



Full wwPDB EM Validation Report ⓘ

Jul 23, 2026 – 03:50 PM JST

PDB ID : 9UJX / pdb_00009ujx
EMDB ID : EMD-64229
Title : CryoEM structure of Brucella melitensis CobS dodecamer 2 without AMPPNP
Authors : Zhou, Y.L.; Chen, X.; Liu, L.
Deposited on : 2025-04-17
Resolution : 4.02 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:

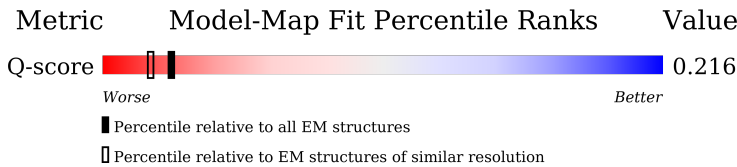
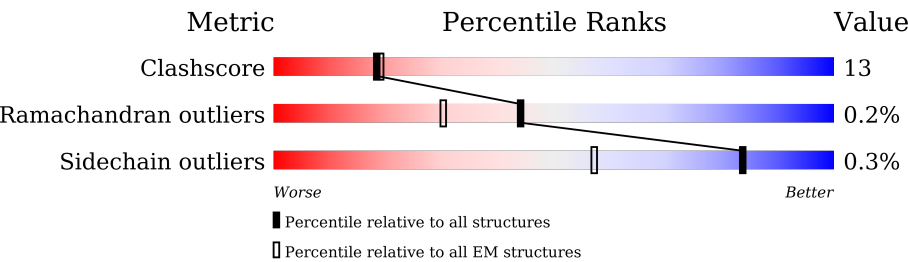
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 4.02 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.



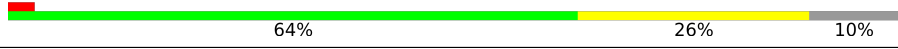
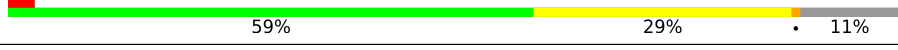
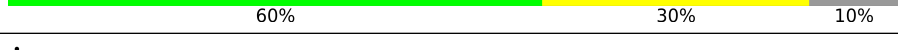
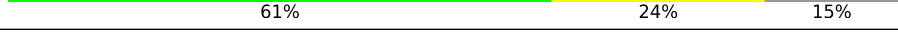
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6727 (3.52 - 4.52)

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	328	6% 66% 23% 10%
1	B	328	62% 27% 11%
1	C	328	59% 30% 10%
1	D	328	64% 25% 11%

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Mol	Chain	Length	Quality of chain
1	E	328	
1	F	328	
1	a	328	
1	b	328	
1	c	328	
1	d	328	
1	e	328	
1	f	328	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 27747 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.

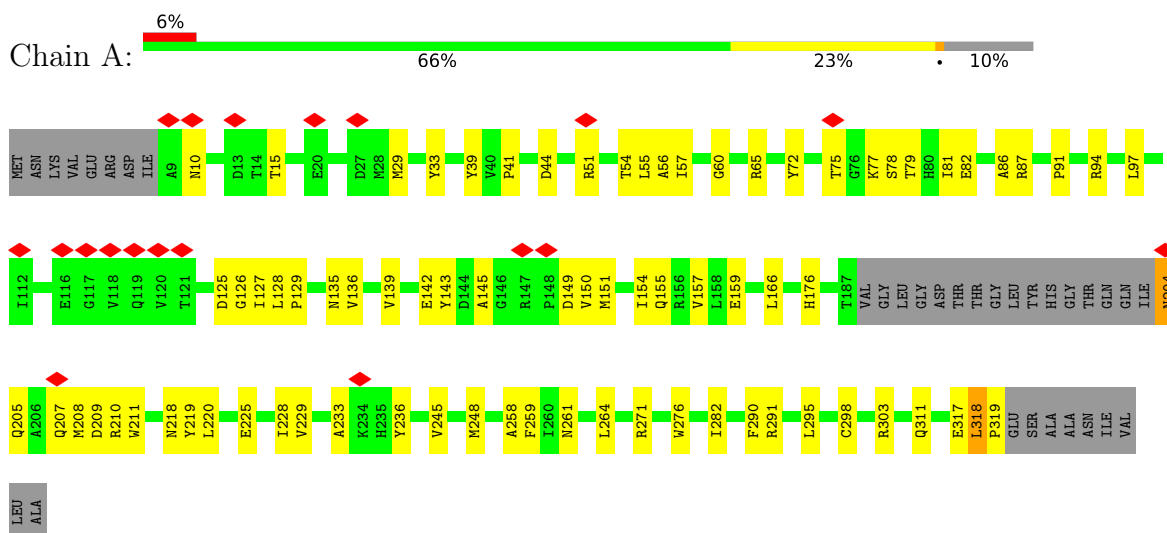
- Molecule 1 is a protein called Cobaltochelataase subunit CobS.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	295	Total	C	N	O	S	0	0
			2342	1486	411	435	10		
1	B	292	Total	C	N	O	S	0	0
			2319	1471	408	430	10		
1	C	294	Total	C	N	O	S	0	0
			2334	1482	410	432	10		
1	D	292	Total	C	N	O	S	0	0
			2319	1471	408	430	10		
1	E	295	Total	C	N	O	S	0	0
			2343	1487	412	434	10		
1	F	280	Total	C	N	O	S	0	0
			2225	1411	394	410	10		
1	a	295	Total	C	N	O	S	0	0
			2342	1486	411	435	10		
1	b	292	Total	C	N	O	S	0	0
			2319	1471	408	430	10		
1	c	294	Total	C	N	O	S	0	0
			2334	1482	410	432	10		
1	d	292	Total	C	N	O	S	0	0
			2318	1472	407	429	10		
1	e	294	Total	C	N	O	S	0	0
			2334	1482	410	432	10		
1	f	279	Total	C	N	O	S	0	0
			2218	1406	393	409	10		

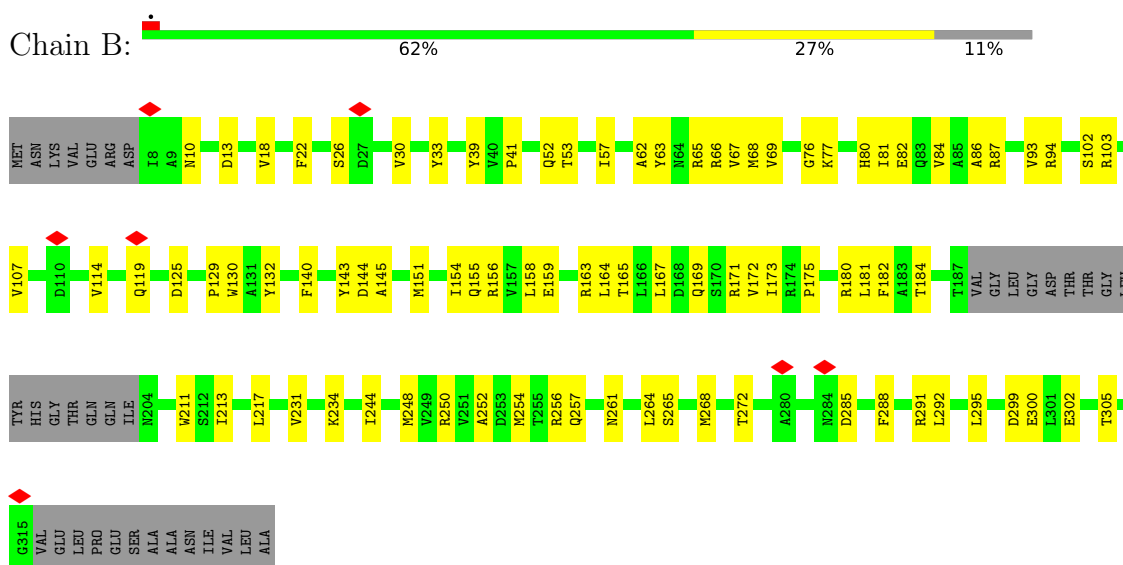
3 Residue-property plots

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.

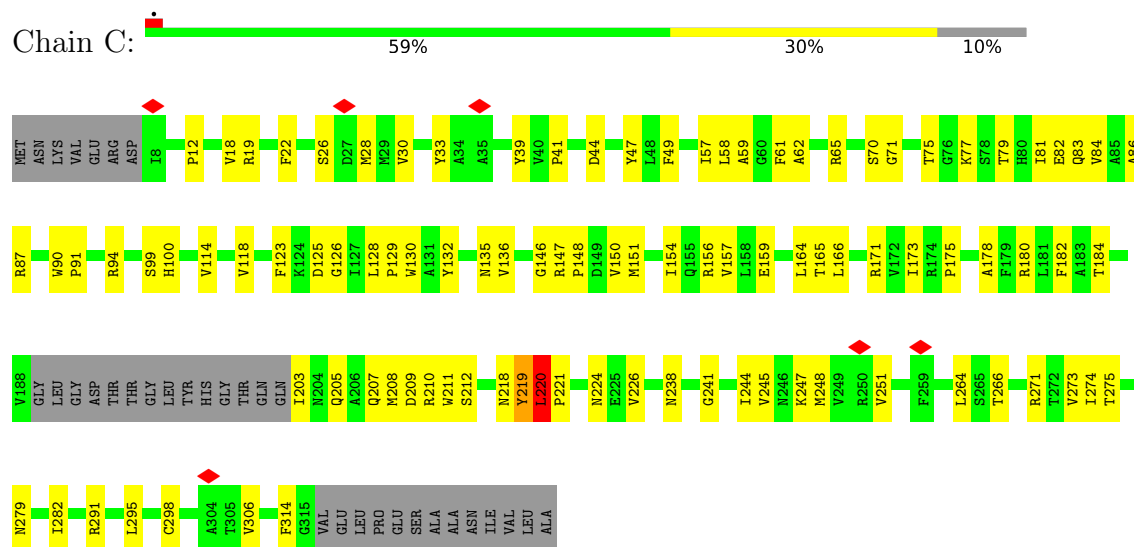
- Molecule 1: Cobaltochelatase subunit CobS



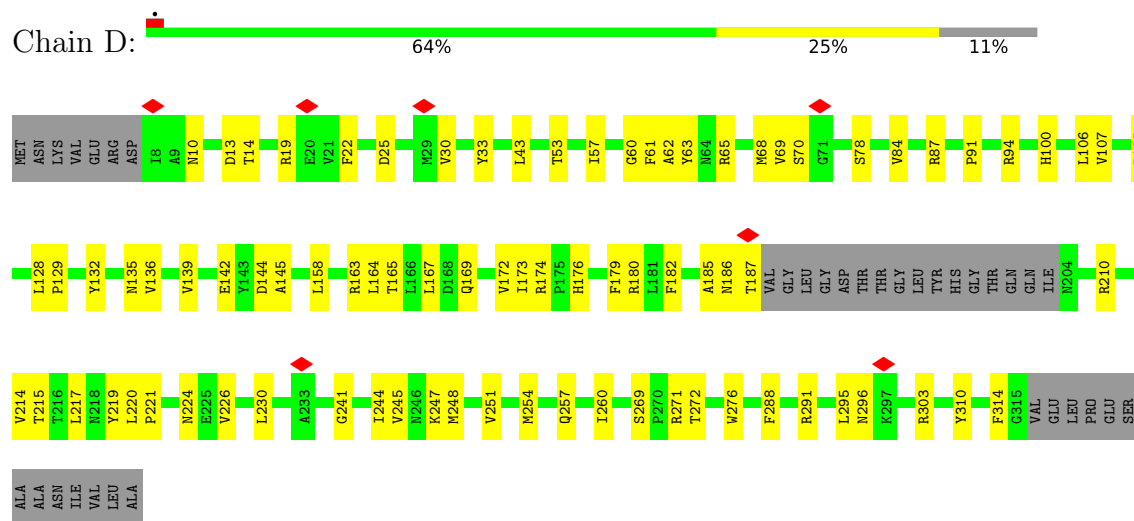
- Molecule 1: Cobaltochelatase subunit CobS



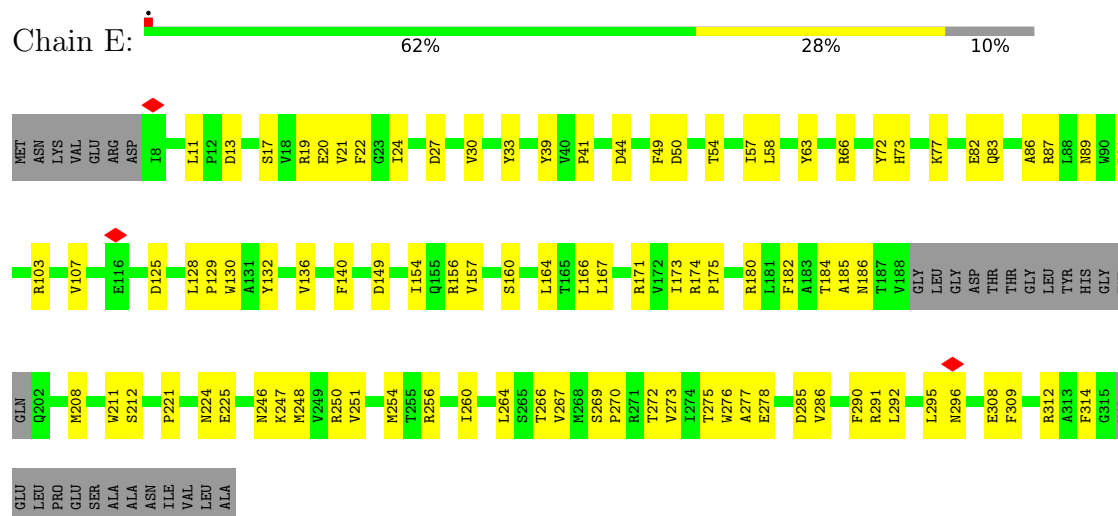
- Molecule 1: Cobaltochelatase subunit CobS



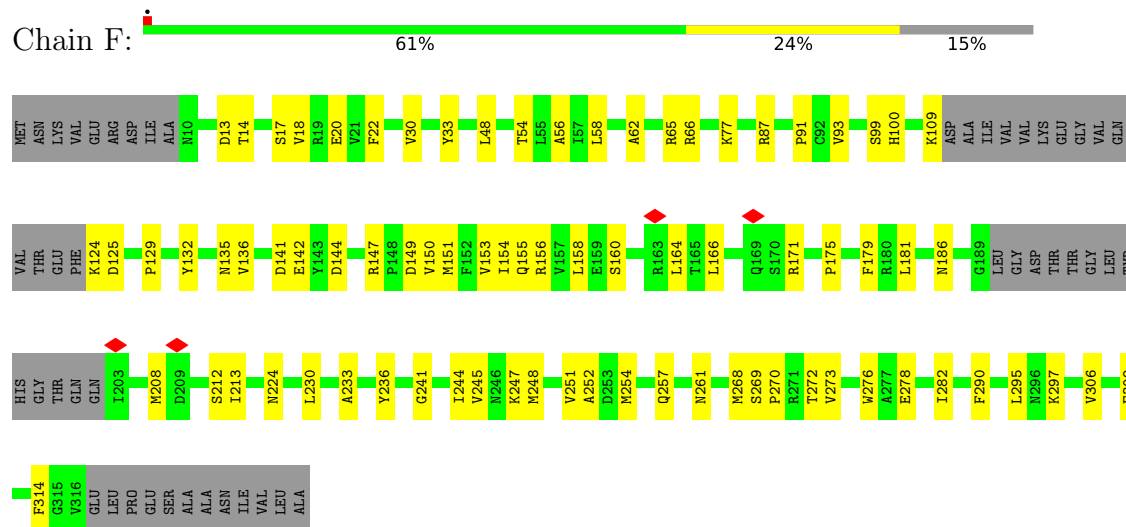
• Molecule 1: Cobaltochelataase subunit CobS



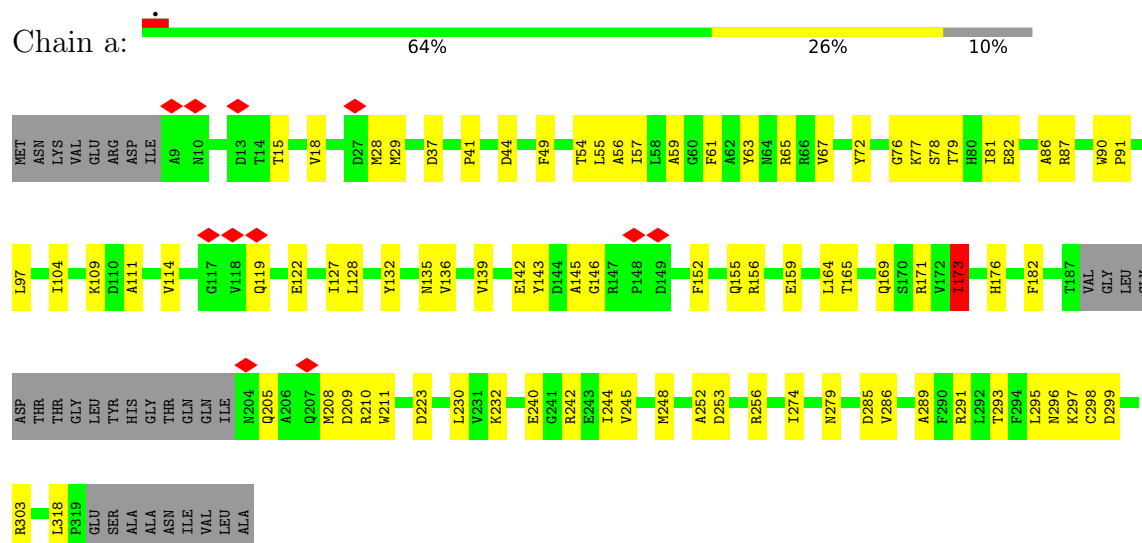
• Molecule 1: Cobaltochelataase subunit CobS



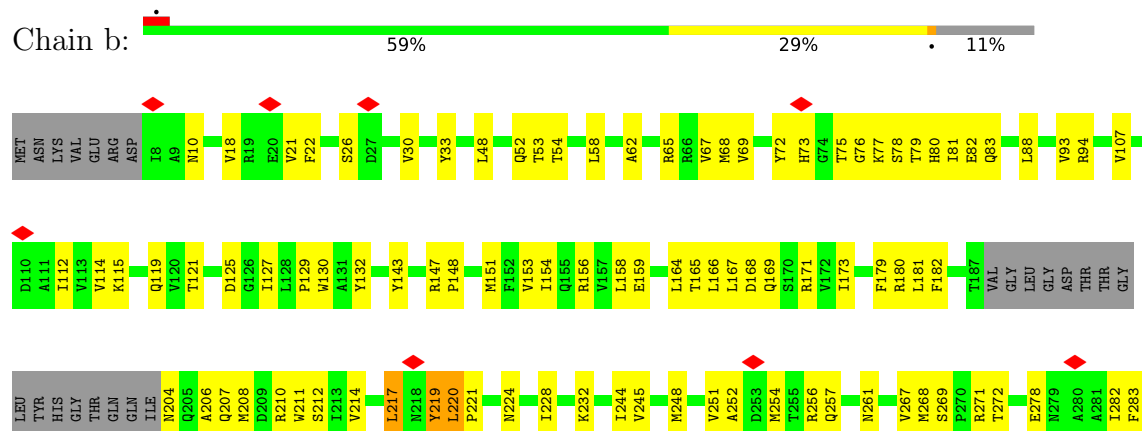
- Molecule 1: Cobaltochelataase subunit CobS



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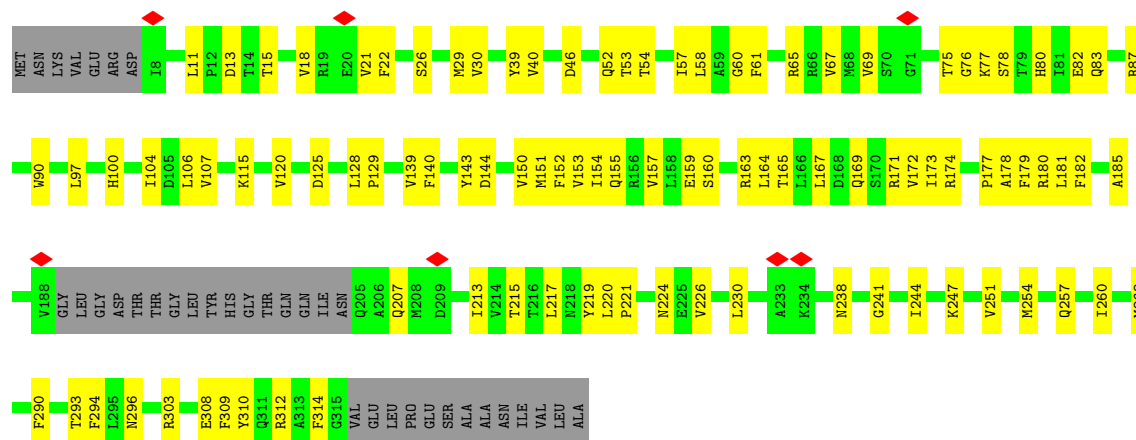




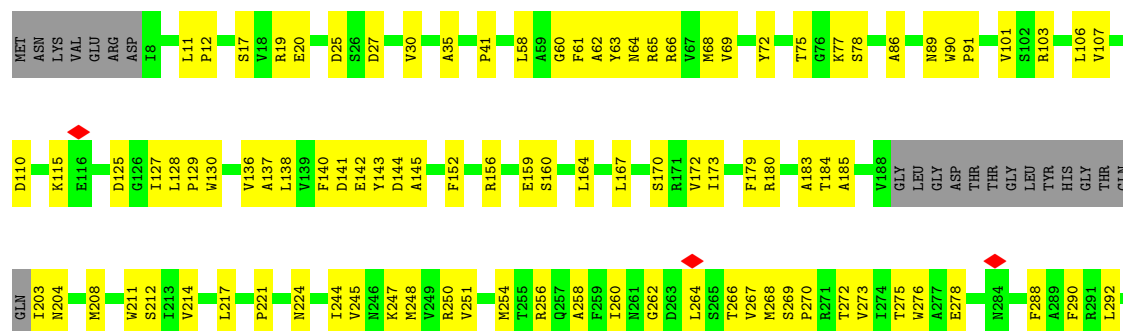
• Molecule 1: Cobaltochelataase subunit CobS



• Molecule 1: Cobaltochelataase subunit CobS



• Molecule 1: Cobaltochelataase subunit CobS



F314	G315
VAL	VAL
GLU	GLU
LEU	LEU
PRO	PRO
GLU	GLU
SER	SER
ALA	ALA
ALA	ASN
ASN	ASN
ILE	ILE
VAL	VAL
LEU	LEU
ALA	ALA

• Molecule 1: Cobaltochelatase subunit CobS



MET	ASN	LYS	VAL	GLY	VAL	GLU	ARG	ASP	ILE	ALA	N10	F22	V30	Y33	D37	S38	Y39	D50	T53	T54	I57	L58	A59	G60	F61	A62	Y63	N64	R65	N68	Y72	H73	G74	K77	H80	R87	P91	N96	S99	H100	V101	K109	ASP	ALA	ILE
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VAL	VAL	LYS	GLY	VAL	GLN	THR	GLU	PHE	K124	D125	G126	I127	L128	P129	Y132	V136	D141	E142	R147	P148	D149	V150	M151	F152	V153	I154	Q155	R163	L166	Q169	S170	R171	P175	T184	G189	LEU	GLY	ASP	THR	THR	GLY	LEU	TYR	HIS	GLY	THR	GLN
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GLN	T203	N204	Q207	N208	D209	R210	N211	S212	I213	D223	N224	E225	N226	I227	L228	V229	L230	V231	N238	A239	I244	V245	M248	T255	T266	V267	N268	S269	P270	R271	T272	V273	N276	A277	E278	I282	A289	F290	T293	F294	K297	G315	VAL	GLU	LEU	PRO
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GLU	SER	ALA	ALA	ASN	ILE	VAL	VAL	LEU	ALA
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	135929	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.110	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.01	Depositor
Map size ($\text{\AA}$)	279.2, 279.2, 279.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.698, 0.698, 0.698	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.14	0/2392	0.30	0/3254
1	B	0.11	0/2368	0.32	0/3220
1	C	0.15	0/2383	0.33	0/3241
1	D	0.10	0/2368	0.29	0/3220
1	E	0.13	0/2392	0.30	0/3253
1	F	0.13	0/2272	0.36	0/3088
1	a	0.17	0/2392	0.39	2/3254 (0.1%)
1	b	0.17	0/2368	0.39	0/3220
1	c	0.15	0/2383	0.30	0/3241
1	d	0.11	0/2367	0.34	0/3219
1	e	0.12	0/2383	0.31	0/3241
1	f	0.12	0/2265	0.34	0/3078
All	All	0.14	0/28333	0.33	2/38529 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	173	ILE	CA-C-N	5.66	128.53	120.49
1	a	173	ILE	C-N-CA	5.66	128.53	120.49

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	A	2342	0	2302	54	0
1	B	2319	0	2280	64	0
1	C	2334	0	2300	72	0
1	D	2319	0	2280	54	0
1	E	2343	0	2308	76	0
1	F	2225	0	2187	62	0
1	a	2342	0	2302	65	0
1	b	2319	0	2280	71	0
1	c	2334	0	2300	50	0
1	d	2318	0	2283	72	0
1	e	2334	0	2300	68	0
1	f	2218	0	2178	62	0
All	All	27747	0	27300	721	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 13.

All (721) 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:111:ALA:HB3	1:a:122:GLU:O	1.62	0.99
1:a:132:TYR:HE2	1:a:173:ILE:HG22	1.39	0.85
1:c:148:PRO:HB3	1:d:100:HIS:HB3	1.62	0.81
1:A:229:VAL:HG11	1:A:248:MET:HE1	1.64	0.79
1:d:60:GLY:HA2	1:d:65:ARG:HB2	1.64	0.79
1:d:164:LEU:HD23	1:d:173:ILE:HD11	1.65	0.78
1:d:163:ARG:HD2	1:d:174:ARG:HH21	1.49	0.77
1:e:250:ARG:HG3	1:e:254:MET:HE1	1.66	0.76
1:B:169:GLN:HE22	1:C:130:TRP:CD1	2.03	0.76
1:B:67:VAL:HG12	1:B:213:ILE:HB	1.67	0.75
1:c:164:LEU:HB3	1:c:173:ILE:HB	1.69	0.75
1:C:148:PRO:HB3	1:D:100:HIS:HB3	1.70	0.74
1:b:151:MET:HG2	1:b:154:ILE:HD11	1.70	0.74
1:f:147:ARG:NH1	1:f:149:ASP:OD1	2.21	0.74
1:d:106:LEU:HB3	1:d:128:LEU:HD23	1.69	0.73
1:F:257:GLN:O	1:F:261:ASN:ND2	2.22	0.73
1:d:215:THR:HG22	1:e:292:LEU:HD22	1.71	0.72
1:A:75:THR:HG22	1:A:219:TYR:HD2	1.55	0.72
1:e:264:LEU:HD23	1:e:266:THR:H	1.56	0.71
1:E:248:MET:HE3	1:E:276:TRP:CD1	2.25	0.71
1:A:56:ALA:HB2	1:B:292:LEU:HD11	1.73	0.71
1:e:68:MET:HB3	1:e:214:VAL:HG22	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:298:CYS:HB2	1:a:303:ARG:HH22	1.56	0.70
1:F:254:MET:HE1	1:F:309:PHE:HD1	1.54	0.70
1:a:291:ARG:HG3	1:a:295:LEU:HD23	1.73	0.70
1:a:253:ASP:OD1	1:a:256:ARG:NH2	2.24	0.69
1:C:18:VAL:HG11	1:C:26:SER:HB3	1.75	0.69
1:b:93:VAL:HG21	1:b:130:TRP:HH2	1.57	0.69
1:f:141:ASP:OD1	1:f:142:GLU:N	2.25	0.69
1:B:107:VAL:HG21	1:B:167:LEU:HB2	1.73	0.69
1:B:268:MET:SD	1:B:272:THR:OG1	2.50	0.69
1:B:299:ASP:OD1	1:B:300:GLU:N	2.26	0.69
1:b:69:VAL:HG21	1:b:81:ILE:HD11	1.74	0.69
1:d:83:GLN:HB3	1:d:87:ARG:HH12	1.56	0.69
1:B:57:ILE:HG21	1:B:84:VAL:HG21	1.74	0.69
1:E:91:PRO:HB2	1:E:136:VAL:HG12	1.74	0.69
1:e:244:ILE:HG22	1:e:248:MET:HE1	1.74	0.68
1:E:41:PRO:HB2	1:E:86:ALA:HB2	1.74	0.68
1:B:69:VAL:HG21	1:B:81:ILE:HD11	1.75	0.68
1:E:264:LEU:HD23	1:E:266:THR:H	1.58	0.68
1:e:90:TRP:HE1	1:e:137:ALA:HB2	1.58	0.68
1:B:41:PRO:HG2	1:B:86:ALA:HB2	1.76	0.68
1:A:128:LEU:HD23	1:A:157:VAL:HG21	1.75	0.68
1:a:114:VAL:HA	1:a:119:GLN:HA	1.76	0.68
1:D:220:LEU:HD12	1:D:221:PRO:HD2	1.76	0.68
1:E:77:LYS:NZ	1:E:185:ALA:O	2.27	0.67
1:a:78:SER:HA	1:a:81:ILE:HD12	1.75	0.67
1:d:220:LEU:HD12	1:d:221:PRO:HD2	1.77	0.67
1:f:72:TYR:O	1:f:77:LYS:NZ	2.28	0.67
1:f:230:LEU:HD21	1:f:245:VAL:HG11	1.77	0.67
1:C:164:LEU:HB3	1:C:173:ILE:HB	1.76	0.67
1:a:59:ALA:HB1	1:b:282:ILE:HD12	1.77	0.66
1:D:33:TYR:OH	1:D:135:ASN:ND2	2.28	0.66
1:a:111:ALA:CB	1:a:122:GLU:O	2.41	0.66
1:a:156:ARG:NH2	1:a:165:THR:OG1	2.29	0.66
1:d:244:ILE:HA	1:d:247:LYS:HG2	1.77	0.66
1:E:248:MET:HE1	1:E:277:ALA:HB2	1.77	0.66
1:A:204:ASN:N	1:A:204:ASN:HD22	1.92	0.66
1:D:60:GLY:HA2	1:D:65:ARG:HB2	1.76	0.66
1:a:171:ARG:HH12	1:a:173:ILE:HG13	1.60	0.66
1:c:128:LEU:HD22	1:c:166:LEU:HD11	1.78	0.66
1:e:11:LEU:HD12	1:e:12:PRO:HD2	1.76	0.66
1:D:291:ARG:HA	1:D:295:LEU:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:141:ASP:HA	1:c:184:THR:HB	1.78	0.66
1:a:104:ILE:O	1:a:109:LYS:NZ	2.29	0.65
1:a:291:ARG:O	1:a:296:ASN:ND2	2.28	0.65
1:B:151:MET:HG2	1:B:154:ILE:HD11	1.78	0.65
1:d:83:GLN:HB3	1:d:87:ARG:NH1	2.11	0.65
1:F:54:THR:C	1:F:56:ALA:H	2.05	0.65
1:f:53:THR:HG23	1:f:57:ILE:HD13	1.77	0.65
1:f:255:THR:HG21	1:f:268:MET:HE3	1.77	0.65
1:A:72:TYR:O	1:A:77:LYS:NZ	2.30	0.65
1:A:291:ARG:HA	1:A:295:LEU:HB3	1.78	0.65
1:a:132:TYR:CE2	1:a:173:ILE:HG22	2.27	0.65
1:A:142:GLU:HB3	1:A:145:ALA:HB3	1.79	0.64
1:b:68:MET:HB2	1:b:214:VAL:HG23	1.79	0.64
1:a:56:ALA:HB2	1:b:292:LEU:HD11	1.78	0.64
1:E:33:TYR:HB2	1:E:89:ASN:HD22	1.63	0.64
1:F:248:MET:HA	1:F:251:VAL:HG12	1.80	0.64
1:D:61:PHE:O	1:D:180:ARG:NH2	2.30	0.64
1:C:128:LEU:HD22	1:C:166:LEU:HD11	1.80	0.64
1:e:30:VAL:HG11	1:e:58:LEU:HD11	1.78	0.64
1:c:24:ILE:HD11	1:c:51:ARG:HG2	1.78	0.64
1:C:61:PHE:HA	1:C:180:ARG:HD3	1.79	0.63
1:F:77:LYS:NZ	1:F:141:ASP:OD2	2.31	0.63
1:F:141:ASP:OD2	1:F:142:GLU:N	2.31	0.63
1:F:66:ARG:NH2	1:F:160:SER:OG	2.31	0.63
1:B:30:VAL:HG23	1:B:62:ALA:HB2	1.81	0.63
1:c:77:LYS:HE3	1:c:184:THR:HG23	1.80	0.63
1:C:30:VAL:HG21	1:C:58:LEU:HG	1.80	0.63
1:a:240:GLU:O	1:a:244:ILE:HD12	1.99	0.63
1:C:203:ILE:N	1:C:207:GLN:OE1	2.31	0.62
1:b:168:ASP:OD2	1:b:171:ARG:NH2	2.32	0.62
1:B:159:GLU:OE2	1:C:94:ARG:NH2	2.33	0.62
1:B:231:VAL:O	1:B:234:LYS:NZ	2.32	0.62
1:b:52:GLN:N	1:b:52:GLN:OE1	2.31	0.62
1:b:65:ARG:NH2	1:b:212:SER:OG	2.33	0.62
1:C:19:ARG:HE	1:C:26:SER:H	1.46	0.62
1:D:106:LEU:HB3	1:D:128:LEU:HD23	1.82	0.61
1:B:77:LYS:HD2	1:B:184:THR:HB	1.83	0.61
1:c:291:ARG:HG2	1:c:295:LEU:HD23	1.83	0.61
1:a:171:ARG:HH22	1:a:173:ILE:HB	1.64	0.61
1:e:159:GLU:OE1	1:f:96:ASN:ND2	2.33	0.61
1:a:142:GLU:HB3	1:a:145:ALA:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:68:MET:HG3	1:f:211:TRP:CZ3	2.36	0.61
1:C:266:THR:OG1	1:C:298:CYS:SG	2.57	0.61
1:B:169:GLN:HE22	1:C:130:TRP:HD1	1.46	0.61
1:D:164:LEU:HD23	1:D:173:ILE:HD11	1.83	0.61
1:A:94:ARG:HG3	1:A:139:VAL:HB	1.82	0.61
1:B:158:LEU:HD21	1:B:211:TRP:NE1	2.16	0.61
1:E:180:ARG:HB3	1:E:182:PHE:HE1	1.66	0.60
1:C:39:TYR:HB2	1:C:91:PRO:HB3	1.83	0.60
1:a:127:ILE:HG23	1:a:128:LEU:HD12	1.83	0.60
1:A:78:SER:HA	1:A:81:ILE:HD12	1.84	0.60
1:c:269:SER:HB3	1:c:272:THR:HG23	1.84	0.60
1:b:158:LEU:HD21	1:b:211:TRP:HE1	1.67	0.59
1:C:114:VAL:HA	1:C:118:VAL:O	2.02	0.59
1:A:311:GLN:HE22	1:A:317:GLU:HB2	1.68	0.59
1:a:139:VAL:HG22	1:a:182:PHE:HB2	1.83	0.59
1:c:22:PHE:HE1	1:c:87:ARG:HE	1.51	0.59
1:B:65:ARG:NH1	1:C:279:ASN:OD1	2.35	0.59
1:b:158:LEU:HD21	1:b:211:TRP:NE1	2.18	0.59
1:e:141:ASP:OD1	1:e:142:GLU:N	2.36	0.59
1:d:67:VAL:HG22	1:d:213:ILE:HB	1.85	0.59
1:F:213:ILE:HG13	1:a:279:ASN:HD21	1.68	0.58
1:e:77:LYS:HD2	1:e:184:THR:OG1	2.03	0.58
1:A:91:PRO:HB2	1:A:136:VAL:HG12	1.84	0.58
1:b:48:LEU:HB2	1:b:228:ILE:HD11	1.84	0.58
1:b:244:ILE:HG22	1:b:248:MET:HE1	1.86	0.58
1:A:298:CYS:H	1:A:303:ARG:HH12	1.50	0.58
1:C:244:ILE:O	1:C:248:MET:N	2.35	0.58
1:E:166:LEU:HB2	1:E:171:ARG:HH22	1.68	0.58
1:B:119:GLN:HG2	1:C:114:VAL:HG21	1.85	0.58
1:B:125:ASP:OD1	1:B:171:ARG:NH2	2.37	0.58
1:f:151:MET:O	1:f:155:GLN:HG2	2.04	0.58
1:c:90:TRP:HE1	1:c:137:ALA:HB2	1.69	0.58
1:f:68:MET:HE1	1:f:208:MET:HG3	1.86	0.58
1:a:295:LEU:O	1:a:303:ARG:NH2	2.37	0.57
1:a:208:MET:HA	1:a:211:TRP:HD1	1.69	0.57
1:f:54:THR:HA	1:f:58:LEU:HD23	1.85	0.57
1:E:19:ARG:NH1	1:E:27:ASP:OD1	2.35	0.57
1:a:72:TYR:O	1:a:77:LYS:NZ	2.36	0.57
1:c:163:ARG:NH2	1:d:40:VAL:O	2.37	0.57
1:E:125:ASP:HB3	1:E:129:PRO:HG2	1.87	0.57
1:F:254:MET:HE1	1:F:309:PHE:CD1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:91:PRO:HB2	1:a:136:VAL:HG12	1.86	0.57
1:e:143:TYR:HB3	1:e:185:ALA:HB2	1.85	0.57
1:D:164:LEU:HB3	1:D:173:ILE:HG13	1.86	0.57
1:F:144:ASP:OD1	1:F:186:ASN:ND2	2.38	0.57
1:b:125:ASP:HB3	1:b:129:PRO:HB2	1.87	0.57
1:e:107:VAL:HG11	1:e:167:LEU:HD12	1.87	0.57
1:F:208:MET:HE2	1:a:297:LYS:HD3	1.87	0.57
1:b:169:GLN:HB3	1:c:130:TRP:CE3	2.39	0.57
1:e:64:ASN:O	1:e:65:ARG:NH1	2.37	0.57
1:E:39:TYR:HB2	1:E:91:PRO:HB3	1.87	0.56
1:d:107:VAL:HG11	1:d:167:LEU:HD12	1.85	0.56
1:A:291:ARG:HG3	1:A:295:LEU:HD23	1.86	0.56
1:B:164:LEU:HB3	1:B:173:ILE:HB	1.87	0.56
1:C:33:TYR:OH	1:C:135:ASN:ND2	2.38	0.56
1:E:103:ARG:HD2	1:E:167:LEU:HD11	1.87	0.56
1:B:22:PHE:HA	1:B:87:ARG:HH22	1.70	0.56
1:a:205:GLN:O	1:a:209:ASP:HB2	2.04	0.56
1:F:248:MET:HE2	1:F:276:TRP:CD1	2.40	0.56
1:e:19:ARG:NH2	1:e:27:ASP:OD1	2.38	0.56
1:B:244:ILE:HG22	1:B:248:MET:HE1	1.86	0.56
1:E:276:TRP:HH2	1:E:290:PHE:HD1	1.53	0.56
1:b:269:SER:O	1:b:272:THR:OG1	2.23	0.56
1:C:49:PHE:HZ	1:C:87:ARG:HH21	1.53	0.56
1:e:152:PHE:O	1:e:156:ARG:HG2	2.05	0.56
1:B:158:LEU:HD21	1:B:211:TRP:HE1	1.71	0.56
1:F:125:ASP:HB3	1:F:129:PRO:HB2	1.88	0.55
1:D:221:PRO:HG2	1:D:224:ASN:HB2	1.88	0.55
1:E:107:VAL:HG11	1:E:167:LEU:HD12	1.89	0.55
1:C:28:MET:HE1	1:C:59:ALA:HA	1.86	0.55
1:D:219:TYR:HE2	1:D:260:ILE:HD11	1.70	0.55
1:F:151:MET:O	1:F:155:GLN:HG2	2.07	0.55
1:f:141:ASP:HA	1:f:184:THR:HB	1.88	0.55
1:E:309:PHE:HD1	1:E:312:ARG:HH22	1.55	0.55
1:d:61:PHE:O	1:d:180:ARG:NH2	2.40	0.55
1:f:30:VAL:HG23	1:f:62:ALA:HB2	1.87	0.55
1:f:248:MET:SD	1:f:276:TRP:NE1	2.80	0.55
1:d:15:THR:HB	1:d:29:MET:HB3	1.89	0.55
1:A:135:ASN:HB3	1:A:176:HIS:CE1	2.42	0.55
1:C:218:ASN:O	1:C:219:TYR:C	2.49	0.55
1:d:90:TRP:HH2	1:d:178:ALA:HB1	1.71	0.55
1:E:30:VAL:HG11	1:E:58:LEU:HG	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:48:LEU:HD22	1:F:224:ASN:HD21	1.72	0.55
1:b:164:LEU:HD23	1:b:173:ILE:HD12	1.89	0.55
1:A:143:TYR:HE1	1:A:154:ILE:HG21	1.72	0.55
1:C:65:ARG:NH2	1:C:212:SER:OG	2.40	0.55
1:D:142:GLU:HB3	1:D:145:ALA:HB3	1.88	0.55
1:b:18:VAL:O	1:b:22:PHE:HB2	2.06	0.55
1:e:125:ASP:HB3	1:e:129:PRO:HG2	1.89	0.55
1:a:97:LEU:HD12	1:a:143:TYR:HA	1.88	0.55
1:D:269:SER:O	1:D:272:THR:OG1	2.21	0.54
1:a:244:ILE:O	1:a:248:MET:HG2	2.07	0.54
1:b:53:THR:HG21	1:b:217:LEU:HD13	1.88	0.54
1:b:75:THR:HG23	1:b:219:TYR:CE1	2.42	0.54
1:c:107:VAL:HG11	1:c:167:LEU:HD12	1.89	0.54
1:E:73:HIS:HB2	1:E:186:ASN:HD21	1.70	0.54
1:E:211:TRP:O	1:F:297:LYS:NZ	2.39	0.54
1:a:41:PRO:HB2	1:a:86:ALA:HB2	1.89	0.54
1:D:254:MET:HA	1:D:257:GLN:HG2	1.89	0.54
1:F:33:TYR:OH	1:F:135:ASN:ND2	2.41	0.54
1:e:72:TYR:O	1:e:75:THR:OG1	2.22	0.54
1:E:167:LEU:H	1:E:171:ARG:HH22	1.55	0.54
1:b:179:PHE:O	1:b:180:ARG:NH1	2.37	0.54
1:c:83:GLN:HG2	1:c:87:ARG:HH22	1.72	0.54
1:e:61:PHE:HE1	1:e:90:TRP:CD1	2.26	0.54
1:E:30:VAL:HG21	1:E:58:LEU:HD11	1.89	0.54
1:d:290:PHE:HA	1:d:293:THR:HG22	1.88	0.54
1:e:41:PRO:HG2	1:e:86:ALA:HB2	1.88	0.54
1:A:204:ASN:N	1:A:204:ASN:ND2	2.49	0.54
1:b:283:PHE:HE2	1:b:292:LEU:HD22	1.72	0.54
1:d:155:GLN:NE2	1:d:207:GLN:OE1	2.41	0.54
1:F:30:VAL:HG23	1:F:62:ALA:HB2	1.89	0.54
1:F:91:PRO:HB2	1:F:136:VAL:HA	1.90	0.54
1:c:68:MET:HE3	1:c:185:ALA:HB2	1.89	0.54
1:d:22:PHE:HE1	1:d:87:ARG:HH21	1.56	0.54
1:B:257:GLN:O	1:B:261:ASN:ND2	2.41	0.53
1:D:139:VAL:HG12	1:D:182:PHE:HB2	1.90	0.53
1:E:54:THR:HA	1:E:57:ILE:HG22	1.90	0.53
1:e:144:ASP:OD1	1:e:145:ALA:N	2.42	0.53
1:B:82:GLU:OE1	1:B:94:ARG:NH2	2.42	0.53
1:F:65:ARG:NH2	1:F:212:SER:HB3	2.24	0.53
1:b:72:TYR:HB2	1:b:219:TYR:CE2	2.43	0.53
1:b:76:GLY:O	1:b:80:HIS:ND1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:291:ARG:HA	1:a:295:LEU:HB3	1.89	0.53
1:C:123:PHE:HD2	1:C:171:ARG:NH1	2.06	0.53
1:D:78:SER:HB2	1:D:94:ARG:HH12	1.74	0.53
1:D:215:THR:HG22	1:E:292:LEU:HD22	1.90	0.53
1:B:18:VAL:HG21	1:B:26:SER:HB3	1.91	0.53
1:B:67:VAL:HG22	1:B:182:PHE:CD1	2.44	0.53
1:d:140:PHE:CE1	1:d:181:LEU:HD11	2.44	0.53
1:e:90:TRP:NE1	1:e:137:ALA:HB2	2.24	0.53
1:e:204:ASN:HD21	1:f:99:SER:HA	1.74	0.53
1:C:248:MET:HE2	1:C:273:VAL:HG13	1.90	0.53
1:D:107:VAL:HG11	1:D:167:LEU:HD12	1.91	0.53
1:a:49:PHE:HB3	1:a:54:THR:HG21	1.90	0.53
1:f:223:ASP:O	1:f:227:ASN:ND2	2.37	0.53
1:C:208:MET:HA	1:C:211:TRP:HD1	1.73	0.52
1:F:306:VAL:HA	1:F:309:PHE:HD2	1.74	0.52
1:F:150:VAL:HA	1:F:153:VAL:HG12	1.91	0.52
1:a:146:GLY:HA3	1:a:152:PHE:HE1	1.75	0.52
1:d:254:MET:HA	1:d:257:GLN:HG2	1.91	0.52
1:e:203:ILE:HG22	1:e:208:MET:HB2	1.91	0.52
1:f:276:TRP:HH2	1:f:290:PHE:HD1	1.58	0.52
1:B:65:ARG:HH22	1:C:275:THR:HG23	1.74	0.52
1:d:219:TYR:HE2	1:d:260:ILE:HD11	1.75	0.52
1:A:205:GLN:O	1:A:209:ASP:HB2	2.09	0.52
1:B:165:THR:OG1	1:B:169:GLN:HG2	2.09	0.52
1:C:125:ASP:HB3	1:C:129:PRO:HB2	1.91	0.52
1:C:91:PRO:HB2	1:C:136:VAL:HG23	1.92	0.52
1:D:288:PHE:HA	1:D:291:ARG:HH12	1.74	0.52
1:E:250:ARG:HH21	1:E:254:MET:HE3	1.73	0.52
1:b:156:ARG:NH2	1:b:165:THR:O	2.42	0.52
1:E:164:LEU:HB3	1:E:173:ILE:HD11	1.91	0.52
1:b:67:VAL:HG22	1:b:182:PHE:CD1	2.45	0.52
1:f:91:PRO:HB2	1:f:136:VAL:HA	1.92	0.52
1:B:264:LEU:HD11	1:B:305:THR:HG21	1.92	0.52
1:f:22:PHE:HE1	1:f:87:ARG:HG2	1.75	0.52
1:f:109:LYS:O	1:f:124:LYS:N	2.43	0.52
1:E:77:LYS:HE2	1:E:184:THR:HB	1.92	0.52
1:a:291:ARG:HD2	1:a:318:LEU:HD13	1.90	0.52
1:B:265:SER:OG	1:B:302:GLU:OE2	2.28	0.51
1:C:221:PRO:HD2	1:C:224:ASN:HD21	1.75	0.51
1:F:248:MET:HE2	1:F:276:TRP:NE1	2.25	0.51
1:b:208:MET:HE2	1:c:297:LYS:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:50:ASP:OD1	1:f:50:ASP:N	2.43	0.51
1:A:41:PRO:HB2	1:A:86:ALA:HB2	1.92	0.51
1:B:63:TYR:O	1:B:65:ARG:HG3	2.11	0.51
1:b:268:MET:SD	1:b:272:THR:OG1	2.68	0.51
1:f:267:VAL:C	1:f:268:MET:HE2	2.35	0.51
1:B:143:TYR:OH	1:B:155:GLN:OE1	2.26	0.51
1:b:79:THR:O	1:b:82:GLU:HG2	2.10	0.51
1:F:290:PHE:CZ	1:F:295:LEU:HD11	2.46	0.51
1:e:208:MET:HG2	1:f:297:LYS:HZ1	1.75	0.51
1:B:52:GLN:N	1:B:52:GLN:OE1	2.44	0.51
1:F:156:ARG:HH11	1:F:164:LEU:HD22	1.75	0.51
1:a:79:THR:HA	1:a:82:GLU:OE1	2.11	0.51
1:d:151:MET:HE3	1:d:155:GLN:HG2	1.91	0.51
1:e:251:VAL:HA	1:e:254:MET:HE2	1.92	0.51
1:f:228:ILE:HA	1:f:231:VAL:HG12	1.93	0.51
1:F:13:ASP:OD1	1:F:14:THR:N	2.44	0.51
1:C:30:VAL:HG22	1:C:62:ALA:HB2	1.93	0.51
1:D:10:ASN:O	1:D:135:ASN:ND2	2.43	0.51
1:a:285:ASP:OD1	1:a:286:VAL:N	2.44	0.51
1:b:114:VAL:HA	1:b:119:GLN:HA	1.92	0.51
1:B:103:ARG:HH21	1:B:167:LEU:HD11	1.76	0.50
1:D:214:VAL:O	1:E:296:ASN:ND2	2.42	0.50
1:E:132:TYR:OH	1:E:175:PRO:HG3	2.11	0.50
1:b:159:GLU:HG2	1:b:210:ARG:HD2	1.92	0.50
1:c:168:ASP:HB3	1:c:171:ARG:NH1	2.25	0.50
1:e:19:ARG:NH1	1:e:25:ASP:OD1	2.43	0.50
1:b:58:LEU:HD11	1:b:88:LEU:HD11	1.92	0.50
1:b:252:ALA:O	1:b:256:ARG:HG3	2.11	0.50
1:c:21:VAL:HG22	1:c:87:ARG:HD2	1.92	0.50
1:A:127:ILE:HG23	1:A:128:LEU:HD12	1.94	0.50
1:E:66:ARG:O	1:E:212:SER:OG	2.27	0.50
1:a:169:GLN:HG3	1:b:127:ILE:HG22	1.94	0.50
1:d:125:ASP:HB3	1:d:129:PRO:HB2	1.92	0.50
1:e:256:ARG:O	1:e:260:ILE:HD12	2.11	0.50
1:C:226:VAL:HG13	1:C:245:VAL:HG12	1.94	0.50
1:F:252:ALA:HA	1:F:268:MET:HG3	1.92	0.50
1:b:251:VAL:HA	1:b:254:MET:HG2	1.94	0.50
1:d:53:THR:HG21	1:d:217:LEU:HD13	1.93	0.50
1:f:37:ASP:OD1	1:f:38:SER:N	2.42	0.50
1:f:150:VAL:O	1:f:154:ILE:HG12	2.12	0.50
1:D:68:MET:HB3	1:D:214:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:180:ARG:HB3	1:E:182:PHE:CE1	2.47	0.50
1:F:149:ASP:OD1	1:F:149:ASP:N	2.43	0.50
1:b:180:ARG:HB3	1:b:182:PHE:CZ	2.47	0.50
1:d:238:ASN:OD1	1:d:241:GLY:N	2.45	0.50
1:A:207:GLN:O	1:A:211:TRP:NE1	2.45	0.50
1:C:75:THR:HG22	1:C:219:TYR:CE1	2.47	0.49
1:d:140:PHE:HE1	1:d:181:LEU:HD11	1.77	0.49
1:A:211:TRP:H	1:A:211:TRP:CD1	2.30	0.49
1:a:104:ILE:HG13	1:a:109:LYS:NZ	2.27	0.49
1:a:135:ASN:HB3	1:a:176:HIS:CE1	2.47	0.49
1:b:77:LYS:O	1:b:81:ILE:HD12	2.12	0.49
1:b:93:VAL:HG21	1:b:130:TRP:CH2	2.43	0.49
1:c:248:MET:SD	1:c:276:TRP:NE1	2.85	0.49
1:d:163:ARG:HD2	1:d:174:ARG:NH2	2.22	0.49
1:d:221:PRO:HG2	1:d:224:ASN:HB2	1.93	0.49
1:A:44:ASP:O	1:A:87:ARG:NH2	2.46	0.49
1:A:149:ASP:HB2	1:A:151:MET:HE1	1.94	0.49
1:D:163:ARG:HG2	1:D:174:ARG:HH21	1.77	0.49
1:d:11:LEU:HD11	1:d:177:PRO:HG2	1.93	0.49
1:D:91:PRO:HG2	1:D:136:VAL:HA	1.94	0.49
1:F:54:THR:C	1:F:56:ALA:N	2.71	0.49
1:d:251:VAL:HA	1:d:254:MET:HG3	1.94	0.49
1:e:245:VAL:HA	1:e:248:MET:HE2	1.93	0.49
1:B:76:GLY:O	1:B:80:HIS:ND1	2.40	0.49
1:F:109:LYS:O	1:F:124:LYS:N	2.45	0.49
1:F:230:LEU:HD21	1:F:245:VAL:HG21	1.94	0.49
1:e:179:PHE:C	1:e:180:ARG:HD2	2.38	0.49
1:D:19:ARG:NH2	1:D:25:ASP:OD1	2.45	0.49
1:B:65:ARG:NH2	1:C:275:THR:HG23	2.28	0.49
1:D:63:TYR:O	1:D:65:ARG:HG2	2.13	0.49
1:D:165:THR:HG23	1:D:172:VAL:HG23	1.94	0.49
1:b:257:GLN:O	1:b:261:ASN:ND2	2.42	0.49
1:c:238:ASN:OD1	1:c:241:GLY:N	2.39	0.49
1:d:171:ARG:HH12	1:d:173:ILE:HG22	1.78	0.49
1:E:166:LEU:H	1:E:171:ARG:HH12	1.61	0.49
1:c:162:GLY:O	1:c:174:ARG:NH2	2.45	0.49
1:e:208:MET:SD	1:f:297:LYS:HB3	2.53	0.49
1:A:271:ARG:NH1	1:f:209:ASP:O	2.45	0.48
1:B:53:THR:HG21	1:B:217:LEU:HB3	1.95	0.48
1:E:256:ARG:O	1:E:260:ILE:HD12	2.13	0.48
1:f:53:THR:HG21	1:f:80:HIS:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ASP:OD1	1:B:13:ASP:N	2.45	0.48
1:a:223:ASP:N	1:a:223:ASP:OD1	2.46	0.48
1:a:232:LYS:HG3	1:a:274:ILE:HD13	1.94	0.48
1:d:18:VAL:HG11	1:d:26:SER:HB3	1.95	0.48
1:e:221:PRO:HG2	1:e:224:ASN:HB2	1.95	0.48
1:E:174:ARG:HD3	1:E:175:PRO:HD2	1.95	0.48
1:e:66:ARG:O	1:e:212:SER:OG	2.31	0.48
1:f:60:GLY:HA2	1:f:65:ARG:HB2	1.94	0.48
1:f:132:TYR:CZ	1:f:175:PRO:HB3	2.49	0.48
1:d:104:ILE:O	1:d:104:ILE:HG13	2.12	0.48
1:e:269:SER:O	1:e:272:THR:OG1	2.20	0.48
1:f:150:VAL:HG13	1:f:151:MET:SD	2.54	0.48
1:d:13:ASP:OD1	1:d:13:ASP:N	2.46	0.48
1:d:69:VAL:HG12	1:d:215:THR:OG1	2.14	0.48
1:d:310:TYR:O	1:d:314:PHE:HB2	2.13	0.48
1:B:250:ARG:O	1:B:254:MET:HG2	2.14	0.48
1:b:153:VAL:HG13	1:b:166:LEU:HB3	1.96	0.48
1:d:241:GLY:HA2	1:d:244:ILE:HG12	1.95	0.48
1:C:82:GLU:OE2	1:C:94:ARG:NE	2.46	0.48
1:D:251:VAL:HA	1:D:254:MET:HG3	1.95	0.48
1:E:154:ILE:HA	1:E:157:VAL:HG12	1.96	0.48
1:F:179:PHE:HE1	1:F:181:LEU:HB2	1.78	0.48
1:F:244:ILE:O	1:F:248:MET:HG2	2.13	0.48
1:b:245:VAL:HA	1:b:248:MET:HE2	1.94	0.48
1:B:66:ARG:HB3	1:B:211:TRP:CZ3	2.49	0.48
1:b:179:PHE:HE1	1:b:181:LEU:HB2	1.77	0.48
1:f:238:ASN:OD1	1:f:239:ALA:N	2.46	0.48
1:f:268:MET:HE1	1:f:294:PHE:CZ	2.48	0.48
1:D:68:MET:HE3	1:D:185:ALA:HB3	1.95	0.48
1:F:17:SER:OG	1:F:20:GLU:OE1	2.30	0.48
1:E:225:GLU:OE1	1:E:256:ARG:NH2	2.44	0.47
1:f:212:SER:HB3	1:f:213:ILE:HD12	1.95	0.47
1:F:278:GLU:O	1:F:282:ILE:HG12	2.14	0.47
1:a:298:CYS:HB2	1:a:303:ARG:NH2	2.27	0.47
1:c:93:VAL:HG23	1:c:136:VAL:HG21	1.95	0.47
1:B:252:ALA:O	1:B:256:ARG:HG3	2.14	0.47
1:F:22:PHE:HE1	1:F:87:ARG:HD2	1.78	0.47
1:d:21:VAL:HG23	1:d:22:PHE:CD2	2.49	0.47
1:E:128:LEU:HD21	1:E:140:PHE:HZ	1.79	0.47
1:E:132:TYR:CD2	1:E:173:ILE:HD12	2.50	0.47
1:F:147:ARG:HG2	1:F:149:ASP:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:70:SER:OG	1:c:71:GLY:N	2.47	0.47
1:c:76:GLY:O	1:c:80:HIS:ND1	2.44	0.47
1:e:269:SER:HB3	1:e:272:THR:HG23	1.96	0.47
1:E:312:ARG:HB2	1:E:312:ARG:NH1	2.29	0.47
1:d:171:ARG:HH12	1:d:173:ILE:CG2	2.28	0.47
1:A:208:MET:HA	1:A:211:TRP:CD1	2.49	0.47
1:D:241:GLY:HA2	1:D:244:ILE:HG12	1.95	0.47
1:E:103:ARG:NH1	1:E:149:ASP:O	2.48	0.47
1:c:150:VAL:O	1:c:154:ILE:HD12	2.13	0.47
1:e:30:VAL:HG23	1:e:62:ALA:HB2	1.96	0.47
1:e:128:LEU:HD21	1:e:140:PHE:HZ	1.79	0.47
1:e:164:LEU:HD23	1:e:173:ILE:HD11	1.96	0.47
1:B:291:ARG:HA	1:B:295:LEU:HB2	1.97	0.47
1:C:156:ARG:NH2	1:C:165:THR:OG1	2.48	0.47
1:b:21:VAL:HG13	1:b:22:PHE:CD1	2.50	0.47
1:b:132:TYR:CD2	1:b:164:LEU:HD22	2.50	0.47
1:A:10:ASN:O	1:A:33:TYR:OH	2.33	0.47
1:B:77:LYS:O	1:B:81:ILE:HD12	2.14	0.47
1:a:159:GLU:OE2	1:b:94:ARG:HD3	2.15	0.47
1:c:30:VAL:HG21	1:c:58:LEU:HD11	1.96	0.47
1:d:159:GLU:CD	1:d:160:SER:H	2.22	0.47
1:C:150:VAL:O	1:C:154:ILE:HD12	2.14	0.47
1:D:144:ASP:OD2	1:D:187:THR:OG1	2.29	0.47
1:e:247:LYS:HB3	1:e:314:PHE:CE1	2.50	0.47
1:B:39:TYR:HE2	1:B:130:TRP:HZ2	1.63	0.46
1:D:296:ASN:HA	1:D:303:ARG:HH21	1.79	0.46
1:E:270:PRO:O	1:E:273:VAL:HG22	2.15	0.46
1:f:166:LEU:HB3	1:f:171:ARG:HG3	1.96	0.46
1:A:39:TYR:HB2	1:A:91:PRO:HB3	1.97	0.46
1:a:230:LEU:HD23	1:a:230:LEU:HA	1.83	0.46
1:c:125:ASP:HB3	1:c:129:PRO:HB2	1.97	0.46
1:e:68:MET:HA	1:e:183:ALA:O	2.15	0.46
1:e:110:ASP:OD1	1:e:110:ASP:N	2.47	0.46
1:e:250:ARG:NE	1:e:254:MET:SD	2.89	0.46
1:A:75:THR:HG22	1:A:219:TYR:CD2	2.43	0.46
1:F:132:TYR:CZ	1:F:175:PRO:HB3	2.49	0.46
1:A:51:ARG:HE	1:A:55:LEU:HD21	1.81	0.46
1:B:132:TYR:OH	1:B:175:PRO:HG3	2.16	0.46
1:b:107:VAL:HG11	1:b:167:LEU:HD12	1.97	0.46
1:d:172:VAL:HG13	1:d:174:ARG:HH22	1.80	0.46
1:e:170:SER:N	1:f:39:TYR:OH	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:289:ALA:O	1:f:293:THR:OG1	2.26	0.46
1:E:107:VAL:HG21	1:E:167:LEU:HB2	1.97	0.46
1:E:248:MET:HE3	1:E:276:TRP:HD1	1.76	0.46
1:F:150:VAL:O	1:F:154:ILE:HG12	2.15	0.46
1:e:106:LEU:HD12	1:e:127:ILE:HB	1.96	0.46
1:C:264:LEU:HD11	1:C:306:VAL:HG22	1.97	0.46
1:D:169:GLN:HG3	1:E:130:TRP:CD2	2.50	0.46
1:a:159:GLU:HA	1:a:210:ARG:HH12	1.81	0.46
1:a:299:ASP:O	1:a:303:ARG:NH1	2.49	0.46
1:A:60:GLY:HA2	1:A:65:ARG:HB2	1.96	0.46
1:D:125:ASP:HB3	1:D:129:PRO:HB2	1.96	0.46
1:b:220:LEU:H	1:b:220:LEU:HG	1.49	0.46
1:f:278:GLU:O	1:f:282:ILE:HG12	2.16	0.46
1:E:49:PHE:HZ	1:E:87:ARG:NH1	2.14	0.46
1:a:44:ASP:O	1:a:87:ARG:NH2	2.48	0.46
1:d:254:MET:HE1	1:d:309:PHE:CG	2.50	0.46
1:f:74:GLY:O	1:f:270:PRO:HD2	2.15	0.46
1:B:125:ASP:HB3	1:B:129:PRO:HB2	1.98	0.46
1:a:208:MET:HA	1:a:211:TRP:CD1	2.49	0.46
1:A:15:THR:HG22	1:A:29:MET:HE3	1.97	0.45
1:F:166:LEU:HB3	1:F:171:ARG:HG3	1.97	0.45
1:F:276:TRP:CH2	1:F:290:PHE:HA	2.52	0.45
1:A:155:GLN:OE1	1:A:155:GLN:N	2.45	0.45
1:D:186:ASN:OD1	1:D:187:THR:N	2.49	0.45
1:F:241:GLY:O	1:F:245:VAL:HG22	2.16	0.45
1:b:204:ASN:ND2	1:c:99:SER:HB2	2.31	0.45
1:A:159:GLU:HA	1:A:210:ARG:NH1	2.31	0.45
1:A:291:ARG:HD3	1:A:319:PRO:HB3	1.99	0.45
1:C:219:TYR:O	1:C:220:LEU:C	2.59	0.45
1:C:238:ASN:OD1	1:C:241:GLY:N	2.36	0.45
1:c:169:GLN:O	1:d:39:TYR:OH	2.25	0.45
1:B:93:VAL:HG21	1:B:130:TRP:HH2	1.81	0.45
1:E:164:LEU:HD23	1:E:173:ILE:HD11	1.98	0.45
1:E:167:LEU:H	1:E:171:ARG:NH2	2.14	0.45
1:a:15:THR:HG22	1:a:29:MET:HE3	1.99	0.45
1:a:76:GLY:O	1:a:79:THR:OG1	2.27	0.45
1:d:115:LYS:HB2	1:d:120:VAL:HG21	1.98	0.45
1:e:160:SER:HB3	1:e:164:LEU:HD13	1.99	0.45
1:A:204:ASN:ND2	1:A:207:GLN:HB2	2.31	0.45
1:D:310:TYR:O	1:D:314:PHE:HB2	2.17	0.45
1:E:63:TYR:CE2	1:F:282:ILE:HD12	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:221:PRO:HG2	1:E:224:ASN:HB2	1.98	0.45
1:F:270:PRO:HA	1:F:273:VAL:HG12	1.99	0.45
1:b:10:ASN:O	1:b:33:TYR:OH	2.34	0.45
1:e:35:ALA:C	1:e:89:ASN:HD21	2.24	0.45
1:e:143:TYR:HE1	1:e:211:TRP:HE1	1.63	0.45
1:A:282:ILE:HD12	1:f:63:TYR:CD2	2.52	0.45
1:B:52:GLN:NE2	1:B:53:THR:HG23	2.31	0.45
1:C:79:THR:HG21	1:C:271:ARG:HH12	1.80	0.45
1:E:246:ASN:O	1:E:250:ARG:HG2	2.17	0.45
1:F:66:ARG:HE	1:F:158:LEU:HD12	1.81	0.45
1:F:99:SER:C	1:F:100:HIS:CD2	2.95	0.45
1:a:159:GLU:HA	1:a:210:ARG:NH1	2.31	0.45
1:c:83:GLN:HG2	1:c:87:ARG:NH2	2.31	0.45
1:d:169:GLN:HG3	1:e:130:TRP:CE3	2.51	0.45
1:f:10:ASN:O	1:f:33:TYR:OH	2.34	0.45
1:B:180:ARG:HB3	1:B:182:PHE:CZ	2.52	0.45
1:E:17:SER:OG	1:E:20:GLU:OE1	2.27	0.45
1:a:37:ASP:HB2	1:a:91:PRO:HG3	1.99	0.45
1:b:112:ILE:HA	1:b:121:THR:HA	1.99	0.45
1:F:93:VAL:HG23	1:F:136:VAL:HG11	1.98	0.45
1:b:79:THR:O	1:b:83:GLN:HG2	2.17	0.45
1:d:152:PHE:CE1	1:e:101:VAL:HG22	2.52	0.45
1:f:127:ILE:HG23	1:f:128:LEU:HD22	1.99	0.45
1:A:125:ASP:HB3	1:A:129:PRO:HG2	2.00	0.44
1:A:258:ALA:HA	1:A:261:ASN:HD22	1.82	0.44
1:E:269:SER:O	1:E:272:THR:OG1	2.20	0.44
1:F:269:SER:OG	1:F:272:THR:HG23	2.18	0.44
1:d:78:SER:O	1:d:82:GLU:HG2	2.17	0.44
1:d:171:ARG:HD2	1:d:171:ARG:HA	1.74	0.44
1:e:63:TYR:CD2	1:f:282:ILE:HD12	2.52	0.44
1:C:83:GLN:HG2	1:C:87:ARG:HH22	1.82	0.44
1:C:90:TRP:CH2	1:C:178:ALA:HB1	2.52	0.44
1:d:144:ASP:OD1	1:d:144:ASP:N	2.51	0.44
1:e:103:ARG:HD2	1:e:167:LEU:HD11	1.99	0.44
1:f:166:LEU:HD23	1:f:171:ARG:HG3	1.99	0.44
1:A:318:LEU:H	1:A:319:PRO:HD2	1.82	0.44
1:b:54:THR:O	1:b:58:LEU:HD23	2.17	0.44
1:E:22:PHE:HB3	1:E:24:ILE:HD12	1.99	0.44
1:C:209:ASP:OD2	1:D:271:ARG:NH2	2.50	0.44
1:B:144:ASP:OD1	1:B:145:ALA:N	2.51	0.44
1:C:12:PRO:HG3	1:C:90:TRP:CZ3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:17:SER:OG	1:e:20:GLU:OE1	2.26	0.44
1:B:169:GLN:NE2	1:C:130:TRP:CD1	2.81	0.44
1:C:132:TYR:CZ	1:C:175:PRO:HB3	2.52	0.44
1:D:248:MET:HE1	1:D:276:TRP:CG	2.53	0.44
1:E:160:SER:HB3	1:E:164:LEU:HD13	2.00	0.44
1:b:278:GLU:O	1:b:282:ILE:HG12	2.18	0.44
1:b:291:ARG:HA	1:b:295:LEU:HB2	2.00	0.44
1:D:70:SER:HA	1:D:185:ALA:O	2.18	0.44
1:D:226:VAL:O	1:D:230:LEU:HD23	2.17	0.44
1:E:270:PRO:HA	1:E:273:VAL:HG22	2.00	0.44
1:F:18:VAL:HG13	1:F:22:PHE:HD2	1.83	0.44
1:a:159:GLU:O	1:a:210:ARG:NH2	2.42	0.44
1:e:78:SER:OG	1:e:141:ASP:OD2	2.28	0.44
1:C:99:SER:O	1:C:100:HIS:ND1	2.51	0.44
1:a:155:GLN:O	1:a:159:GLU:N	2.51	0.44
1:c:108:GLY:O	1:c:109:LYS:HE2	2.18	0.44
1:c:128:LEU:HD21	1:c:157:VAL:HG21	2.00	0.44
1:d:308:GLU:OE1	1:d:312:ARG:NH1	2.51	0.44
1:B:63:TYR:CE2	1:C:282:ILE:HD12	2.53	0.43
1:d:30:VAL:HG11	1:d:58:LEU:HD12	2.00	0.43
1:e:115:LYS:HD3	1:e:115:LYS:HA	1.85	0.43
1:e:258:ALA:O	1:e:262:GLY:N	2.51	0.43
1:C:47:TYR:HB2	1:C:83:GLN:HE22	1.83	0.43
1:C:247:LYS:NZ	1:C:314:PHE:HA	2.32	0.43
1:D:158:LEU:HD21	1:D:210:ARG:HB3	1.99	0.43
1:d:226:VAL:O	1:d:230:LEU:HD23	2.17	0.43
1:e:275:THR:HA	1:e:278:GLU:HG2	2.01	0.43
1:f:244:ILE:O	1:f:248:MET:HG2	2.18	0.43
1:C:44:ASP:HB3	1:C:83:GLN:NE2	2.33	0.43
1:a:289:ALA:O	1:a:293:THR:OG1	2.29	0.43
1:C:128:LEU:HD11	1:C:157:VAL:HG11	2.00	0.43
1:E:44:ASP:O	1:E:83:GLN:NE2	2.52	0.43
1:b:164:LEU:HB3	1:b:173:ILE:HB	2.00	0.43
1:c:41:PRO:HB2	1:c:86:ALA:HB2	1.99	0.43
1:E:248:MET:O	1:E:251:VAL:HG12	2.18	0.43
1:A:245:VAL:HG13	1:A:248:MET:HE2	2.01	0.43
1:B:163:ARG:HG3	1:B:172:VAL:HG23	2.00	0.43
1:d:53:THR:O	1:d:57:ILE:HG12	2.18	0.43
1:C:159:GLU:HG3	1:C:210:ARG:HD3	2.00	0.43
1:D:30:VAL:HG12	1:D:62:ALA:HB2	1.99	0.43
1:D:248:MET:HE1	1:D:276:TRP:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:28:MET:HE2	1:a:55:LEU:HD13	2.01	0.43
1:f:125:ASP:HB3	1:f:129:PRO:HB2	2.00	0.43
1:D:43:LEU:HG	1:D:87:ARG:NH2	2.34	0.43
1:D:132:TYR:HA	1:D:179:PHE:CE1	2.54	0.43
1:E:89:ASN:O	1:E:89:ASN:ND2	2.51	0.43
1:c:298:CYS:SG	1:c:302:GLU:HG3	2.59	0.43
1:d:90:TRP:CH2	1:d:178:ALA:HB1	2.51	0.43
1:C:100:HIS:HA	1:C:147:ARG:HH22	1.84	0.43
1:E:156:ARG:HA	1:E:156:ARG:HD2	1.89	0.43
1:E:285:ASP:OD1	1:E:286:VAL:N	2.52	0.43
1:F:147:ARG:NH1	1:F:149:ASP:OD1	2.52	0.43
1:F:147:ARG:O	1:F:149:ASP:N	2.46	0.43
1:a:63:TYR:O	1:a:65:ARG:NH1	2.51	0.43
1:b:219:TYR:HD1	1:b:219:TYR:HA	1.73	0.43
1:e:60:GLY:HA2	1:e:65:ARG:HB2	2.00	0.43
1:e:172:VAL:HG11	1:f:38:SER:HB2	2.00	0.43
1:f:266:THR:OG1	1:f:294:PHE:HZ	2.01	0.43
1:C:100:HIS:HA	1:C:147:ARG:NH2	2.34	0.43
1:c:75:THR:HG22	1:c:219:TYR:CD1	2.54	0.43
1:D:69:VAL:HG13	1:D:217:LEU:HD23	2.00	0.42
1:D:244:ILE:HG13	1:D:245:VAL:N	2.34	0.42
1:F:18:VAL:HG13	1:F:22:PHE:CD2	2.54	0.42
1:B:68:MET:HE3	1:B:211:TRP:CE2	2.54	0.42
1:C:291:ARG:HG2	1:C:295:LEU:HD23	2.01	0.42
1:E:73:HIS:HB3	1:E:267:VAL:HG11	2.01	0.42
1:E:83:GLN:HG2	1:E:87:ARG:NH1	2.34	0.42
1:c:91:PRO:HB2	1:c:136:VAL:HG23	2.01	0.42
1:e:63:TYR:CE2	1:f:282:ILE:HD12	2.54	0.42
1:f:150:VAL:HA	1:f:153:VAL:HG12	2.01	0.42
1:f:270:PRO:HA	1:f:273:VAL:HG22	2.00	0.42
1:D:179:PHE:C	1:D:180:ARG:HD2	2.43	0.42
1:E:276:TRP:CH2	1:E:290:PHE:HA	2.54	0.42
1:F:156:ARG:NE	1:F:166:LEU:HB2	2.35	0.42
1:e:91:PRO:HB2	1:e:136:VAL:HA	2.02	0.42
1:e:91:PRO:HB2	1:e:136:VAL:HG12	2.01	0.42
1:e:267:VAL:O	1:e:268:MET:HE2	2.19	0.42
1:F:251:VAL:HA	1:F:254:MET:HG3	2.01	0.42
1:a:54:THR:HA	1:a:57:ILE:HG12	2.00	0.42
1:b:232:LYS:HD2	1:b:232:LYS:HA	1.85	0.42
1:d:61:PHE:HE2	1:d:90:TRP:CG	2.38	0.42
1:d:76:GLY:O	1:d:80:HIS:ND1	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:97:LEU:HD12	1:d:143:TYR:HA	2.01	0.42
1:A:225:GLU:HA	1:A:228:ILE:HD12	2.01	0.42
1:C:146:GLY:C	1:C:151:MET:HE1	2.44	0.42
1:E:83:GLN:HG2	1:E:87:ARG:HH11	1.84	0.42
1:F:269:SER:O	1:F:272:THR:OG1	2.26	0.42
1:c:75:THR:HG22	1:c:219:TYR:CE1	2.55	0.42
1:d:179:PHE:CE2	1:d:181:LEU:HB2	2.55	0.42
1:B:66:ARG:HB3	1:B:211:TRP:CE3	2.55	0.42
1:C:271:ARG:HA	1:C:274:ILE:HD13	2.01	0.42
1:b:18:VAL:HG21	1:b:26:SER:HB3	2.02	0.42
1:b:221:PRO:HD2	1:b:224:ASN:HB2	2.02	0.42
1:d:143:TYR:HB3	1:d:185:ALA:HB2	2.00	0.42
1:f:77:LYS:HD2	1:f:184:THR:HG23	2.01	0.42
1:A:79:THR:HA	1:A:82:GLU:CD	2.45	0.42
1:C:164:LEU:HG	1:C:166:LEU:HG	2.02	0.42
1:C:208:MET:HA	1:C:211:TRP:CD1	2.54	0.42
1:D:13:ASP:OD1	1:D:14:THR:N	2.52	0.42
1:E:41:PRO:HB3	1:E:82:GLU:HG3	2.02	0.42
1:F:290:PHE:CE2	1:F:295:LEU:HD11	2.55	0.42
1:A:54:THR:HA	1:A:57:ILE:HG12	2.00	0.42
1:A:126:GLY:C	1:A:129:PRO:HD2	2.45	0.42
1:C:291:ARG:HA	1:C:295:LEU:HB3	2.00	0.42
1:E:13:ASP:OD1	1:E:13:ASP:N	2.49	0.42
1:c:219:TYR:O	1:c:220:LEU:C	2.63	0.42
1:d:54:THR:O	1:d:58:LEU:HD23	2.20	0.42
1:d:268:MET:HE1	1:d:294:PHE:CG	2.55	0.42
1:d:296:ASN:HA	1:d:303:ARG:HH21	1.83	0.42
1:e:69:VAL:HG13	1:e:217:LEU:HD23	2.02	0.42
1:f:269:SER:OG	1:f:272:THR:HG23	2.19	0.42
1:A:154:ILE:HD12	1:A:154:ILE:H	1.85	0.42
1:B:285:ASP:HB3	1:B:288:PHE:HB3	2.01	0.42
1:C:58:LEU:HD12	1:C:58:LEU:HA	1.91	0.42
1:b:78:SER:CB	1:b:94:ARG:HH21	2.32	0.42
1:F:247:LYS:HB3	1:F:314:PHE:CE1	2.55	0.41
1:a:242:ARG:HA	1:a:245:VAL:HG12	2.02	0.41
1:d:46:ASP:N	1:d:46:ASP:OD1	2.53	0.41
1:d:75:THR:HG23	1:d:77:LYS:HG3	2.02	0.41
1:f:50:ASP:O	1:f:54:THR:OG1	2.33	0.41
1:f:207:GLN:HG2	1:f:208:MET:SD	2.60	0.41
1:B:93:VAL:HG21	1:B:130:TRP:CH2	2.55	0.41
1:C:81:ILE:HD12	1:C:81:ILE:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:55:LEU:HD23	1:c:55:LEU:HA	1.91	0.41
1:d:52:GLN:HB3	1:e:288:PHE:HE1	1.85	0.41
1:d:150:VAL:HG12	1:d:154:ILE:HG12	2.00	0.41
1:f:155:GLN:NE2	1:f:207:GLN:HB2	2.35	0.41
1:C:251:VAL:HG11	1:C:314:PHE:CZ	2.54	0.41
1:D:22:PHE:HZ	1:D:84:VAL:HA	1.84	0.41
1:E:247:LYS:HB3	1:E:314:PHE:CE1	2.55	0.41
1:b:67:VAL:HG22	1:b:182:PHE:HD1	1.84	0.41
1:c:302:GLU:O	1:c:305:THR:OG1	2.37	0.41
1:e:128:LEU:HD23	1:e:138:LEU:HD21	2.03	0.41
1:e:270:PRO:HA	1:e:273:VAL:HG22	2.02	0.41
1:e:276:TRP:HH2	1:e:290:PHE:CD1	2.39	0.41
1:A:166:LEU:HD23	1:A:166:LEU:HA	1.91	0.41
1:B:10:ASN:O	1:B:33:TYR:OH	2.33	0.41
1:c:70:SER:OG	1:c:187:THR:O	2.36	0.41
1:d:163:ARG:CD	1:d:174:ARG:HH21	2.27	0.41
1:A:97:LEU:HD12	1:A:143:TYR:HA	2.02	0.41
1:A:276:TRP:CZ3	1:A:290:PHE:HA	2.56	0.41
1:C:57:ILE:HG21	1:C:84:VAL:HG11	2.02	0.41
1:C:180:ARG:HB3	1:C:182:PHE:CE2	2.56	0.41
1:b:73:HIS:HB2	1:b:267:VAL:HG21	2.03	0.41
1:c:49:PHE:HZ	1:c:87:ARG:NH2	2.18	0.41
1:A:259:PHE:HA	1:A:264:LEU:HB2	2.03	0.41
1:E:50:ASP:O	1:E:54:THR:HG22	2.21	0.41
1:E:308:GLU:HB3	1:E:312:ARG:HH21	1.85	0.41
1:c:132:TYR:HA	1:c:179:PHE:CD1	2.55	0.41
1:c:139:VAL:HG22	1:c:182:PHE:HB2	2.02	0.41
1:d:139:VAL:HG12	1:d:182:PHE:HB2	2.01	0.41
1:e:77:LYS:HG3	1:e:78:SER:N	2.35	0.41
1:B:65:ARG:NH1	1:B:213:ILE:HD11	2.35	0.41
1:b:73:HIS:CG	1:b:267:VAL:HG11	2.55	0.41
1:b:143:TYR:OH	1:b:207:GLN:OE1	2.29	0.41
1:b:147:ARG:HA	1:b:148:PRO:HD3	1.95	0.41
1:b:164:LEU:HG	1:b:166:LEU:HG	2.02	0.41
1:b:206:ALA:O	1:b:210:ARG:HG2	2.21	0.41
1:b:214:VAL:HG13	1:c:296:ASN:HB2	2.03	0.41
1:f:212:SER:CB	1:f:213:ILE:HD12	2.51	0.41
1:C:18:VAL:HA	1:C:22:PHE:HB3	2.03	0.41
1:C:41:PRO:HB2	1:C:86:ALA:HB2	2.02	0.41
1:E:208:MET:CE	1:F:297:LYS:HB3	2.50	0.41
1:F:233:ALA:O	1:F:236:TYR:N	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:18:VAL:HG21	1:a:28:MET:HE3	2.01	0.41
1:a:252:ALA:HB1	1:a:256:ARG:NH1	2.36	0.41
1:b:269:SER:C	1:b:271:ARG:H	2.29	0.41
1:d:164:LEU:HB3	1:d:173:ILE:HG13	2.03	0.41
1:f:225:GLU:O	1:f:228:ILE:HG22	2.20	0.41
1:A:79:THR:HA	1:A:82:GLU:OE2	2.21	0.41
1:D:53:THR:O	1:D:57:ILE:HG12	2.20	0.41
1:E:275:THR:HA	1:E:278:GLU:HG2	2.02	0.41
1:a:67:VAL:HB	1:a:182:PHE:CD1	2.56	0.41
1:a:132:TYR:CZ	1:a:164:LEU:HB2	2.56	0.41
1:c:271:ARG:HA	1:c:274:ILE:HB	2.03	0.41
1:d:165:THR:HG23	1:d:172:VAL:HG23	2.03	0.41
1:A:15:THR:CG2	1:A:29:MET:HG3	2.51	0.40
1:A:150:VAL:HG11	1:B:102:SER:HB3	2.03	0.40
1:C:156:ARG:HD2	1:C:156:ARG:HA	1.92	0.40
1:D:135:ASN:HB3	1:D:176:HIS:CE1	2.55	0.40
1:F:99:SER:C	1:F:100:HIS:HD2	2.29	0.40
1:c:94:ARG:NH2	1:c:141:ASP:OD2	2.54	0.40
1:C:77:LYS:HB2	1:C:184:THR:OG1	2.21	0.40
1:D:169:GLN:HG3	1:E:130:TRP:CE3	2.56	0.40
1:E:208:MET:HE1	1:F:297:LYS:HB3	2.03	0.40
1:E:276:TRP:HH2	1:E:290:PHE:CD1	2.37	0.40
1:a:244:ILE:HG23	1:a:248:MET:HE3	2.03	0.40
1:b:148:PRO:HB3	1:c:100:HIS:CE1	2.56	0.40
1:f:101:VAL:O	1:f:147:ARG:NH2	2.54	0.40
1:D:247:LYS:HE2	1:D:314:PHE:CE2	2.57	0.40
1:E:11:LEU:H	1:E:11:LEU:HD23	1.86	0.40
1:b:30:VAL:HG13	1:b:62:ALA:HB2	2.03	0.40
1:c:70:SER:HB2	1:c:185:ALA:HB3	2.03	0.40
1:d:153:VAL:O	1:d:157:VAL:HG12	2.21	0.40
1:B:103:ARG:O	1:B:107:VAL:HG12	2.21	0.40
1:B:140:PHE:CE2	1:B:181:LEU:HD11	2.56	0.40
1:B:156:ARG:NH2	1:B:165:THR:O	2.54	0.40
1:C:126:GLY:C	1:C:129:PRO:HD2	2.46	0.40
1:E:21:VAL:HG13	1:E:22:PHE:CD2	2.57	0.40
1:F:22:PHE:HE2	1:F:58:LEU:HD11	1.85	0.40
1:A:233:ALA:HB1	1:A:236:TYR:HB3	2.04	0.40
1:C:70:SER:OG	1:C:71:GLY:N	2.54	0.40
1:E:291:ARG:HA	1:E:295:LEU:HD23	2.03	0.40
1:a:61:PHE:HZ	1:a:90:TRP:CE3	2.39	0.40
1:c:10:ASN:O	1:c:33:TYR:OH	2.26	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:50:ASP:OD1	1:f:53:THR:HB	2.21	0.40
1:f:268:MET:HE2	1:f:268:MET:N	2.37	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	291/328 (89%)	275 (94%)	14 (5%)	2 (1%)	18	54
1	B	288/328 (88%)	272 (94%)	15 (5%)	1 (0%)	36	70
1	C	290/328 (88%)	275 (95%)	12 (4%)	3 (1%)	12	45
1	D	288/328 (88%)	269 (93%)	19 (7%)	0	100	100
1	E	291/328 (89%)	281 (97%)	10 (3%)	0	100	100
1	F	274/328 (84%)	248 (90%)	26 (10%)	0	100	100
1	a	291/328 (89%)	272 (94%)	19 (6%)	0	100	100
1	b	288/328 (88%)	266 (92%)	21 (7%)	1 (0%)	36	70
1	c	290/328 (88%)	275 (95%)	14 (5%)	1 (0%)	36	70
1	d	288/328 (88%)	269 (93%)	19 (7%)	0	100	100
1	e	290/328 (88%)	275 (95%)	15 (5%)	0	100	100
1	f	273/328 (83%)	249 (91%)	24 (9%)	0	100	100
All	All	3442/3936 (87%)	3226 (94%)	208 (6%)	8 (0%)	44	75

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	b	115	LYS
1	A	318	LEU

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Mol	Chain	Res	Type
1	C	205	GLN
1	A	220	LEU
1	C	219	TYR
1	B	114	VAL
1	c	219	TYR
1	C	220	LEU

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	252/278 (91%)	250 (99%)	2 (1%)	73	78
1	B	249/278 (90%)	249 (100%)	0	100	100
1	C	251/278 (90%)	250 (100%)	1 (0%)	84	84
1	D	249/278 (90%)	249 (100%)	0	100	100
1	E	252/278 (91%)	251 (100%)	1 (0%)	84	84
1	F	239/278 (86%)	239 (100%)	0	100	100
1	a	252/278 (91%)	251 (100%)	1 (0%)	84	84
1	b	249/278 (90%)	246 (99%)	3 (1%)	63	73
1	c	251/278 (90%)	249 (99%)	2 (1%)	73	78
1	d	249/278 (90%)	249 (100%)	0	100	100
1	e	251/278 (90%)	251 (100%)	0	100	100
1	f	238/278 (86%)	238 (100%)	0	100	100
All	All	2982/3336 (89%)	2972 (100%)	10 (0%)	84	85

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	ASN
1	A	218	ASN
1	C	220	LEU
1	E	72	TYR

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Mol	Chain	Res	Type
1	a	173	ILE
1	b	217	LEU
1	b	219	TYR
1	b	220	LEU
1	c	219	TYR
1	c	220	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	100	HIS
1	A	133	GLN
1	A	204	ASN
1	A	261	ASN
1	A	311	GLN
1	B	119	GLN
1	B	133	GLN
1	B	134	HIS
1	B	257	GLN
1	C	83	GLN
1	C	96	ASN
1	C	169	GLN
1	C	207	GLN
1	C	246	ASN
1	C	257	GLN
1	C	311	GLN
1	D	64	ASN
1	D	96	ASN
1	D	135	ASN
1	D	169	GLN
1	D	205	GLN
1	D	222	HIS
1	D	296	ASN
1	E	186	ASN
1	E	227	ASN
1	F	135	ASN
1	F	155	GLN
1	F	224	ASN
1	F	261	ASN
1	a	83	GLN
1	b	96	ASN

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Mol	Chain	Res	Type
1	b	133	GLN
1	b	134	HIS
1	b	205	GLN
1	b	257	GLN
1	b	296	ASN
1	c	96	ASN
1	c	100	HIS
1	c	227	ASN
1	c	257	GLN
1	c	296	ASN
1	c	311	GLN
1	d	10	ASN
1	d	135	ASN
1	d	155	GLN
1	d	207	GLN
1	e	227	ASN
1	e	257	GLN
1	f	169	GLN
1	f	296	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

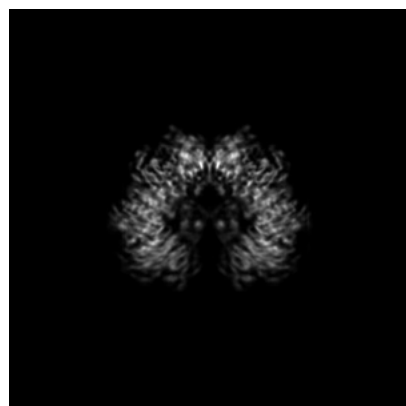
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64229. These allow visual inspection of the internal detail of the map and identification of artifacts.

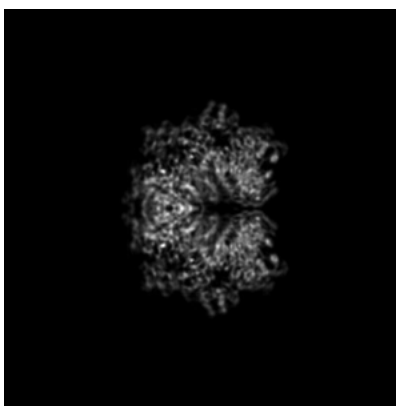
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

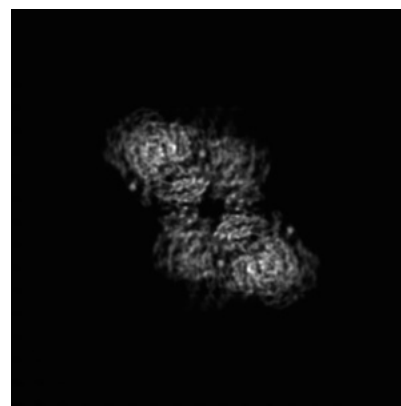
6.1.1 Primary map



X

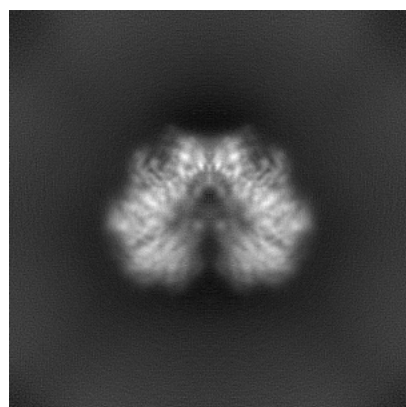


Y

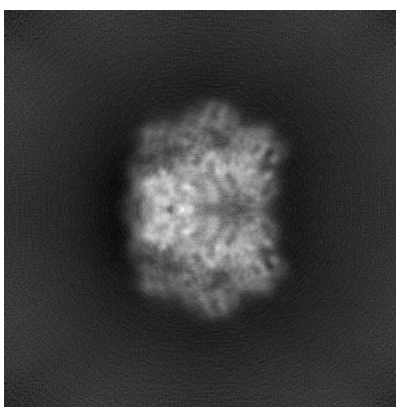


Z

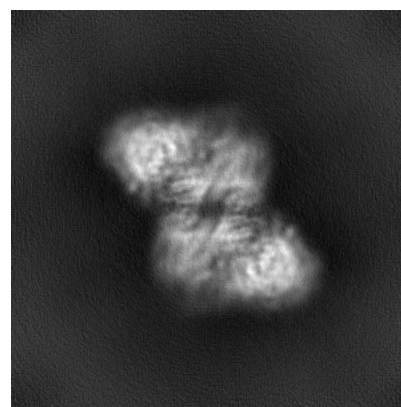
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

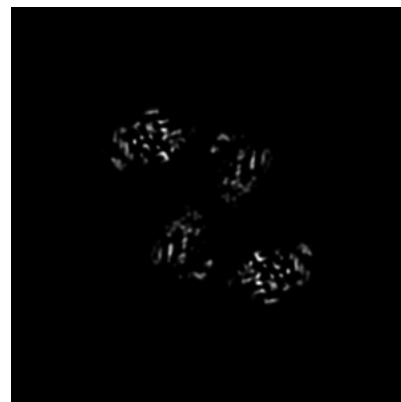
6.2.1 Primary map



X Index: 200

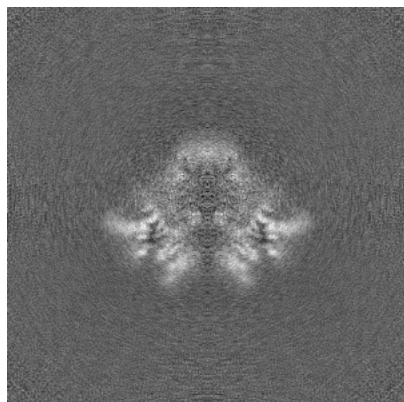


Y Index: 200

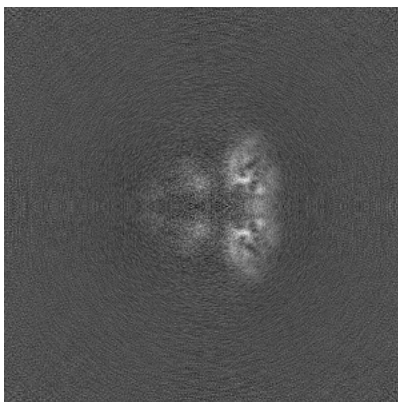


Z Index: 200

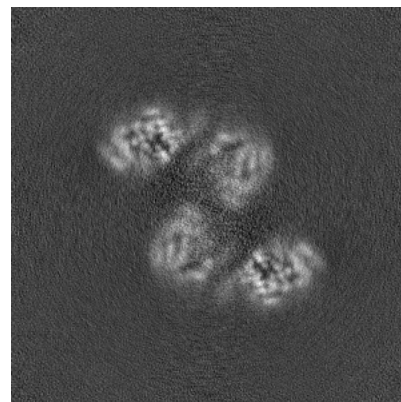
6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

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: 170

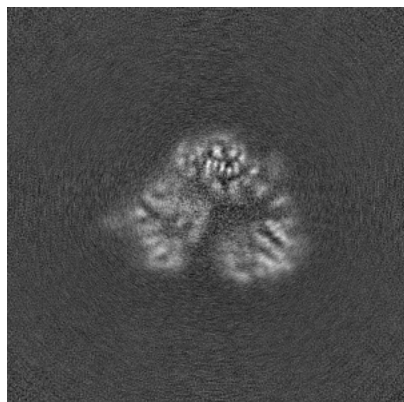


Y Index: 146

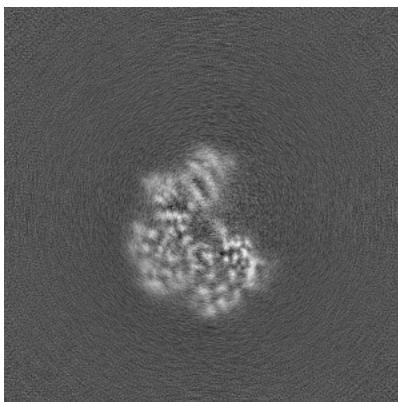


Z Index: 236

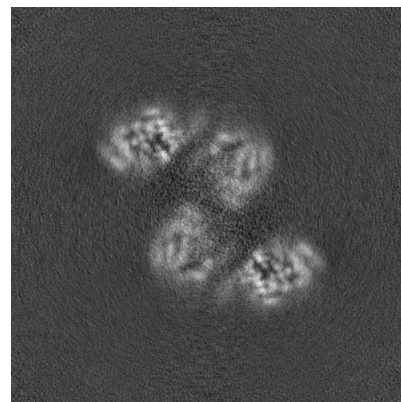
6.3.2 Raw map



X Index: 174



Y Index: 255

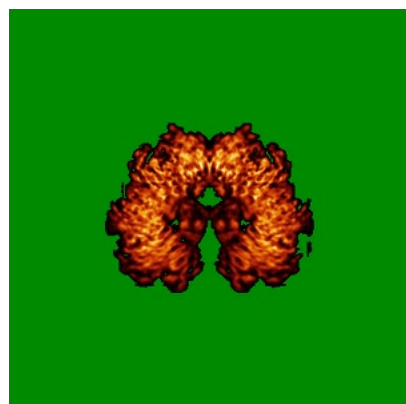


Z Index: 200

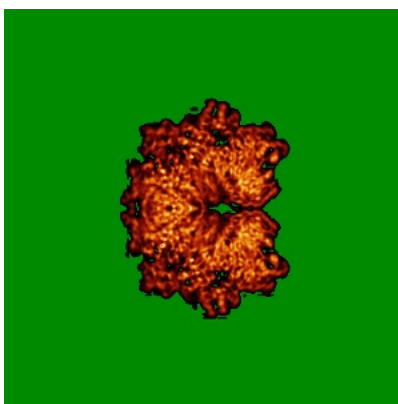
The images above show the largest variance slices of the map in three orthogonal directions.

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

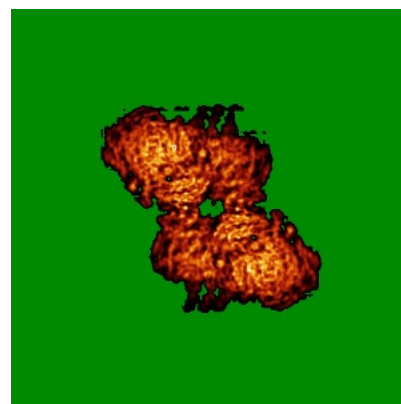
6.4.1 Primary map



X

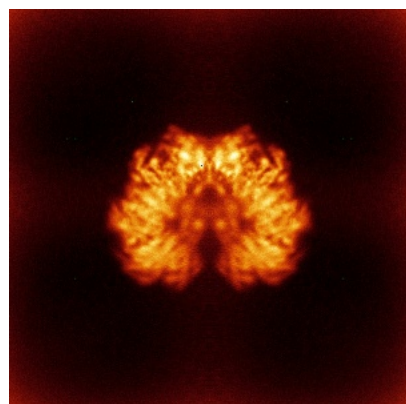


Y

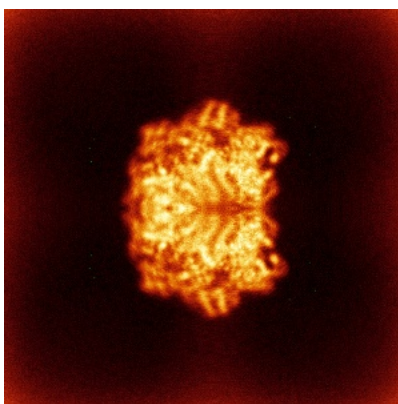


Z

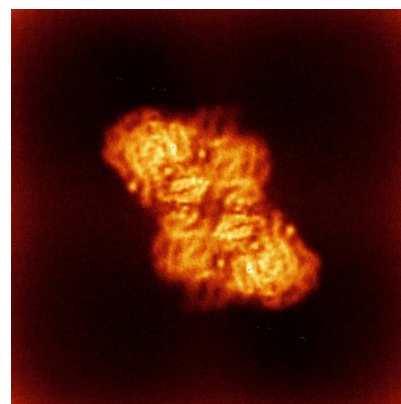
6.4.2 Raw map



X



Y



Z

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

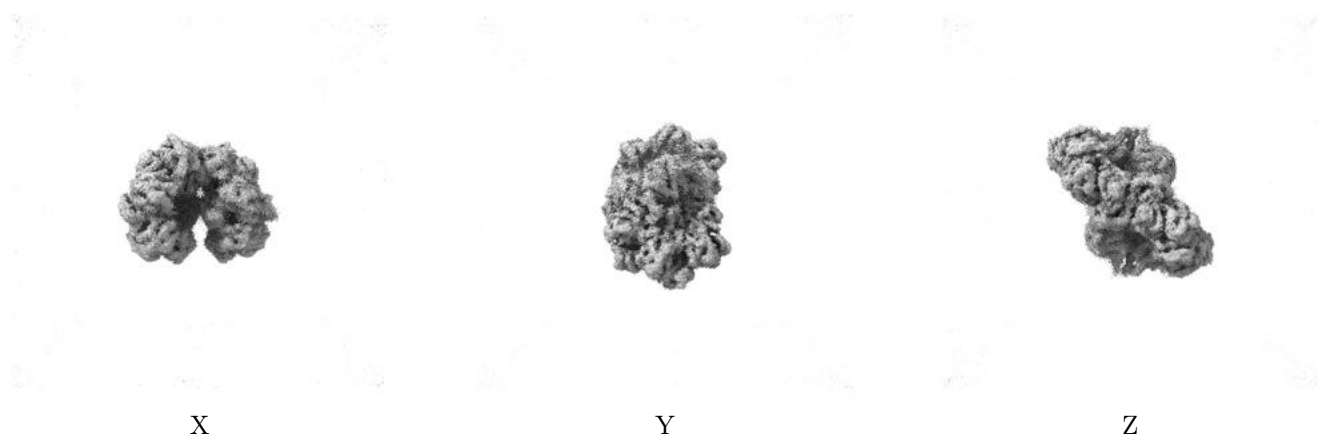
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

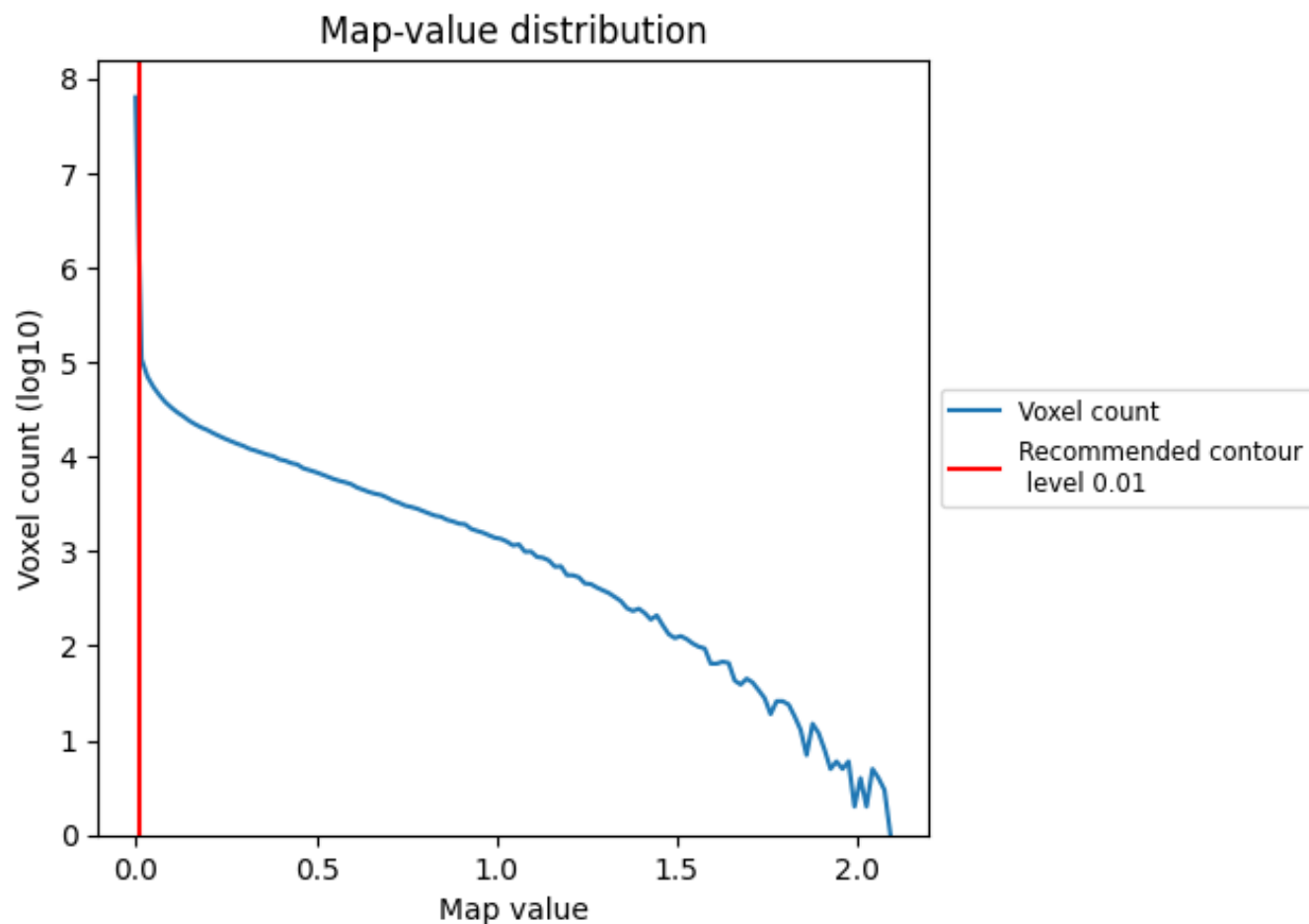
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

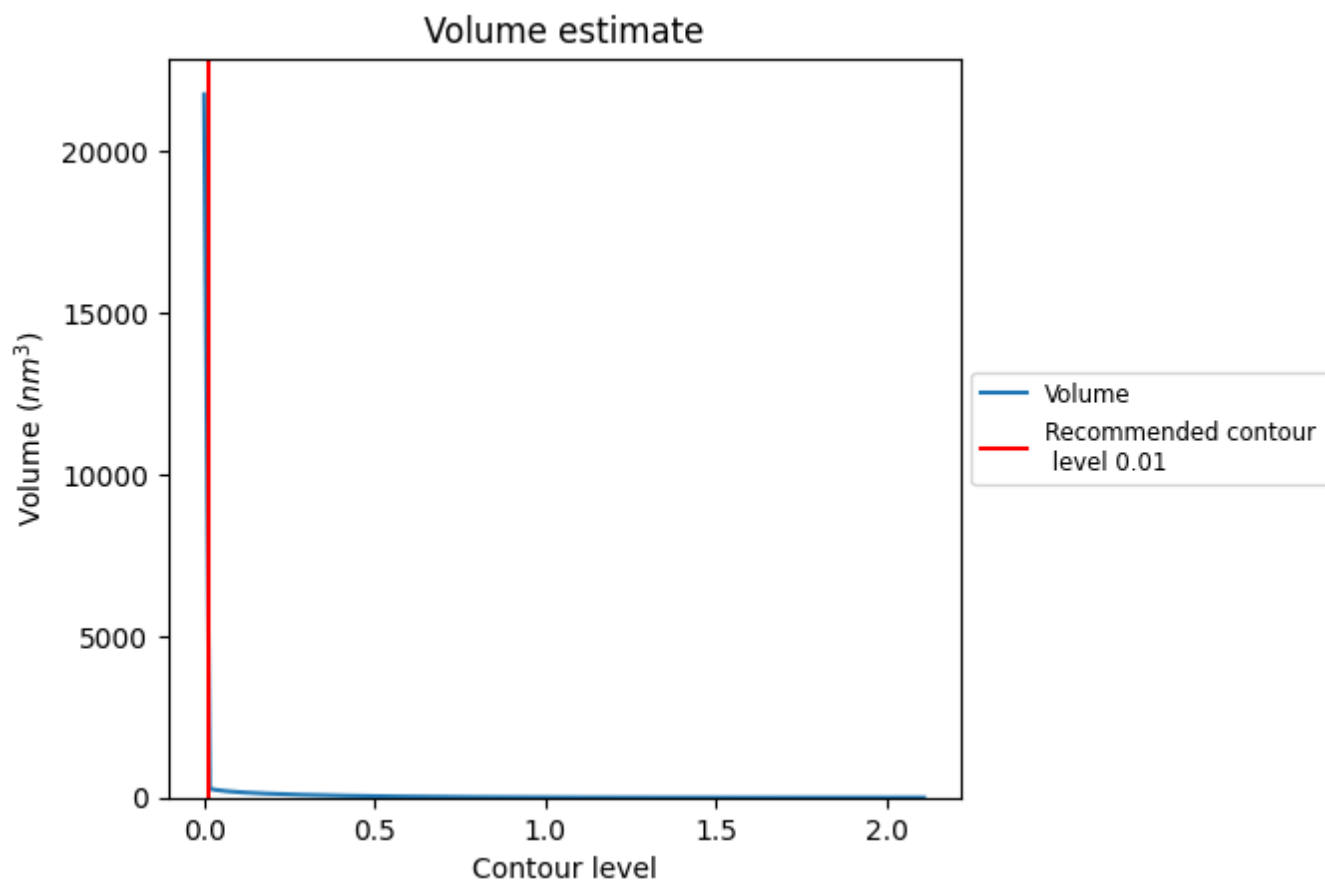
This section contains the results of statistical analysis of the map.

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.

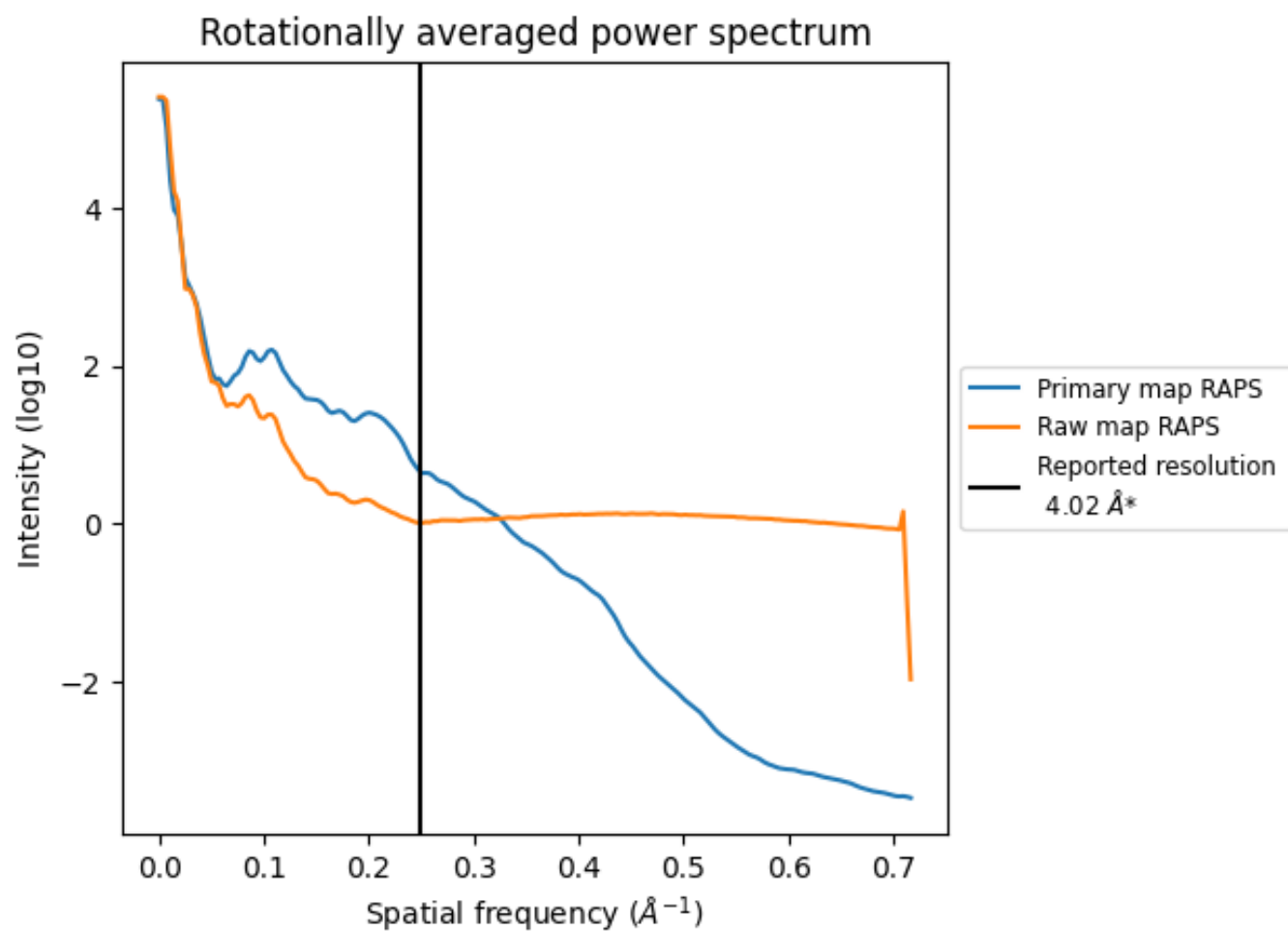
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6560 nm³; this corresponds to an approximate mass of 5926 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 ⓘ

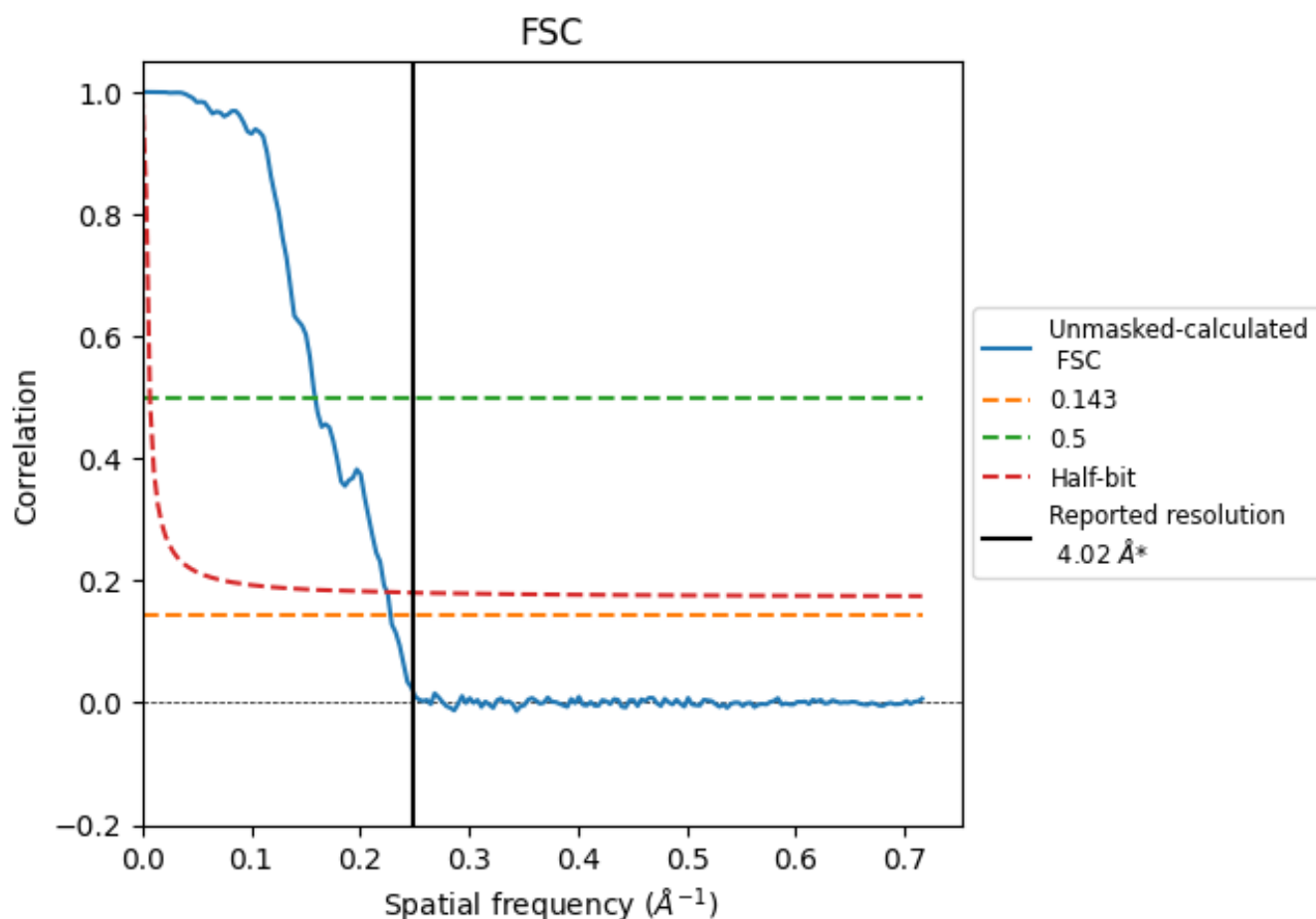


*Reported resolution corresponds to spatial frequency of 0.249 $\text{\AA}^{-1}$

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 0.249 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

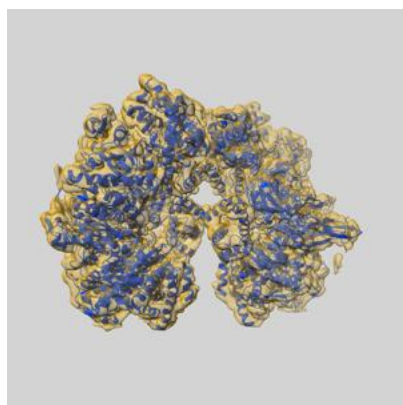
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.02	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.38	6.30	4.45

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

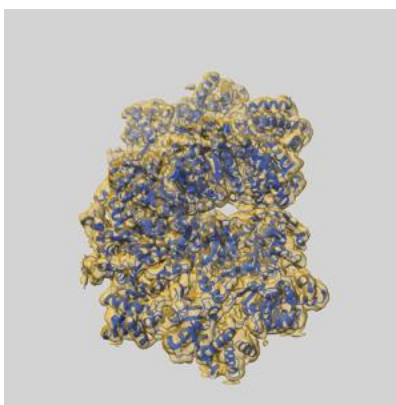
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-64229 and PDB model 9UJX. Per-residue inclusion information can be found in section [3](#) on page [5](#).

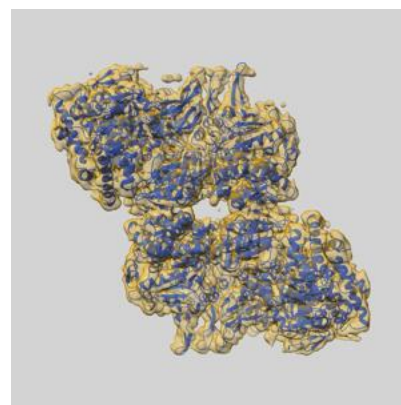
9.1 Map-model overlay [i](#)



X



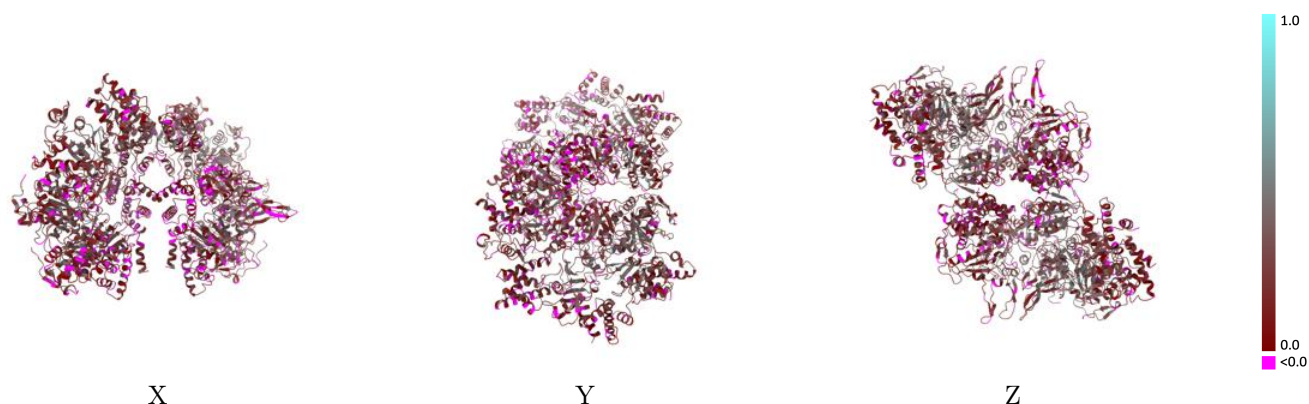
Y



Z

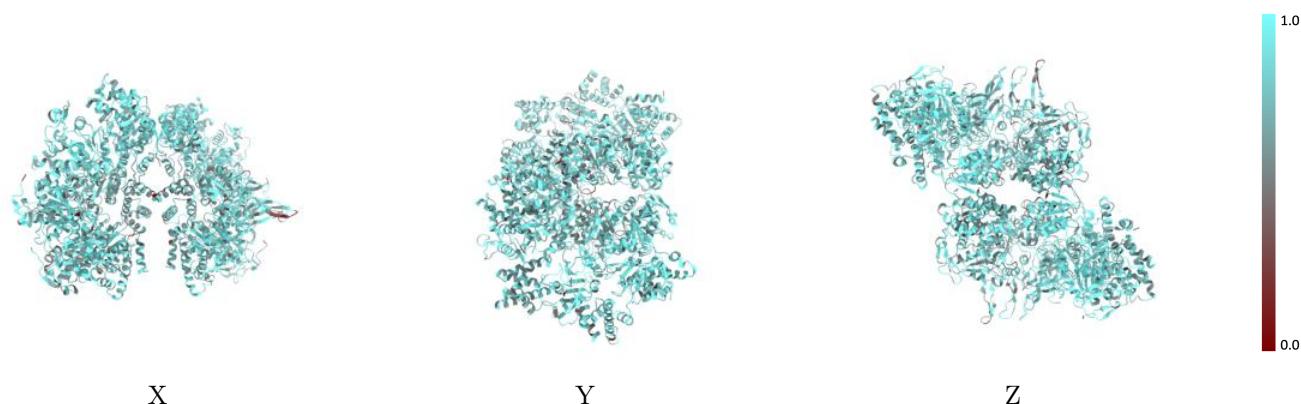
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



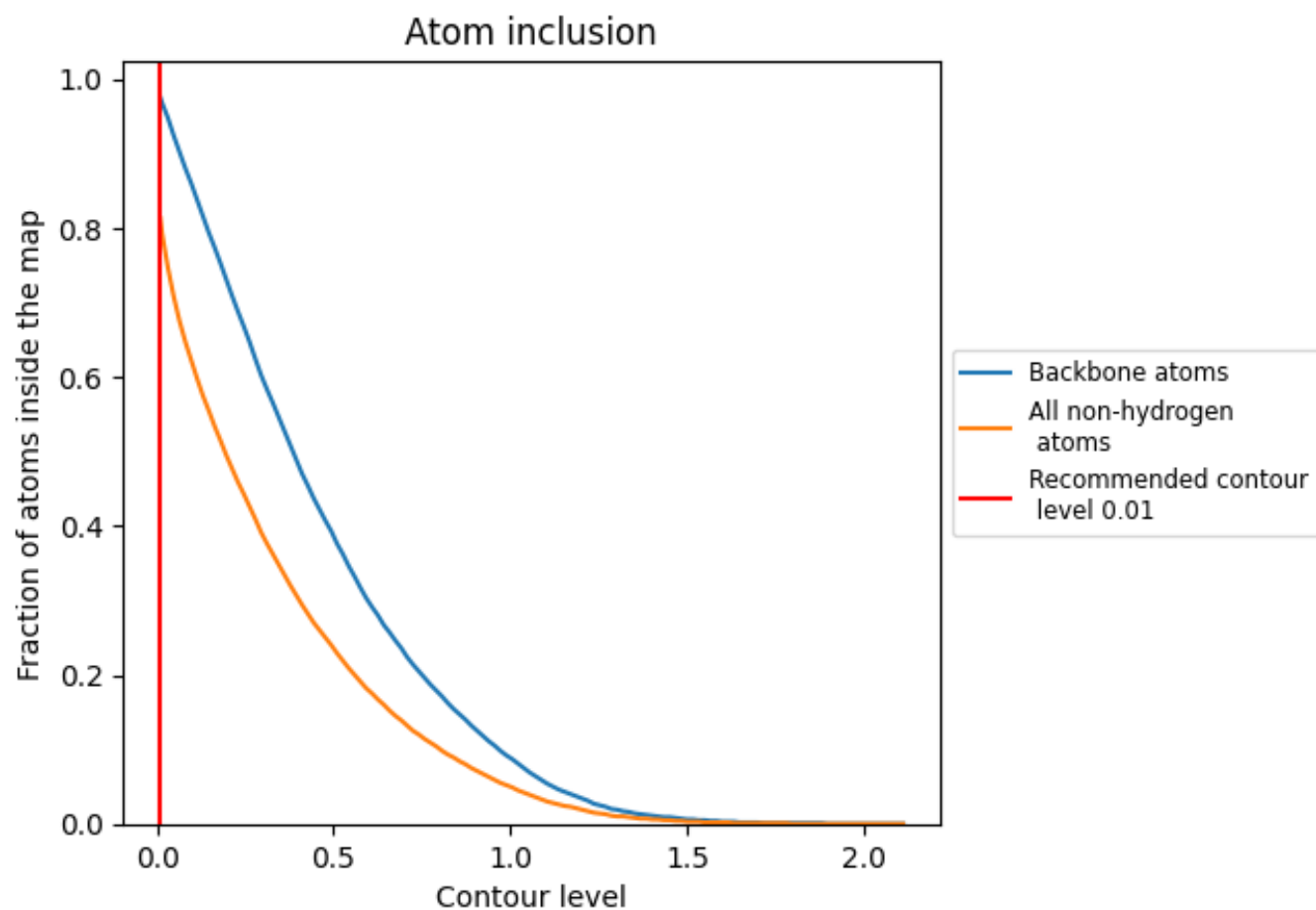
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 81% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8130	0.2160
A	0.7610	0.1570
B	0.7930	0.1720
C	0.8150	0.2190
D	0.8250	0.2390
E	0.8460	0.2650
F	0.8400	0.2480
a	0.7770	0.1660
b	0.7900	0.1800
c	0.8190	0.2140
d	0.8140	0.2270
e	0.8430	0.2650
f	0.8300	0.2390

