



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 10:09 AM UTC

PDB ID : 7OMM / pdb_00007omm
EMDB ID : EMD-12990
Title : Cryo-EM structure of *N. gonorrhoeae* LptDE in complex with ProMacrobodies (MBPs have not been built de novo)
Authors : Botte, M.; Ni, D.; Schenck, S.; Zimmermann, I.; Chami, M.; Bocquet, N.; Egloff, P.; Bucher, D.; Trabuco, M.; Cheng, R.K.Y.; Brunner, J.D.; Seeger, M.A.; Stahlberg, H.; Hennig, M.
Deposited on : 2021-05-24
Resolution : 3.40 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.dev132
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) : 2.49

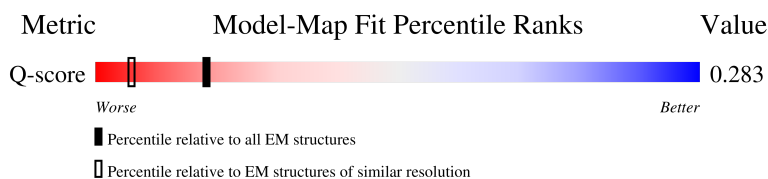
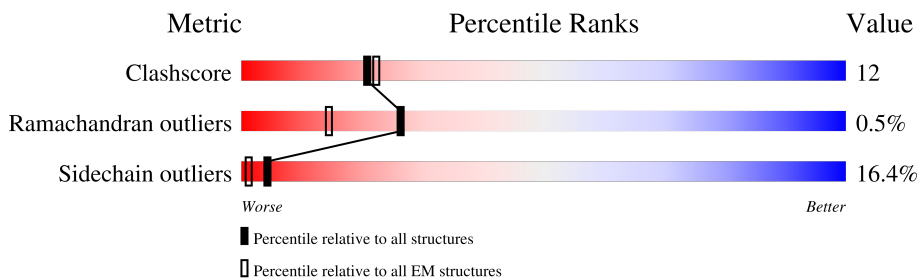
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	801	
2	B	165	
3	C	520	
4	D	526	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13981 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 LPS-assembly protein LptD.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	698	Total	C	N	O	S	0	0
			5462	3430	985	1038	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	SER	ALA	conflict	UNP Q5F651

- Molecule 2 is a protein called LPS-assembly lipoprotein LptE.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	128	Total	C	N	O	S	0	0
			1020	640	179	198	3		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	160	HIS	-	expression tag	UNP A0A5K1Q6A7
B	161	HIS	-	expression tag	UNP A0A5K1Q6A7
B	162	HIS	-	expression tag	UNP A0A5K1Q6A7
B	163	HIS	-	expression tag	UNP A0A5K1Q6A7
B	164	HIS	-	expression tag	UNP A0A5K1Q6A7
B	165	HIS	-	expression tag	UNP A0A5K1Q6A7

- Molecule 3 is a protein called ProMacrobody 21,Maltodextrin-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	479	Total	C	N	O	S	0	0
			3731	2397	614	710	10		

There are 37 discrepancies between the modelled and reference sequences:

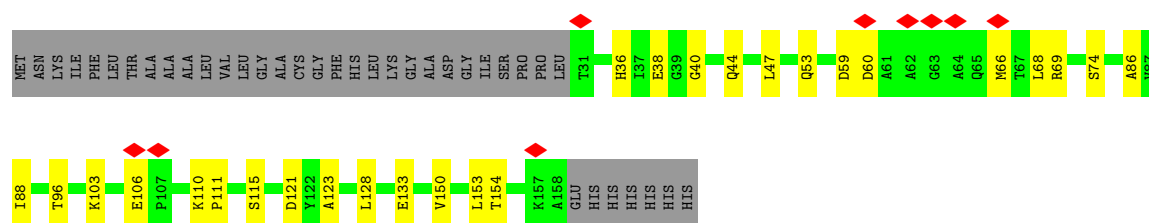
Chain	Residue	Modelled	Actual	Comment	Reference
C	484	PRO	-	expression tag	UNP A0A0F8L1I7
C	485	GLY	-	expression tag	UNP A0A0F8L1I7
C	486	SER	-	expression tag	UNP A0A0F8L1I7
C	487	GLY	-	expression tag	UNP A0A0F8L1I7
C	488	GLY	-	expression tag	UNP A0A0F8L1I7
C	489	GLY	-	expression tag	UNP A0A0F8L1I7
C	490	SER	-	expression tag	UNP A0A0F8L1I7
C	491	ALA	-	expression tag	UNP A0A0F8L1I7
C	492	TRP	-	expression tag	UNP A0A0F8L1I7
C	493	SER	-	expression tag	UNP A0A0F8L1I7
C	494	HIS	-	expression tag	UNP A0A0F8L1I7
C	495	PRO	-	expression tag	UNP A0A0F8L1I7
C	496	GLN	-	expression tag	UNP A0A0F8L1I7
C	497	PHE	-	expression tag	UNP A0A0F8L1I7
C	498	GLU	-	expression tag	UNP A0A0F8L1I7
C	499	LYS	-	expression tag	UNP A0A0F8L1I7
C	500	GLY	-	expression tag	UNP A0A0F8L1I7
C	501	GLY	-	expression tag	UNP A0A0F8L1I7
C	502	GLY	-	expression tag	UNP A0A0F8L1I7
C	503	SER	-	expression tag	UNP A0A0F8L1I7
C	504	GLY	-	expression tag	UNP A0A0F8L1I7
C	505	GLY	-	expression tag	UNP A0A0F8L1I7
C	506	GLY	-	expression tag	UNP A0A0F8L1I7
C	507	SER	-	expression tag	UNP A0A0F8L1I7
C	508	GLY	-	expression tag	UNP A0A0F8L1I7
C	509	GLY	-	expression tag	UNP A0A0F8L1I7
C	510	SER	-	expression tag	UNP A0A0F8L1I7
C	511	ALA	-	expression tag	UNP A0A0F8L1I7
C	512	TRP	-	expression tag	UNP A0A0F8L1I7
C	513	SER	-	expression tag	UNP A0A0F8L1I7
C	514	HIS	-	expression tag	UNP A0A0F8L1I7
C	515	PRO	-	expression tag	UNP A0A0F8L1I7
C	516	GLN	-	expression tag	UNP A0A0F8L1I7
C	517	PHE	-	expression tag	UNP A0A0F8L1I7
C	518	GLU	-	expression tag	UNP A0A0F8L1I7
C	519	LYS	-	expression tag	UNP A0A0F8L1I7
C	520	ALA	-	expression tag	UNP A0A0F8L1I7

- Molecule 4 is a protein called ProMacrobody 51,Maltodextrin-binding protein.

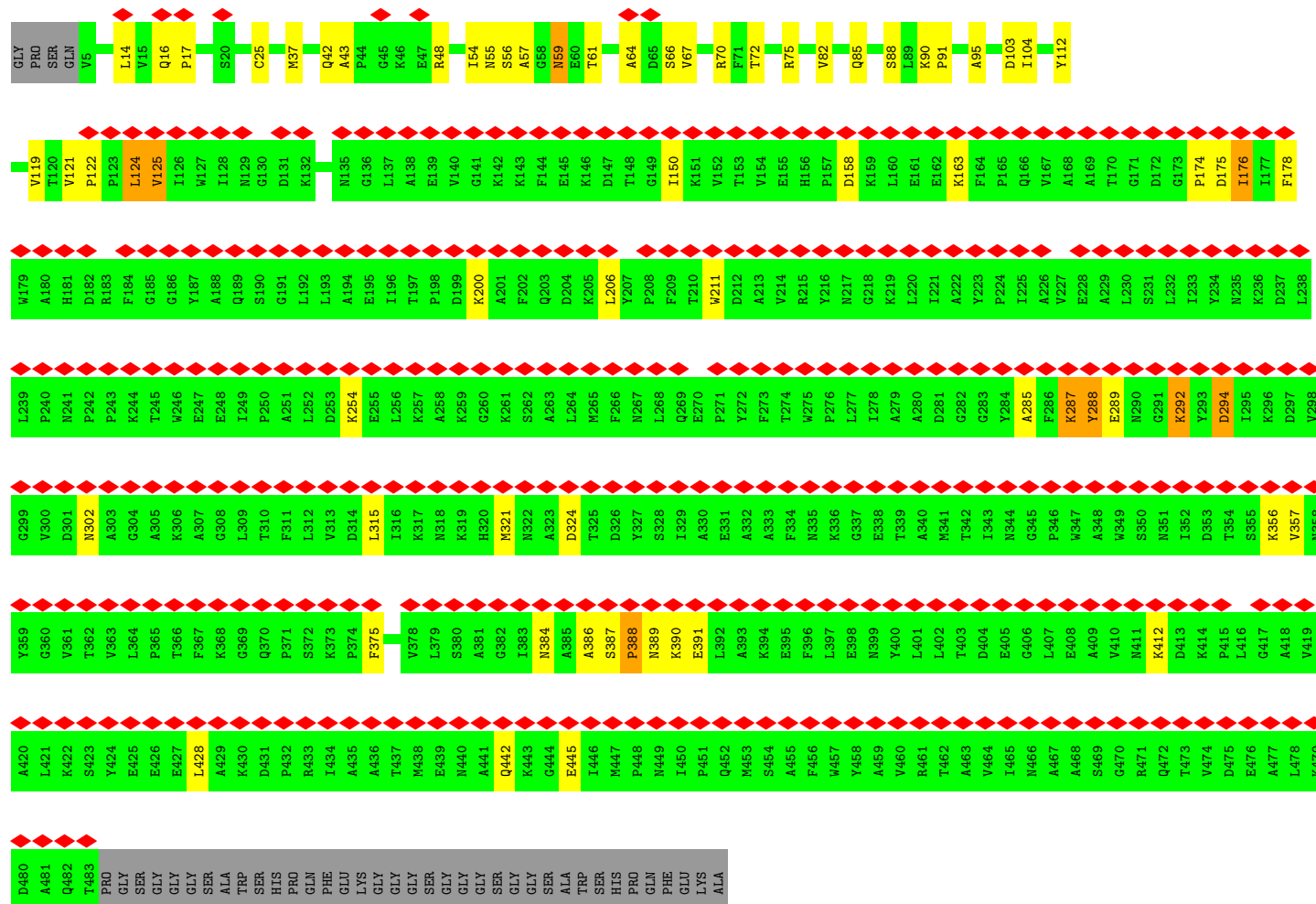
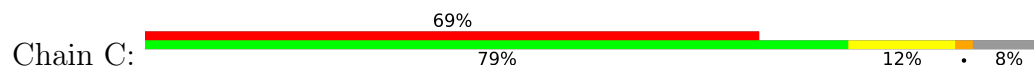
Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	489	Total	C	N	O	S	0	0
			3768	2422	614	723	9		

There are 37 discrepancies between the modelled and reference sequences:

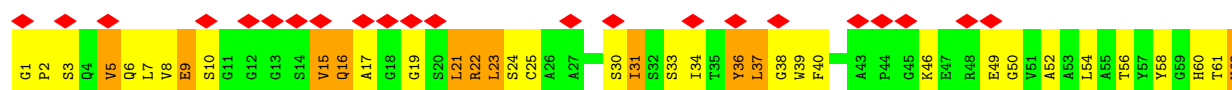
Chain	Residue	Modelled	Actual	Comment	Reference
D	490	PRO	-	expression tag	UNP A0A0F8L1I7
D	491	GLY	-	expression tag	UNP A0A0F8L1I7
D	492	SER	-	expression tag	UNP A0A0F8L1I7
D	493	GLY	-	expression tag	UNP A0A0F8L1I7
D	494	GLY	-	expression tag	UNP A0A0F8L1I7
D	495	GLY	-	expression tag	UNP A0A0F8L1I7
D	496	SER	-	expression tag	UNP A0A0F8L1I7
D	497	ALA	-	expression tag	UNP A0A0F8L1I7
D	498	TRP	-	expression tag	UNP A0A0F8L1I7
D	499	SER	-	expression tag	UNP A0A0F8L1I7
D	500	HIS	-	expression tag	UNP A0A0F8L1I7
D	501	PRO	-	expression tag	UNP A0A0F8L1I7
D	502	GLN	-	expression tag	UNP A0A0F8L1I7
D	503	PHE	-	expression tag	UNP A0A0F8L1I7
D	504	GLU	-	expression tag	UNP A0A0F8L1I7
D	505	LYS	-	expression tag	UNP A0A0F8L1I7
D	506	GLY	-	expression tag	UNP A0A0F8L1I7
D	507	GLY	-	expression tag	UNP A0A0F8L1I7
D	508	GLY	-	expression tag	UNP A0A0F8L1I7
D	509	SER	-	expression tag	UNP A0A0F8L1I7
D	510	GLY	-	expression tag	UNP A0A0F8L1I7
D	511	GLY	-	expression tag	UNP A0A0F8L1I7
D	512	GLY	-	expression tag	UNP A0A0F8L1I7
D	513	SER	-	expression tag	UNP A0A0F8L1I7
D	514	GLY	-	expression tag	UNP A0A0F8L1I7
D	515	GLY	-	expression tag	UNP A0A0F8L1I7
D	516	SER	-	expression tag	UNP A0A0F8L1I7
D	517	ALA	-	expression tag	UNP A0A0F8L1I7
D	518	TRP	-	expression tag	UNP A0A0F8L1I7
D	519	SER	-	expression tag	UNP A0A0F8L1I7
D	520	HIS	-	expression tag	UNP A0A0F8L1I7
D	521	PRO	-	expression tag	UNP A0A0F8L1I7
D	522	GLN	-	expression tag	UNP A0A0F8L1I7
D	523	PHE	-	expression tag	UNP A0A0F8L1I7
D	524	GLU	-	expression tag	UNP A0A0F8L1I7
D	525	LYS	-	expression tag	UNP A0A0F8L1I7
D	526	ALA	-	expression tag	UNP A0A0F8L1I7



• Molecule 3: ProMacrobody 21,Maltodextrin-binding protein



• Molecule 4: ProMacrobody 51,Maltodextrin-binding protein



PRO	Y430	L370	G310	K250	F190	L130	Y63
GLY	E431	P371	A311	T251	G191	L131	A64
SER	E432	T372	K312	W252	G192	V131	D65
GLY	E433	F373	A313	E253	Y193	I132	S66
GLY	E434	K374	G314	E254	A194	W133	V67
SER	A435	G375	L315	E255	Q195	I134	K68
ALA	K436	Q376	T316	P256	S196	G136	
TRP	D437	P377	F317	A257	G197	D137	F71
SER	F438	S378	L318	L258	L198	K138	T72
PRO	R439	K379	V319	D259	L199	V139	V73
GLN	T440	P380	D320	K260	A200	G139	S74
PHE	T440	F381	L321	E261	E201	N141	L75
LYS	A441	V382	I322	L262	I202	G142	D76
GLY	T442	G383	K323	K263	T203	L143	N77
GLY	T443	V384	N324	A264	T203	A144	A78
GLY	M444	L385	K325	K265	D205	E145	M80
SER	E445	L386	K326	K266	K206	V146	T81
GLY	M446	S387	H327	G267	A207	G147	V82
GLY	A447	A387	M327	K267	F208	K148	Y83
SER	Q448	G388	N328	S268	Q209	K149	L84
GLY	K449	T389	A329	A269	D210	F150	Q85
GLY	G450	N390	D330	L270	K211	E151	M86
SER	E451	A391	T331	M271	L212	K152	L89
ALA	A451	A392	D332	F272	Y213	D153	K90
TRP	T452	S393	Y333	N273	P214	T154	P91
SER	M453	P394	S334	L274	F215	G155	E92
HIS	F454	N395	I335	Q275	T216	I156	D93
PRO	N455	K396	A336	E276	W217	K157	L96
GLN	T456	E397	E337	E277	W218	V158	Y97
PHE	P457	L398	A338	P277	D218	T159	Y98
GLU	T458	A399	A339	Y278	A219	V160	C99
LYS	Y459	K400	F340	F279	V220	E161	A100
	S460	E401	N341	T280	R221	H162	A101
	A461	F402	K342	W281	Y222	P163	S104
	F462	L403	K343	P282	N223	D164	G105
	V463	E404	G344	L283	G224	K165	I106
	Y464	N405	E344	I284	K225	L166	L110
	A465	Y406	T345	A285	K226	E167	G111
	V466	L407	A346	A286	L226	K169	V112
	R467	L408	M347	D287	I227	F170	V113
	T468	T409	T348	G288	A228	P171	A114
	A469	D410	I349	G289	Y229	Q172	T115
	V470	E411	N350	Y290	P230	V173	Y116
	T471	G412	G351	A291	I231	A174	E117
	N472	L413	P352	F292	A232	A175	Y118
	A473	E414	W353	K293	V233	T176	W119
	A474	A415	A354	Y294	E234	G177	G120
	S475	V416	W355	E295	A235	D178	Q121
	G476	N417	S356	N296	L236	G179	V125
	R477	K418	N357	G297	S237	P180	T126
	Q478	D419	I358	K298	L238	D181	V127
	T479	K420	D359	Y299	I239	I182	P128
	V480	P421	T360	D300	Y240	I183	P129
	D481	L422	S361	I301	N241	F184	
	E482	G423	K362	K302	D242	W185	
	A483	A424	V363	D303	D243	A186	
	L484	V425	N364	V304	L244	H187	
	K485	A426	Y365	G305	L245	D188	
	D486	L427	G366	V306	P246	R189	
	A487	K428	V367	D307	N247		
	Q488	S429	T368	N308	P248		
	T489		V369	A309	P249		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	184206	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.965	Depositor
Minimum map value	-1.718	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.45	Depositor
Map size ($\text{\AA}$)	344.4, 344.4, 344.4	wwPDB
Map dimensions	390, 390, 390	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8830769, 0.8830769, 0.8830769	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	0.44	0/5594	0.73	8/7569 (0.1%)
2	B	0.15	0/1034	0.36	0/1400
3	C	0.79	0/3829	1.40	6/5208 (0.1%)
4	D	0.98	0/3865	1.30	8/5260 (0.2%)
All	All	0.71	0/14322	1.10	22/19437 (0.1%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	181	ASP	N-CA-C	9.31	121.03	111.07
4	D	137	ASP	N-CA-C	-8.71	101.78	111.28
1	A	662	ARG	CB-CA-C	-7.34	103.83	110.44
4	D	402	PHE	CA-CB-CG	7.00	120.80	113.80
4	D	78	ALA	N-CA-C	-6.93	104.64	113.23
3	C	384	ASN	CA-CB-CG	6.27	118.87	112.60
3	C	122	PRO	N-CA-C	6.03	118.06	110.70
1	A	738	GLY	N-CA-C	-5.89	105.82	114.90
1	A	261	PRO	N-CA-C	5.85	124.53	112.47
1	A	739	CYS	CA-C-N	-5.76	115.59	122.44
1	A	739	CYS	C-N-CA	-5.76	115.59	122.44
4	D	471	ILE	N-CA-C	-5.75	104.74	111.00
4	D	325	LYS	O-C-N	5.69	129.14	121.97
1	A	206	GLY	CA-C-O	-5.62	116.17	122.24
1	A	473	ARG	CA-C-O	-5.52	115.70	121.06
4	D	421	PRO	N-CA-C	5.34	119.48	111.14
1	A	394	ASN	CA-C-O	-5.33	115.75	121.45
4	D	138	LYS	N-CA-C	-5.32	100.51	108.96
3	C	388	PRO	N-CA-C	-5.26	107.34	114.80
3	C	119	VAL	CA-C-N	-5.15	115.73	123.00
3	C	119	VAL	C-N-CA	-5.15	115.73	123.00
3	C	302	ASN	CA-CB-CG	5.08	117.68	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	5462	0	5221	131	0
2	B	1020	0	1024	20	0
3	C	3731	0	3645	33	0
4	D	3768	0	3692	158	0
All	All	13981	0	13582	331	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 12.

All (331) 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)
4:D:131:VAL:HB	4:D:180:PRO:HB3	1.36	1.07
4:D:333:TYR:O	4:D:333:TYR:HD1	1.40	1.04
4:D:401:GLU:OE1	4:D:401:GLU:O	1.82	0.97
4:D:333:TYR:CD1	4:D:333:TYR:C	2.43	0.91
4:D:333:TYR:O	4:D:333:TYR:CD1	2.28	0.87
3:C:57:ALA:HB3	3:C:59:ASN:ND2	1.90	0.85
4:D:262:LEU:HD23	4:D:267:LYS:O	1.78	0.84
4:D:1:GLY:N	4:D:2:PRO:CD	2.41	0.83
3:C:57:ALA:HB3	3:C:59:ASN:HD21	1.45	0.81
4:D:333:TYR:HD1	4:D:333:TYR:C	1.84	0.80
1:A:378:ARG:HH11	1:A:403:GLN:HB2	1.48	0.77
4:D:107:TRP:HD1	4:D:112:VAL:HG22	1.49	0.76
1:A:256:SER:HB2	1:A:279:ASN:HB3	1.68	0.74
4:D:1:GLY:H3	4:D:2:PRO:HD3	1.52	0.74
1:A:680:LYS:HD2	2:B:123:ALA:HB1	1.69	0.74
4:D:40:PHE:HA	4:D:50:GLY:HA3	1.70	0.73
4:D:296:ASN:OD1	4:D:297:GLY:N	2.22	0.72
4:D:262:LEU:HB3	4:D:267:LYS:O	1.88	0.72
4:D:1:GLY:H2	4:D:2:PRO:HD2	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:THR:HG21	1:A:135:VAL:HB	1.74	0.70
4:D:286:ALA:HB2	4:D:378:SER:HA	1.72	0.69
4:D:133:TRP:CG	4:D:180:PRO:HD2	2.27	0.69
1:A:151:GLU:HB2	1:A:165:HIS:HB2	1.76	0.68
4:D:1:GLY:H2	4:D:2:PRO:CD	2.03	0.68
3:C:91:PRO:CG	3:C:150:ILE:HG23	2.23	0.68
4:D:105:GLY:HA3	4:D:114:ALA:HB2	1.76	0.68
4:D:139:GLY:H	4:D:420:LYS:HB2	1.59	0.68
4:D:202:ILE:HG23	4:D:389:ILE:HD11	1.74	0.68
4:D:16:GLN:HA	4:D:128:PRO:HD2	1.75	0.67
4:D:135:ASN:H	4:D:166:LEU:HD22	1.59	0.67
4:D:262:LEU:CD2	4:D:267:LYS:O	2.43	0.67
2:B:66:MET:HG2	2:B:103:LYS:HD3	1.76	0.66
4:D:16:GLN:HB2	4:D:394:PRO:HD2	1.75	0.66
4:D:1:GLY:N	4:D:2:PRO:HD3	2.07	0.66
1:A:662:ARG:HG3	1:A:668:VAL:HG12	1.77	0.65
4:D:434:LEU:HD13	4:D:440:ILE:HG21	1.78	0.63
1:A:404:THR:HG21	1:A:415:PRO:HD2	1.80	0.63
2:B:68:LEU:HD22	2:B:153:LEU:HD11	1.81	0.63
4:D:387:ALA:HB1	4:D:403:LEU:HD22	1.79	0.63
3:C:175:ASP:HA	3:C:387:SER:HB2	1.81	0.62
4:D:208:PHE:HZ	4:D:408:LEU:HD13	1.64	0.62
1:A:276:TYR:CD1	1:A:278:PHE:HD2	2.16	0.62
1:A:624:ASP:HA	1:A:646:ASN:HA	1.82	0.62
3:C:91:PRO:HD2	3:C:150:ILE:HG12	1.82	0.61
4:D:399:ALA:O	4:D:403:LEU:HG	2.01	0.61
1:A:119:LEU:HD13	1:A:141:LEU:HD12	1.82	0.61
1:A:362:ARG:HG3	1:A:751:THR:HB	1.81	0.61
4:D:425:VAL:HG21	4:D:430:TYR:HB3	1.83	0.60
3:C:206:LEU:HD12	3:C:211:TRP:CZ2	2.36	0.60
2:B:69:ARG:NH2	2:B:106:GLU:OE2	2.34	0.60
1:A:88:TYR:OH	1:A:90:ARG:NH2	2.33	0.60
3:C:66:SER:O	3:C:70:ARG:NH2	2.34	0.60
4:D:15:VAL:HG21	4:D:19:GLY:HA3	1.82	0.60
1:A:636:ARG:HB2	1:A:661:TYR:HD1	1.67	0.60
1:A:418:ILE:HG23	1:A:442:THR:HG23	1.83	0.59
1:A:419:MET:HB2	1:A:420:PRO:HD3	1.85	0.59
3:C:91:PRO:HG2	3:C:150:ILE:HG23	1.83	0.59
1:A:265:ALA:HB1	1:A:761:PHE:HA	1.85	0.59
1:A:498:ARG:NH1	1:A:540:GLN:OE1	2.36	0.58
1:A:301:ASP:N	1:A:301:ASP:OD1	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:LEU:HG	1:A:276:TYR:HD2	1.69	0.58
4:D:353:TRP:HB2	4:D:420:LYS:HG2	1.86	0.58
1:A:454:ARG:NH1	1:A:568:ASP:OD1	2.37	0.58
4:D:380:PRO:HG3	4:D:446:ASN:HB3	1.85	0.58
1:A:162:GLY:H	1:A:187:MET:HB3	1.67	0.57
3:C:88:SER:O	3:C:90:LYS:NZ	2.37	0.57
4:D:91:PRO:HG2	4:D:157:LYS:H	1.69	0.57
4:D:170:PHE:HB3	4:D:193:TYR:CE1	2.39	0.57
4:D:5:VAL:HG23	4:D:119:TRP:HB3	1.86	0.57
1:A:311:TYR:HB3	1:A:340:HIS:CD2	2.39	0.57
1:A:496:VAL:HG11	1:A:543:LEU:HD11	1.87	0.57
4:D:107:TRP:CD1	4:D:112:VAL:HG22	2.35	0.57
3:C:42:GLN:HB2	3:C:48:ARG:HG3	1.86	0.57
4:D:139:GLY:H	4:D:420:LYS:CB	2.18	0.56
4:D:189:ARG:HB3	4:D:193:TYR:CZ	2.40	0.56
4:D:372:THR:HA	4:D:377:PRO:HA	1.86	0.56
2:B:36:HIS:ND1	2:B:59:ASP:O	2.39	0.56
4:D:154:THR:HG23	4:D:156:ILE:HB	1.87	0.56
4:D:181:ASP:HA	4:D:390:ASN:HB3	1.86	0.56
4:D:208:PHE:CZ	4:D:408:LEU:HD13	2.41	0.56
4:D:132:ILE:HG23	4:D:182:ILE:HG12	1.86	0.56
4:D:167:GLU:HB3	4:D:185:TRP:HE1	1.70	0.55
4:D:270:LEU:HD21	4:D:349:ILE:HG13	1.89	0.55
1:A:196:THR:HA	1:A:216:SER:HA	1.89	0.55
4:D:255:ILE:HD11	4:D:371:PRO:HG2	1.88	0.55
4:D:129:PRO:HB3	4:D:157:LYS:C	2.31	0.55
4:D:401:GLU:OE1	4:D:401:GLU:C	2.50	0.55
1:A:88:TYR:HE1	1:A:90:ARG:HD2	1.71	0.55
1:A:664:ALA:HB1	1:A:665:PRO:HD2	1.88	0.55
4:D:389:ILE:HG23	4:D:399:ALA:HB3	1.89	0.55
4:D:402:PHE:HD1	4:D:406:TYR:HB2	1.73	0.54
1:A:144:ASP:N	1:A:144:ASP:OD1	2.41	0.54
4:D:369:VAL:HG11	4:D:449:LYS:NZ	2.23	0.54
4:D:401:GLU:O	4:D:401:GLU:CD	2.51	0.54
1:A:625:TRP:HB2	1:A:645:TYR:HB3	1.89	0.53
1:A:765:GLN:HG3	1:A:787:TYR:CE2	2.44	0.53
1:A:287:THR:HG23	1:A:303:GLN:HG2	1.91	0.53
4:D:23:LEU:HD13	4:D:86:MET:HE1	1.90	0.53
1:A:322:HIS:HA	1:A:329:ASN:HA	1.89	0.53
1:A:301:ASP:HB3	1:A:318:THR:HG23	1.89	0.53
4:D:417:ASN:HA	4:D:421:PRO:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ASP:OD1	1:A:448:GLY:N	2.40	0.53
1:A:552:SER:HB3	2:B:121:ASP:HB2	1.89	0.53
4:D:356:SER:HB2	4:D:421:PRO:HD3	1.89	0.53
1:A:751:THR:OG1	1:A:755:THR:OG1	2.27	0.52
2:B:40:GLY:O	2:B:44:GLN:NE2	2.35	0.52
1:A:255:LYS:HG3	1:A:258:LEU:HB2	1.91	0.52
1:A:387:ARG:O	1:A:389:ALA:N	2.42	0.52
1:A:421:ARG:NH2	1:A:442:THR:OG1	2.42	0.52
1:A:438:SER:OG	1:A:439:ALA:N	2.43	0.52
1:A:463:TRP:H	1:A:463:TRP:CD1	2.25	0.52
4:D:167:GLU:HG2	4:D:168:GLU:H	1.74	0.52
4:D:189:ARG:HB3	4:D:193:TYR:CE1	2.44	0.52
4:D:231:ILE:HB	4:D:385:LEU:HD23	1.92	0.52
4:D:22:ARG:HG2	4:D:83:TYR:HB3	1.92	0.52
1:A:371:ALA:HB2	2:B:88:ILE:HD13	1.92	0.52
4:D:133:TRP:CE3	4:D:179:GLY:HA2	2.45	0.52
4:D:133:TRP:CD2	4:D:180:PRO:HD2	2.45	0.52
1:A:248:PHE:HB3	1:A:795:ALA:HB2	1.92	0.52
4:D:294:TYR:HD1	4:D:298:LYS:HG2	1.75	0.52
1:A:750:VAL:HG13	2:B:86:ALA:HB2	1.92	0.51
1:A:92:VAL:H	1:A:111:ILE:HG22	1.76	0.51
1:A:235:PHE:HB3	1:A:240:LEU:HD22	1.92	0.51
4:D:135:ASN:HA	4:D:163:PRO:HD2	1.93	0.51
4:D:183:ILE:O	4:D:387:ALA:HA	2.11	0.51
4:D:233:VAL:HG13	4:D:384:VAL:HG23	1.93	0.51
1:A:93:ALA:HB2	1:A:110:VAL:HG12	1.93	0.51
3:C:91:PRO:CD	3:C:150:ILE:HG12	2.40	0.51
4:D:291:ALA:HB2	4:D:381:PHE:HZ	1.76	0.51
1:A:454:ARG:NH2	1:A:547:ASP:OD2	2.44	0.51
4:D:231:ILE:HA	4:D:408:LEU:HG	1.93	0.51
1:A:183:ARG:HB3	1:A:197:GLU:HB3	1.93	0.50
1:A:483:TYR:OH	1:A:568:ASP:OD1	2.29	0.50
1:A:641:SER:OG	1:A:642:SER:N	2.43	0.50
3:C:72:THR:HG23	3:C:85:GLN:HB3	1.93	0.50
1:A:498:ARG:HD2	1:A:500:LEU:HD13	1.94	0.50
1:A:260:VAL:HG23	1:A:275:PRO:HB2	1.94	0.50
2:B:110:LYS:HD2	2:B:111:PRO:HD2	1.93	0.50
1:A:466:SER:OG	2:B:53:GLN:NE2	2.40	0.50
1:A:371:ALA:O	1:A:373:ASN:ND2	2.43	0.50
1:A:219:ALA:HB1	1:A:799:LYS:HE3	1.92	0.50
4:D:231:ILE:HD11	4:D:407:LEU:HD23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:416:VAL:HB	4:D:422:LEU:HD11	1.93	0.50
4:D:38:GLY:H	4:D:100:ALA:HB3	1.77	0.50
2:B:36:HIS:NE2	2:B:38:GLU:OE2	2.40	0.49
3:C:75:ARG:HB2	3:C:82:VAL:HG12	1.94	0.49
4:D:403:LEU:HA	4:D:407:LEU:HB2	1.94	0.49
1:A:637:PHE:H	1:A:661:TYR:HB2	1.76	0.49
4:D:131:VAL:CB	4:D:180:PRO:HB3	2.26	0.49
1:A:565:TYR:CE2	2:B:133:GLU:HA	2.47	0.49
4:D:79:LYS:C	4:D:81:THR:H	2.21	0.49
4:D:353:TRP:HA	4:D:421:PRO:HD2	1.95	0.49
3:C:104:ILE:HD11	3:C:112:TYR:CD1	2.48	0.49
4:D:36:TYR:HB2	4:D:56:THR:HG22	1.93	0.49
3:C:25:CYS:HB3	3:C:82:VAL:HG22	1.95	0.49
4:D:222:TYR:HB3	4:D:227:ILE:HG12	1.95	0.49
1:A:358:SER:O	1:A:362:ARG:NH1	2.46	0.48
1:A:765:GLN:HG3	1:A:787:TYR:CD2	2.48	0.48
4:D:16:GLN:HB3	4:D:17:ALA:H	1.49	0.48
4:D:187:HIS:HE1	4:D:453:MET:HG3	1.78	0.48
4:D:62:TYR:CG	4:D:111:GLY:HA2	2.49	0.48
1:A:360:TYR:CZ	1:A:364:PHE:HE2	2.31	0.48
3:C:17:PRO:HB2	3:C:389:ASN:HD21	1.79	0.48
4:D:291:ALA:HB2	4:D:381:PHE:CZ	2.48	0.48
1:A:263:VAL:HG23	1:A:273:SER:HB3	1.95	0.48
4:D:183:ILE:HD11	4:D:185:TRP:HB2	1.95	0.48
1:A:91:ILE:HG22	1:A:93:ALA:H	1.79	0.47
4:D:16:GLN:HG2	4:D:128:PRO:HG2	1.96	0.47
1:A:153:LEU:HD21	1:A:155:TYR:CZ	2.49	0.47
4:D:131:VAL:O	4:D:181:ASP:HB2	2.14	0.47
1:A:146:THR:O	1:A:146:THR:OG1	2.32	0.47
2:B:96:THR:HG22	2:B:115:SER:HB2	1.96	0.47
1:A:139:PHE:CE1	1:A:153:LEU:HD22	2.49	0.47
1:A:502:VAL:HG22	1:A:535:ILE:HG12	1.95	0.47
1:A:267:SER:HB3	1:A:759:ALA:HA	1.96	0.47
1:A:276:TYR:CE1	1:A:278:PHE:HD2	2.33	0.47
1:A:767:LYS:HG2	1:A:768:ASP:OD1	2.15	0.47
4:D:355:TRP:HA	4:D:358:ILE:HD12	1.95	0.47
4:D:401:GLU:C	4:D:401:GLU:CD	2.83	0.47
2:B:74:SER:HG	2:B:96:THR:HG1	1.61	0.47
3:C:91:PRO:CD	3:C:150:ILE:HG23	2.45	0.47
1:A:577:SER:HA	1:A:601:LYS:HA	1.96	0.46
1:A:765:GLN:OE1	1:A:770:SER:OG	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:62:TYR:HB3	4:D:112:VAL:HG23	1.97	0.46
3:C:176:ILE:HD11	3:C:178:PHE:CE1	2.50	0.46
1:A:668:VAL:HG11	1:A:782:VAL:HG21	1.97	0.46
4:D:40:PHE:HB2	4:D:98:TYR:HB2	1.97	0.46
4:D:117:GLU:HB3	4:D:119:TRP:CE2	2.50	0.46
4:D:253:GLU:O	4:D:256:PRO:HD2	2.15	0.46
1:A:249:PRO:HD2	1:A:794:SER:OG	2.16	0.46
4:D:9:GLU:H	4:D:121:GLN:HB3	1.80	0.46
4:D:231:ILE:HB	4:D:385:LEU:HB3	1.96	0.46
4:D:152:LYS:HE2	4:D:152:LYS:HB3	1.74	0.46
4:D:427:LEU:HD13	4:D:427:LEU:HA	1.80	0.46
1:A:90:ARG:HE	1:A:91:ILE:H	1.63	0.46
3:C:54:ILE:HD12	3:C:61:THR:HG22	1.97	0.46
1:A:345:THR:OG1	1:A:346:LEU:HD12	2.16	0.46
4:D:323:LYS:HA	4:D:323:LYS:HD3	1.63	0.46
1:A:782:VAL:HG23	1:A:783:ALA:N	2.31	0.45
3:C:43:ALA:HA	3:C:95:ALA:HA	1.97	0.45
4:D:40:PHE:HA	4:D:50:GLY:CA	2.42	0.45
1:A:156:ASN:O	1:A:157:LEU:HG	2.17	0.45
4:D:79:LYS:HG2	4:D:83:TYR:HE1	1.82	0.45
4:D:242:LYS:HB3	4:D:242:LYS:HE3	1.72	0.45
4:D:31:ILE:H	4:D:31:ILE:HG13	1.35	0.45
1:A:681:ILE:HG22	1:A:682:TYR:HB3	1.99	0.45
4:D:17:ALA:HB1	4:D:156:ILE:HG12	1.97	0.45
3:C:125:VAL:HB	3:C:174:PRO:HA	1.99	0.45
4:D:37:LEU:HB3	4:D:101:ALA:H	1.82	0.45
4:D:434:LEU:HD22	4:D:440:ILE:HD13	1.99	0.45
1:A:278:PHE:O	1:A:278:PHE:CD1	2.70	0.45
4:D:390:ASN:O	4:D:396:LYS:HB3	2.17	0.45
1:A:483:TYR:HB2	1:A:496:VAL:HG22	1.99	0.44
1:A:625:TRP:N	1:A:645:TYR:O	2.43	0.44
1:A:723:LYS:HD3	3:C:103:ASP:O	2.17	0.44
4:D:135:ASN:N	4:D:166:LEU:HD22	2.29	0.44
1:A:791:HIS:CE1	1:A:797:ARG:HH22	2.35	0.44
1:A:139:PHE:CZ	1:A:153:LEU:HD13	2.53	0.44
4:D:239:ILE:HG23	4:D:367:VAL:HG22	1.98	0.44
4:D:347:MET:HE3	4:D:347:MET:HB2	1.86	0.44
1:A:547:ASP:HB2	2:B:128:LEU:HB3	1.98	0.44
4:D:21:LEU:HD13	4:D:21:LEU:HA	1.73	0.44
4:D:283:LEU:HD23	4:D:283:LEU:HA	1.74	0.44
1:A:356:SER:OG	1:A:357:ASP:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:ASP:OD1	1:A:507:GLY:N	2.51	0.44
1:A:143:GLN:HG3	1:A:144:ASP:OD1	2.17	0.44
4:D:367:VAL:HB	4:D:439:ARG:HA	1.98	0.44
1:A:210:TRP:CH2	1:A:769:LEU:HD21	2.52	0.44
3:C:124:LEU:HD22	3:C:124:LEU:HA	1.77	0.44
4:D:144:ALA:O	4:D:148:LYS:N	2.47	0.44
4:D:187:HIS:HB2	4:D:455:ASN:HB3	2.00	0.44
4:D:362:LYS:HB2	4:D:362:LYS:HE2	1.60	0.44
1:A:361:TYR:C	1:A:363:ASP:H	2.27	0.43
2:B:150:VAL:O	2:B:154:THR:HG23	2.18	0.43
3:C:386:ALA:O	3:C:388:PRO:HD3	2.18	0.43
3:C:75:ARG:HA	3:C:82:VAL:HA	1.99	0.43
4:D:68:LYS:HB2	4:D:68:LYS:HE2	1.42	0.43
4:D:184:PHE:HA	4:D:386:SER:O	2.18	0.43
1:A:706:THR:O	1:A:707:ARG:C	2.62	0.43
4:D:39:TRP:O	4:D:50:GLY:HA3	2.18	0.43
3:C:288:TYR:HB2	3:C:294:ASP:HB2	2.01	0.43
4:D:189:ARG:N	4:D:189:ARG:HD3	2.34	0.43
4:D:19:GLY:O	4:D:89:LEU:HB2	2.18	0.43
3:C:292:LYS:NZ	3:C:294:ASP:HB2	2.34	0.43
3:C:64:ALA:HB3	3:C:67:VAL:HG22	2.01	0.43
4:D:374:LYS:HB3	4:D:374:LYS:HE3	1.59	0.43
4:D:385:LEU:HD12	4:D:385:LEU:HA	1.75	0.43
1:A:298:ALA:O	1:A:321:PRO:HD2	2.19	0.43
2:B:47:LEU:HD23	2:B:47:LEU:HA	1.94	0.43
4:D:167:GLU:HG2	4:D:168:GLU:N	2.33	0.43
4:D:322:ILE:HD13	4:D:474:ALA:HA	2.01	0.43
1:A:514:ASN:O	1:A:517:LEU:HD23	2.19	0.42
1:A:667:LYS:HG2	1:A:704:PRO:HD2	2.01	0.42
4:D:63:TYR:CE1	4:D:72:THR:HA	2.54	0.42
4:D:262:LEU:HD23	4:D:267:LYS:HB2	1.99	0.42
1:A:358:SER:HB3	1:A:406:ALA:H	1.84	0.42
1:A:725:ILE:HG22	1:A:726:GLU:HG3	2.01	0.42
1:A:462:LYS:HE3	1:A:462:LYS:HB3	1.54	0.42
1:A:242:TYR:HB3	4:D:107:TRP:HB3	2.02	0.42
1:A:308:ARG:HG3	1:A:311:TYR:CZ	2.55	0.42
4:D:206:LYS:HA	4:D:206:LYS:HD2	1.64	0.42
4:D:232:ALA:HB1	4:D:425:VAL:HA	2.01	0.42
3:C:315:LEU:HD13	3:C:321:MET:HE3	2.02	0.42
4:D:183:ILE:HG12	4:D:193:TYR:HE2	1.85	0.42
4:D:420:LYS:HZ3	4:D:420:LYS:HG3	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:425:VAL:HG11	4:D:430:TYR:HD2	1.84	0.42
1:A:220:ASP:OD1	1:A:221:ARG:N	2.52	0.42
1:A:274:VAL:HG13	1:A:274:VAL:O	2.20	0.42
3:C:37:MET:HG3	3:C:82:VAL:HG11	2.02	0.42
4:D:385:LEU:HD21	4:D:422:LEU:HD22	2.02	0.42
1:A:221:ARG:HG2	1:A:799:LYS:NZ	2.35	0.42
1:A:255:LYS:HA	1:A:255:LYS:HD2	1.86	0.42
1:A:647:GLN:OE1	1:A:647:GLN:N	2.44	0.42
4:D:413:LEU:HD13	4:D:413:LEU:HA	1.72	0.42
1:A:89:THR:HA	1:A:113:GLU:HB3	2.00	0.42
2:B:36:HIS:CE1	2:B:60:ASP:HA	2.54	0.42
4:D:202:ILE:HG22	4:D:400:LYS:HG2	2.02	0.42
4:D:434:LEU:HD23	4:D:434:LEU:HA	1.83	0.42
1:A:517:LEU:HB2	1:A:522:VAL:HG23	2.01	0.42
4:D:271:MET:HB2	4:D:345:THR:HG21	2.02	0.42
4:D:282:PRO:HA	4:D:379:LYS:O	2.18	0.42
4:D:463:TRP:HA	4:D:463:TRP:CE3	2.54	0.42
1:A:661:TYR:CZ	1:A:663:PRO:HG3	2.55	0.42
3:C:37:MET:HB2	3:C:54:ILE:HG22	2.02	0.42
4:D:199:LEU:HA	4:D:199:LEU:HD22	1.77	0.42
4:D:403:LEU:HG	4:D:403:LEU:H	1.74	0.42
1:A:314:GLN:HE21	1:A:314:GLN:HB2	1.61	0.41
1:A:643:ILE:HG13	1:A:655:TYR:HB3	2.01	0.41
4:D:165:LYS:O	4:D:169:LYS:HB2	2.20	0.41
1:A:148:ILE:HG23	1:A:167:VAL:HG13	2.01	0.41
3:C:56:SER:HA	3:C:75:ARG:NH1	2.36	0.41
1:A:767:LYS:HG3	1:A:788:ILE:HG21	2.01	0.41
4:D:238:LEU:HG	4:D:371:PRO:HD3	2.01	0.41
4:D:357:ASN:HB2	4:D:420:LYS:HZ1	1.85	0.41
1:A:239:PRO:HG3	4:D:60:HIS:CE1	2.55	0.41
1:A:257:GLY:H	1:A:278:PHE:HA	1.86	0.41
1:A:379:ARG:NH1	1:A:398:SER:OG	2.53	0.41
1:A:707:ARG:H	1:A:707:ARG:HG2	1.51	0.41
4:D:52:ALA:HB1	4:D:73:VAL:HG22	2.02	0.41
4:D:276:GLU:HB2	4:D:279:PHE:HB2	2.03	0.41
4:D:433:GLU:H	4:D:433:GLU:HG3	1.75	0.41
1:A:105:ARG:HG3	1:A:124:ALA:O	2.20	0.41
1:A:184:THR:O	1:A:196:THR:OG1	2.38	0.41
1:A:343:SER:C	1:A:345:THR:H	2.28	0.41
1:A:737:CYS:C	1:A:767:LYS:HE2	2.45	0.41
4:D:306:VAL:HA	4:D:484:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:CYS:HB2	1:A:737:CYS:HB3	1.53	0.41
1:A:704:PRO:HA	1:A:710:SER:HA	2.03	0.41
4:D:183:ILE:HG12	4:D:193:TYR:CE2	2.56	0.41
4:D:356:SER:CB	4:D:421:PRO:HD3	2.51	0.41
2:B:128:LEU:HD23	2:B:128:LEU:HA	1.87	0.41
4:D:434:LEU:HB3	4:D:440:ILE:HG21	2.02	0.41
1:A:242:TYR:CE1	4:D:58:TYR:HD1	2.39	0.41
4:D:75:LEU:HD13	4:D:75:LEU:HA	1.90	0.41
4:D:132:ILE:HB	4:D:160:VAL:HG13	2.03	0.41
1:A:256:SER:HB2	1:A:279:ASN:CB	2.45	0.41
1:A:289:ALA:HB3	1:A:301:ASP:O	2.20	0.41
4:D:263:LYS:HD3	4:D:263:LYS:HA	1.68	0.41
1:A:192:ARG:HG2	1:A:220:ASP:OD1	2.20	0.40
1:A:404:THR:HG21	1:A:414:GLU:HA	2.04	0.40
4:D:401:GLU:OE1	4:D:401:GLU:CA	2.69	0.40
1:A:147:LEU:HD21	1:A:149:ARG:HH22	1.86	0.40
1:A:359:GLY:HA2	1:A:362:ARG:NH1	2.36	0.40
4:D:183:ILE:HG13	4:D:184:PHE:N	2.35	0.40
4:D:451:GLU:H	4:D:451:GLU:HG3	1.67	0.40
1:A:276:TYR:CE1	1:A:278:PHE:CD2	3.09	0.40
4:D:270:LEU:HA	4:D:347:MET:O	2.21	0.40
1:A:407:ASN:OD1	1:A:408:GLN:N	2.50	0.40
1:A:800:ARG:HE	1:A:801:PRO:HD2	1.87	0.40
4:D:444:MET:HE2	4:D:444:MET:HB2	1.81	0.40
3:C:287:LYS:HD3	3:C:287:LYS:HA	1.88	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	671/801 (84%)	551 (82%)	116 (17%)	4 (1%)	21 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	126/165 (76%)	118 (94%)	8 (6%)	0	100	100
3	C	477/520 (92%)	457 (96%)	17 (4%)	3 (1%)	21	50
4	D	487/526 (93%)	464 (95%)	21 (4%)	2 (0%)	30	59
All	All	1761/2012 (88%)	1590 (90%)	162 (9%)	9 (0%)	26	54

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	PRO
3	C	390	LYS
4	D	163	PRO
1	A	207	ASP
1	A	265	ALA
4	D	294	TYR
1	A	388	ALA
3	C	285	ALA
3	C	294	ASP

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	556/632 (88%)	509 (92%)	47 (8%)	10	33
2	B	108/136 (79%)	108 (100%)	0	100	100
3	C	384/409 (94%)	359 (94%)	25 (6%)	15	42
4	D	387/409 (95%)	223 (58%)	164 (42%)	0	0
All	All	1435/1586 (90%)	1199 (84%)	236 (16%)	4	10

All (236) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	159	GLN

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Mol	Chain	Res	Type
1	A	176	ARG
1	A	177	ARG
1	A	178	LEU
1	A	203	CYS
1	A	255	LYS
1	A	256	SER
1	A	259	LEU
1	A	260	VAL
1	A	261	PRO
1	A	263	VAL
1	A	264	SER
1	A	270	VAL
1	A	285	ASP
1	A	287	THR
1	A	292	ILE
1	A	301	ASP
1	A	304	ILE
1	A	309	PRO
1	A	312	SER
1	A	315	THR
1	A	393	LEU
1	A	462	LYS
1	A	463	TRP
1	A	473	ARG
1	A	510	THR
1	A	512	GLU
1	A	524	GLN
1	A	526	ILE
1	A	562	ASN
1	A	576	LEU
1	A	577	SER
1	A	580	VAL
1	A	582	SER
1	A	584	ILE
1	A	600	GLN
1	A	657	VAL
1	A	661	TYR
1	A	669	LEU
1	A	670	ASN
1	A	709	LEU
1	A	710	SER
1	A	712	VAL

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Mol	Chain	Res	Type
1	A	713	VAL
1	A	736	SER
1	A	747	GLN
3	C	14	LEU
3	C	16	GLN
3	C	55	ASN
3	C	59	ASN
3	C	121	VAL
3	C	124	LEU
3	C	125	VAL
3	C	158	ASP
3	C	163	LYS
3	C	176	ILE
3	C	200	LYS
3	C	254	LYS
3	C	287	LYS
3	C	288	TYR
3	C	289	GLU
3	C	292	LYS
3	C	324	ASP
3	C	356	LYS
3	C	357	VAL
3	C	375	PHE
3	C	391	GLU
3	C	412	LYS
3	C	428	LEU
3	C	442	GLN
3	C	445	GLU
4	D	3	SER
4	D	5	VAL
4	D	6	GLN
4	D	7	LEU
4	D	8	VAL
4	D	9	GLU
4	D	10	SER
4	D	15	VAL
4	D	16	GLN
4	D	21	LEU
4	D	22	ARG
4	D	23	LEU
4	D	24	SER
4	D	25	CYS

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Mol	Chain	Res	Type
4	D	30	SER
4	D	31	ILE
4	D	33	SER
4	D	34	ILE
4	D	36	TYR
4	D	37	LEU
4	D	46	LYS
4	D	49	GLU
4	D	54	LEU
4	D	61	THR
4	D	62	TYR
4	D	65	ASP
4	D	66	SER
4	D	67	VAL
4	D	68	LYS
4	D	72	THR
4	D	73	VAL
4	D	75	LEU
4	D	76	ASP
4	D	79	LYS
4	D	81	THR
4	D	82	VAL
4	D	84	LEU
4	D	86	MET
4	D	92	GLU
4	D	96	LEU
4	D	104	SER
4	D	110	LEU
4	D	115	THR
4	D	117	GLU
4	D	121	GLN
4	D	125	VAL
4	D	126	THR
4	D	127	VAL
4	D	130	LEU
4	D	131	VAL
4	D	133	TRP
4	D	134	ILE
4	D	143	LEU
4	D	145	GLU
4	D	146	VAL
4	D	148	LYS

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Mol	Chain	Res	Type
4	D	149	LYS
4	D	151	GLU
4	D	152	LYS
4	D	156	ILE
4	D	157	LYS
4	D	158	VAL
4	D	159	THR
4	D	160	VAL
4	D	166	LEU
4	D	182	ILE
4	D	183	ILE
4	D	184	PHE
4	D	187	HIS
4	D	188	ASP
4	D	189	ARG
4	D	195	GLN
4	D	196	SER
4	D	198	LEU
4	D	199	LEU
4	D	202	ILE
4	D	203	THR
4	D	206	LYS
4	D	221	ARG
4	D	233	VAL
4	D	237	SER
4	D	238	LEU
4	D	239	ILE
4	D	241	ASN
4	D	242	LYS
4	D	243	ASP
4	D	244	LEU
4	D	247	ASN
4	D	250	LYS
4	D	251	THR
4	D	255	ILE
4	D	258	LEU
4	D	262	LEU
4	D	263	LYS
4	D	268	SER
4	D	270	LEU
4	D	276	GLU
4	D	283	LEU

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Mol	Chain	Res	Type
4	D	287	ASP
4	D	293	LYS
4	D	301	ILE
4	D	302	LYS
4	D	304	VAL
4	D	308	ASN
4	D	318	LEU
4	D	321	LEU
4	D	323	LYS
4	D	325	LYS
4	D	327	MET
4	D	328	ASN
4	D	330	ASP
4	D	331	THR
4	D	333	TYR
4	D	334	SER
4	D	335	ILE
4	D	342	LYS
4	D	350	ASN
4	D	362	LYS
4	D	369	VAL
4	D	370	LEU
4	D	374	LYS
4	D	376	GLN
4	D	378	SER
4	D	379	LYS
4	D	381	PHE
4	D	384	VAL
4	D	385	LEU
4	D	386	SER
4	D	389	ILE
4	D	393	SER
4	D	396	LYS
4	D	400	LYS
4	D	401	GLU
4	D	403	LEU
4	D	407	LEU
4	D	408	LEU
4	D	409	THR
4	D	410	ASP
4	D	411	GLU
4	D	413	LEU

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Mol	Chain	Res	Type
4	D	416	VAL
4	D	417	ASN
4	D	418	LYS
4	D	420	LYS
4	D	422	LEU
4	D	427	LEU
4	D	429	SER
4	D	437	ASP
4	D	443	THR
4	D	445	GLU
4	D	448	GLN
4	D	451	GLU
4	D	452	ILE
4	D	453	MET
4	D	455	ASN
4	D	456	ILE
4	D	467	ARG
4	D	468	THR
4	D	479	THR
4	D	480	VAL
4	D	482	GLU
4	D	484	LEU
4	D	485	LYS
4	D	488	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	201	ASN
1	A	230	HIS
1	A	314	GLN
1	A	337	GLN
1	A	338	HIS
1	A	434	GLN
1	A	440	GLN
1	A	581	GLN
1	A	791	HIS
2	B	53	GLN
3	C	59	ASN
3	C	118	GLN
3	C	217	ASN

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Mol	Chain	Res	Type
3	C	466	ASN
3	C	472	GLN
4	D	4	GLN
4	D	60	HIS
4	D	87	ASN
4	D	187	HIS
4	D	195	GLN
4	D	328	ASN
4	D	350	ASN
4	D	458	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 oligosaccharides 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-12990. These allow visual inspection of the internal detail of the map and identification of artifacts.

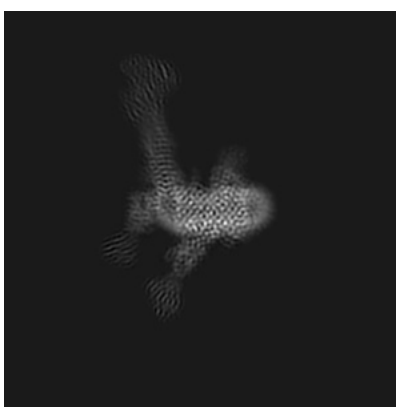
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

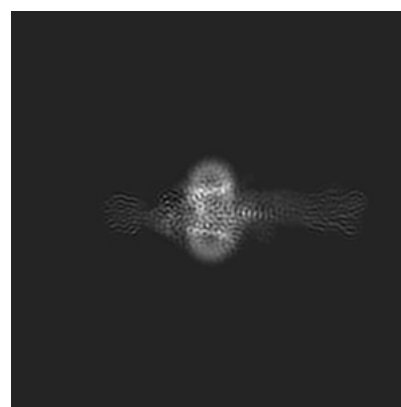
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

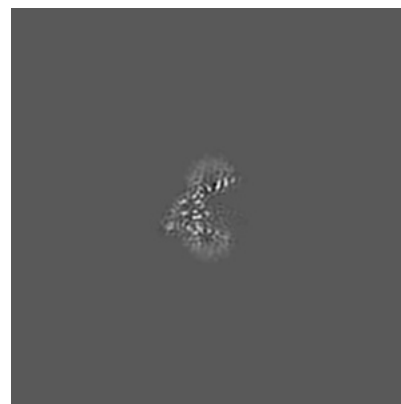
6.2.1 Primary map



X Index: 195



Y Index: 195



Z Index: 195

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

6.3 Largest variance slices [i](#)

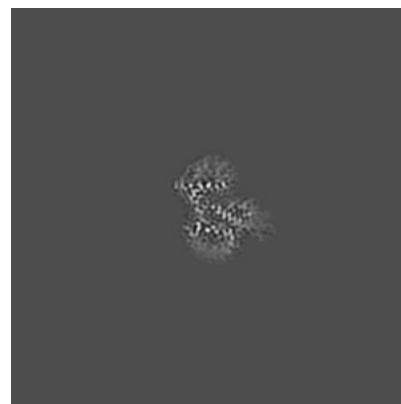
6.3.1 Primary map



X Index: 185



Y Index: 189



Z Index: 216

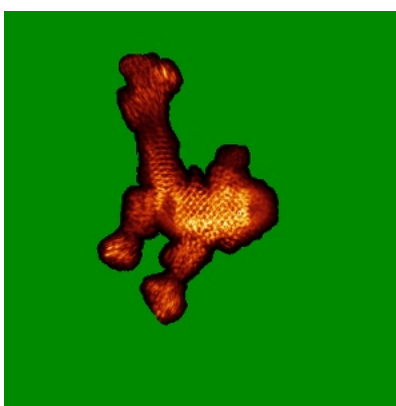
The images above show the largest variance slices of the map in three orthogonal directions.

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

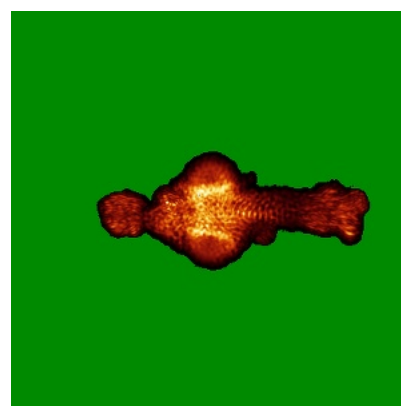
6.4.1 Primary map



X



Y



Z

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 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

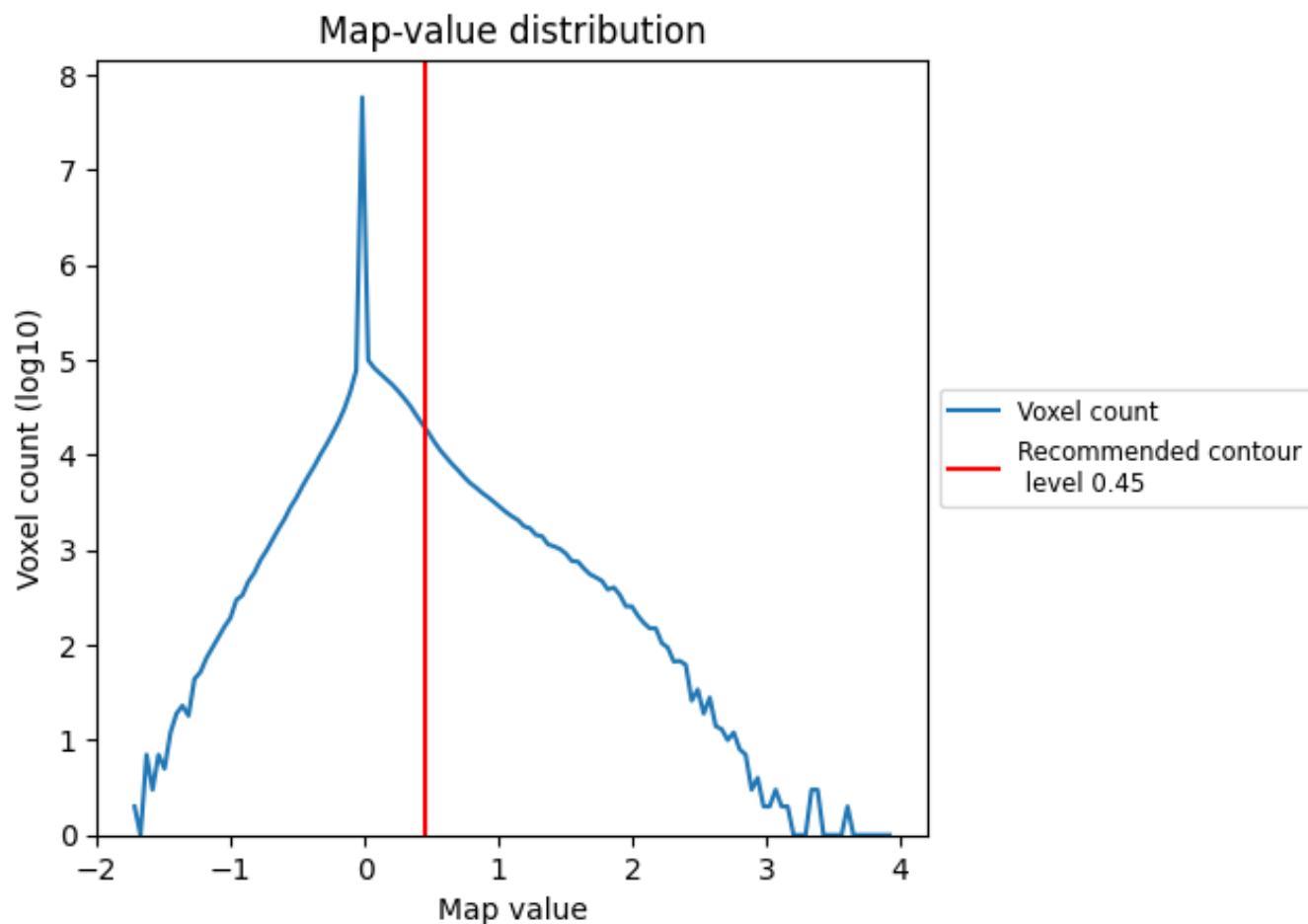
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

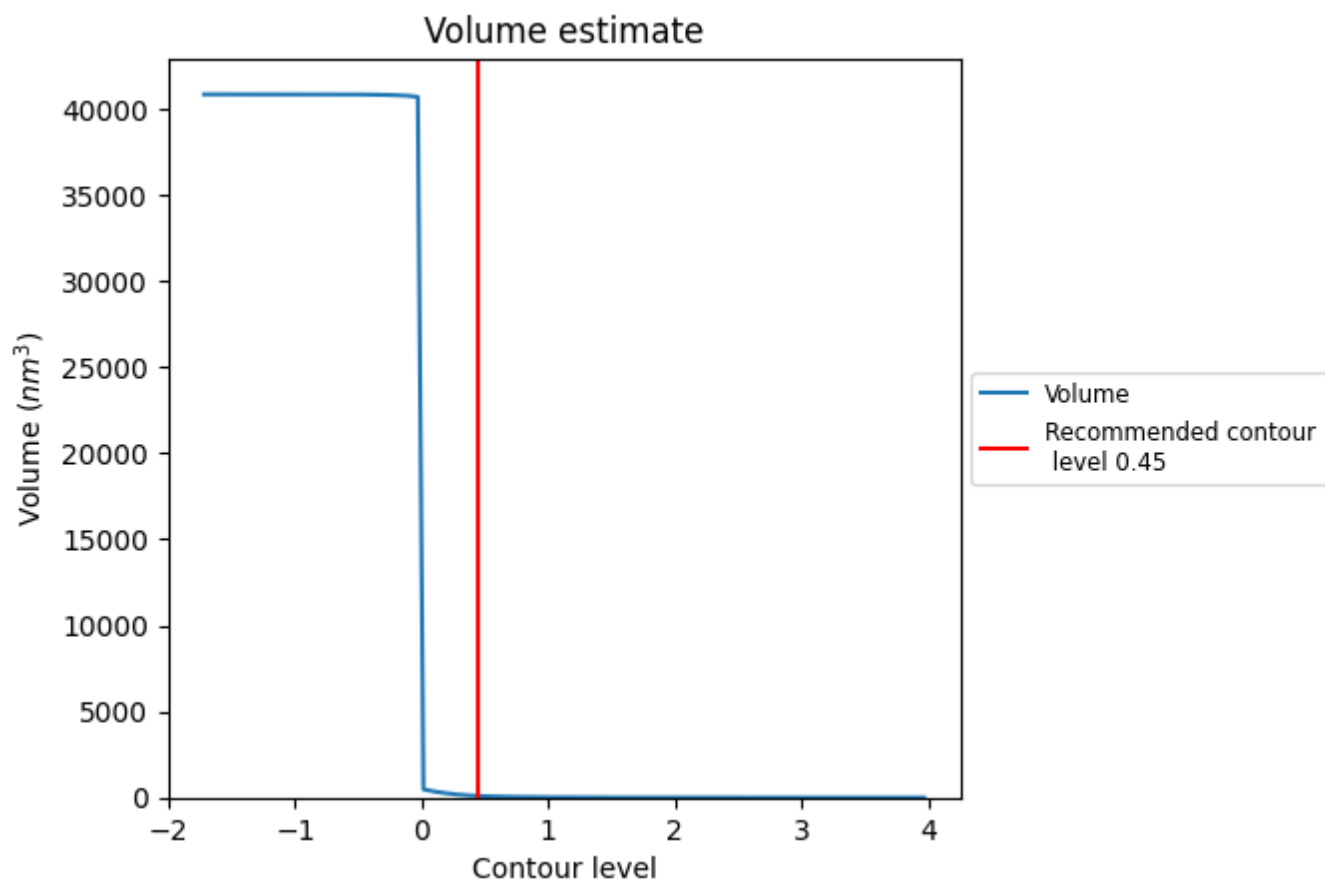
This section contains the results of statistical analysis of the map.

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.

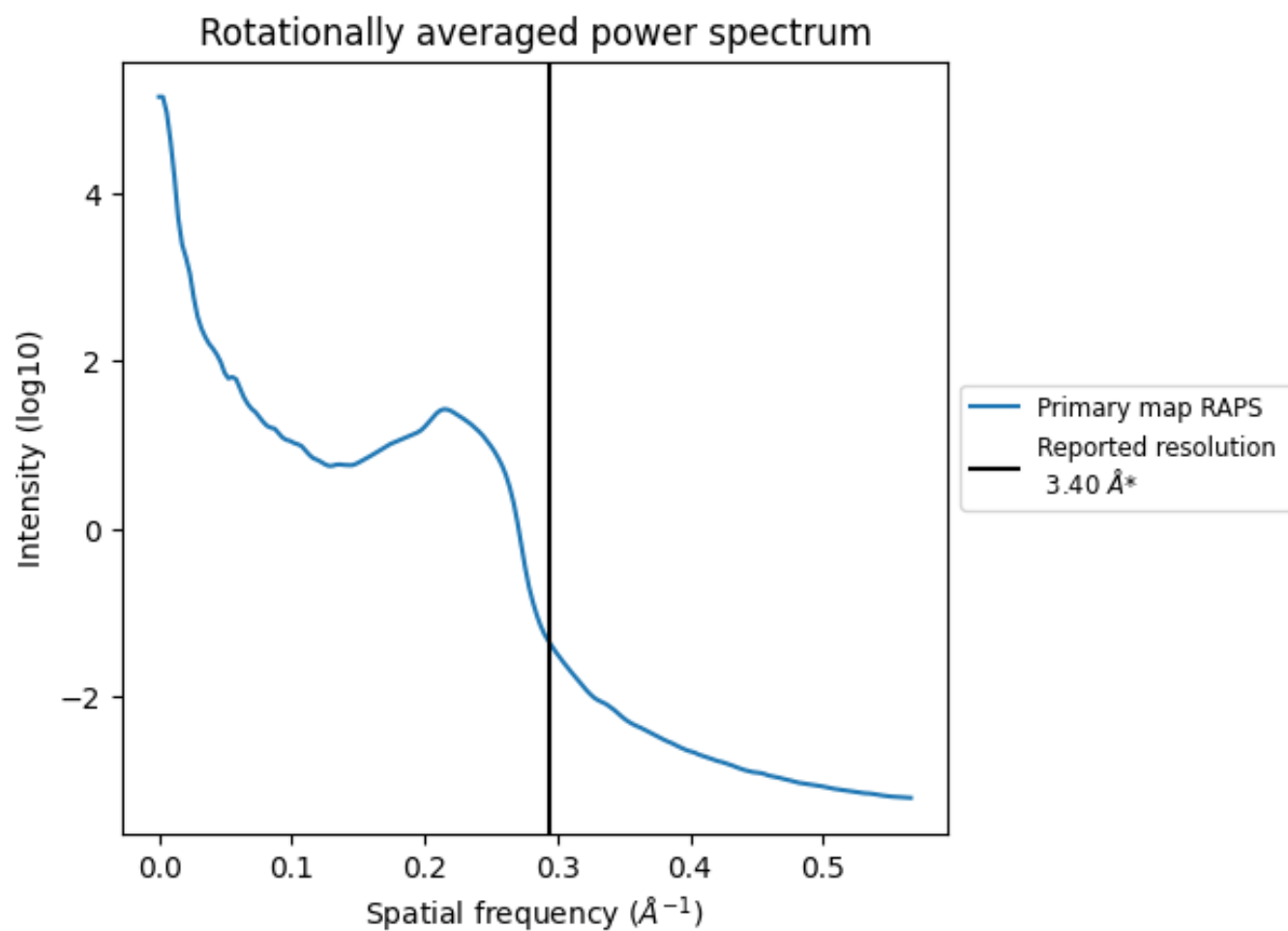
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 91 nm^3 ; this corresponds to an approximate mass of 82 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 0.294 Å⁻¹

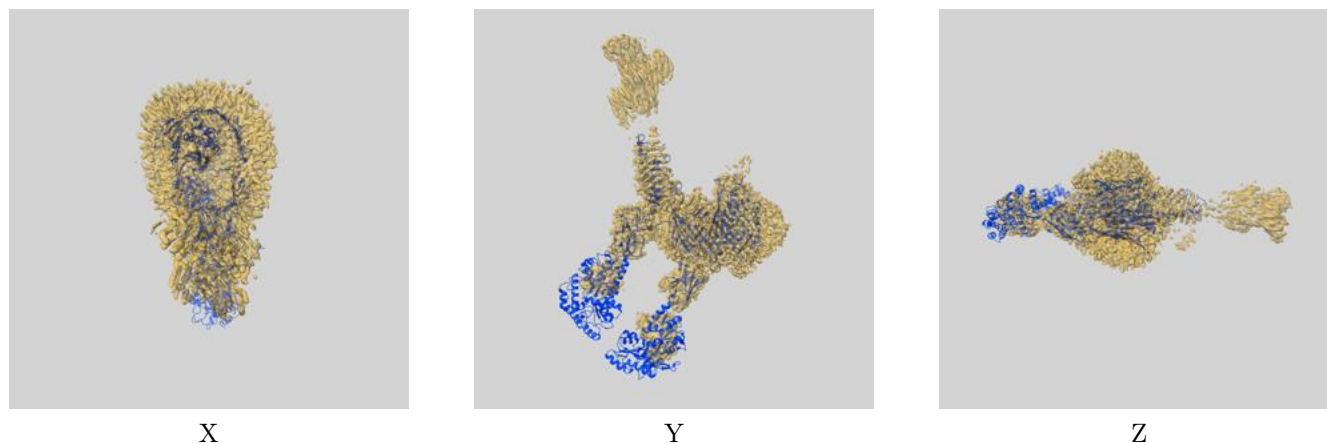
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

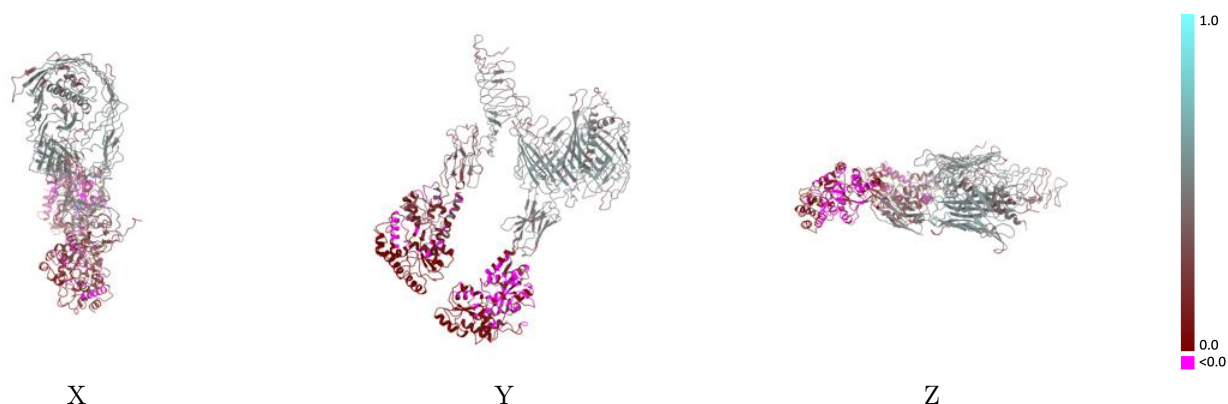
This section contains information regarding the fit between EMDB map EMD-12990 and PDB model 7OMM. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.45 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](#)

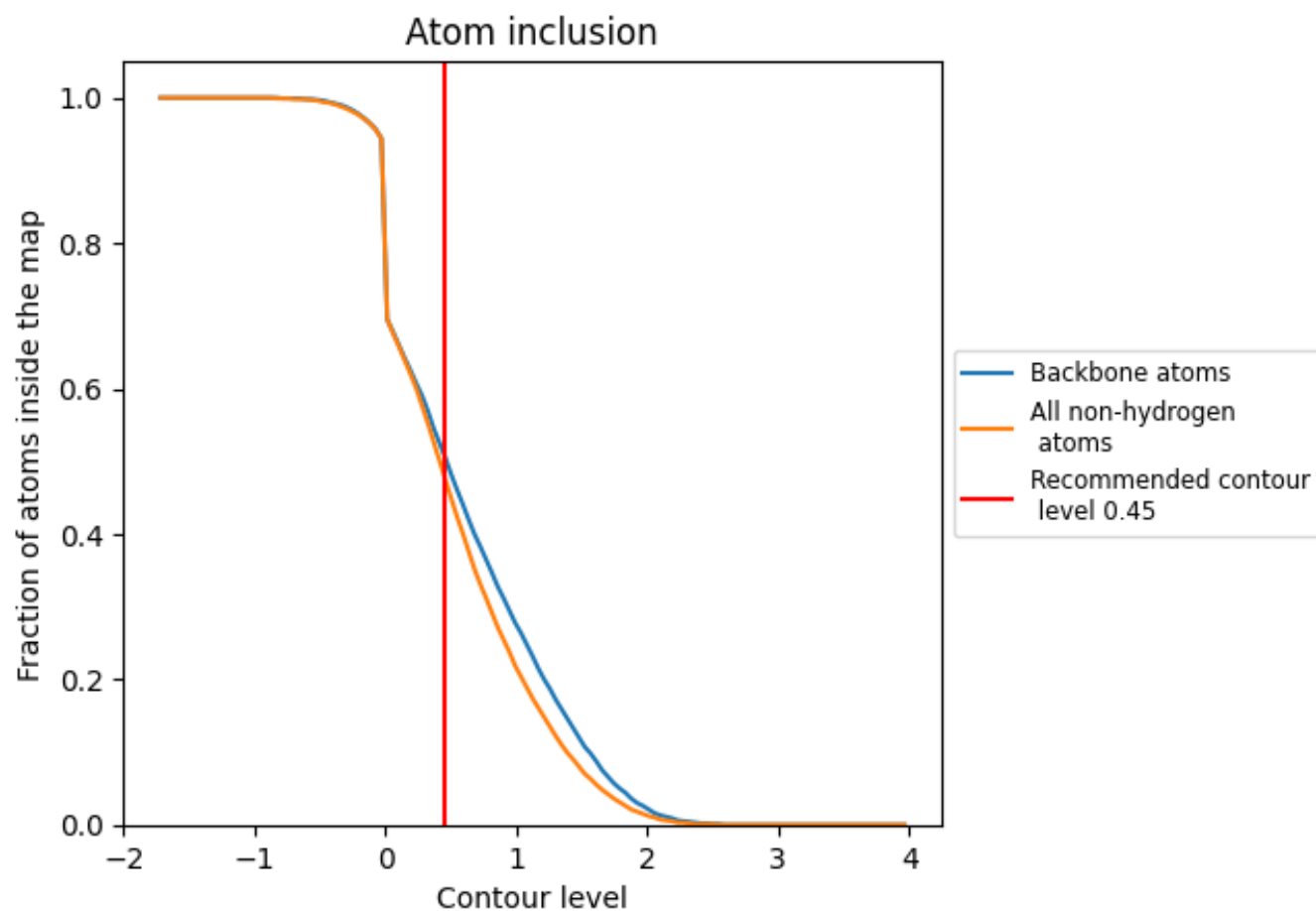


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 51% of all backbone atoms, 48% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4780	0.2830
A	0.7840	0.4720
B	0.7480	0.4570
C	0.2330	0.1050
D	0.2110	0.1380

