

#### Jun 24, 2024 – 01:06 PM JST

PDB ID	:	8JWE
EMDB ID	:	EMD-36680
Title	:	The open structure of the mechanosensitive channel MSL10 in Arabidopsis
		thaliana
Authors	:	Sun, L.; Liu, X.; Li, X.
Deposited on	:	2023-06-28
Resolution	:	2.74  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 (i) 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 (1)) were used in the production of this report:

:	0.0.1. dev 92
:	4.02b-467
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	1.9.13
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.37.1
	: : : : :

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.74 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	$egin{array}{c} { m Whole \ archive}\ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
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 <=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	А	734	28% 9% • 62%						
1	В	734	<b>28%</b> 9% • 62%						
1	С	734							
1	D	734	28% 10% · 62%						
1	Е	734	28% 9% • 62%						
1	F	734	<b>2</b> 8% 9% • 62%						
1	G	734	28% 9% • 62%						



# 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 14861 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.

Mol	Chain	Residues		At	oms			AltConf	Trace			
1	Λ	281	Total	С	Ν	0	$\mathbf{S}$	0	0			
1	Л	201	2123	1369	355	389	10	0	0			
1	Р	201	Total	С	Ν	0	S	0	0			
1	D	201	2123	1369	355	389	10	0	0			
1	С	281	Total	С	Ν	0	$\mathbf{S}$	0	0			
1	U	U	U	201	2123	1369	355	389	10	0	0	
1	Л	281	Total	С	Ν	0	$\mathbf{S}$	0	0			
1	D	201	2123	1369	355	389	10	0	0			
1	F	981	Total	С	Ν	0	$\mathbf{S}$	0	0			
1	Ľ	201	2123	1369	355	389	10	0	0			
1	Б	Б	Б	Б	281	Total	С	Ν	0	$\mathbf{S}$	0	0
1	Ľ	201	2123	1369	355	389	10	0	0			
1	C	281	Total	C	N	0	S	0	0			
	G	201	2123	1369	355	389	10	0				

• Molecule 1 is a protein called Mechanosensitive ion channel protein 10.



# 3 Residue-property plots (i)

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: Mechanosensitive ion channel protein 10







# 15.25 V6.26 V5.36 A5.36 A5.37 B5.36 B5.36 B5.36 B5.37 B5.36 B5.36 B5.37 B5.36 B5.36 B5.37 B5.37 B5.37 B5.37<

# • Molecule 1: Mechanosensitive ion channel protein 10 Chain D: 28% 10% 62% VAL VAL LYSS LYSS CGLY VAL LYSS CJN C LYSS C LYSS CJN C LYSS CJN C LYSS CJN C LYSS C LYSS CJN C LYSS C L • Molecule 1: Mechanosensitive ion channel protein 10 Chain E: 28% 62% PERFECTION OF A STREAM OF A ST







# V614 1615 1615 1615 1615 1623 8624 8631 8632 8633 8636 8636 8636 8636 8637 8655 8656 8657 8658 8659 8659 8656 8656 8656 8656 8656 86576 8658 8659 8705

• Molecule 1: Mechanosensitive ion channel protein 10





# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	111376	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)	1500	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	6.001	Depositor
Minimum map value	-3.854	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.154	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	303.0, 303.0, 303.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	Depositor



# 5 Model quality (i)

#### 5.1 Standard geometry (i)

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

Mal	Chain	В	ond lengths	Bond angles		
	Ullaili	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	1.99	76/2159~(3.5%)	1.10	10/2942~(0.3%)	
1	В	1.99	75/2159~(3.5%)	1.10	10/2942~(0.3%)	
1	С	1.99	77/2159~(3.6%)	1.10	10/2942~(0.3%)	
1	D	1.99	77/2159~(3.6%)	1.10	10/2942~(0.3%)	
1	Е	1.99	76/2159~(3.5%)	1.10	10/2942~(0.3%)	
1	F	1.99	78/2159~(3.6%)	1.10	10/2942~(0.3%)	
1	G	1.99	77/2159~(3.6%)	1.10	10/2942~(0.3%)	
All	All	1.99	536/15113~(3.5%)	1.10	70/20594~(0.3%)	

All (536) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	С	591	GLU	CG-CD	-12.07	1.33	1.51
1	А	591	GLU	CG-CD	-12.07	1.33	1.51
1	В	591	GLU	CG-CD	-12.06	1.33	1.51
1	G	591	GLU	CG-CD	-12.03	1.33	1.51
1	Ε	591	GLU	CG-CD	-12.01	1.33	1.51
1	D	591	GLU	CG-CD	-11.99	1.33	1.51
1	F	591	GLU	CG-CD	-11.99	1.33	1.51
1	В	671	VAL	CB-CG1	-9.13	1.33	1.52
1	А	671	VAL	CB-CG1	-9.13	1.33	1.52
1	С	671	VAL	CB-CG1	-9.12	1.33	1.52
1	Ε	671	VAL	CB-CG1	-9.12	1.33	1.52
1	D	671	VAL	CB-CG1	-9.12	1.33	1.52
1	F	671	VAL	CB-CG1	-9.11	1.33	1.52
1	G	671	VAL	CB-CG1	-9.09	1.33	1.52
1	В	705	GLU	CB-CG	-9.01	1.35	1.52
1	D	705	GLU	CB-CG	-9.01	1.35	1.52
1	Е	705	GLU	CB-CG	-9.01	1.35	1.52
1	F	705	GLU	CB-CG	-9.00	1.35	1.52
1	G	705	GLU	CB-CG	-9.00	1.35	1.52
1	С	705	GLU	CB-CG	-8.99	1.35	1.52
1	А	705	GLU	CB-CG	-8.99	1.35	1.52



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
1	D	623	TYR	CD2-CE2	-8.85	1.26	1.39
1	В	623	TYR	CD2-CE2	-8.82	1.26	1.39
1	С	623	TYR	CD2-CE2	-8.82	1.26	1.39
1	G	623	TYR	CD2-CE2	-8.80	1.26	1.39
1	F	623	TYR	CD2-CE2	-8.80	1.26	1.39
1	А	623	TYR	CD2-CE2	-8.74	1.26	1.39
1	Е	623	TYR	CD2-CE2	-8.71	1.26	1.39
1	F	591	GLU	CB-CG	-8.70	1.35	1.52
1	G	591	GLU	CB-CG	-8.69	1.35	1.52
1	А	591	GLU	CB-CG	-8.67	1.35	1.52
1	В	634	GLU	CB-CG	-8.67	1.35	1.52
1	А	634	GLU	CB-CG	-8.67	1.35	1.52
1	G	634	GLU	CB-CG	-8.67	1.35	1.52
1	С	634	GLU	CB-CG	-8.67	1.35	1.52
1	В	591	GLU	CB-CG	-8.66	1.35	1.52
1	D	591	GLU	CB-CG	-8.66	1.35	1.52
1	D	634	GLU	CB-CG	-8.66	1.35	1.52
1	F	634	GLU	CB-CG	-8.66	1.35	1.52
1	С	591	GLU	CB-CG	-8.65	1.35	1.52
1	Ε	591	GLU	CB-CG	-8.64	1.35	1.52
1	Ε	634	GLU	CB-CG	-8.63	1.35	1.52
1	D	676	GLU	CG-CD	-8.62	1.39	1.51
1	F	676	GLU	CG-CD	-8.62	1.39	1.51
1	Ε	676	GLU	CG-CD	-8.61	1.39	1.51
1	В	676	GLU	CG-CD	-8.59	1.39	1.51
1	С	676	GLU	CG-CD	-8.59	1.39	1.51
1	G	676	GLU	CG-CD	-8.57	1.39	1.51
1	А	676	GLU	CG-CD	-8.55	1.39	1.51
1	F	609	TYR	CD2-CE2	-8.46	1.26	1.39
1	D	609	TYR	CD2-CE2	-8.45	1.26	1.39
1	В	582	VAL	CB-CG2	-8.43	1.35	1.52
1	D	582	VAL	CB-CG2	-8.43	1.35	1.52
1	А	609	TYR	CD2-CE2	-8.43	1.26	1.39
1	Е	582	VAL	CB-CG2	-8.42	1.35	1.52
1	G	582	VAL	CB-CG2	-8.42	1.35	1.52
1	F	582	VAL	CB-CG2	-8.42	1.35	1.52
1	С	582	VAL	CB-CG2	-8.41	1.35	1.52
1	C	609	TYR	CD2-CE2	-8.41	1.26	1.39
1	E	609	TYR	CD2-CE2	-8.41	1.26	1.39
1	В	609	TYR	CD2-CE2	-8.40	1.26	1.39
1	G	609	TYR	CD2-CE2	-8.39	1.26	1.39
1	A	582	VAL	CB-CG2	-8.38	1.35	1.52



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Е	564	GLU	CB-CG	-8.34	1.36	1.52
1	F	564	GLU	CB-CG	-8.33	1.36	1.52
1	С	564	GLU	CB-CG	-8.32	1.36	1.52
1	А	581	CYS	CB-SG	-8.32	1.68	1.82
1	D	564	GLU	CB-CG	-8.31	1.36	1.52
1	А	564	GLU	CB-CG	-8.31	1.36	1.52
1	В	581	CYS	CB-SG	-8.30	1.68	1.82
1	G	564	GLU	CB-CG	-8.29	1.36	1.52
1	С	581	CYS	CB-SG	-8.28	1.68	1.82
1	Е	581	CYS	CB-SG	-8.27	1.68	1.82
1	В	564	GLU	CB-CG	-8.27	1.36	1.52
1	D	581	CYS	CB-SG	-8.27	1.68	1.82
1	F	581	CYS	CB-SG	-8.26	1.68	1.82
1	F	609	TYR	CD1-CE1	-8.26	1.26	1.39
1	G	581	CYS	CB-SG	-8.25	1.68	1.82
1	С	609	TYR	CD1-CE1	-8.23	1.26	1.39
1	В	609	TYR	CD1-CE1	-8.22	1.27	1.39
1	G	609	TYR	CD1-CE1	-8.22	1.27	1.39
1	А	609	TYR	CD1-CE1	-8.20	1.27	1.39
1	Е	609	TYR	CD1-CE1	-8.19	1.27	1.39
1	D	609	TYR	CD1-CE1	-8.17	1.27	1.39
1	С	655	GLU	CB-CG	-8.13	1.36	1.52
1	В	655	GLU	CB-CG	-8.12	1.36	1.52
1	F	655	GLU	CB-CG	-8.12	1.36	1.52
1	Ε	655	GLU	CB-CG	-8.12	1.36	1.52
1	F	575	TYR	CD1-CE1	-8.12	1.27	1.39
1	D	655	GLU	CB-CG	-8.11	1.36	1.52
1	А	655	GLU	CB-CG	-8.11	1.36	1.52
1	С	575	TYR	CD1-CE1	-8.11	1.27	1.39
1	G	655	GLU	CB-CG	-8.11	1.36	1.52
1	В	575	TYR	CD1-CE1	-8.10	1.27	1.39
1	F	610	TYR	CD1-CE1	-8.09	1.27	1.39
1	D	575	TYR	CD1-CE1	-8.09	1.27	1.39
1	А	575	TYR	CD1-CE1	-8.08	1.27	1.39
1	G	575	TYR	CD1-CE1	-8.07	1.27	1.39
1	Е	575	TYR	CD1-CE1	-8.07	1.27	1.39
1	А	610	TYR	CD1-CE1	-8.05	1.27	1.39
1	С	610	TYR	CD1-CE1	-8.01	1.27	1.39
1	G	610	TYR	CD1-CE1	-7.99	1.27	1.39
1	В	610	TYR	CD1-CE1	-7.98	1.27	1.39
1	D	610	TYR	CD1-CE1	-7.93	1.27	1.39
1	$\mathbf{E}$	610	$\perp TYR$	CD1-CE1	-7.92	1.27	1.39



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	С	698	GLU	CB-CG	-7.71	1.37	1.52
1	В	698	GLU	CB-CG	-7.69	1.37	1.52
1	Е	698	GLU	CB-CG	-7.69	1.37	1.52
1	А	698	GLU	CB-CG	-7.68	1.37	1.52
1	F	698	GLU	CB-CG	-7.68	1.37	1.52
1	G	698	GLU	CB-CG	-7.68	1.37	1.52
1	В	703	ARG	CG-CD	-7.67	1.32	1.51
1	Е	703	ARG	CG-CD	-7.67	1.32	1.51
1	А	703	ARG	CG-CD	-7.66	1.32	1.51
1	D	698	GLU	CB-CG	-7.65	1.37	1.52
1	D	703	ARG	CG-CD	-7.65	1.32	1.51
1	G	606	GLU	CB-CG	-7.64	1.37	1.52
1	F	703	ARG	CG-CD	-7.63	1.32	1.51
1	G	703	ARG	CG-CD	-7.62	1.32	1.51
1	Е	606	GLU	CB-CG	-7.61	1.37	1.52
1	С	703	ARG	CG-CD	-7.61	1.32	1.51
1	D	606	GLU	CB-CG	-7.60	1.37	1.52
1	F	606	GLU	CB-CG	-7.60	1.37	1.52
1	С	606	GLU	CB-CG	-7.60	1.37	1.52
1	В	606	GLU	CB-CG	-7.59	1.37	1.52
1	А	606	GLU	CB-CG	-7.57	1.37	1.52
1	D	715	GLU	CB-CG	-7.51	1.37	1.52
1	А	715	GLU	CB-CG	-7.51	1.37	1.52
1	Ε	715	GLU	CB-CG	-7.50	1.37	1.52
1	G	715	GLU	CB-CG	-7.50	1.38	1.52
1	В	715	GLU	CB-CG	-7.47	1.38	1.52
1	F	715	GLU	CB-CG	-7.47	1.38	1.52
1	С	715	GLU	CB-CG	-7.47	1.38	1.52
1	D	582	VAL	CB-CG1	-7.36	1.37	1.52
1	E	582	VAL	CB-CG1	-7.36	1.37	1.52
1	G	582	VAL	CB-CG1	-7.35	1.37	1.52
1	D	575	TYR	CE2-CZ	-7.35	1.28	1.38
1	E	575	TYR	CE2-CZ	-7.33	1.29	1.38
1	F	582	VAL	CB-CG1	-7.33	1.37	1.52
1	G	575	TYR	CE2-CZ	-7.33	1.29	1.38
1	С	575	TYR	CE2-CZ	-7.33	1.29	1.38
1	В	582	VAL	CB-CG1	-7.33	1.37	1.52
1	A	575	TYR	CE2-CZ	-7.31	1.29	1.38
1	A	582	VAL	CB-CG1	-7.30	1.37	1.52
1	С	582	VAL	CB-CG1	-7.29	1.37	1.52
1	B	575	TYR	CE2-CZ	-7.29	1.29	1.38
1	C	602	LYS	CB-CG	-7.28	1.32	1.52



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	В	602	LYS	CB-CG	-7.26	1.32	1.52
1	Е	602	LYS	CB-CG	-7.26	1.32	1.52
1	F	575	TYR	CE2-CZ	-7.25	1.29	1.38
1	G	602	LYS	CB-CG	-7.25	1.32	1.52
1	Е	695	GLU	CB-CG	-7.25	1.38	1.52
1	F	602	LYS	CB-CG	-7.24	1.32	1.52
1	D	602	LYS	CB-CG	-7.24	1.33	1.52
1	Е	608	VAL	CB-CG2	-7.24	1.37	1.52
1	С	695	GLU	CB-CG	-7.24	1.38	1.52
1	F	608	VAL	CB-CG2	-7.24	1.37	1.52
1	А	651	GLU	CB-CG	-7.23	1.38	1.52
1	D	651	GLU	CB-CG	-7.23	1.38	1.52
1	А	602	LYS	CB-CG	-7.23	1.33	1.52
1	А	695	GLU	CB-CG	-7.22	1.38	1.52
1	G	695	GLU	CB-CG	-7.22	1.38	1.52
1	С	651	GLU	CB-CG	-7.22	1.38	1.52
1	Е	651	GLU	CB-CG	-7.21	1.38	1.52
1	G	651	GLU	CB-CG	-7.21	1.38	1.52
1	F	695	GLU	CB-CG	-7.21	1.38	1.52
1	В	651	GLU	CB-CG	-7.21	1.38	1.52
1	D	695	GLU	CB-CG	-7.20	1.38	1.52
1	В	695	GLU	CB-CG	-7.19	1.38	1.52
1	В	608	VAL	CB-CG2	-7.19	1.37	1.52
1	D	608	VAL	CB-CG2	-7.19	1.37	1.52
1	G	608	VAL	CB-CG2	-7.19	1.37	1.52
1	С	608	VAL	CB-CG2	-7.18	1.37	1.52
1	А	608	VAL	CB-CG2	-7.18	1.37	1.52
1	F	651	GLU	CB-CG	-7.16	1.38	1.52
1	С	609	TYR	CE1-CZ	-7.15	1.29	1.38
1	G	609	TYR	CE1-CZ	-7.14	1.29	1.38
1	Е	609	TYR	CE1-CZ	-7.14	1.29	1.38
1	Е	676	GLU	CB-CG	-7.13	1.38	1.52
1	D	676	GLU	CB-CG	-7.12	1.38	1.52
1	А	676	GLU	CB-CG	-7.12	1.38	1.52
1	В	609	TYR	CE1-CZ	-7.12	1.29	1.38
1	А	609	TYR	CE1-CZ	-7.12	1.29	1.38
1	G	676	GLU	CB-CG	-7.11	1.38	1.52
1	В	676	GLU	CB-CG	-7.11	1.38	1.52
1	С	676	GLU	CB-CG	-7.10	1.38	1.52
1	D	609	TYR	CE1-CZ	-7.10	1.29	1.38
1	F	609	TYR	CE1-CZ	-7.09	1.29	1.38
1	В	602	LYS	CD-CE	-7.07	1.33	1.51



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	676	GLU	CB-CG	-7.07	1.38	1.52
1	G	602	LYS	CD-CE	-7.06	1.33	1.51
1	D	602	LYS	CD-CE	-7.05	1.33	1.51
1	А	602	LYS	CD-CE	-7.04	1.33	1.51
1	F	602	LYS	CD-CE	-7.04	1.33	1.51
1	Е	602	LYS	CD-CE	-7.04	1.33	1.51
1	С	602	LYS	CD-CE	-7.03	1.33	1.51
1	D	575	TYR	CD2-CE2	-6.91	1.28	1.39
1	В	575	TYR	CD2-CE2	-6.91	1.28	1.39
1	G	575	TYR	CD2-CE2	-6.90	1.28	1.39
1	Е	575	TYR	CD2-CE2	-6.90	1.29	1.39
1	С	575	TYR	CD2-CE2	-6.88	1.29	1.39
1	F	575	TYR	CD2-CE2	-6.86	1.29	1.39
1	А	575	TYR	CD2-CE2	-6.84	1.29	1.39
1	Е	634	GLU	CG-CD	-6.70	1.42	1.51
1	С	634	GLU	CG-CD	-6.68	1.42	1.51
1	G	634	GLU	CG-CD	-6.68	1.42	1.51
1	В	634	GLU	CG-CD	-6.65	1.42	1.51
1	D	634	GLU	CG-CD	-6.65	1.42	1.51
1	А	634	GLU	CG-CD	-6.64	1.42	1.51
1	D	631	GLU	CB-CG	-6.63	1.39	1.52
1	F	634	GLU	CG-CD	-6.62	1.42	1.51
1	G	631	GLU	CB-CG	-6.62	1.39	1.52
1	В	631	GLU	CB-CG	-6.59	1.39	1.52
1	Е	631	GLU	CB-CG	-6.59	1.39	1.52
1	F	631	GLU	CB-CG	-6.58	1.39	1.52
1	С	631	GLU	CB-CG	-6.57	1.39	1.52
1	А	631	GLU	CB-CG	-6.56	1.39	1.52
1	С	721	TYR	CD2-CE2	-6.55	1.29	1.39
1	А	721	TYR	CD2-CE2	-6.55	1.29	1.39
1	G	652	ARG	CB-CG	-6.54	1.34	1.52
1	F	721	TYR	CD2-CE2	-6.54	1.29	1.39
1	В	652	ARG	CB-CG	-6.53	1.34	1.52
1	С	652	ARG	CB-CG	-6.53	1.34	1.52
1	E	721	TYR	CD2-CE2	-6.53	1.29	1.39
1	E	652	ARG	CB-CG	-6.53	1.34	1.52
1	G	721	TYR	CD2-CE2	-6.53	1.29	1.39
1	D	721	TYR	CD2-CE2	-6.52	1.29	1.39
1	D	652	ARG	CB-CG	-6.51	1.34	1.52
1	F	652	ARG	CB-CG	-6.50	1.34	1.52
1	А	652	ARG	CB-CG	-6.50	1.34	1.52
1	B	721	TYR.	CD2-CE2	-6.47	1.29	1.39



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
1	А	610	TYR	CD2-CE2	-6.39	1.29	1.39
1	G	610	TYR	CD2-CE2	-6.39	1.29	1.39
1	Е	610	TYR	CD2-CE2	-6.34	1.29	1.39
1	С	610	TYR	CD2-CE2	-6.33	1.29	1.39
1	В	610	TYR	CD2-CE2	-6.31	1.29	1.39
1	D	610	TYR	CD2-CE2	-6.30	1.29	1.39
1	F	610	TYR	CD2-CE2	-6.25	1.29	1.39
1	G	599	VAL	CB-CG2	-6.24	1.39	1.52
1	Ε	599	VAL	CB-CG2	-6.23	1.39	1.52
1	F	599	VAL	CB-CG2	-6.22	1.39	1.52
1	С	599	VAL	CB-CG2	-6.22	1.39	1.52
1	В	599	VAL	CB-CG2	-6.21	1.39	1.52
1	А	599	VAL	CB-CG2	-6.19	1.39	1.52
1	D	599	VAL	CB-CG2	-6.18	1.39	1.52
1	А	599	VAL	CB-CG1	-6.09	1.40	1.52
1	В	614	VAL	CB-CG2	-6.07	1.40	1.52
1	С	614	VAL	CB-CG2	-6.07	1.40	1.52
1	D	614	VAL	CB-CG2	-6.07	1.40	1.52
1	Е	614	VAL	CB-CG2	-6.07	1.40	1.52
1	А	614	VAL	CB-CG2	-6.07	1.40	1.52
1	G	614	VAL	CB-CG2	-6.06	1.40	1.52
1	Е	599	VAL	CB-CG1	-6.06	1.40	1.52
1	В	599	VAL	CB-CG1	-6.06	1.40	1.52
1	С	599	VAL	CB-CG1	-6.05	1.40	1.52
1	F	614	VAL	CB-CG2	-6.04	1.40	1.52
1	G	599	VAL	CB-CG1	-6.04	1.40	1.52
1	D	599	VAL	CB-CG1	-6.04	1.40	1.52
1	F	599	VAL	CB-CG1	-6.03	1.40	1.52
1	G	592	GLU	CB-CG	-5.99	1.40	1.52
1	D	592	GLU	CB-CG	-5.99	1.40	1.52
1	D	652	ARG	CG-CD	-5.98	1.37	1.51
1	А	652	ARG	CG-CD	-5.97	1.37	1.51
1	G	652	ARG	CG-CD	-5.97	1.37	1.51
1	С	592	GLU	CB-CG	-5.95	1.40	1.52
1	G	656	TYR	CD2-CE2	-5.95	1.30	1.39
1	B	652	ARG	CG-CD	-5.95	1.37	1.51
1	С	652	ARG	CG-CD	-5.95	1.37	1.51
1	A	592	GLU	CB-CG	-5.94	1.40	1.52
1	E	592	GLU	CB-CG	-5.94	1.40	1.52
1	Е	652	ARG	CG-CD	-5.94	1.37	1.51
1	В	579	ASP	CB-CG	-5.94	1.39	1.51
1	Е	602	LYS	CG-CD	-5.93	1.32	1.52



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	625	ARG	CZ-NH1	-5.93	1.25	1.33
1	F	592	GLU	CB-CG	-5.93	1.40	1.52
1	F	652	ARG	CG-CD	-5.93	1.37	1.51
1	В	592	GLU	CB-CG	-5.93	1.40	1.52
1	F	579	ASP	CB-CG	-5.93	1.39	1.51
1	F	602	LYS	CG-CD	-5.92	1.32	1.52
1	G	579	ASP	CB-CG	-5.92	1.39	1.51
1	D	602	LYS	CG-CD	-5.92	1.32	1.52
1	D	579	ASP	CB-CG	-5.92	1.39	1.51
1	С	602	LYS	CG-CD	-5.92	1.32	1.52
1	G	602	LYS	CG-CD	-5.92	1.32	1.52
1	С	579	ASP	CB-CG	-5.91	1.39	1.51
1	В	602	LYS	CG-CD	-5.91	1.32	1.52
1	А	579	ASP	CB-CG	-5.91	1.39	1.51
1	С	625	ARG	CZ-NH1	-5.91	1.25	1.33
1	Е	579	ASP	CB-CG	-5.91	1.39	1.51
1	С	590	VAL	CB-CG2	-5.90	1.40	1.52
1	В	590	VAL	CB-CG2	-5.89	1.40	1.52
1	А	602	LYS	CG-CD	-5.89	1.32	1.52
1	D	705	GLU	CG-CD	-5.89	1.43	1.51
1	Е	590	VAL	CB-CG2	-5.89	1.40	1.52
1	Е	625	ARG	CZ-NH1	-5.89	1.25	1.33
1	А	590	VAL	CB-CG2	-5.88	1.40	1.52
1	G	590	VAL	CB-CG2	-5.88	1.40	1.52
1	F	590	VAL	CB-CG2	-5.88	1.40	1.52
1	В	569	VAL	CB-CG2	-5.88	1.40	1.52
1	D	609	TYR	CE2-CZ	-5.87	1.30	1.38
1	G	625	ARG	CZ-NH1	-5.87	1.25	1.33
1	А	569	VAL	CB-CG2	-5.87	1.40	1.52
1	D	625	ARG	CZ-NH1	-5.87	1.25	1.33
1	E	656	TYR	CD2-CE2	-5.87	1.30	1.39
1	F	664	TRP	CE3-CZ3	-5.87	1.28	1.38
1	A	656	TYR	CD2-CE2	-5.86	1.30	1.39
1	Ε	705	GLU	CG-CD	-5.86	1.43	1.51
1	F	656	TYR	CD2-CE2	-5.86	1.30	1.39
1	E	609	TYR	CE2-CZ	-5.86	1.30	1.38
1	D	590	VAL	CB-CG2	-5.85	1.40	1.52
1	G	705	GLU	CG-CD	-5.85	1.43	1.51
1	В	705	GLU	CG-CD	-5.85	1.43	1.51
1	С	705	GLU	CG-CD	-5.85	1.43	1.51
1	F	625	ARG	CZ-NH1	-5.85	1.25	1.33
1	F	609	TYR	CE2-CZ	-5.85	1.30	1.38



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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	С	609	TYR	CE2-CZ	-5.84	1.30	1.38
1	А	664	TRP	CE3-CZ3	-5.84	1.28	1.38
1	С	569	VAL	CB-CG2	-5.83	1.40	1.52
1	F	705	GLU	CG-CD	-5.83	1.43	1.51
1	F	569	VAL	CB-CG2	-5.83	1.40	1.52
1	С	656	TYR	CD2-CE2	-5.83	1.30	1.39
1	В	664	TRP	CE3-CZ3	-5.83	1.28	1.38
1	D	569	VAL	CB-CG2	-5.83	1.40	1.52
1	G	569	VAL	CB-CG2	-5.83	1.40	1.52
1	G	609	TYR	CE2-CZ	-5.82	1.30	1.38
1	Е	664	TRP	CE3-CZ3	-5.82	1.28	1.38
1	А	609	TYR	CE2-CZ	-5.81	1.30	1.38
1	В	656	TYR	CD2-CE2	-5.81	1.30	1.39
1	В	625	ARG	CZ-NH1	-5.81	1.25	1.33
1	D	664	TRP	CE3-CZ3	-5.81	1.28	1.38
1	С	664	TRP	CE3-CZ3	-5.80	1.28	1.38
1	D	721	TYR	CD1-CE1	-5.80	1.30	1.39
1	А	721	TYR	CD1-CE1	-5.80	1.30	1.39
1	Е	569	VAL	CB-CG2	-5.80	1.40	1.52
1	G	664	TRP	CE3-CZ3	-5.80	1.28	1.38
1	С	695	GLU	CG-CD	-5.80	1.43	1.51
1	D	656	TYR	CD2-CE2	-5.80	1.30	1.39
1	А	705	GLU	CG-CD	-5.78	1.43	1.51
1	В	609	TYR	CE2-CZ	-5.78	1.31	1.38
1	G	721	TYR	CD1-CE1	-5.78	1.30	1.39
1	С	591	GLU	CD-OE1	-5.77	1.19	1.25
1	А	695	GLU	CG-CD	-5.77	1.43	1.51
1	А	591	GLU	CD-OE1	-5.77	1.19	1.25
1	Е	695	GLU	CG-CD	-5.76	1.43	1.51
1	G	591	GLU	CD-OE1	-5.76	1.19	1.25
1	В	695	GLU	CG-CD	-5.76	1.43	1.51
1	В	721	TYR	CD1-CE1	-5.76	1.30	1.39
1	Е	721	TYR	CD1-CE1	-5.76	1.30	1.39
1	G	695	GLU	CG-CD	-5.76	1.43	1.51
1	F	695	GLU	CG-CD	-5.75	1.43	1.51
1	F	591	GLU	CD-OE1	-5.75	1.19	1.25
1	С	721	TYR	CD1-CE1	-5.74	1.30	1.39
1	D	591	GLU	CD-OE1	-5.74	1.19	1.25
1	D	695	GLU	CG-CD	-5.74	1.43	1.51
1	F	721	TYR	CD1-CE1	-5.74	1.30	1.39

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VAL

GLU

CB-CG2

CD-OE1

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-5.73

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	577	VAL	CB-CG2	-5.72	1.40	1.52
1	С	577	VAL	CB-CG2	-5.71	1.40	1.52
1	G	577	VAL	CB-CG2	-5.71	1.40	1.52
1	А	577	VAL	CB-CG2	-5.70	1.40	1.52
1	F	626	SER	CB-OG	-5.70	1.34	1.42
1	В	577	VAL	CB-CG2	-5.70	1.40	1.52
1	В	591	GLU	CD-OE1	-5.69	1.19	1.25
1	С	626	SER	CB-OG	-5.69	1.34	1.42
1	G	671	VAL	CB-CG2	-5.68	1.41	1.52
1	D	577	VAL	CB-CG2	-5.68	1.41	1.52
1	А	626	SER	CB-OG	-5.68	1.34	1.42
1	F	671	VAL	CB-CG2	-5.67	1.41	1.52
1	С	671	VAL	CB-CG2	-5.65	1.41	1.52
1	G	626	SER	CB-OG	-5.65	1.34	1.42
1	D	626	SER	CB-OG	-5.65	1.34	1.42
1	Ε	671	VAL	CB-CG2	-5.65	1.41	1.52
1	D	671	VAL	CB-CG2	-5.64	1.41	1.52
1	Ε	626	SER	CB-OG	-5.64	1.34	1.42
1	А	671	VAL	CB-CG2	-5.62	1.41	1.52
1	В	671	VAL	CB-CG2	-5.62	1.41	1.52
1	А	568	PHE	CD1-CE1	-5.59	1.28	1.39
1	D	568	PHE	CD1-CE1	-5.59	1.28	1.39
1	В	626	SER	CB-OG	-5.59	1.34	1.42
1	F	568	PHE	CD1-CE1	-5.58	1.28	1.39
1	С	568	PHE	CD1-CE1	-5.58	1.28	1.39
1	G	575	TYR	CE1-CZ	-5.54	1.31	1.38
1	В	568	PHE	CD1-CE1	-5.54	1.28	1.39
1	G	568	PHE	CD1-CE1	-5.54	1.28	1.39
1	E	568	PHE	CD1-CE1	-5.53	1.28	1.39
1	Е	575	TYR	CE1-CZ	-5.53	1.31	1.38
1	F	575	TYR	CE1-CZ	-5.51	1.31	1.38
1	A	575	TYR	CE1-CZ	-5.49	1.31	1.38
1	В	575	TYR	CE1-CZ	-5.47	1.31	1.38
1	С	575	TYR	CE1-CZ	-5.47	1.31	1.38
1	D	575	TYR	CE1-CZ	-5.46	1.31	1.38
1	G	673	LYS	CB-CG	-5.41	1.38	1.52
	В	673	LYS	CB-CG	-5.40	1.38	1.52
1	A	673	LYS	CB-CG	-5.40	1.38	1.52
1	G	568	PHE	CD2-CE2	-5.39	1.28	1.39
1	F	568	PHE	CD2-CE2	-5.39	1.28	1.39
1	C	568	PHE	CD2-CE2	-5.39	1.28	1.39
1	C	673	LYS	CB-CG	-5.39	1.38	1.52



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Е	568	PHE	CD2-CE2	-5.39	1.28	1.39
1	Е	670	VAL	CB-CG1	-5.39	1.41	1.52
1	А	568	PHE	CD2-CE2	-5.39	1.28	1.39
1	В	568	PHE	CD2-CE2	-5.39	1.28	1.39
1	D	568	PHE	CD2-CE2	-5.38	1.28	1.39
1	F	673	LYS	CB-CG	-5.38	1.38	1.52
1	Е	673	LYS	CB-CG	-5.38	1.38	1.52
1	G	670	VAL	CB-CG1	-5.38	1.41	1.52
1	D	673	LYS	CB-CG	-5.37	1.38	1.52
1	А	670	VAL	CB-CG1	-5.37	1.41	1.52
1	G	703	ARG	CB-CG	-5.36	1.38	1.52
1	С	670	VAL	CB-CG1	-5.36	1.41	1.52
1	В	670	VAL	CB-CG1	-5.36	1.41	1.52
1	F	672	VAL	CB-CG2	-5.35	1.41	1.52
1	С	703	ARG	CB-CG	-5.35	1.38	1.52
1	D	670	VAL	CB-CG1	-5.35	1.41	1.52
1	F	703	ARG	CB-CG	-5.34	1.38	1.52
1	А	703	ARG	CB-CG	-5.34	1.38	1.52
1	D	703	ARG	CB-CG	-5.33	1.38	1.52
1	В	703	ARG	CB-CG	-5.33	1.38	1.52
1	С	672	VAL	CB-CG2	-5.33	1.41	1.52
1	Е	703	ARG	CB-CG	-5.33	1.38	1.52
1	G	672	VAL	CB-CG2	-5.33	1.41	1.52
1	F	606	GLU	CD-OE1	-5.32	1.19	1.25
1	В	614	VAL	CB-CG1	-5.32	1.41	1.52
1	F	670	VAL	CB-CG1	-5.32	1.41	1.52
1	G	590	VAL	CB-CG1	-5.32	1.41	1.52
1	D	672	VAL	CB-CG2	-5.31	1.41	1.52
1	А	614	VAL	CB-CG1	-5.31	1.41	1.52
1	А	672	VAL	CB-CG2	-5.31	1.41	1.52
1	С	590	VAL	CB-CG1	-5.31	1.41	1.52
1	Е	606	GLU	CD-OE1	-5.31	1.19	1.25
1	A	590	VAL	CB-CG1	-5.31	1.41	1.52
1	D	590	VAL	CB-CG1	-5.31	1.41	1.52
1	F	590	VAL	CB-CG1	-5.31	1.41	1.52
1	Е	590	VAL	CB-CG1	-5.31	1.41	1.52
1	E	567	VAL	CB-CG1	-5.30	1.41	1.52
1	F	567	VAL	CB-CG1	-5.30	1.41	1.52
1	В	590	VAL	CB-CG1	-5.30	1.41	1.52

VAL

VAL

VAL

614

614

672

С

Е

В

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CB-CG1

CB-CG1

CB-CG2

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-5.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	614	VAL	CB-CG1	-5.29	1.41	1.52
1	G	614	VAL	CB-CG1	-5.29	1.41	1.52
1	А	567	VAL	CB-CG1	-5.29	1.41	1.52
1	D	567	VAL	CB-CG1	-5.28	1.41	1.52
1	Е	672	VAL	CB-CG2	-5.27	1.41	1.52
1	С	567	VAL	CB-CG1	-5.27	1.41	1.52
1	В	567	VAL	CB-CG1	-5.26	1.41	1.52
1	F	614	VAL	CB-CG1	-5.26	1.41	1.52
1	G	567	VAL	CB-CG1	-5.26	1.41	1.52
1	А	606	GLU	CD-OE1	-5.23	1.19	1.25
1	С	606	GLU	CD-OE1	-5.23	1.19	1.25
1	В	606	GLU	CD-OE1	-5.22	1.20	1.25
1	D	606	GLU	CD-OE1	-5.21	1.20	1.25
1	G	606	GLU	CD-OE1	-5.21	1.20	1.25
1	Е	569	VAL	CB-CG1	-5.18	1.42	1.52
1	В	623	TYR	CD1-CE1	-5.18	1.31	1.39
1	А	623	TYR	CD1-CE1	-5.18	1.31	1.39
1	G	625	ARG	C-N	-5.17	1.22	1.34
1	Е	623	TYR	CD1-CE1	-5.17	1.31	1.39
1	А	625	ARG	C-N	-5.17	1.22	1.34
1	В	625	ARG	C-N	-5.17	1.22	1.34
1	D	625	ARG	C-N	-5.17	1.22	1.34
1	Ε	625	ARG	C-N	-5.17	1.22	1.34
1	F	597	THR	CB-CG2	-5.17	1.35	1.52
1	В	569	VAL	CB-CG1	-5.17	1.42	1.52
1	D	623	TYR	CD1-CE1	-5.17	1.31	1.39
1	Е	597	THR	CB-CG2	-5.16	1.35	1.52
1	F	625	ARG	C-N	-5.16	1.22	1.34
1	С	625	ARG	C-N	-5.16	1.22	1.34
1	F	623	TYR	CD1-CE1	-5.16	1.31	1.39
1	А	569	VAL	CB-CG1	-5.16	1.42	1.52
1	В	597	THR	CB-CG2	-5.16	1.35	1.52
1	D	569	VAL	CB-CG1	-5.16	1.42	1.52
1	G	597	THR	CB-CG2	-5.16	1.35	1.52
1	G	569	VAL	CB-CG1	-5.15	1.42	1.52
1	С	569	VAL	CB-CG1	-5.15	1.42	1.52
1	А	597	THR	CB-CG2	-5.15	1.35	1.52
1	С	597	THR	CB-CG2	-5.15	1.35	1.52
1	G	623	TYR	CD1-CE1	-5.15	1.31	1.39
1	F	569	VAL	CB-CG1	-5.14	1.42	1.52
1	С	623	TYR	CD1-CE1	-5.14	1.31	1.39
1	D	597	L THR	CB-CG2	-5.14	1.35	1.52



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	608	VAL	CB-CG1	-5.12	1.42	1.52
1	G	682	LYS	CB-CG	-5.12	1.38	1.52
1	В	608	VAL	CB-CG1	-5.11	1.42	1.52
1	F	608	VAL	CB-CG1	-5.11	1.42	1.52
1	D	608	VAL	CB-CG1	-5.11	1.42	1.52
1	А	682	LYS	CB-CG	-5.11	1.38	1.52
1	А	608	VAL	CB-CG1	-5.10	1.42	1.52
1	Е	608	VAL	CB-CG1	-5.10	1.42	1.52
1	С	608	VAL	CB-CG1	-5.09	1.42	1.52
1	Е	682	LYS	CB-CG	-5.09	1.38	1.52
1	С	682	LYS	CB-CG	-5.08	1.38	1.52
1	F	682	LYS	CB-CG	-5.08	1.38	1.52
1	Е	623	TYR	CE2-CZ	-5.07	1.31	1.38
1	D	682	LYS	CB-CG	-5.07	1.38	1.52
1	А	574	PRO	CB-CG	-5.06	1.24	1.50
1	Е	574	PRO	CB-CG	-5.06	1.24	1.50
1	F	574	PRO	CB-CG	-5.06	1.24	1.50
1	F	645	LYS	CB-CG	-5.06	1.38	1.52
1	В	574	PRO	CB-CG	-5.06	1.24	1.50
1	В	682	LYS	CB-CG	-5.05	1.39	1.52
1	F	575	TYR	CZ-OH	-5.05	1.29	1.37
1	В	577	VAL	CB-CG1	-5.05	1.42	1.52
1	D	574	PRO	CB-CG	-5.05	1.24	1.50
1	С	574	PRO	CB-CG	-5.05	1.24	1.50
1	А	575	TYR	CZ-OH	-5.05	1.29	1.37
1	А	623	TYR	CE2-CZ	-5.04	1.31	1.38
1	G	623	TYR	CE2-CZ	-5.04	1.31	1.38
1	G	645	LYS	CB-CG	-5.04	1.39	1.52
1	С	575	TYR	CZ-OH	-5.04	1.29	1.37
1	G	574	PRO	CB-CG	-5.04	1.24	1.50
1	G	575	TYR	CZ-OH	-5.04	1.29	1.37
1	D	575	TYR	CZ-OH	-5.04	1.29	1.37
1	G	670	VAL	CB-CG2	-5.04	1.42	1.52
1	F	577	VAL	CB-CG1	-5.03	1.42	1.52
1	D	670	VAL	CB-CG2	-5.03	1.42	1.52
1	G	577	VAL	CB-CG1	-5.03	1.42	1.52
1	В	575	TYR	CZ-OH	-5.03	1.29	1.37
1	D	645	LYS	CB-CG	-5.03	1.39	1.52
1	A	577	VAL	CB-CG1	-5.03	1.42	1.52
1	A	645	LYS	CB-CG	-5.03	1.39	1.52
1	E	645	LYS	CB-CG	-5.02	1.39	1.52
1	F,	623	I TYR	CE2-CZ	-5.02	1.32	1.38



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	В	645	LYS	CB-CG	-5.02	1.39	1.52
1	D	577	VAL	CB-CG1	-5.02	1.42	1.52
1	С	577	VAL	CB-CG1	-5.02	1.42	1.52
1	F	670	VAL	CB-CG2	-5.02	1.42	1.52
1	С	645	LYS	CB-CG	-5.02	1.39	1.52
1	С	670	VAL	CB-CG2	-5.02	1.42	1.52
1	Е	577	VAL	CB-CG1	-5.02	1.42	1.52
1	D	623	TYR	CE2-CZ	-5.01	1.32	1.38
1	F	568	PHE	CE2-CZ	-5.01	1.27	1.37
1	Ē	575	TYR	CZ-OH	-5.00	1.29	1.37
1	С	623	TYR	CE2-CZ	-5.00	1.32	1.38

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Е	531	LEU	CA-CB-CG	6.99	131.38	115.30
1	В	531	LEU	CA-CB-CG	6.98	131.36	115.30
1	D	531	LEU	CA-CB-CG	6.98	131.36	115.30
1	А	531	LEU	CA-CB-CG	6.98	131.36	115.30
1	G	531	LEU	CA-CB-CG	6.98	131.35	115.30
1	F	531	LEU	CA-CB-CG	6.97	131.32	115.30
1	С	531	LEU	CA-CB-CG	6.96	131.31	115.30
1	В	703	ARG	NE-CZ-NH1	-6.66	116.97	120.30
1	F	703	ARG	NE-CZ-NH1	-6.64	116.98	120.30
1	А	703	ARG	NE-CZ-NH1	-6.63	116.99	120.30
1	Е	703	ARG	NE-CZ-NH1	-6.62	116.99	120.30
1	D	703	ARG	NE-CZ-NH1	-6.59	117.00	120.30
1	G	703	ARG	NE-CZ-NH1	-6.55	117.02	120.30
1	D	445	PRO	N-CA-CB	6.55	111.16	103.30
1	В	445	PRO	N-CA-CB	6.54	111.15	103.30
1	F	445	PRO	N-CA-CB	6.53	111.14	103.30
1	С	445	PRO	N-CA-CB	6.53	111.13	103.30
1	А	445	PRO	N-CA-CB	6.52	111.12	103.30
1	Е	445	PRO	N-CA-CB	6.52	111.12	103.30
1	G	445	PRO	N-CA-CB	6.51	111.12	103.30
1	С	703	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	G	595	LEU	CB-CG-CD2	-6.20	100.46	111.00
1	Е	595	LEU	CB-CG-CD2	-6.20	100.47	111.00
1	D	595	LEU	CB-CG-CD2	-6.19	100.48	111.00
1	В	595	LEU	CB-CG-CD2	-6.19	100.48	111.00
1	С	595	LEU	CB-CG-CD2	-6.18	100.49	111.00
1	F	595	LEU	CB-CG-CD2	-6.18	100.49	111.00



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	595	LEU	CB-CG-CD2	-6.17	100.50	111.00
1	G	701	LEU	CB-CG-CD2	-5.67	101.37	111.00
1	С	701	LEU	CB-CG-CD2	-5.66	101.38	111.00
1	D	701	LEU	CB-CG-CD2	-5.63	101.42	111.00
1	В	701	LEU	CB-CG-CD2	-5.63	101.43	111.00
1	Е	701	LEU	CB-CG-CD2	-5.62	101.44	111.00
1	А	701	LEU	CB-CG-CD2	-5.62	101.44	111.00
1	F	701	LEU	CB-CG-CD2	-5.61	101.47	111.00
1	F	530	LEU	CA-CB-CG	5.55	128.07	115.30
1	А	530	LEU	CA-CB-CG	5.55	128.07	115.30
1	D	530	LEU	CA-CB-CG	5.55	128.07	115.30
1	G	530	LEU	CA-CB-CG	5.54	128.05	115.30
1	С	530	LEU	CA-CB-CG	5.54	128.04	115.30
1	В	530	LEU	CA-CB-CG	5.54	128.03	115.30
1	Е	530	LEU	CA-CB-CG	5.54	128.03	115.30
1	D	551	LEU	CA-CB-CG	5.47	127.87	115.30
1	Е	551	LEU	CA-CB-CG	5.46	127.87	115.30
1	А	551	LEU	CA-CB-CG	5.46	127.85	115.30
1	G	551	LEU	CA-CB-CG	5.46	127.86	115.30
1	С	551	LEU	CA-CB-CG	5.45	127.83	115.30
1	В	551	LEU	CA-CB-CG	5.44	127.81	115.30
1	F	551	LEU	CA-CB-CG	5.44	127.81	115.30
1	G	589	LEU	CB-CG-CD2	-5.44	101.76	111.00
1	В	589	LEU	CB-CG-CD2	-5.43	101.77	111.00
1	А	589	LEU	CB-CG-CD2	-5.42	101.79	111.00
1	D	589	LEU	CB-CG-CD2	-5.42	101.79	111.00
1	Е	589	LEU	CB-CG-CD2	-5.41	101.80	111.00
1	F	589	LEU	CB-CG-CD2	-5.41	101.80	111.00
1	С	589	LEU	CB-CG-CD2	-5.40	101.82	111.00
1	А	723	LEU	CA-CB-CG	5.31	127.52	115.30
1	В	723	LEU	CA-CB-CG	5.31	127.50	115.30
1	G	723	LEU	CA-CB-CG	5.30	127.49	115.30
1	D	723	LEU	CA-CB-CG	5.30	127.49	115.30
1	Е	723	LEU	CA-CB-CG	5.30	127.49	115.30
1	F	723	LEU	CA-CB-CG	5.29	127.47	115.30
1	С	723	LEU	CA-CB-CG	5.28	127.44	115.30
1	В	576	ASP	CB-CG-OD1	5.28	123.05	118.30
1	Е	576	ASP	CB-CG-OD1	5.26	123.03	118.30
1	C	576	ASP	CB-CG-OD1	5.24	123.01	118.30
1	G	576	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	576	ASP	CB-CG-OD1	5.21	122.99	118.30
1	D	576	ASP	CB-CG-OD1	5.21	122.99	118.30



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Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^{o})$	$Ideal(^{o})$
1	F	576	ASP	CB-CG-OD1	5.20	122.98	118.30

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2123	0	2064	22	0
1	В	2123	0	2064	20	0
1	С	2123	0	2064	21	0
1	D	2123	0	2064	24	0
1	Е	2123	0	2064	21	0
1	F	2123	0	2064	21	0
1	G	2123	0	2064	21	0
All	All	14861	0	14448	138	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 5.

All (138) 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:C:631:GLU:CD	1:C:703:ARG:HD2	2.05	0.77
1:A:631:GLU:CD	1:A:703:ARG:HD2	2.06	0.76
1:B:631:GLU:CD	1:B:703:ARG:HD2	2.06	0.76
1:E:631:GLU:CD	1:E:703:ARG:HD2	2.06	0.76
1:G:631:GLU:CD	1:G:703:ARG:HD2	2.05	0.75
1:D:631:GLU:CD	1:D:703:ARG:HD2	2.05	0.75
1:F:631:GLU:CD	1:F:703:ARG:HD2	2.06	0.75
1:E:506:THR:HG22	1:E:508:THR:H	1.61	0.66
1:A:506:THR:HG22	1:A:508:THR:H	1.61	0.66
1:C:506:THR:HG22	1:C:508:THR:H	1.61	0.65
1:G:506:THR:HG22	1:G:508:THR:H	1.61	0.65
1:D:506:THR:HG22	1:D:508:THR:H	1.61	0.65



	to ac pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:506:THR:HG22	1:B:508:THR:H	1.61	0.65
1:F:506:THR:HG22	1:F:508:THR:H	1.61	0.64
1:G:610:TYR:OH	1:G:615:LEU:HA	2.00	0.62
1:D:610:TYR:OH	1:D:615:LEU:HA	2.00	0.62
1:A:610:TYR:OH	1:A:615:LEU:HA	2.00	0.61
1:F:610:TYR:OH	1:F:615:LEU:HA	2.00	0.61
1:C:610:TYR:OH	1:C:615:LEU:HA	2.00	0.60
1:B:610:TYR:OH	1:B:615:LEU:HA	2.00	0.60
1:E:610:TYR:OH	1:E:615:LEU:HA	2.00	0.60
1:F:631:GLU:OE2	1:F:703:ARG:HD2	2.02	0.60
1:A:631:GLU:OE2	1:A:703:ARG:HD2	2.02	0.60
1:E:631:GLU:OE2	1:E:703:ARG:HD2	2.02	0.60
1:C:631:GLU:OE2	1:C:703:ARG:HD2	2.02	0.60
1:B:631:GLU:OE2	1:B:703:ARG:HD2	2.02	0.60
1:G:631:GLU:OE2	1:G:703:ARG:HD2	2.02	0.59
1:A:631:GLU:OE1	1:A:703:ARG:NE	2.36	0.59
1:B:631:GLU:OE1	1:B:703:ARG:NE	2.36	0.59
1:E:631:GLU:OE1	1:E:703:ARG:NE	2.36	0.59
1:D:631:GLU:OE2	1:D:703:ARG:HD2	2.02	0.58
1:D:631:GLU:OE1	1:D:703:ARG:NE	2.36	0.58
1:F:631:GLU:OE1	1:F:703:ARG:NE	2.36	0.58
1:B:696:ASN:O	1:B:699:ARG:HG2	2.05	0.57
1:E:539:LYS:HD2	1:E:540:VAL:HG13	1.86	0.57
1:C:631:GLU:OE1	1:C:703:ARG:NE	2.36	0.57
1:D:696:ASN:O	1:D:699:ARG:HG2	2.05	0.57
1:E:696:ASN:O	1:E:699:ARG:HG2	2.04	0.57
1:D:539:LYS:HD2	1:D:540:VAL:HG13	1.86	0.57
1:F:539:LYS:HD2	1:F:540:VAL:HG13	1.86	0.57
1:G:631:GLU:OE1	1:G:703:ARG:NE	2.36	0.57
1:G:696:ASN:O	1:G:699:ARG:HG2	2.05	0.57
1:A:539:LYS:HD2	1:A:540:VAL:HG13	1.86	0.56
1:A:696:ASN:O	1:A:699:ARG:HG2	2.05	0.56
1:C:539:LYS:HD2	1:C:540:VAL:HG13	1.86	0.56
1:F:696:ASN:O	1:F:699:ARG:HG2	2.04	0.56
1:G:610:TYR:OH	1:G:615:LEU:HD23	2.06	0.56
1:B:539:LYS:HD2	1:B:540:VAL:HG13	1.86	0.56
1:C:696:ASN:O	1:C:699:ARG:HG2	2.04	0.56
1:D:580:ARG:H	1:D:694:GLN:HE22	1.54	0.56
1:G:539:LYS:HD2	1:G:540:VAL:HG13	1.86	0.56
1:F:610:TYR:OH	1:F:615:LEU:HD23	2.06	0.56
1:E:580:ARG:H	1:E:694:GLN:HE22	1.54	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:580:ARG:H	1:F:694:GLN:HE22	1.53	0.55
1:E:610:TYR:OH	1:E:615:LEU:HD23	2.06	0.55
1:C:580:ARG:H	1:C:694:GLN:HE22	1.54	0.55
1:G:580:ARG:H	1:G:694:GLN:HE22	1.54	0.55
1:A:610:TYR:OH	1:A:615:LEU:HD23	2.06	0.54
1:A:580:ARG:H	1:A:694:GLN:HE22	1.54	0.54
1:B:580:ARG:H	1:B:694:GLN:HE22	1.53	0.54
1:C:610:TYR:OH	1:C:615:LEU:HD23	2.06	0.54
1:D:610:TYR:OH	1:D:615:LEU:HD23	2.06	0.53
1:A:489:VAL:HA	1:A:492:VAL:HG22	1.91	0.53
1:G:489:VAL:HA	1:G:492:VAL:HG22	1.91	0.53
1:B:489:VAL:HA	1:B:492:VAL:HG22	1.91	0.53
1:C:489:VAL:HA	1:C:492:VAL:HG22	1.91	0.52
1:F:489:VAL:HA	1:F:492:VAL:HG22	1.91	0.52
1:E:489:VAL:HA	1:E:492:VAL:HG22	1.91	0.51
1:D:489:VAL:HA	1:D:492:VAL:HG22	1.91	0.51
1:E:610:TYR:OH	1:E:615:LEU:CA	2.59	0.51
1:D:610:TYR:OH	1:D:615:LEU:CA	2.59	0.51
1:F:610:TYR:OH	1:F:615:LEU:CA	2.58	0.51
1:G:610:TYR:OH	1:G:615:LEU:CA	2.58	0.51
1:B:610:TYR:OH	1:B:615:LEU:HD23	2.06	0.51
1:A:610:TYR:OH	1:A:615:LEU:CA	2.59	0.51
1:B:610:TYR:OH	1:B:615:LEU:CA	2.59	0.51
1:C:610:TYR:OH	1:C:615:LEU:CA	2.59	0.51
1:A:558:THR:CG2	1:F:564:GLU:HG2	2.42	0.50
1:A:564:GLU:HG2	1:B:558:THR:CG2	2.42	0.50
1:C:558:THR:CG2	1:G:564:GLU:HG2	2.43	0.49
1:C:564:GLU:HG2	1:D:558:THR:CG2	2.43	0.48
1:D:564:GLU:HG2	1:E:558:THR:CG2	2.43	0.48
1:E:505:ASP:O	1:E:506:THR:OG1	2.32	0.47
1:E:564:GLU:HG2	1:F:558:THR:CG2	2.45	0.47
1:B:564:GLU:HG2	1:G:558:THR:CG2	2.45	0.46
1:D:505:ASP:O	1:D:506:THR:OG1	2.32	0.46
1:C:505:ASP:O	1:C:506:THR:OG1	2.32	0.46
1:A:551:LEU:O	1:A:555:ILE:HG12	2.17	0.46
1:G:551:LEU:O	1:G:555:ILE:HG12	2.17	0.45
1:G:505:ASP:O	1:G:506:THR:OG1	2.32	0.45
1:D:551:LEU:O	1:D:555:ILE:HG12	2.17	0.45
1:E:551:LEU:O	1:E:555:ILE:HG12	2.16	0.45
1:B:505:ASP:O	1:B:506:THR:OG1	2.32	0.45
1:B:546:THR:O	1:B:550:ALA:N	2.50	0.44



	ious puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:551:LEU:O	1:B:555:ILE:HG12	2.17	0.44
1:F:551:LEU:O	1:F:555:ILE:HG12	2.17	0.44
1:C:551:LEU:O	1:C:555:ILE:HG12	2.16	0.44
1:A:546:THR:O	1:A:550:ALA:N	2.50	0.44
1:F:546:THR:O	1:F:550:ALA:N	2.50	0.44
1:D:546:THR:O	1:D:550:ALA:N	2.50	0.44
1:C:546:THR:O	1:C:550:ALA:N	2.50	0.43
1:E:484:ALA:HB2	1:E:525:THR:HG21	2.00	0.43
1:E:546:THR:O	1:E:550:ALA:N	2.50	0.43
1:G:546:THR:O	1:G:550:ALA:N	2.50	0.43
1:D:484:ALA:HB2	1:D:525:THR:HG21	2.00	0.43
1:F:484:ALA:HB2	1:F:525:THR:HG21	2.00	0.43
1:C:484:ALA:HB2	1:C:525:THR:HG21	2.00	0.43
1:G:484:ALA:HB2	1:G:525:THR:HG21	2.00	0.43
1:A:638:SER:HB2	1:A:721:TYR:HA	2.01	0.43
1:F:638:SER:HB2	1:F:721:TYR:HA	2.01	0.43
1:A:484:ALA:HB2	1:A:525:THR:HG21	2.00	0.42
1:E:638:SER:HB2	1:E:721:TYR:HA	2.01	0.42
1:B:484:ALA:HB2	1:B:525:THR:HG21	2.00	0.42
1:D:564:GLU:HG2	1:E:558:THR:HG22	2.02	0.42
1:G:631:GLU:CD	1:G:703:ARG:CD	2.85	0.42
1:C:638:SER:HB2	1:C:721:TYR:HA	2.01	0.42
1:G:638:SER:HB2	1:G:721:TYR:HA	2.01	0.42
1:A:505:ASP:O	1:A:506:THR:OG1	2.32	0.42
1:B:638:SER:HB2	1:B:721:TYR:HA	2.01	0.42
1:A:524:VAL:HA	1:A:527:VAL:HG12	2.02	0.42
1:F:524:VAL:HA	1:F:527:VAL:HG12	2.02	0.42
1:G:524:VAL:HA	1:G:527:VAL:HG12	2.02	0.42
1:B:524:VAL:HA	1:B:527:VAL:HG12	2.02	0.41
1:C:524:VAL:HA	1:C:527:VAL:HG12	2.02	0.41
1:D:638:SER:HB2	1:D:721:TYR:HA	2.01	0.41
1:A:558:THR:HG22	1:F:564:GLU:HG2	2.01	0.41
1:A:564:GLU:HG2	1:B:558:THR:HG22	2.01	0.41
1:D:524:VAL:HA	1:D:527:VAL:HG12	2.02	0.41
1:E:524:VAL:HA	1:E:527:VAL:HG12	2.02	0.41
1:F:507:LYS:HA	1:F:507:LYS:HD2	1.83	0.41
1:C:564:GLU:HG2	1:D:558:THR:HG22	2.03	0.41
1:C:558:THR:HG22	1:G:564:GLU:HG2	2.03	0.41
1:A:631:GLU:HG2	1:A:689:HIS:NE2	2.36	0.41
1:D:631:GLU:HG2	1:D:689:HIS:NE2	2.36	0.41
1:D:545:SER:O	1:D:545:SER:OG	2.37	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:631:GLU:HG2	1:F:689:HIS:NE2	2.36	0.40
1:D:507:LYS:HD2	1:D:507:LYS:HA	1.83	0.40
1:E:631:GLU:HG2	1:E:689:HIS:NE2	2.36	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	Perc	entiles
1	А	275/734~(38%)	257 (94%)	17 (6%)	1 (0%)	34	55
1	В	275/734~(38%)	257~(94%)	17 (6%)	1 (0%)	34	55
1	С	275/734~(38%)	257 (94%)	17 (6%)	1 (0%)	34	55
1	D	275/734~(38%)	257 (94%)	17 (6%)	1 (0%)	34	55
1	Е	275/734~(38%)	257 (94%)	17 (6%)	1 (0%)	34	55
1	F	275/734~(38%)	257 (94%)	17 (6%)	1 (0%)	34	55
1	G	275/734~(38%)	257 (94%)	17 (6%)	1 (0%)	34	55
All	All	1925/5138~(38%)	1799 (94%)	119 (6%)	7 (0%)	38	55

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	445	PRO
1	В	445	PRO
1	С	445	PRO
1	D	445	PRO
1	Е	445	PRO
1	F	445	PRO
1	G	445	PRO



#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	218/657~(33%)	218 (100%)	0	100 100
1	В	218/657~(33%)	218 (100%)	0	100 100
1	С	218/657~(33%)	218 (100%)	0	100 100
1	D	218/657~(33%)	218 (100%)	0	100 100
1	Ε	218/657~(33%)	218 (100%)	0	100 100
1	F	218/657~(33%)	218 (100%)	0	100 100
1	G	218/657~(33%)	218 (100%)	0	100 100
All	All	1526/4599~(33%)	1526 (100%)	0	100 100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	561	ASN
1	А	612	ASN
1	А	660	ASN
1	А	663	HIS
1	А	677	ASN
1	А	679	ASN
1	А	694	GLN
1	В	561	ASN
1	В	612	ASN
1	В	660	ASN
1	В	663	HIS
1	В	677	ASN
1	В	679	ASN
1	В	694	GLN
1	С	561	ASN
1	С	612	ASN
1	С	660	ASN
1	С	663	HIS



Mol	Chain	Res	Type
1	С	677	ASN
1	С	679	ASN
1	С	694	GLN
1	D	561	ASN
1	D	612	ASN
1	D	660	ASN
1	D	663	HIS
1	D	677	ASN
1	D	679	ASN
1	D	694	GLN
1	Е	561	ASN
1	Е	612	ASN
1	Е	660	ASN
1	Е	663	HIS
1	Е	677	ASN
1	Е	679	ASN
1	Е	694	GLN
1	F	561	ASN
1	F	612	ASN
1	F	660	ASN
1	F	663	HIS
1	F	677	ASN
1	F	679	ASN
1	F	694	GLN
1	G	561	ASN
1	G	612	ASN
1	G	660	ASN
1	G	663	HIS
1	G	677	ASN
1	G	679	ASN
1	G	694	GLN

#### 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-36680. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

#### 6.1 Orthogonal projections (i)

#### 6.1.1 Primary map



6.1.2 Raw map



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



#### 6.2 Central slices (i)

#### 6.2.1 Primary map



X Index: 150



Y Index: 150



Z Index: 150

#### 6.2.2 Raw map



X Index: 150

Y Index: 150

Z Index: 150

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: 138



Y Index: 166



Z Index: 126

#### 6.3.2 Raw map



X Index: 138

Y Index: 166



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



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

#### 6.4.1 Primary map



6.4.2 Raw map



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



#### 6.5 Orthogonal surface views (i)

#### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

#### 6.5.2 Raw map



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

#### 6.6 Mask visualisation (i)

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



# 7 Map analysis (i)

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

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



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



#### 7.2 Volume estimate (i)



The volume at the recommended contour level is  $454 \text{ nm}^3$ ; this corresponds to an approximate mass of 410 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 0.365  ${\rm \AA^{-1}}$ 



### 8 Fourier-Shell correlation (i)

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

#### 8.1 FSC (i)



\*Reported resolution corresponds to spatial frequency of 0.365  $\mathrm{\AA^{-1}}$ 



#### 8.2 Resolution estimates (i)

$\begin{bmatrix} Bosolution ostimato (Å) \end{bmatrix}$	Estimation criterion (FSC cut-off)			
Resolution estimate (A)	0.143	0.5	Half-bit	
Reported by author	2.74	-	-	
Author-provided FSC curve	2.74	3.08	2.80	
Unmasked-calculated*	3.11	3.47	3.14	

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.11 differs from the reported value 2.74 by more than 10 %



## 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-36680 and PDB model 8JWE. Per-residue inclusion information can be found in section 3 on page 4.

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



The images above show the 3D surface view of the map at the recommended contour level 0.3 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 (0.3).



#### 9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.



#### 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	
All	0.9260	0.6120	
А	0.9260	0.6130	
В	0.9260	0.6120	
С	0.9250	0.6110	
D	0.9250	0.6120	
Е	0.9260	0.6120	
F	0.9250	0.6110	
G	0.9270	0.6110	

