96	0.46
1:I:33:ARG:HD3	1:I:143:SER:HB3	1.97	0.46
2:R:902:SER:OG	2:R:903:ASP:N	2.48	0.46
2:R:991:GLN:HB2	2:R:1004:VAL:HG12	1.96	0.46
2:U:997:ASP:OD1	2:U:1023:GLY:N	2.46	0.46
2:V:797:GLN:HA	2:V:800:LEU:HB2	1.98	0.46
2:V:942:ASP:O	2:V:946:THR:OG1	2.23	0.46
2:W:887:TRP:HE3	2:W:912:TYR:HD2	1.63	0.46
2:W:980:GLU:OE1	2:W:1083:ARG:NH2	2.48	0.46
2:W:811:PRO:HG2	2:W:813:ALA:HB3	1.97	0.46
2:W:880:ARG:NE	2:W:1103:GLU:OE2	2.45	0.46
2:W:901:SER:HA	2:W:1049:ARG:HH22	1.81	0.46
1:G:52:TYR:HE2	1:G:68:LEU:HD21	1.80	0.46
1:N:89:GLN:HE22	2:X:1031:THR:HB	1.81	0.46
2:R:1030:SER:OG	2:R:1033:ALA:N	2.44	0.46
2:U:852:GLY:HA2	2:U:855:VAL:HG12	1.97	0.46
2:V:887:TRP:HE3	2:V:912:TYR:HD2	1.63	0.46
2:W:995:ILE:HG12	2:W:1000:LYS:HG2	1.96	0.46
2:S:624:ARG:NH1	2:S:724:VAL:O	2.43	0.46
2:T:823:LEU:HD22	2:T:945:ASN:HB3	1.97	0.46
2:V:579:ASP:OD2	2:V:669:ARG:NH1	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:878:ARG:NH2	2:V:927:ASN:OD1	2.39	0.46
2:V:997:ASP:OD1	2:V:1023:GLY:N	2.46	0.46
2:Y:880:ARG:NE	2:Y:1103:GLU:OE2	2.44	0.46
2:P:829:ASP:HB2	2:P:832:ASP:HB3	1.98	0.46
2:R:1027:SER:HA	2:R:1037:GLN:HA	1.98	0.46
2:V:715:LEU:HD11	2:V:855:VAL:HG23	1.97	0.46
2:Y:1030:SER:HB3	2:Y:1033:ALA:H	1.80	0.46
2:R:982:ARG:NH1	2:W:1018:ASP:OD2	2.43	0.45
2:V:581:MET:O	2:V:585:LYS:NZ	2.48	0.45
2:X:814:MET:HA	2:X:817:LEU:HB2	1.98	0.45
1:J:72:ASP:OD1	1:J:72:ASP:N	2.47	0.45
2:Q:579:ASP:H	2:Q:582:LEU:HD13	1.82	0.45
2:Q:1036:ARG:HH21	2:Q:1073:GLN:HE21	1.64	0.45
2:U:991:GLN:O	2:U:1029:VAL:N	2.46	0.45
2:U:995:ILE:HG12	2:U:1000:LYS:HG2	1.98	0.45
2:W:871:ALA:O	2:W:875:LEU:N	2.47	0.45
1:F:33:ARG:HD3	1:F:143:SER:HB3	1.98	0.45
1:N:32:ALA:HB2	1:N:88:LEU:HD12	1.97	0.45
2:X:1019:THR:OG1	2:X:1020:GLU:N	2.49	0.45
2:Y:820:GLN:HG2	2:Y:824:GLN:HE21	1.81	0.45
2:Y:991:GLN:O	2:Y:1029:VAL:N	2.47	0.45
1:B:60:PHE:O	1:B:124:ARG:NH1	2.50	0.45
2:T:624:ARG:NH1	2:T:724:VAL:O	2.43	0.45
2:V:639:ILE:HD11	2:V:667:ARG:HG3	1.96	0.45
2:W:698:SER:OG	2:W:699:ASP:N	2.49	0.45
2:Y:904:ALA:O	2:Y:1045:TRP:NE1	2.43	0.45
2:S:793:THR:HA	2:S:796:THR:HG22	1.97	0.45
2:X:811:PRO:HG2	2:X:813:ALA:HB3	1.98	0.45
1:A:60:PHE:O	1:A:124:ARG:NH1	2.50	0.45
1:B:53:GLN:HE22	1:B:100:LEU:HA	1.81	0.45
1:I:66:GLN:O	1:I:70:THR:OG1	2.30	0.45
2:Q:902:SER:OG	2:Q:903:ASP:N	2.48	0.45
2:R:605:ASP:OD1	2:R:605:ASP:N	2.49	0.45
2:R:809:SER:OG	2:R:810:ASP:OD2	2.31	0.45
2:S:613:PHE:HB3	2:S:692:ARG:HH21	1.81	0.45
2:U:824:GLN:O	2:U:826:LYS:N	2.47	0.45
2:U:878:ARG:NH2	2:U:927:ASN:OD1	2.38	0.45
2:U:913:LEU:HD22	2:U:962:LEU:HD22	1.97	0.45
1:A:153:LYS:HE2	1:A:153:LYS:HB3	1.89	0.45
2:P:816:GLN:O	2:P:820:GLN:N	2.48	0.45
2:R:585:LYS:HB3	2:R:589:ARG:HH21	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:797:GLN:HA	2:X:800:LEU:HB2	1.99	0.45
1:F:41:ALA:HB2	2:U:1021:ALA:HB2	1.99	0.45
2:S:608:VAL:HG22	2:S:714:PRO:HG3	1.98	0.45
2:V:980:GLU:OE1	2:V:1083:ARG:NH2	2.49	0.45
2:V:1064:SER:O	2:V:1064:SER:OG	2.35	0.45
2:X:777:ASP:OD1	2:X:779:GLN:N	2.48	0.45
2:Y:903:ASP:HB3	2:Y:1045:TRP:HD1	1.82	0.45
1:B:153:LYS:HE2	1:B:153:LYS:HB3	1.87	0.45
1:D:29:ASP:N	1:D:29:ASP:OD1	2.50	0.45
1:J:52:TYR:HE2	1:J:68:LEU:HD21	1.82	0.45
1:L:32:ALA:HB2	1:L:88:LEU:HD12	1.97	0.45
1:E:153:LYS:HE2	1:E:153:LYS:HB3	1.87	0.44
1:I:52:TYR:HE2	1:I:68:LEU:HD21	1.82	0.44
2:R:631:VAL:HA	2:R:634:SER:HB3	1.99	0.44
1:A:27:HIS:ND1	1:A:97:ASP:OD1	2.46	0.44
1:A:31:ARG:NH2	1:F:90:PRO:O	2.50	0.44
1:O:107:THR:OG1	1:O:127:LEU:O	2.35	0.44
2:R:624:ARG:NH1	2:R:724:VAL:O	2.44	0.44
2:U:670:LEU:HA	2:U:673:ARG:HE	1.83	0.44
2:V:811:PRO:HG2	2:V:813:ALA:HB3	1.98	0.44
2:W:820:GLN:HG2	2:W:824:GLN:HE21	1.82	0.44
2:X:698:SER:OG	2:X:699:ASP:N	2.50	0.44
2:R:1036:ARG:HH21	2:R:1073:GLN:HE21	1.64	0.44
2:U:1019:THR:OG1	2:U:1020:GLU:N	2.50	0.44
2:W:852:GLY:HA2	2:W:855:VAL:HG12	1.98	0.44
2:W:1028:TRP:HB3	2:W:1078:LEU:HD21	1.99	0.44
2:Y:708:ALA:HB2	2:Y:792:LEU:HD12	1.99	0.44
1:C:60:PHE:O	1:C:124:ARG:NH1	2.51	0.44
1:F:27:HIS:HB3	1:F:137:PRO:HB3	2.00	0.44
1:K:86:VAL:HG11	1:K:94:VAL:HG11	1.99	0.44
2:W:670:LEU:HA	2:W:673:ARG:HE	1.82	0.44
1:O:117:ASP:OD2	1:O:145:ASN:ND2	2.51	0.44
2:P:844:LEU:HD23	2:P:844:LEU:HA	1.85	0.44
2:U:811:PRO:HG2	2:U:813:ALA:HB3	1.98	0.44
2:X:670:LEU:HA	2:X:673:ARG:HE	1.82	0.44
2:X:887:TRP:HE3	2:X:912:TYR:HD2	1.64	0.44
2:Y:1028:TRP:HB3	2:Y:1078:LEU:HD21	1.99	0.44
1:O:32:ALA:HB2	1:O:88:LEU:HD12	1.98	0.44
2:V:670:LEU:HA	2:V:673:ARG:HE	1.83	0.44
2:W:777:ASP:OD2	2:W:779:GLN:N	2.49	0.44
2:Y:615:ASP:OD1	2:Y:615:ASP:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ASP:OD1	1:B:29:ASP:N	2.51	0.44
1:C:153:LYS:HE2	1:C:153:LYS:HB3	1.88	0.44
1:F:28:LEU:HD23	1:F:28:LEU:HA	1.82	0.44
1:F:52:TYR:HE2	1:F:68:LEU:HD21	1.82	0.44
1:H:52:TYR:HE2	1:H:68:LEU:HD21	1.82	0.44
1:H:53:GLN:HB2	1:H:82:ALA:HB3	1.99	0.44
2:P:809:SER:OG	2:P:810:ASP:OD2	2.31	0.44
2:R:800:LEU:HD23	2:R:800:LEU:HA	1.84	0.44
2:V:698:SER:OG	2:V:699:ASP:N	2.49	0.44
2:V:1068:LEU:HD23	2:V:1068:LEU:HA	1.88	0.44
2:X:913:LEU:HD22	2:X:962:LEU:HD22	1.99	0.44
1:D:53:GLN:HE22	1:D:100:LEU:HA	1.82	0.44
1:M:117:ASP:OD2	1:M:145:ASN:ND2	2.51	0.44
2:Q:800:LEU:HD23	2:Q:800:LEU:HA	1.82	0.44
2:U:820:GLN:HG2	2:U:824:GLN:HE21	1.82	0.44
2:T:1074:ASP:OD1	2:T:1074:ASP:N	2.51	0.44
2:U:708:ALA:HB2	2:U:792:LEU:HD12	2.00	0.44
1:I:27:HIS:HB3	1:I:137:PRO:HB3	2.00	0.43
2:S:829:ASP:HB2	2:S:832:ASP:HB3	2.01	0.43
1:H:66:GLN:O	1:H:70:THR:OG1	2.30	0.43
1:I:41:ALA:HB2	2:X:1021:ALA:HB2	1.98	0.43
1:L:117:ASP:OD2	1:L:145:ASN:ND2	2.50	0.43
2:R:816:GLN:O	2:R:820:GLN:N	2.50	0.43
2:V:852:GLY:HA2	2:V:855:VAL:HG12	1.99	0.43
2:Y:698:SER:O	2:Y:701:THR:OG1	2.35	0.43
2:Q:956:LEU:HD23	2:Q:956:LEU:HA	1.84	0.43
2:Q:982:ARG:NH1	2:V:1018:ASP:OD2	2.43	0.43
2:Q:1035:THR:O	2:Q:1035:THR:OG1	2.26	0.43
2:S:816:GLN:O	2:S:820:GLN:N	2.49	0.43
2:S:1050:LEU:HD12	2:S:1050:LEU:HA	1.79	0.43
2:X:852:GLY:HA2	2:X:855:VAL:HG12	1.99	0.43
2:U:597:MET:HB3	2:U:618:VAL:HG13	2.01	0.43
2:V:957:LYS:HA	2:V:957:LYS:HD3	1.81	0.43
2:X:1028:TRP:HB3	2:X:1078:LEU:HD21	1.99	0.43
1:H:50:ARG:HD3	1:H:83:GLN:HE21	1.84	0.43
2:V:913:LEU:HD22	2:V:962:LEU:HD22	1.99	0.43
1:C:68:LEU:HD12	1:C:123:TRP:HH2	1.84	0.43
1:G:41:ALA:HB2	2:V:1021:ALA:HB2	2.01	0.43
1:I:66:GLN:HG3	2:R:1037:GLN:HE22	1.84	0.43
1:J:27:HIS:HB3	1:J:137:PRO:HB3	2.01	0.43
2:P:666:LEU:HA	2:P:669:ARG:HB2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:605:ASP:OD1	2:Q:605:ASP:N	2.51	0.43
2:P:605:ASP:OD1	2:P:605:ASP:N	2.49	0.43
2:S:823:LEU:HD22	2:S:945:ASN:HB3	2.00	0.43
2:W:955:PHE:HA	2:W:1102:PRO:HG2	2.01	0.43
2:X:820:GLN:HG2	2:X:824:GLN:HE21	1.84	0.43
2:Y:777:ASP:OD2	2:Y:779:GLN:N	2.52	0.43
2:Y:914:ASN:ND2	2:Y:973:GLY:O	2.49	0.43
1:C:29:ASP:OD1	1:C:29:ASP:N	2.50	0.43
1:D:51:ILE:HB	1:D:84:LYS:HB3	2.00	0.43
2:P:894:ARG:NH1	2:Q:1085:GLU:O	2.52	0.43
2:V:820:GLN:HG2	2:V:824:GLN:HE21	1.82	0.43
2:X:901:SER:HA	2:X:1049:ARG:HH22	1.84	0.43
2:Y:599:LEU:HD23	2:Y:599:LEU:HA	1.90	0.43
1:C:53:GLN:HB2	1:C:82:ALA:H	1.83	0.43
1:D:52:TYR:N	1:D:108:GLY:O	2.50	0.43
1:E:68:LEU:HD12	1:E:123:TRP:HH2	1.84	0.43
2:Q:624:ARG:NH1	2:Q:724:VAL:O	2.42	0.43
2:T:723:ALA:HA	2:T:773:LEU:HD11	2.01	0.43
2:V:708:ALA:HB2	2:V:792:LEU:HD12	2.00	0.43
1:A:68:LEU:HD12	1:A:123:TRP:HH2	1.84	0.42
1:F:141:GLU:O	1:F:148:THR:OG1	2.34	0.42
1:M:93:SER:OG	1:M:94:VAL:N	2.52	0.42
2:P:723:ALA:HA	2:P:773:LEU:HD11	2.00	0.42
2:P:982:ARG:NH1	2:U:1018:ASP:OD2	2.42	0.42
2:T:613:PHE:HB3	2:T:692:ARG:HH21	1.84	0.42
2:V:880:ARG:NE	2:V:1103:GLU:OE2	2.44	0.42
2:W:991:GLN:O	2:W:1029:VAL:N	2.48	0.42
2:Y:670:LEU:HA	2:Y:673:ARG:HE	1.83	0.42
1:L:38:THR:HB	1:L:42:GLY:HA2	2.02	0.42
2:S:982:ARG:NH1	2:X:1018:ASP:OD2	2.42	0.42
2:T:800:LEU:HD23	2:T:800:LEU:HA	1.83	0.42
2:Y:858:ARG:HA	2:Y:858:ARG:HD2	1.87	0.42
1:A:53:GLN:HE22	1:A:100:LEU:HA	1.84	0.42
1:J:132:LEU:HD23	1:J:132:LEU:HA	1.89	0.42
1:K:117:ASP:OD2	1:K:145:ASN:ND2	2.52	0.42
1:N:93:SER:OG	1:N:94:VAL:N	2.53	0.42
1:O:93:SER:OG	1:O:94:VAL:N	2.51	0.42
2:T:956:LEU:HD23	2:T:956:LEU:HA	1.82	0.42
2:Y:990:MET:N	2:Y:1029:VAL:O	2.41	0.42
1:J:41:ALA:HB2	2:Y:1021:ALA:HB2	2.02	0.42
1:K:89:GLN:HE22	2:U:1031:THR:HB	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:1025:SER:OG	2:Q:1040:ASP:OD2	2.37	0.42
2:U:942:ASP:O	2:U:946:THR:OG1	2.23	0.42
2:W:716:VAL:HA	2:W:719:MET:HB2	2.00	0.42
2:W:985:THR:OG1	2:W:986:ALA:N	2.52	0.42
2:X:880:ARG:NE	2:X:1103:GLU:OE2	2.43	0.42
1:C:65:TYR:OH	1:C:113:PHE:O	2.38	0.42
1:D:65:TYR:OH	1:D:113:PHE:O	2.37	0.42
1:H:132:LEU:HD23	1:H:132:LEU:HA	1.86	0.42
1:M:121:ASN:HD21	1:M:124:ARG:NH2	2.17	0.42
2:P:624:ARG:NH1	2:P:724:VAL:O	2.43	0.42
2:Q:916:ASP:OD1	2:Q:916:ASP:N	2.51	0.42
2:S:702:GLU:O	2:S:705:THR:OG1	2.37	0.42
2:U:1051:LEU:HD23	2:U:1051:LEU:HA	1.89	0.42
2:Y:707:MET:HG3	2:Y:715:LEU:HD23	2.01	0.42
2:Q:666:LEU:HA	2:Q:669:ARG:HB2	2.02	0.42
2:Q:1050:LEU:HA	2:Q:1050:LEU:HD12	1.82	0.42
2:R:611:LEU:HD23	2:R:611:LEU:HA	1.89	0.42
2:T:1050:LEU:HD12	2:T:1050:LEU:HA	1.85	0.42
2:V:674:TYR:O	2:V:678:PHE:N	2.53	0.42
2:X:957:LYS:HA	2:X:957:LYS:HD3	1.81	0.42
2:Y:880:ARG:HH21	2:Y:1103:GLU:HG3	1.85	0.42
1:B:31:ARG:NH2	1:G:90:PRO:O	2.52	0.42
1:I:61:ASP:O	1:I:124:ARG:NH2	2.53	0.42
1:O:89:GLN:HE22	2:Y:1031:THR:HB	1.85	0.42
2:Q:583:TYR:HB2	2:Q:670:LEU:HD11	2.01	0.42
2:R:1091:LEU:HD23	2:R:1091:LEU:HA	1.89	0.42
2:S:601:ASP:OD1	2:S:601:ASP:N	2.50	0.42
2:U:821:THR:HG23	2:U:826:LYS:HB2	2.02	0.42
1:A:29:ASP:OD1	1:A:29:ASP:N	2.52	0.42
1:B:65:TYR:OH	1:B:113:PHE:O	2.37	0.42
1:B:68:LEU:HD12	1:B:123:TRP:HH2	1.85	0.42
2:P:909:LEU:HG	2:P:913:LEU:HD21	2.00	0.42
2:T:850:GLY:O	2:T:854:THR:OG1	2.27	0.42
2:V:794:ARG:HD3	2:V:794:ARG:HA	1.86	0.42
1:E:72:ASP:OD1	1:E:72:ASP:N	2.53	0.42
1:F:50:ARG:HD3	1:F:83:GLN:HE21	1.83	0.42
1:G:27:HIS:HB3	1:G:137:PRO:HB3	2.00	0.42
1:G:141:GLU:O	1:G:148:THR:OG1	2.34	0.42
2:Y:822:VAL:HG11	2:Y:868:LEU:HD12	2.02	0.42
1:C:72:ASP:OD1	1:C:72:ASP:N	2.53	0.42
1:D:131:GLU:O	1:D:138:ARG:NH1	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:53:GLN:HB2	1:F:82:ALA:HB3	2.02	0.42
1:N:121:ASN:HD21	1:N:124:ARG:NH2	2.18	0.42
2:P:1063:ALA:HA	2:P:1064:SER:HA	1.81	0.42
2:T:1096:LEU:HD23	2:T:1096:LEU:HA	1.91	0.42
2:U:599:LEU:HA	2:U:602:MET:HB2	2.01	0.42
2:V:908:LEU:HD12	2:V:908:LEU:HA	1.87	0.42
2:W:903:ASP:HB3	2:W:1045:TRP:HD1	1.84	0.42
2:X:720:ASN:HD22	2:X:720:ASN:HA	1.65	0.42
1:D:68:LEU:HD12	1:D:123:TRP:HH2	1.85	0.41
2:U:997:ASP:HB3	2:U:1017:ALA:HB3	2.02	0.41
2:V:991:GLN:O	2:V:1029:VAL:N	2.48	0.41
2:X:997:ASP:OD1	2:X:1023:GLY:N	2.48	0.41
2:Y:675:PHE:HA	2:Y:678:PHE:HB2	2.02	0.41
1:A:52:TYR:N	1:A:108:GLY:O	2.49	0.41
1:N:54:LEU:O	1:N:105:LYS:N	2.53	0.41
1:N:117:ASP:OD2	1:N:145:ASN:ND2	2.54	0.41
2:Q:829:ASP:HB2	2:Q:832:ASP:HB3	2.02	0.41
2:T:1036:ARG:HH21	2:T:1073:GLN:HE21	1.68	0.41
2:X:997:ASP:HB3	2:X:1017:ALA:HB3	2.02	0.41
1:A:39:SER:HB3	1:A:45:LEU:HD13	2.02	0.41
1:E:28:LEU:HD12	1:E:28:LEU:HA	1.92	0.41
1:I:28:LEU:HD23	1:I:28:LEU:HA	1.82	0.41
2:P:611:LEU:HD23	2:P:611:LEU:HA	1.90	0.41
2:V:955:PHE:HA	2:V:1102:PRO:HG2	2.03	0.41
2:V:956:LEU:HD23	2:V:956:LEU:HA	1.89	0.41
2:W:997:ASP:HB3	2:W:1017:ALA:HB3	2.02	0.41
2:W:1019:THR:OG1	2:W:1020:GLU:N	2.53	0.41
2:X:995:ILE:HD12	2:X:1000:LYS:HG2	2.02	0.41
2:Y:814:MET:H	2:Y:817:LEU:HD13	1.86	0.41
2:Y:1026:LEU:HD21	2:Y:1078:LEU:HD22	2.02	0.41
1:E:65:TYR:OH	1:E:113:PHE:O	2.39	0.41
2:Q:589:ARG:NH1	2:Q:637:THR:OG1	2.53	0.41
2:S:585:LYS:HD2	2:S:585:LYS:HA	1.81	0.41
2:U:822:VAL:HG11	2:U:868:LEU:HD12	2.02	0.41
2:U:1030:SER:OG	2:U:1031:THR:N	2.53	0.41
2:W:708:ALA:HB2	2:W:792:LEU:HD12	2.01	0.41
2:Y:811:PRO:HG2	2:Y:813:ALA:HB3	2.02	0.41
2:Y:1019:THR:OG1	2:Y:1020:GLU:N	2.52	0.41
1:C:50:ARG:HG3	1:C:85:ASP:HB3	2.02	0.41
1:H:150:LEU:HD23	1:H:150:LEU:HA	1.93	0.41
1:M:38:THR:HB	1:M:42:GLY:HA2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:875:LEU:HD11	2:P:927:ASN:HB3	2.02	0.41
2:R:829:ASP:OD2	2:R:829:ASP:N	2.49	0.41
2:U:615:ASP:OD1	2:U:615:ASP:N	2.51	0.41
2:V:1019:THR:OG1	2:V:1020:GLU:N	2.54	0.41
2:X:858:ARG:HD2	2:X:858:ARG:HA	1.85	0.41
2:X:962:LEU:HD23	2:X:962:LEU:HA	1.89	0.41
2:Y:709:ASP:OD1	2:Y:710:VAL:N	2.54	0.41
2:Y:955:PHE:HA	2:Y:1102:PRO:HG2	2.02	0.41
1:B:51:ILE:HB	1:B:84:LYS:HB3	2.01	0.41
1:E:29:ASP:OD1	1:E:29:ASP:N	2.52	0.41
1:I:48:VAL:HG22	1:I:87:TRP:CD1	2.55	0.41
1:I:53:GLN:HB2	1:I:82:ALA:HB3	2.02	0.41
2:R:723:ALA:HA	2:R:773:LEU:HD11	2.02	0.41
2:T:875:LEU:HD11	2:T:927:ASN:HB3	2.01	0.41
2:X:822:VAL:HG11	2:X:868:LEU:HD12	2.03	0.41
2:Y:1041:LEU:HD13	2:Y:1049:ARG:HB3	2.02	0.41
2:Y:1068:LEU:HD23	2:Y:1068:LEU:HA	1.93	0.41
1:L:89:GLN:HE22	2:V:1031:THR:HB	1.86	0.41
1:M:89:GLN:HA	1:M:90:PRO:HD3	1.94	0.41
2:P:982:ARG:NH2	2:U:1018:ASP:OD1	2.50	0.41
2:S:909:LEU:HD12	2:S:909:LEU:HA	1.90	0.41
2:U:955:PHE:HA	2:U:1102:PRO:HG2	2.01	0.41
2:V:904:ALA:O	2:V:1045:TRP:NE1	2.46	0.41
2:X:955:PHE:HA	2:X:1102:PRO:HG2	2.03	0.41
1:A:65:TYR:OH	1:A:113:PHE:O	2.38	0.41
1:D:153:LYS:HE2	1:D:153:LYS:HB3	1.88	0.41
2:P:793:THR:O	2:P:793:THR:OG1	2.38	0.41
2:R:916:ASP:OD1	2:R:916:ASP:N	2.52	0.41
2:T:589:ARG:NH1	2:T:637:THR:OG1	2.53	0.41
2:V:822:VAL:HG11	2:V:868:LEU:HD12	2.02	0.41
2:W:858:ARG:HD2	2:W:858:ARG:HA	1.84	0.41
2:W:1068:LEU:HD23	2:W:1068:LEU:HA	1.93	0.41
1:C:31:ARG:NH2	1:H:90:PRO:O	2.53	0.41
1:F:66:GLN:O	1:F:70:THR:OG1	2.31	0.41
1:F:145:ASN:OD1	1:F:145:ASN:N	2.54	0.41
1:H:41:ALA:HB2	2:W:1021:ALA:HB2	2.03	0.41
1:J:28:LEU:HD23	1:J:28:LEU:HA	1.81	0.41
1:M:89:GLN:HE22	2:W:1031:THR:HB	1.86	0.41
1:O:121:ASN:HD21	1:O:124:ARG:NH2	2.18	0.41
2:R:844:LEU:HA	2:R:844:LEU:HD23	1.85	0.41
2:S:632:LEU:HD23	2:S:632:LEU:HA	1.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:844:LEU:HD23	2:T:844:LEU:HA	1.84	0.41
2:V:777:ASP:OD2	2:V:779:GLN:N	2.52	0.41
2:V:824:GLN:O	2:V:826:LYS:N	2.47	0.41
2:V:905:SER:O	2:V:905:SER:OG	2.38	0.41
2:W:794:ARG:HD3	2:W:794:ARG:HA	1.86	0.41
2:W:913:LEU:HD22	2:W:962:LEU:HD22	2.02	0.41
2:X:1030:SER:HG	2:X:1076:ARG:HH21	1.67	0.41
2:Y:997:ASP:HB3	2:Y:1017:ALA:HB3	2.02	0.41
1:E:52:TYR:N	1:E:108:GLY:O	2.51	0.41
1:N:38:THR:HB	1:N:42:GLY:HA2	2.03	0.41
2:Q:875:LEU:HD11	2:Q:927:ASN:HB3	2.03	0.41
1:J:113:PHE:HB2	1:J:116:PRO:HB3	2.03	0.40
1:L:121:ASN:HD21	1:L:124:ARG:NH2	2.18	0.40
2:Q:1094:LEU:HD23	2:Q:1094:LEU:HA	1.91	0.40
2:T:611:LEU:HD12	2:T:714:PRO:HG2	2.04	0.40
2:U:901:SER:HA	2:U:1049:ARG:HH22	1.87	0.40
2:U:1026:LEU:HD21	2:U:1078:LEU:HD22	2.03	0.40
2:V:995:ILE:HD12	2:V:1000:LYS:HG2	2.03	0.40
2:W:821:THR:HG23	2:W:826:LYS:HB2	2.03	0.40
2:Y:794:ARG:HD3	2:Y:794:ARG:HA	1.87	0.40
1:N:54:LEU:HB2	1:N:106:PHE:HB2	2.04	0.40
2:U:698:SER:O	2:U:701:THR:OG1	2.38	0.40
2:W:895:TYR:OH	2:W:1052:GLU:OE1	2.30	0.40
2:X:880:ARG:HH21	2:X:1103:GLU:HG3	1.86	0.40
1:K:54:LEU:HD12	1:K:54:LEU:HA	1.91	0.40
1:K:107:THR:OG1	1:K:127:LEU:O	2.34	0.40
1:K:121:ASN:HD21	1:K:124:ARG:NH2	2.18	0.40
1:M:142:VAL:HG22	1:M:147:LEU:HD23	2.03	0.40
2:P:875:LEU:HD13	2:P:875:LEU:HA	1.92	0.40
2:R:589:ARG:NH1	2:R:637:THR:OG1	2.53	0.40
2:R:932:LEU:HD12	2:R:932:LEU:HA	1.91	0.40
2:T:982:ARG:NH1	2:Y:1018:ASP:OD2	2.45	0.40
2:X:581:MET:O	2:X:585:LYS:NZ	2.53	0.40
2:X:1026:LEU:HD21	2:X:1078:LEU:HD22	2.02	0.40
2:Y:816:GLN:HA	2:Y:819:ALA:HB3	2.03	0.40
2:Y:997:ASP:OD1	2:Y:1023:GLY:N	2.46	0.40
1:H:48:VAL:HG22	1:H:87:TRP:CD1	2.57	0.40
1:K:138:ARG:H	1:K:138:ARG:HG2	1.74	0.40
2:R:632:LEU:HD23	2:R:632:LEU:HA	1.89	0.40
2:S:589:ARG:NH1	2:S:637:THR:OG1	2.54	0.40
2:T:607:ASP:OD2	2:U:778:ASN:ND2	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:675:PHE:HA	2:W:678:PHE:HB2	2.04	0.40
2:W:698:SER:O	2:W:701:THR:OG1	2.37	0.40
1:F:48:VAL:HG22	1:F:87:TRP:CD1	2.56	0.40
2:Q:932:LEU:HD12	2:Q:932:LEU:HA	1.90	0.40
2:W:942:ASP:O	2:W:946:THR:OG1	2.24	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	133/178 (75%)	127 (96%)	6 (4%)	0	100	100
1	B	133/178 (75%)	126 (95%)	7 (5%)	0	100	100
1	C	133/178 (75%)	126 (95%)	7 (5%)	0	100	100
1	D	133/178 (75%)	127 (96%)	6 (4%)	0	100	100
1	E	133/178 (75%)	127 (96%)	6 (4%)	0	100	100
1	F	131/178 (74%)	123 (94%)	8 (6%)	0	100	100
1	G	131/178 (74%)	125 (95%)	6 (5%)	0	100	100
1	H	131/178 (74%)	125 (95%)	6 (5%)	0	100	100
1	I	131/178 (74%)	126 (96%)	5 (4%)	0	100	100
1	J	131/178 (74%)	125 (95%)	6 (5%)	0	100	100
1	K	119/178 (67%)	115 (97%)	4 (3%)	0	100	100
1	L	119/178 (67%)	113 (95%)	6 (5%)	0	100	100
1	M	119/178 (67%)	115 (97%)	4 (3%)	0	100	100
1	N	119/178 (67%)	114 (96%)	5 (4%)	0	100	100
1	O	119/178 (67%)	114 (96%)	5 (4%)	0	100	100
2	P	479/1129 (42%)	439 (92%)	39 (8%)	1 (0%)	47	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Q	479/1129 (42%)	436 (91%)	41 (9%)	2 (0%)	34	71
2	R	479/1129 (42%)	439 (92%)	39 (8%)	1 (0%)	47	79
2	S	479/1129 (42%)	432 (90%)	45 (9%)	2 (0%)	34	71
2	T	479/1129 (42%)	437 (91%)	41 (9%)	1 (0%)	47	79
2	U	475/1129 (42%)	427 (90%)	44 (9%)	4 (1%)	19	58
2	V	475/1129 (42%)	428 (90%)	43 (9%)	4 (1%)	19	58
2	W	475/1129 (42%)	429 (90%)	42 (9%)	4 (1%)	19	58
2	X	475/1129 (42%)	427 (90%)	44 (9%)	4 (1%)	19	58
2	Y	475/1129 (42%)	430 (90%)	41 (9%)	4 (1%)	19	58
All	All	6685/13960 (48%)	6152 (92%)	506 (8%)	27 (0%)	38	71

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	U	786	LEU
2	V	786	LEU
2	W	786	LEU
2	X	786	LEU
2	Y	786	LEU
2	X	711	ARG
2	U	711	ARG
2	V	711	ARG
2	W	711	ARG
2	W	823	LEU
2	U	823	LEU
2	V	823	LEU
2	X	823	LEU
2	Y	711	ARG
2	Y	823	LEU
2	P	788	LEU
2	Q	788	LEU
2	R	788	LEU
2	S	788	LEU
2	T	788	LEU
2	U	844	LEU
2	V	844	LEU
2	W	844	LEU
2	X	844	LEU
2	Y	844	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Q	845	GLY
2	S	845	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	106/145 (73%)	106 (100%)	0	100	100
1	B	106/145 (73%)	106 (100%)	0	100	100
1	C	106/145 (73%)	106 (100%)	0	100	100
1	D	106/145 (73%)	106 (100%)	0	100	100
1	E	106/145 (73%)	106 (100%)	0	100	100
1	F	104/145 (72%)	103 (99%)	1 (1%)	76	86
1	G	104/145 (72%)	103 (99%)	1 (1%)	76	86
1	H	104/145 (72%)	104 (100%)	0	100	100
1	I	104/145 (72%)	103 (99%)	1 (1%)	76	86
1	J	104/145 (72%)	103 (99%)	1 (1%)	76	86
1	K	96/145 (66%)	96 (100%)	0	100	100
1	L	96/145 (66%)	96 (100%)	0	100	100
1	M	96/145 (66%)	96 (100%)	0	100	100
1	N	96/145 (66%)	96 (100%)	0	100	100
1	O	96/145 (66%)	96 (100%)	0	100	100
2	P	399/949 (42%)	396 (99%)	3 (1%)	81	89
2	Q	399/949 (42%)	394 (99%)	5 (1%)	69	82
2	R	399/949 (42%)	396 (99%)	3 (1%)	81	89
2	S	399/949 (42%)	395 (99%)	4 (1%)	76	86
2	T	399/949 (42%)	394 (99%)	5 (1%)	69	82
2	U	394/949 (42%)	393 (100%)	1 (0%)	92	95
2	V	394/949 (42%)	392 (100%)	2 (0%)	88	93

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	W	394/949 (42%)	393 (100%)	1 (0%)	92	95
2	X	394/949 (42%)	392 (100%)	2 (0%)	88	93
2	Y	394/949 (42%)	393 (100%)	1 (0%)	92	95
All	All	5495/11665 (47%)	5464 (99%)	31 (1%)	86	92

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	136	THR
1	G	136	THR
1	I	136	THR
1	J	136	THR
2	P	711	ARG
2	P	913	LEU
2	P	1074	ASP
2	Q	606	THR
2	Q	673	ARG
2	Q	711	ARG
2	Q	913	LEU
2	Q	1066	TRP
2	R	673	ARG
2	R	711	ARG
2	R	913	LEU
2	S	587	LEU
2	S	711	ARG
2	S	913	LEU
2	S	1035	THR
2	T	606	THR
2	T	673	ARG
2	T	711	ARG
2	T	913	LEU
2	T	1066	TRP
2	U	621	MET
2	V	621	MET
2	V	1082	LEU
2	W	621	MET
2	X	621	MET
2	X	869	THR
2	Y	711	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64)

such sidechains are listed below:

Mol	Chain	Res	Type
1	F	121	ASN
1	G	121	ASN
1	H	121	ASN
1	I	121	ASN
1	J	121	ASN
1	K	83	GLN
1	L	83	GLN
1	M	83	GLN
1	N	83	GLN
1	N	89	GLN
1	O	83	GLN
2	P	787	ASN
2	P	803	GLN
2	P	862	GLN
2	P	866	GLN
2	P	999	GLN
2	Q	680	ASN
2	Q	781	ASN
2	Q	787	ASN
2	Q	862	GLN
2	Q	866	GLN
2	Q	978	HIS
2	Q	1073	GLN
2	R	781	ASN
2	R	787	ASN
2	R	862	GLN
2	R	866	GLN
2	R	978	HIS
2	R	1073	GLN
2	S	781	ASN
2	S	787	ASN
2	S	862	GLN
2	S	866	GLN
2	S	999	GLN
2	S	1073	GLN
2	T	680	ASN
2	T	778	ASN
2	T	781	ASN
2	T	787	ASN
2	T	862	GLN
2	T	999	GLN
2	T	1073	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	U	720	ASN
2	U	779	GLN
2	U	820	GLN
2	U	862	GLN
2	U	1079	ASN
2	V	779	GLN
2	V	820	GLN
2	V	862	GLN
2	W	720	ASN
2	W	779	GLN
2	W	820	GLN
2	W	862	GLN
2	W	1079	ASN
2	X	720	ASN
2	X	779	GLN
2	X	820	GLN
2	X	862	GLN
2	X	1079	ASN
2	Y	779	GLN
2	Y	824	GLN
2	Y	862	GLN
2	Y	1079	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.

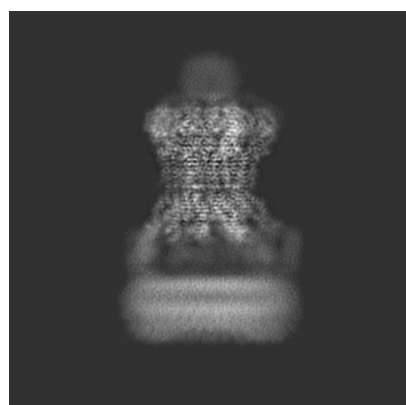
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9747. These allow visual inspection of the internal detail of the map and identification of artifacts.

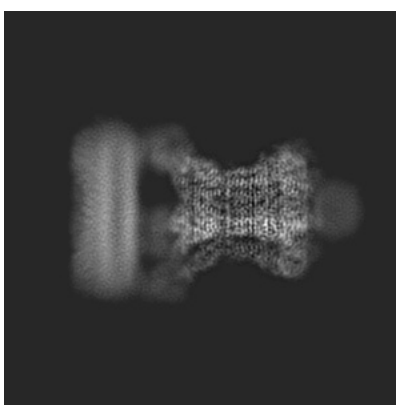
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

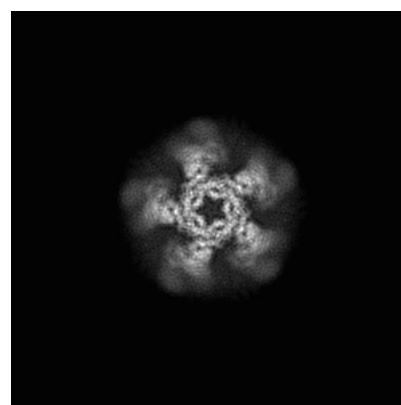
6.1.1 Primary map



X



Y

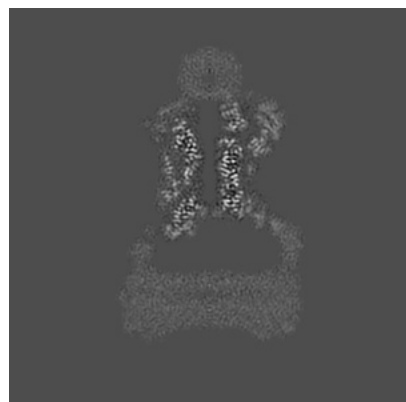


Z

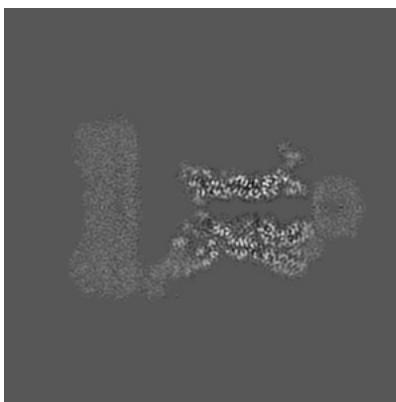
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

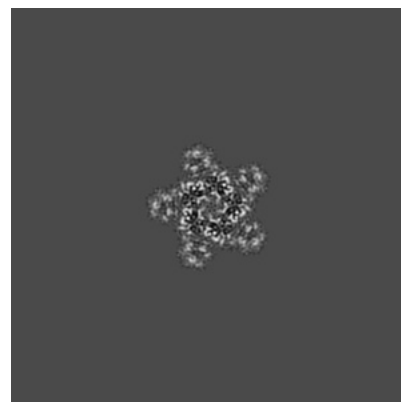
6.2.1 Primary map



X Index: 170



Y Index: 170

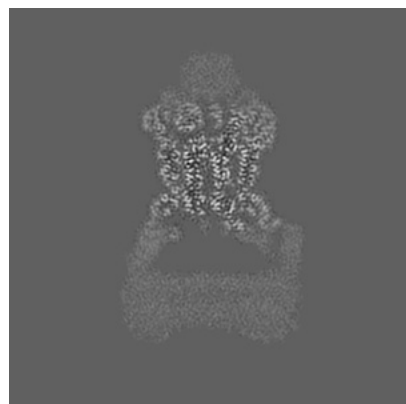


Z Index: 170

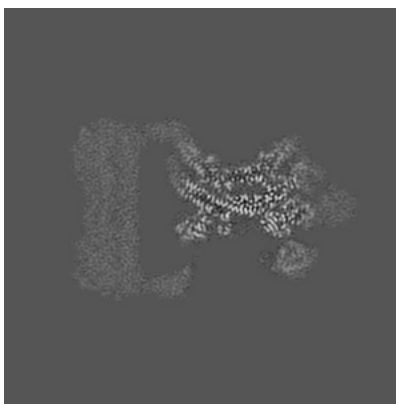
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 158



Y Index: 191



Z Index: 222

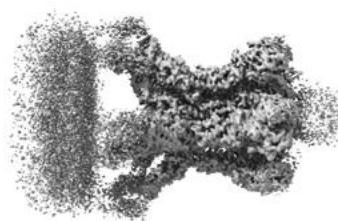
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

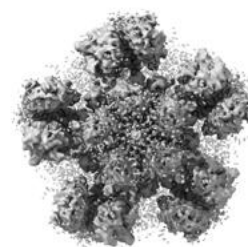
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

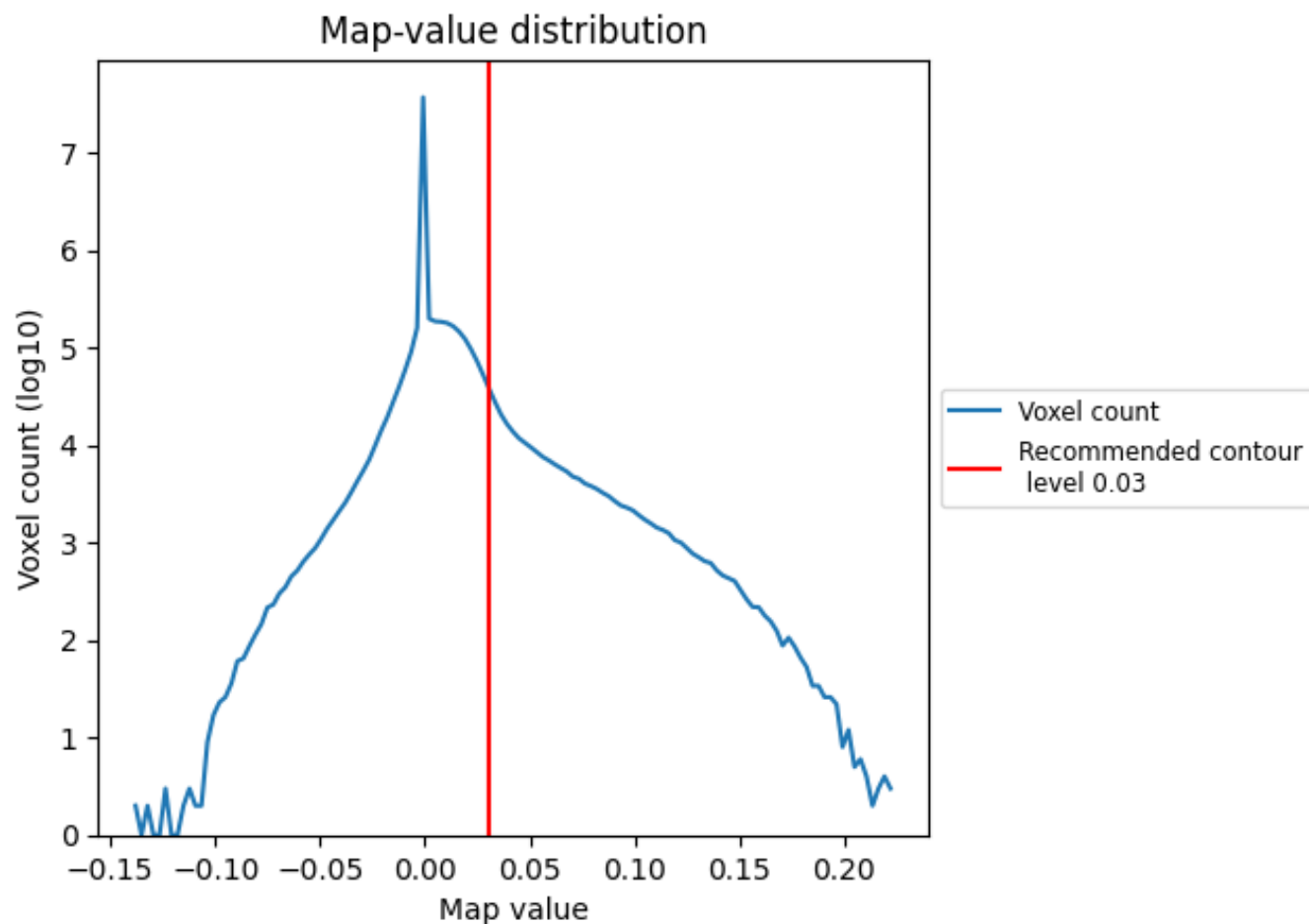
6.5 Mask visualisation

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

7 Map analysis [i](#)

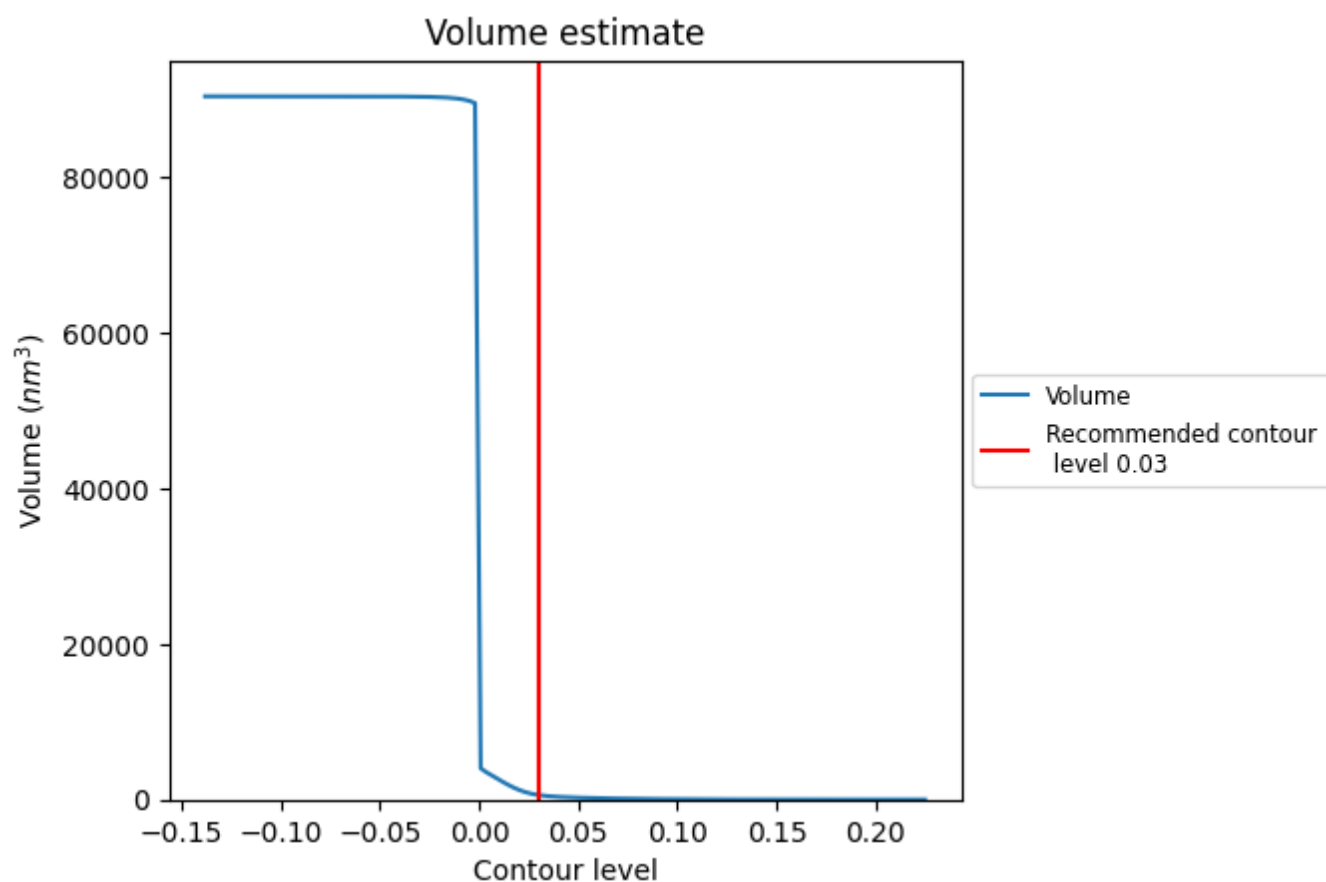
This section contains the results of statistical analysis of the map.

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.

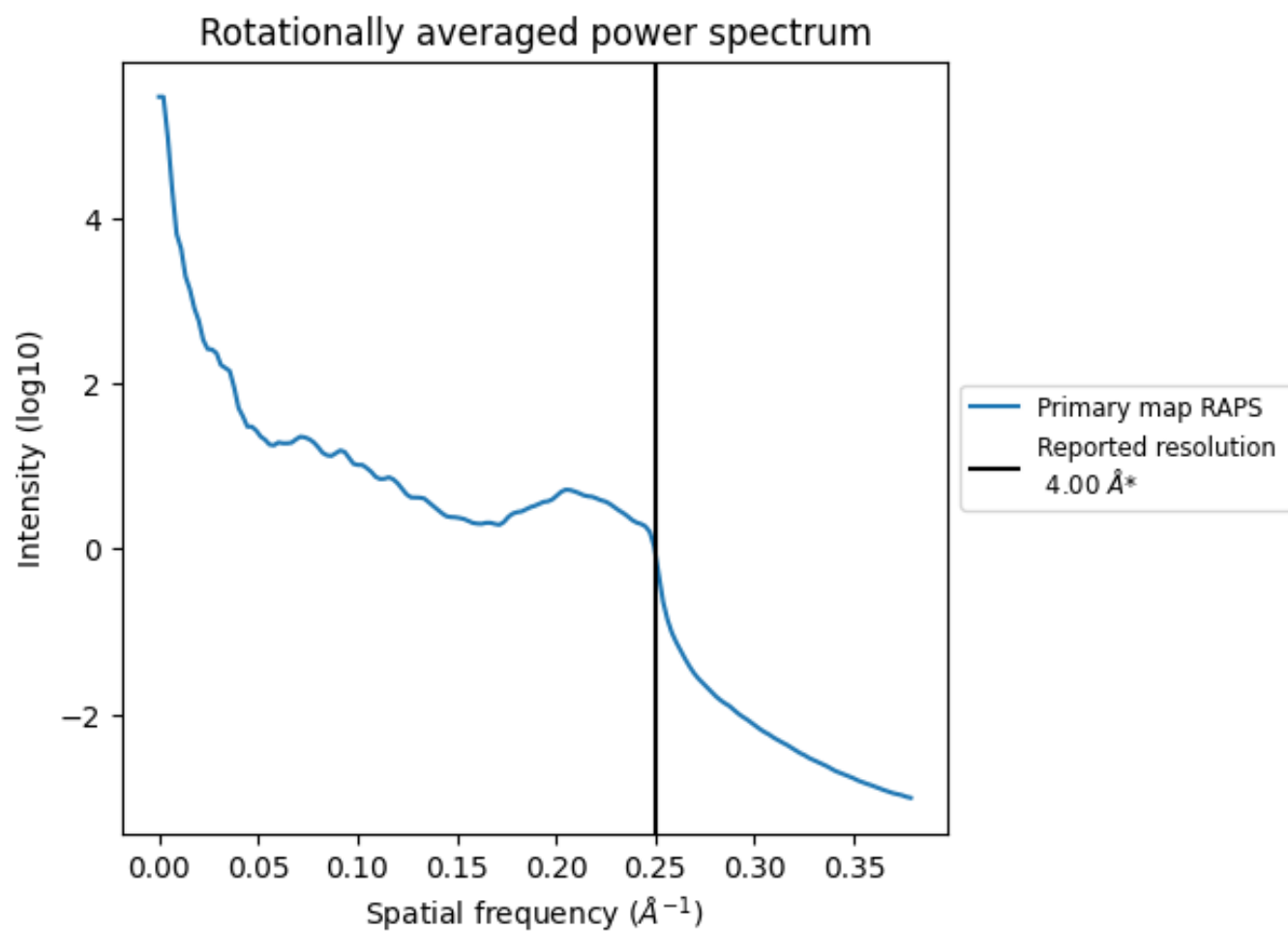
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 588 nm³; this corresponds to an approximate mass of 531 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 0.250 \AA^{-1}

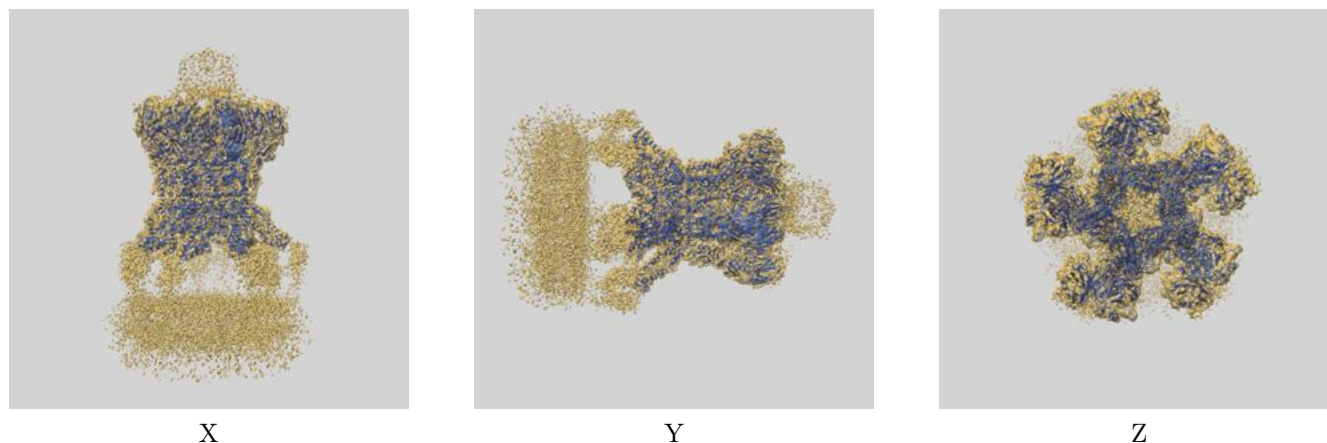
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

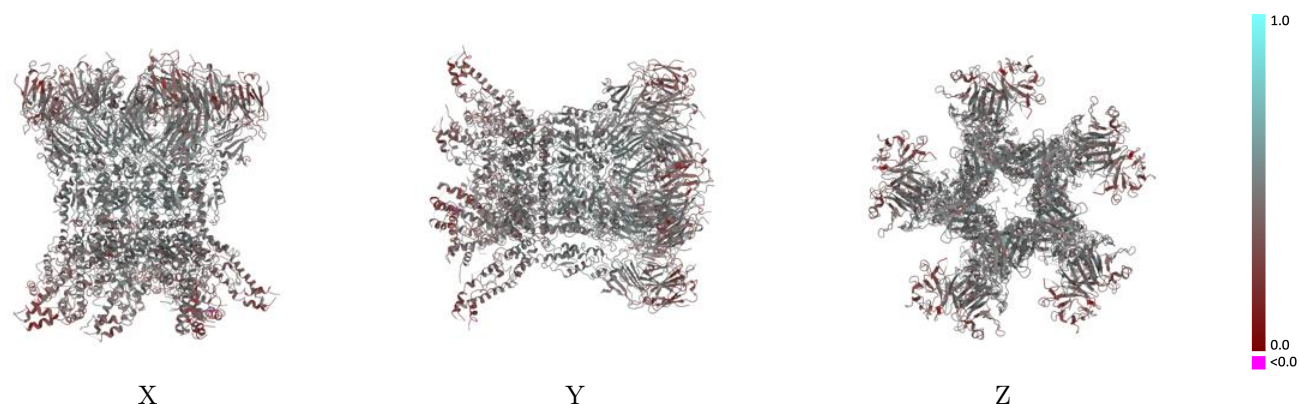
This section contains information regarding the fit between EMDB map EMD-9747 and PDB model 6IXH. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



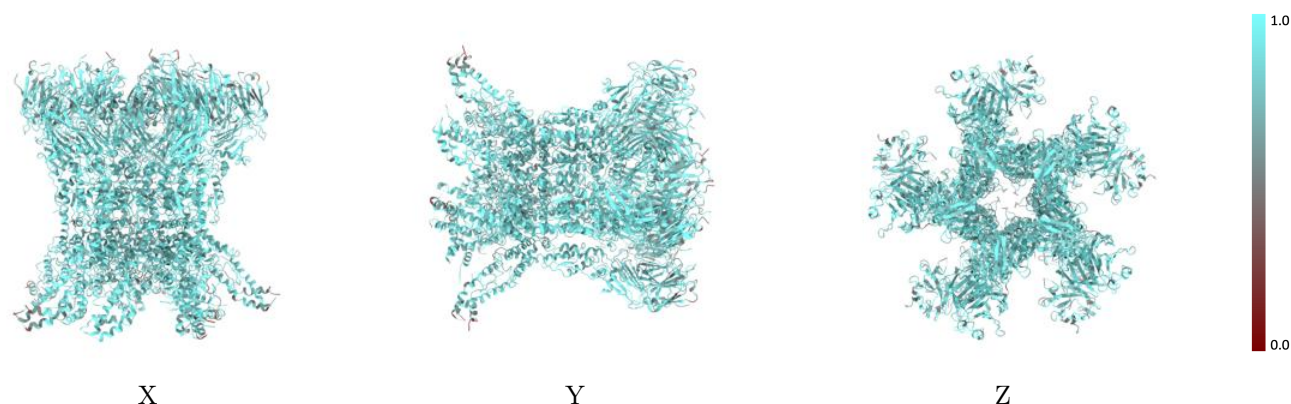
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



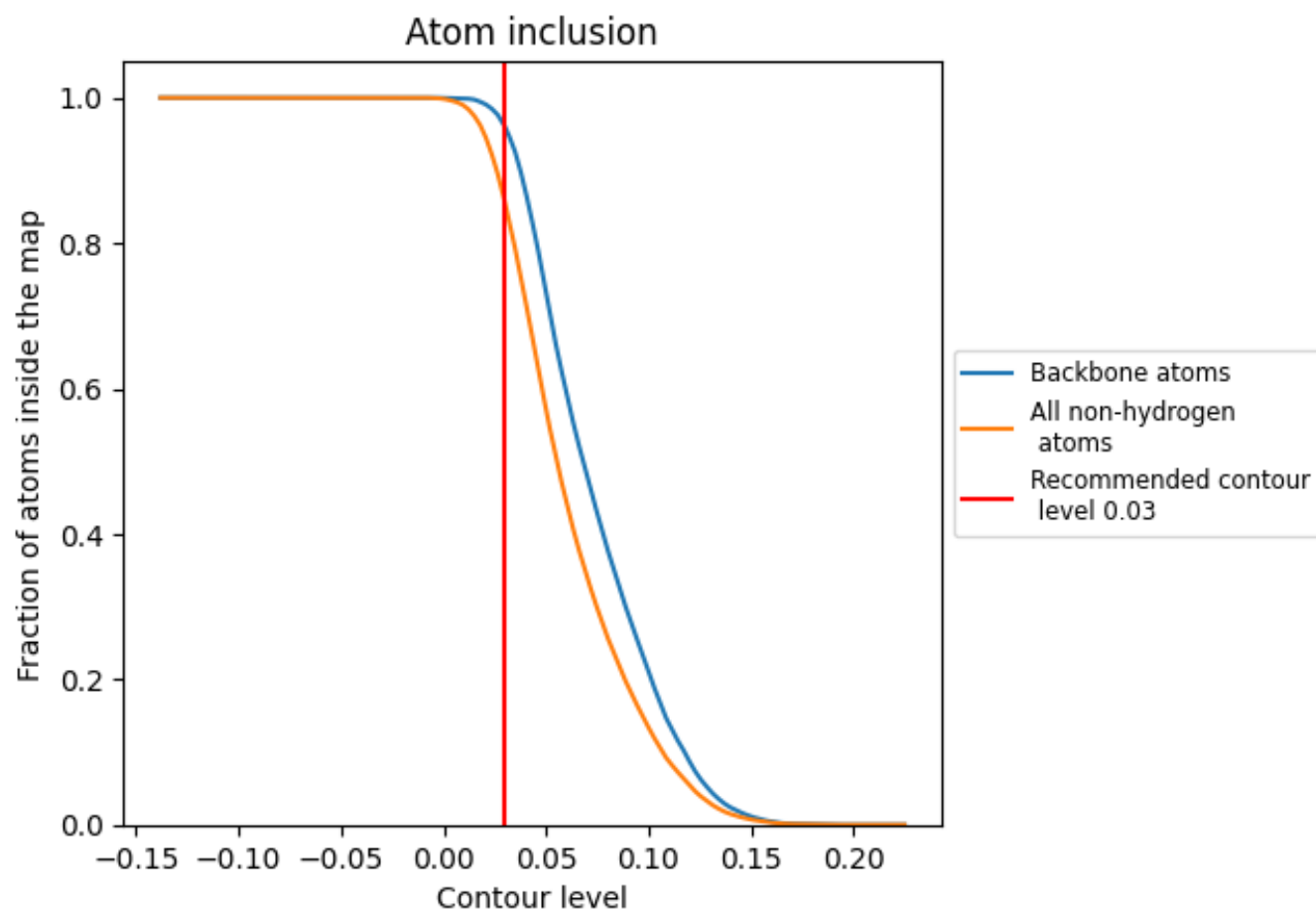
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).





















































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 86% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8559	 0.4420
A	 0.8134	 0.4240
B	 0.8094	 0.4260
C	 0.8044	 0.4260
D	 0.8114	 0.4210
E	 0.8054	 0.4230
F	 0.8419	 0.4600
G	 0.8409	 0.4600
H	 0.8389	 0.4590
I	 0.8460	 0.4610
J	 0.8419	 0.4590
K	 0.7731	 0.3530
L	 0.7797	 0.3520
M	 0.7819	 0.3540
N	 0.7764	 0.3540
O	 0.7775	 0.3560
P	 0.8908	 0.4780
Q	 0.8908	 0.4790
R	 0.8894	 0.4790
S	 0.8927	 0.4770
T	 0.8902	 0.4770
U	 0.8561	 0.4300
V	 0.8586	 0.4300
W	 0.8548	 0.4270
X	 0.8561	 0.4260
Y	 0.8580	 0.4270

