Full wwPDB EM Validation Report ⓘ

May 14, 2024 – 12:20 am BST

PDB ID	:	6YS8
EMDB ID	:	EMD-10893
Title	:	Structure of GldLM, the proton-powered motor that drives protein transport and gliding motility
Authors	:	Hennell James, R.; Deme, J.C.; Lea, S.M.
Deposited on	:	2020-04-21
Resolution	:	3.90 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:

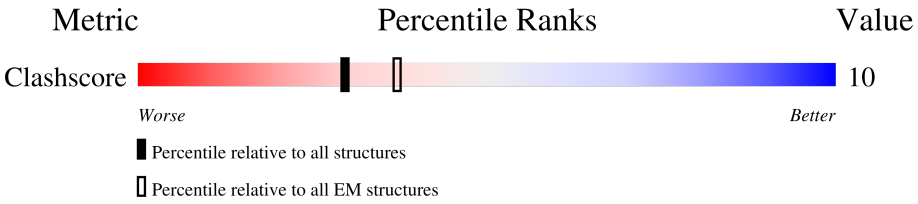
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.90 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

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%

Mol	Chain	Length	Quality of chain
1	A	513	36% 6% 58%
1	B	513	37% 6% 57%
2	C	215	19% 8% 72%
2	D	215	23% 5% 72%
2	E	215	23% 5% 72%
2	F	215	25% • 72%
2	G	215	27% 72%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5624 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 GldM.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	218	Total	C	N	O	S	0	0
			1695	1080	275	333	7		
1	B	219	Total	C	N	O	S	0	0
			1704	1086	277	334	7		

- Molecule 2 is a protein called GldL.

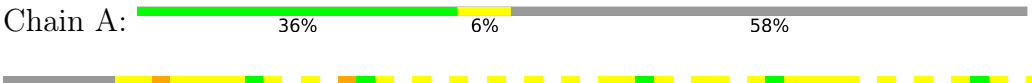
Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	60	Total	C	N	O	S	0	0
			445	299	66	77	3		
2	F	60	Total	C	N	O	S	0	0
			445	299	66	77	3		
2	E	60	Total	C	N	O	S	0	0
			445	299	66	77	3		
2	D	60	Total	C	N	O	S	0	0
			445	299	66	77	3		
2	C	60	Total	C	N	O	S	0	0
			445	299	66	77	3		

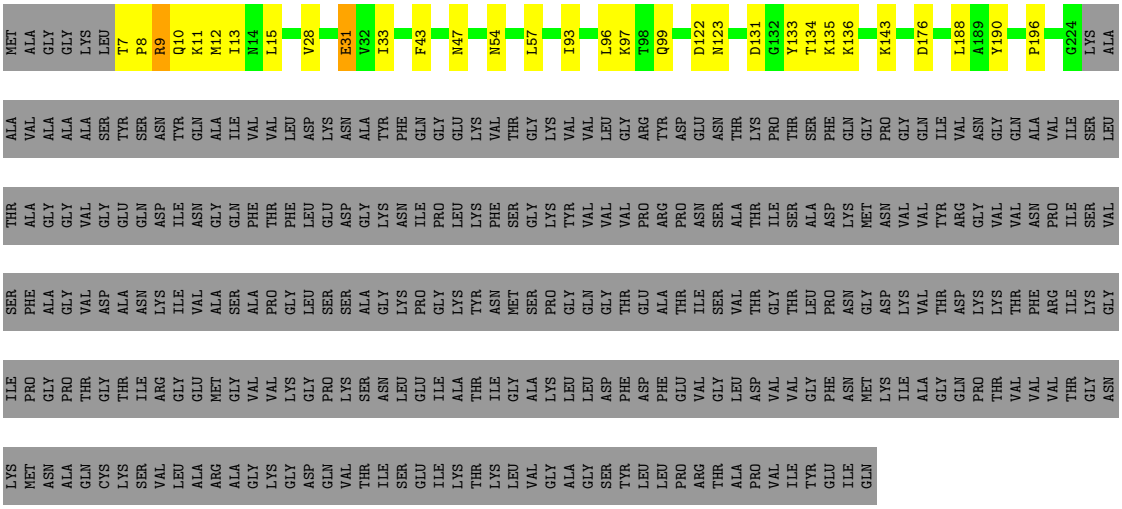
3 Residue-property plots (i)

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. 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. 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: GldM

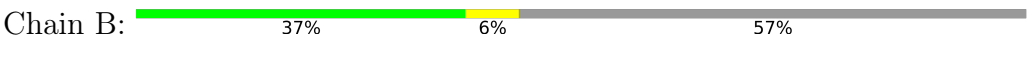
Chain A:

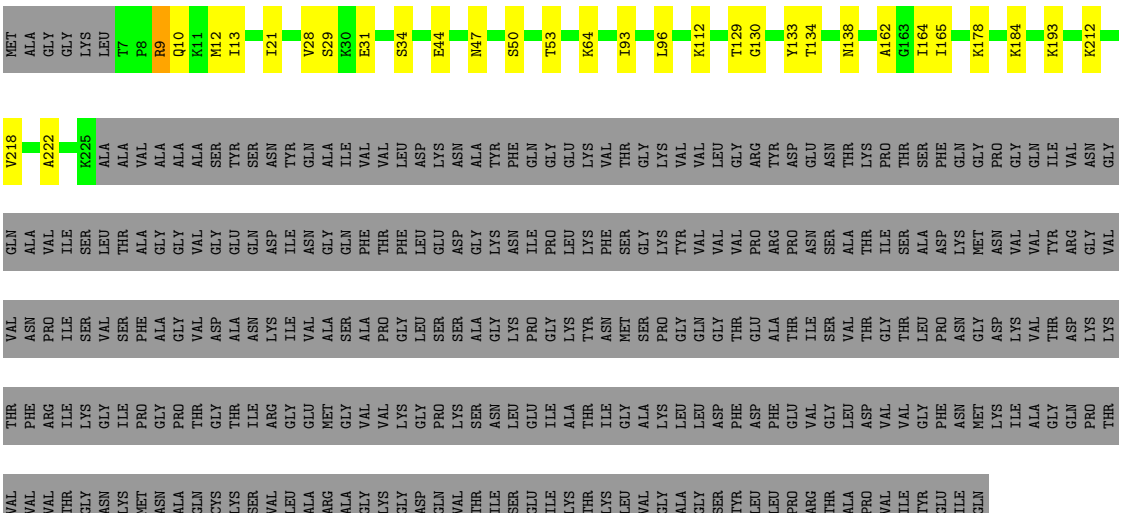




- Molecule 1: GldM

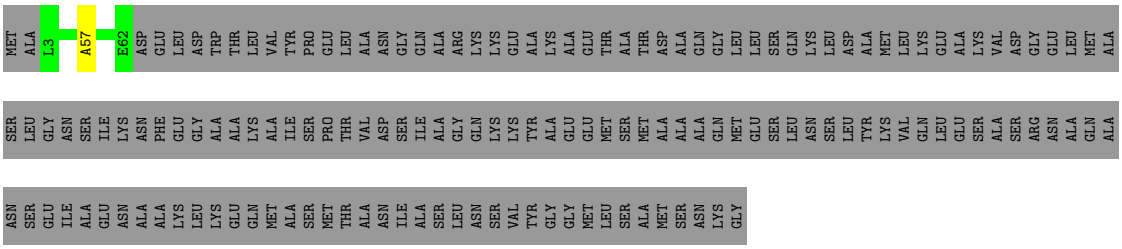
Chain B:





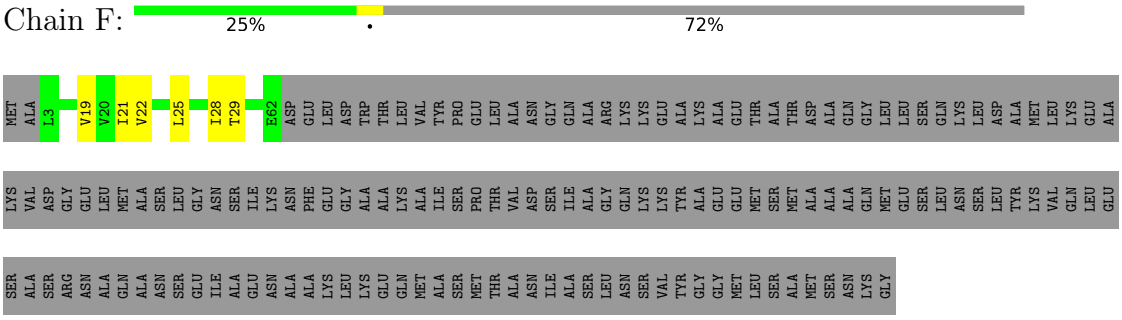
- Molecule 2: GldL

Chain G:



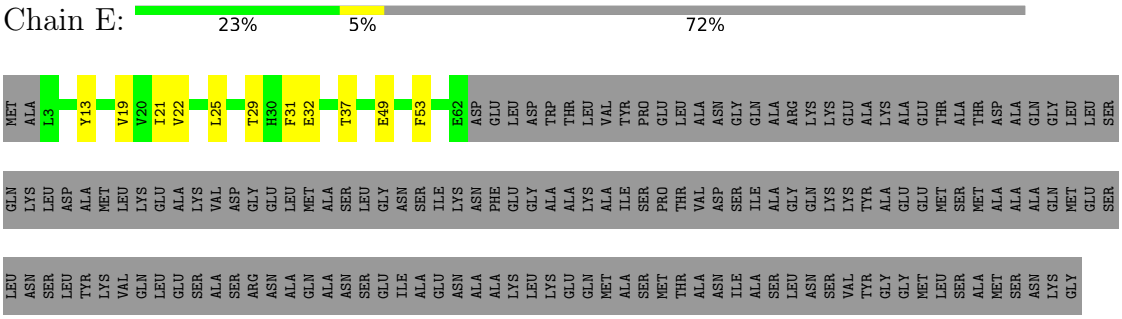
• Molecule 2: GldL

Chain F:



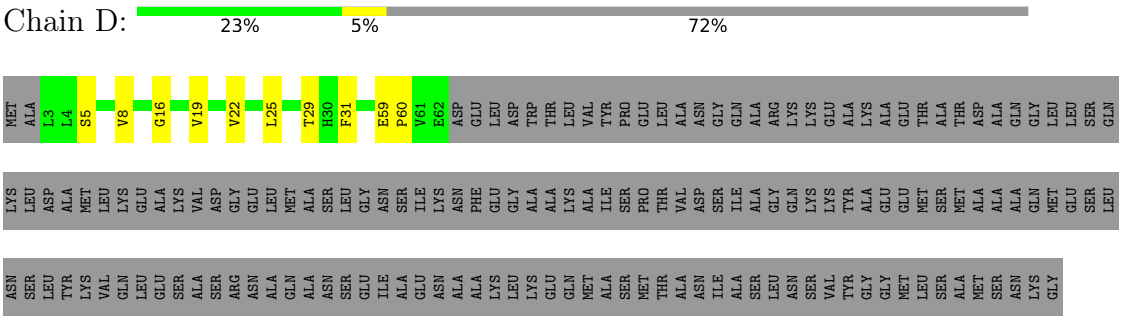
• Molecule 2: GldL

Chain E:



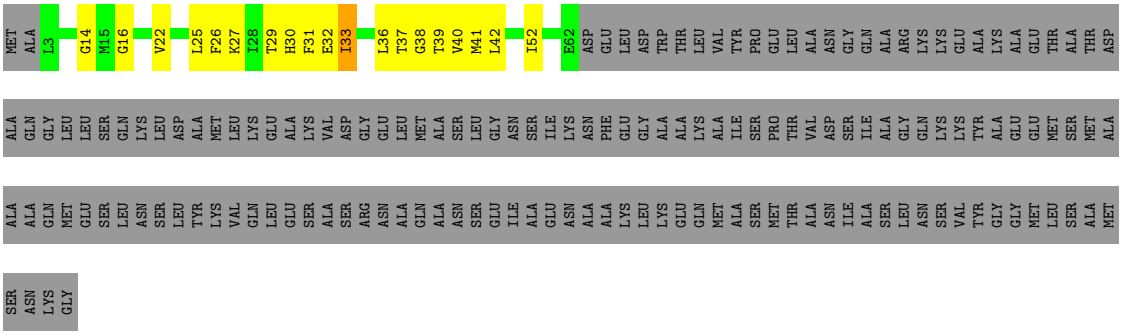
• Molecule 2: GldL

Chain D:



• Molecule 2: GldL

Chain C:


MET ALA L3 G14 M15 G16 V22 L25 F26 K27 I28 T29 H30 F31 E32 I33 L36 T37 G38 T39 V40 M41 L42 I52 E62 ASP GLU LEU ASP TRP THR LEU VAL TYR PRO GLU LEU ALA ASN GLY GLN ALA ARG LYS LYS GLU ALA LYS ALA GLU THR ALA THR ASP
ALA GLN GLY LEU LEU SER GLN LYS LEU ASP ALA MET LEU LYS GLU ALA LYS VAL ASP GLY GLU LEU MET ALA SER LEU GLY ASN SER ILE LYS ASN PHE GLU GLY ALA ALA LYS ALA ILE SER PRO THR VAL ASP SER ILE ALA GLY GLN LYS LYS TYR ALA GLU GLU MET SER MET ALA
ALA ALA GLN MET GLU SER LEU ASN SER LEU TYR LYS VAL GLN LEU GLU SER ALA SER ARG ASN ALA GLN ALA ASN SER GLU ILE ALA GLU ASN ALA ALA LYS LEU LYS GLU GLN MET ALA SER MET THR ALA ASN ILE ALA SER LEU ASN SER VAL TYR GLY GLY MET LEU SER ALA MET
SER ASN LYS GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	119230	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	0.1	Depositor
Maximum defocus (nm)	0.3	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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	0.39	0/1723	0.53	0/2312
1	B	0.35	0/1732	0.49	0/2323
2	C	0.38	0/453	0.76	1/613 (0.2%)
2	D	0.34	0/453	0.59	0/613
2	E	0.31	0/453	0.54	0/613
2	F	0.33	0/446	0.57	0/605
2	G	0.33	0/453	0.58	0/613
All	All	0.36	0/5713	0.55	1/7692 (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.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
2	D	0	1
2	E	0	1
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	33	ILE	CB-CA-C	12.03	135.66	111.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	31	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	A	9	ARG	Sidechain
1	B	9	ARG	Sidechain
2	D	31	PHE	Peptide
2	E	31	PHE	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	1695	0	1698	39	0
1	B	1704	0	1710	34	0
2	C	445	0	474	33	0
2	D	445	0	474	5	0
2	E	445	0	474	19	0
2	F	445	0	474	6	0
2	G	445	0	474	1	0
All	All	5624	0	5778	115	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 10.

All (115) 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:A:9:ARG:HD2	2:E:53:PHE:CE1	1.54	1.41
1:A:12:MET:CE	2:E:49:GLU:OE1	1.80	1.27
1:A:10:GLN:OE1	1:B:10:GLN:NE2	1.69	1.24
2:C:26:PHE:CD1	2:C:31:PHE:HD1	1.58	1.20
1:A:9:ARG:CD	2:E:53:PHE:HE1	1.57	1.17
1:A:12:MET:HE3	2:E:49:GLU:OE1	0.99	1.17
1:B:9:ARG:HH21	1:B:12:MET:CE	1.60	1.14
1:B:9:ARG:NH2	1:B:12:MET:CE	2.11	1.13
2:C:26:PHE:CE1	2:C:31:PHE:CD1	2.40	1.09
2:C:26:PHE:CD1	2:C:31:PHE:CD1	2.45	1.03
1:B:9:ARG:NH2	1:B:12:MET:HE3	1.72	1.02
2:C:38:GLY:HA2	2:C:41:MET:SD	2.08	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:38:GLY:H	2:C:41:MET:CE	1.82	0.93
2:C:38:GLY:O	2:C:40:VAL:HG23	1.71	0.90
2:C:36:LEU:HB2	2:C:41:MET:HE3	1.54	0.90
2:C:26:PHE:HE1	2:C:31:PHE:CE1	1.93	0.87
1:B:9:ARG:HH21	1:B:12:MET:HE3	1.28	0.85
1:A:8:PRO:O	2:E:13:TYR:OH	1.93	0.85
1:A:7:THR:HB	1:A:10:GLN:HB3	1.58	0.85
1:B:9:ARG:NH2	1:B:12:MET:HE1	1.91	0.84
2:C:38:GLY:CA	2:C:41:MET:SD	2.65	0.84
1:B:31:GLU:CG	1:B:34:SER:HB3	2.09	0.82
2:C:26:PHE:CE1	2:C:31:PHE:CE1	2.68	0.79
1:B:31:GLU:HG3	1:B:34:SER:HB3	1.66	0.77
1:A:12:MET:CE	2:E:49:GLU:CD	2.53	0.77
2:C:38:GLY:N	2:C:41:MET:SD	2.58	0.76
2:C:26:PHE:HD1	2:C:31:PHE:HD1	1.35	0.73
2:C:32:GLU:HA	2:C:37:THR:HG22	1.68	0.73
1:A:10:GLN:NE2	1:A:10:GLN:HA	2.03	0.71
1:A:12:MET:HE3	2:E:49:GLU:CD	2.04	0.71
2:C:16:GLY:HA3	2:C:52:ILE:HD11	1.76	0.67
1:A:10:GLN:HA	1:A:10:GLN:HE21	1.59	0.67
1:B:31:GLU:HG2	1:B:34:SER:HB3	1.77	0.66
1:B:9:ARG:O	1:B:12:MET:HB3	1.96	0.66
2:C:36:LEU:CB	2:C:41:MET:HE3	2.26	0.65
1:A:190:TYR:CE2	1:B:31:GLU:OE1	2.49	0.65
1:B:28:VAL:O	1:B:29:SER:O	2.16	0.64
1:B:10:GLN:HA	1:B:10:GLN:OE1	1.96	0.64
2:E:32:GLU:HB2	2:E:37:THR:HA	1.79	0.64
1:A:9:ARG:HD2	2:E:53:PHE:HE1	0.63	0.62
2:C:38:GLY:C	2:C:40:VAL:H	2.01	0.62
2:C:36:LEU:HB2	2:C:41:MET:CE	2.30	0.61
1:A:9:ARG:CD	2:E:53:PHE:CE1	2.49	0.60
1:A:134:THR:HG23	1:A:136:LYS:H	1.65	0.60
1:B:28:VAL:HG21	2:F:28:ILE:HG22	1.84	0.59
1:B:28:VAL:HG11	2:F:28:ILE:HA	1.85	0.58
2:C:36:LEU:HA	2:C:40:VAL:HG11	1.86	0.58
2:C:36:LEU:O	2:C:40:VAL:HG21	2.05	0.57
1:B:134:THR:O	1:B:138:ASN:ND2	2.38	0.56
1:A:12:MET:HE1	2:E:49:GLU:OE2	2.05	0.56
2:C:38:GLY:C	2:C:40:VAL:N	2.59	0.55
2:E:49:GLU:O	2:E:53:PHE:HB2	2.06	0.54
1:B:129:THR:HG23	1:B:134:THR:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ASN:HA	1:A:57:LEU:HD12	1.90	0.54
2:F:19:VAL:HA	2:F:22:VAL:HG12	1.89	0.53
1:A:131:ASP:N	1:A:131:ASP:OD1	2.38	0.53
1:A:10:GLN:HE21	1:A:10:GLN:CA	2.20	0.53
2:C:38:GLY:O	2:C:40:VAL:N	2.42	0.52
1:A:99:GLN:NE2	1:A:123:ASN:O	2.40	0.51
1:B:10:GLN:O	1:B:13:ILE:HG22	2.11	0.50
2:C:32:GLU:O	2:C:33:ILE:C	2.49	0.50
2:C:26:PHE:HD2	2:C:41:MET:HG3	1.76	0.49
1:A:93:ILE:HD13	1:A:96:LEU:HD12	1.94	0.49
2:D:25:LEU:O	2:D:29:THR:OG1	2.26	0.48
1:A:28:VAL:HG11	1:A:196:PRO:HG3	1.96	0.48
1:A:190:TYR:CZ	1:B:31:GLU:OE1	2.66	0.48
2:C:27:LYS:HD2	2:C:42:LEU:HD22	1.96	0.48
1:B:10:GLN:O	1:B:13:ILE:N	2.46	0.48
1:A:31:GLU:O	1:A:33:ILE:N	2.47	0.47
1:A:15:LEU:HD11	2:E:21:ILE:HD11	1.94	0.47
2:E:25:LEU:O	2:E:29:THR:OG1	2.28	0.47
1:B:162:ALA:HA	1:B:165:ILE:HD12	1.96	0.47
1:A:12:MET:CE	2:E:49:GLU:OE2	2.62	0.47
2:D:5:SER:HB3	2:D:8:VAL:HG23	1.97	0.47
1:B:218:VAL:O	1:B:222:ALA:HB2	2.15	0.47
2:F:22:VAL:HG23	2:F:25:LEU:HD23	1.97	0.47
1:A:176:ASP:OD1	1:A:176:ASP:N	2.46	0.46
2:C:36:LEU:O	2:C:40:VAL:CG2	2.63	0.46
1:A:122:ASP:OD2	2:C:39:THR:OG1	2.27	0.46
1:B:93:ILE:HD13	1:B:96:LEU:HD12	1.97	0.46
2:F:21:ILE:HD12	2:E:53:PHE:HD2	1.81	0.45
1:A:9:ARG:O	1:A:9:ARG:HG3	2.17	0.45
2:C:36:LEU:HA	2:C:40:VAL:CB	2.47	0.45
2:D:59:GLU:HA	2:D:60:PRO:HD3	1.87	0.45
1:A:11:LYS:HB3	1:A:11:LYS:HE3	1.87	0.44
1:B:130:GLY:O	1:B:193:LYS:NZ	2.50	0.44
2:C:38:GLY:H	2:C:41:MET:HE1	1.73	0.44
1:B:164:ILE:HD12	1:B:164:ILE:HA	1.90	0.44
2:C:36:LEU:HA	2:C:40:VAL:CG1	2.47	0.44
1:B:112:LYS:HB3	1:B:112:LYS:HE2	1.82	0.44
2:C:30:HIS:CD2	2:C:30:HIS:N	2.86	0.43
1:A:133:TYR:HE1	1:A:188:LEU:HB2	1.83	0.43
1:A:12:MET:HE1	2:E:49:GLU:CD	2.37	0.43
2:C:22:VAL:HG23	2:C:25:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LYS:HD3	1:A:135:LYS:HA	1.88	0.43
1:A:143:LYS:HD3	1:A:143:LYS:HA	1.85	0.43
1:A:43:PHE:O	1:A:47:ASN:ND2	2.52	0.42
1:A:97:LYS:HB2	1:A:97:LYS:HE3	1.93	0.42
2:G:57:ALA:HB2	2:C:14:GLY:HA3	2.02	0.42
2:D:19:VAL:HA	2:D:22:VAL:HG12	2.01	0.42
1:B:178:LYS:HD3	1:B:184:LYS:HD2	2.02	0.41
1:B:129:THR:OG1	1:B:133:TYR:O	2.30	0.41
1:B:212:LYS:HD3	1:B:212:LYS:HA	1.85	0.41
2:F:28:ILE:HG13	2:F:29:THR:HG23	2.01	0.41
1:B:64:LYS:HA	1:B:64:LYS:HD2	1.74	0.41
2:E:19:VAL:HA	2:E:22:VAL:HG12	2.03	0.41
1:B:44:GLU:HA	1:B:47:ASN:HD22	1.86	0.41
1:B:50:SER:HA	1:B:53:THR:HG22	2.02	0.41
1:A:12:MET:O	1:A:15:LEU:HB3	2.21	0.41
2:D:16:GLY:HA2	2:D:19:VAL:HG12	2.03	0.40
2:C:29:THR:O	2:C:30:HIS:O	2.39	0.40
1:A:12:MET:SD	2:E:49:GLU:OE1	2.75	0.40
1:B:21:ILE:HD13	1:B:21:ILE:HA	1.96	0.40
1:B:31:GLU:CG	1:B:34:SER:CB	2.91	0.40
1:A:13:ILE:H	1:A:13:ILE:HG12	1.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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

This section contains visualisations of the EMDB entry EMD-10893. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

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

9 Map-model fit

This section was not generated.