WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB EM Validation Report ⓘ

Dec 23, 2024 – 12:27 PM JST

PDB ID	:	9IXM
EMDB ID	:	EMD-60973
Title	:	Cryo-EM structure of Lactobacillus casei DdmDE bound with DNA
Authors	:	Huang, P.P.; Chen, M.R.; Xiao, Y.B.
Deposited on	:	2024-07-29
Resolution	:	3.26 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:
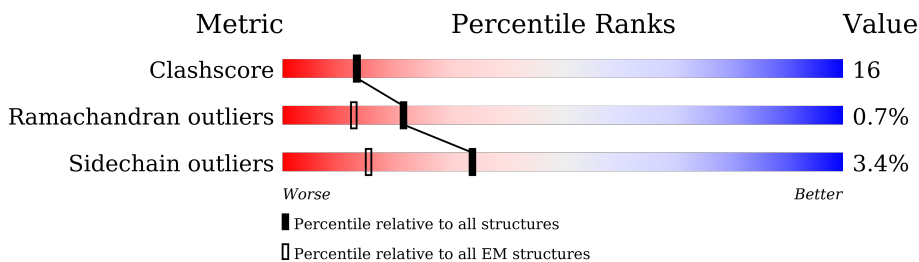
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.26 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	Percentile Ranks	Value
Clashscore		16
Ramachandran outliers		0.7%
Sidechain outliers		3.4%

Worse — *Better*

■ Percentile relative to all structures
❚ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1192	5% / 69% / 27% / · ·
1	C	1192	5% / 26% / 16% · / 56%
2	B	715	· / 73% / 25% / ·
3	E	30	23% / · / 97%
4	D	15	20% / 80%
5	F	30	27% / 30% / 60% / 10%

2 Entity composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 20925 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 DdmD.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1169	Total 9459	C 6029	N 1635	O 1766	S 29	0	0
1	C	521	Total 4076	C 2606	N 706	O 752	S 12	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	SER	LEU	conflict	UNP A0A5R8LS59
A	46	ILE	VAL	conflict	UNP A0A5R8LS59
A	115	SER	ASN	conflict	UNP A0A5R8LS59
A	154	GLU	ASP	conflict	UNP A0A5R8LS59
A	174	LYS	ARG	conflict	UNP A0A5R8LS59
A	179	ALA	GLU	conflict	UNP A0A5R8LS59
A	187	ASP	ASN	conflict	UNP A0A5R8LS59
A	313	PHE	SER	conflict	UNP A0A5R8LS59
A	468	HIS	TYR	conflict	UNP A0A5R8LS59
A	575	GLU	GLN	conflict	UNP A0A5R8LS59
A	681	ASP	GLU	conflict	UNP A0A5R8LS59
A	704	ILE	VAL	conflict	UNP A0A5R8LS59
A	762	ARG	PRO	conflict	UNP A0A5R8LS59
A	859	PRO	THR	conflict	UNP A0A5R8LS59
A	1090	VAL	ALA	conflict	UNP A0A5R8LS59
A	1101	ASP	ASN	conflict	UNP A0A5R8LS59
A	1106	ALA	VAL	conflict	UNP A0A5R8LS59
A	1140	ARG	GLN	conflict	UNP A0A5R8LS59
A	1165	THR	MET	conflict	UNP A0A5R8LS59
C	7	SER	LEU	conflict	UNP A0A5R8LS59
C	46	ILE	VAL	conflict	UNP A0A5R8LS59
C	115	SER	ASN	conflict	UNP A0A5R8LS59
C	154	GLU	ASP	conflict	UNP A0A5R8LS59
C	174	LYS	ARG	conflict	UNP A0A5R8LS59
C	179	ALA	GLU	conflict	UNP A0A5R8LS59
C	187	ASP	ASN	conflict	UNP A0A5R8LS59

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Chain	Residue	Modelled	Actual	Comment	Reference
C	313	PHE	SER	conflict	UNP A0A5R8LS59
C	468	HIS	TYR	conflict	UNP A0A5R8LS59
C	575	GLU	GLN	conflict	UNP A0A5R8LS59
C	681	ASP	GLU	conflict	UNP A0A5R8LS59
C	704	ILE	VAL	conflict	UNP A0A5R8LS59
C	762	ARG	PRO	conflict	UNP A0A5R8LS59
C	859	PRO	THR	conflict	UNP A0A5R8LS59
C	1090	VAL	ALA	conflict	UNP A0A5R8LS59
C	1101	ASP	ASN	conflict	UNP A0A5R8LS59
C	1106	ALA	VAL	conflict	UNP A0A5R8LS59
C	1140	ARG	GLN	conflict	UNP A0A5R8LS59
C	1165	THR	MET	conflict	UNP A0A5R8LS59

- Molecule 2 is a protein called DdmE.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	713	Total 5848	C 3737	N 1025	O 1064	S 22	0	0

- Molecule 3 is a DNA chain called DNA (30-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	30	Total 614	C 293	N 115	O 176	P 30	0	0

- Molecule 4 is a DNA chain called DNA (5'-D(P*TP*GP*AP*CP*GP*GP*CP*TP*CP*TP *AP*AP*TP*CP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	15	Total 305	C 146	N 52	O 92	P 15	0	0

- Molecule 5 is a DNA chain called DNA (30-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	30	Total 622	C 296	N 118	O 178	P 30	0	0

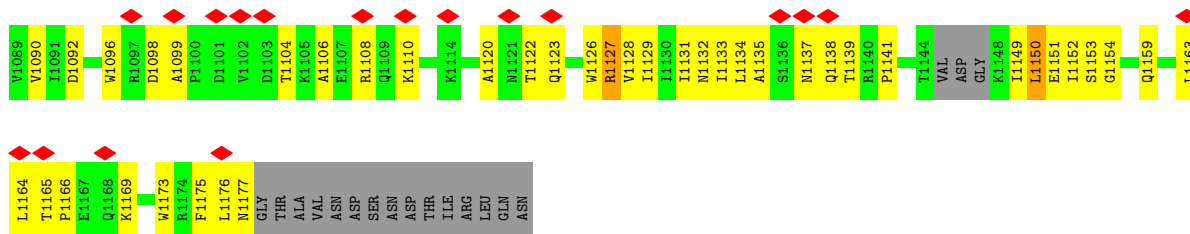- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

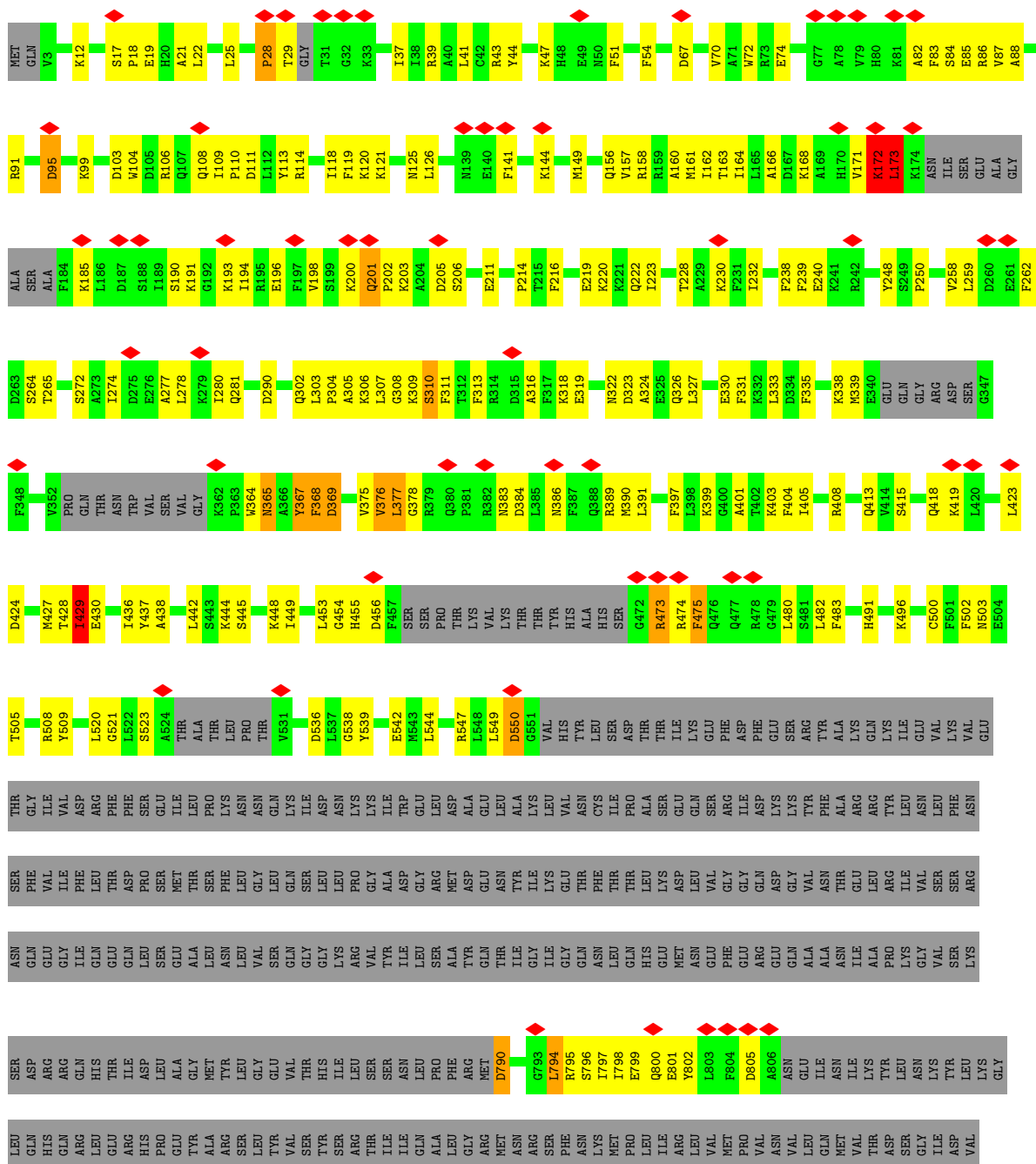| Mol	Chain	Residues	Atoms		AltConf
6	D	1	Total 1	Mg 1	0

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.
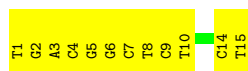
● Molecule 1: DdmD

Chain A:

• Molecule 1: DdmD

Chain C:

GLU LYS THR SER GLN GLU TYR ARG CYS LEU LEU THR ALA ALA LYS ASP ARG TRP GLU ARG ASP PHE GLU LYS PRO SER ALA GLU ILE ALA LYS GLN ASN ALA THR PHE ASN THR PHE ARG ASP TYR ARG PHE VAL LEU ALA TYR LEU GLN THR LYS SER TRP ALA GLN ILE ILE TYR HIS ASP

THR ARG TRP PHE TYR VAL ARG HIS PRO THR VAL SER ASP LYS ASP LYS SER GLN VAL PHE GLN GLN ARG ASP ASP GLU PHE GLY LEU LEU GLN TYR LEU LEU ASN GLU LEU ASP VAL SER TYR GLU VAL LYS PRO ILE ASN HIS ASP ASN GLY PHE ASP SER PHE SER GLY THR

GLY MET GLU VAL SER ALA GLU ALA ALA GLY LEU VAL ALA MET CYS ARG TYR PRO GLY LEU LYS GLU LYS ALA PHE GLU GLU SER LEU ASP ILE LEU PRO THR LYS TRP GLU PRO ASN GLU ARG ILE LEU ASN PRO ALA GLN PHE TYR ASN TYR ARG GLY LEU LEU GLY VAL SER GLN PHE ILE

PHE GLN ASN GLN TRP SER LYS LEU ALA ASP PHE LYS PRO ASN TYR GLU LEU PHE PHE ASP HIS TRP GLU GLY LYS VAL VAL ILE ILE ASP PHE ASN TRP ASP ALA ASP VAL THR LYS ALA ARG GLN LYS VAL GLU LYS LEU ALA LYS LEU GLN ALA

ASN THR GLN GLU ARG GLU TRP ARG VAL VAL ILE ILE ILE ASN ILE LEU ALA SER ASN GLN THR ARG PRO VAL MET THR VAL ASP GLY LYS ILE LEU GLU ILE SER GLY LEU ILE ASP ASP HIS GLN GLY LYS PHE LEU THR PRO GLU GLN LYS LEU ASN VAL TRP ARG PHE LEU ASN GLY THR ALA

VAL ASN ASP ASN SER ASP ASP THR ILE ARG LEU GLN ASN

• Molecule 2: DdmE

Chain B: 73%   25%

MET GLU Q3 D13 Y14 K15 M18 M19 Q20 D24 F25 K26 K31 L44 S49 P50 E51 T54 S55 I56 Y60 D64 Y65 L66 L72 E82 Y97 P98 N99 H100 L106 N107 Q108 K114 S115 L116 K121 E131 R134 R137 D138 M139

Q142 M158 T162 F163 T164 Q165 E168 F169 Q170 W171 D172 K173 Q174 I175 Y176 R184 I195 Y196 F197 V198 Q199 G200 N201 N205 L212 S213 L214 F220 Y221 G226 D233 L244 H250 K251 S252 R259 I268 Q271 I279 Q282 D285

R286 L287 S288 Q289 E290 L291 Q303 R306 R314 K317 I318 Q319 N323 I324 D329 R333 A334 A335 E336 A342 V348 Q349 H350 L351 T352 V353 E354 N355 F356 Q360 K364 E365 I366 V383 A384 I385 L388 I389 Q390 I394 L398 K402 V406

E407 P408 Y421 K427 D430 L438 E443 M444 E445 S449 N456 S460 D461 Y464 T465 Q466 L475 Y481 S482 A483 S493 K496 R505 T506 I507 M508 P509 R515 R522 K525 R529 D530 K531 R540 S544 G545 D546 S547 D548 Y549

V550 E554 R564 P565 D573 G580 L581 K584 R585 R586 D587 M588 N598 A599 T600 L603 K604 D613 L616 K620 T625 R626 I627 E628 E629 H633 T636 F637 V640 D643 L646 K647 P648 V649 V650 V654 R657 D665 I668 I669

M680 E683 Q689 Y690 T691 V692 Y695 P696 Y699 L700 R701 E702 Y705 R709 P712 R715

• Molecule 3: DNA (30-MER)

Chain E: 23%   97%

C24 A25 C26 T27 A28 A29 T30 A31 G32 A33 T34 T35 A36 G37 A38 G39 C40 C41 G42 T43 C44 A45 C46 G47 T48 A49 T50 C51 A52 A53

• Molecule 4: DNA (5'-D(P*TP*GP*AP*CP*GP*GP*CP*TP*CP*TP*AP*AP*TP*CP*T)-3')

Chain D: 20%   80%

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T1 G2 A3 C4 G5 G6 C7 T8 C9 T10 C14 T15

• Molecule 5: DNA (30-MER)

Chain F:

27%

30% 60% 10%

T7 T8 G9 A10 T11 A12 C13 G14 A15 C16 T17 G18 G21 A22 A27 G28 A29 T30 A31 A32 A33 G34 T35 G36

4   Experimental information   ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94045	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	45	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.736	Depositor
Minimum map value	-0.356	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	357.888, 357.888, 357.888	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.932, 0.932, 0.932	Depositor

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.27	0/9652	0.56	12/13017 (0.1%)
1	C	0.29	0/4143	0.62	8/5573 (0.1%)
2	B	0.26	0/5972	0.56	7/8060 (0.1%)
3	E	0.59	0/689	0.95	0/1060
4	D	0.52	0/340	0.83	0/522
5	F	0.73	4/699 (0.6%)	0.87	0/1078
All	All	0.32	4/21495 (0.0%)	0.61	27/29310 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	30	DT	C1'-N1	5.91	1.56	1.49
5	F	17	DT	C1'-N1	5.54	1.56	1.49
5	F	16	DC	C1'-N1	5.03	1.55	1.49
5	F	7	DT	C1'-N1	5.01	1.55	1.49

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	427	MET	CB-CA-C	-15.31	79.79	110.40
1	A	139	ASN	N-CA-C	10.53	139.44	111.00
2	B	407	GLU	CB-CA-C	7.66	125.71	110.40
1	A	139	ASN	CB-CA-C	-7.38	95.64	110.40
1	C	429	ILE	CB-CA-C	-7.32	96.96	111.60
1	A	430	GLU	N-CA-C	-6.81	92.61	111.00
2	B	60	TYR	N-CA-C	-6.76	92.74	111.00
2	B	64	ASP	CB-CA-C	-6.62	97.16	110.40
1	C	28	PRO	CB-CA-C	-6.61	95.47	112.00
1	C	172	LYS	N-CA-C	-6.38	93.76	111.00
1	A	460	PRO	N-CA-CB	6.34	110.91	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	65	TYR	N-CA-CB	6.16	121.68	110.60
1	C	28	PRO	N-CA-CB	5.97	110.47	103.30
1	C	430	GLU	N-CA-C	-5.97	94.88	111.00
1	A	626	ASP	N-CA-C	-5.90	95.07	111.00
2	B	620	LYS	CB-CA-C	-5.85	98.71	110.40
1	C	376	VAL	N-CA-C	5.82	126.71	111.00
1	A	517	ALA	N-CA-CB	5.80	118.22	110.10
1	C	18	PRO	N-CA-CB	5.77	110.22	103.30
1	C	29	THR	N-CA-CB	-5.58	99.69	110.30
2	B	158	MET	N-CA-C	-5.22	96.91	111.00
2	B	598	ASN	CB-CA-C	-5.17	100.07	110.40
1	A	516	LYS	CB-CA-C	-5.10	100.20	110.40
1	A	429	ILE	CB-CA-C	-5.08	101.43	111.60
1	A	428	THR	N-CA-CB	-5.08	100.65	110.30
1	A	78	ALA	CB-CA-C	-5.06	102.52	110.10
1	A	456	ASP	N-CA-C	5.01	124.52	111.00

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	9459	0	9382	273	0
1	C	4076	0	3971	166	0
2	B	5848	0	5916	139	0
3	E	614	0	338	67	0
4	D	305	0	171	14	0
5	F	622	0	339	58	0
6	D	1	0	0	0	0
All	All	20925	0	20117	653	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 16.

All (653) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:480:LEU:CD1	1:C:797:ILE:HG21	1.55	1.35
1:A:186:LEU:HD11	1:A:239:PHE:CD2	1.67	1.27
1:C:473:ARG:NH1	1:C:805:ASP:O	1.65	1.27
1:C:480:LEU:CD1	1:C:797:ILE:CG2	2.12	1.27
1:C:480:LEU:HD11	1:C:797:ILE:CG2	1.65	1.26
5:F:34:DG:N2	5:F:35:DT:C2	2.16	1.13
1:C:480:LEU:HD12	1:C:797:ILE:HG22	1.35	1.07
1:A:186:LEU:CD1	1:A:239:PHE:CD2	2.37	1.07
1:C:274:ILE:HD11	1:C:794:LEU:HD22	1.13	1.07
5:F:34:DG:N2	5:F:35:DT:O2	1.87	1.07
3:E:45:DA:H61	5:F:15:DA:H62	1.06	1.02
1:C:480:LEU:HD12	1:C:797:ILE:CG2	1.88	1.01
1:A:137:LYS:HE3	1:A:143:LEU:HB2	1.41	1.00
1:A:365:ASN:HB3	1:A:383:ASN:HB3	1.41	1.00
2:B:584:LYS:HE3	5:F:14:DG:H2"	1.42	1.00
1:C:429:ILE:HG23	1:C:429:ILE:O	1.60	1.00
1:A:186:LEU:HD21	1:A:239:PHE:HB3	1.43	0.99
1:A:137:LYS:O	1:A:141:PHE:HE1	1.45	0.98
1:C:172:LYS:O	1:C:173:LEU:HD23	1.61	0.98
1:C:475:PHE:CD2	1:C:801:GLU:HB3	2.00	0.96
1:A:186:LEU:HD11	1:A:239:PHE:CE2	2.01	0.96
3:E:50:DT:H71	5:F:10:DA:N6	1.81	0.95
1:A:826:LEU:HD23	5:F:18:DG:H21	1.30	0.95
1:A:406:LEU:HD22	1:A:455:HIS:O	1.65	0.95
1:A:429:ILE:HG23	1:A:429:ILE:O	1.66	0.92
1:C:274:ILE:CD1	1:C:794:LEU:HD22	2.00	0.92
1:C:106:ARG:O	3:E:26:DC:H5	1.53	0.91
5:F:29:DA:H2'	5:F:30:DT:H4'	1.53	0.90
1:A:137:LYS:O	1:A:141:PHE:CE1	2.25	0.89
3:E:45:DA:H61	5:F:15:DA:N6	1.70	0.89
1:A:1122:THR:HG1	1:A:1126:TRP:HE1	0.93	0.88
5:F:17:DT:H2'	5:F:17:DT:O2	1.71	0.88
1:A:186:LEU:CD1	1:A:239:PHE:CE2	2.57	0.87
1:C:475:PHE:HD2	1:C:801:GLU:HB3	1.36	0.86
2:B:64:ASP:O	2:B:65:TYR:CD1	2.27	0.86
1:C:274:ILE:HD11	1:C:794:LEU:CD2	2.04	0.86
3:E:50:DT:H71	5:F:10:DA:H62	1.41	0.85
1:C:480:LEU:CD1	1:C:797:ILE:HG22	1.95	0.83
1:A:625:ILE:HD13	1:A:625:ILE:N	1.93	0.82
1:C:475:PHE:HB2	1:C:805:ASP:OD2	1.78	0.82
1:A:823:HIS:HD2	1:A:825:ARG:NH2	1.77	0.82
1:A:826:LEU:HD23	5:F:18:DG:N2	1.93	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:586:ARG:HE	3:E:50:DT:H4'	1.46	0.80
5:F:16:DC:H2'	5:F:16:DC:O2	1.80	0.80
1:A:622:GLN:O	1:A:622:GLN:NE2	2.15	0.80
3:E:43:DT:H1'	3:E:44:DC:OP1	1.82	0.79
1:C:413:GLN:NE2	1:C:427:MET:O	2.15	0.79
2:B:407:GLU:HG2	2:B:408:PRO:CD	2.13	0.78
1:A:493:LEU:HD22	1:C:304:PRO:HG3	1.66	0.78
2:B:689:GLN:NE2	3:E:44:DC:OP1	2.17	0.78
1:A:406:LEU:CD2	1:A:455:HIS:O	2.33	0.77
1:A:72:TRP:O	1:A:76:SER:HB2	1.83	0.77
2:B:689:GLN:NE2	3:E:44:DC:P	2.59	0.76
1:A:136:MET:HE1	1:A:140:GLU:HG2	1.67	0.76
1:A:626:ASP:N	1:A:626:ASP:OD1	2.16	0.76
1:C:480:LEU:HD11	1:C:797:ILE:HG21	0.80	0.75
1:C:99:LYS:HZ1	1:C:211:GLU:HG2	1.52	0.75
1:C:429:ILE:O	1:C:429:ILE:CG2	2.33	0.75
1:A:625:ILE:HD13	1:A:625:ILE:H	1.50	0.74
1:C:473:ARG:HB3	1:C:805:ASP:HB3	1.69	0.74
3:E:50:DT:H72	5:F:9:DG:H1	1.53	0.74
5:F:13:DC:H2"	5:F:14:DG:C8	2.23	0.74
1:A:474:ARG:HH11	1:A:478:ARG:HH12	1.34	0.73
1:C:106:ARG:O	3:E:26:DC:C5	2.41	0.73
5:F:27:DA:H2"	5:F:28:DG:H5"	1.71	0.72
1:A:825:ARG:O	1:A:825:ARG:HG3	1.88	0.72
3:E:31:DA:H4'	3:E:32:DG:OP1	1.89	0.72
1:A:137:LYS:HE3	1:A:143:LEU:CB	2.19	0.72
1:A:914:THR:HG22	1:A:1041:ASN:HB2	1.70	0.71
1:A:694:ARG:NH1	1:A:710:GLU:OE2	2.24	0.71
1:A:1139:THR:HB	1:A:1163:LEU:HD23	1.71	0.71
1:C:278:LEU:CD2	1:C:794:LEU:HD13	2.21	0.71
3:E:51:DC:H2"	3:E:52:DA:H5"	1.72	0.71
2:B:475:LEU:HD12	2:B:483:ALA:HB1	1.73	0.71
5:F:29:DA:C4	5:F:30:DT:H1'	2.25	0.70
3:E:24:DC:H2"	3:E:25:DA:H5'	1.73	0.70
1:C:278:LEU:HD21	1:C:794:LEU:CD1	2.21	0.70
1:C:365:ASN:O	1:C:377:LEU:HA	1.90	0.70
1:A:1120:ALA:O	1:A:1123:GLN:NE2	2.25	0.70
1:A:823:HIS:HD2	1:A:825:ARG:HH22	1.37	0.69
1:A:985:VAL:HG23	1:A:997:PHE:HA	1.73	0.69
3:E:52:DA:H2"	3:E:53:DA:H5'	1.72	0.69
1:A:186:LEU:H	1:A:186:LEU:HD23	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:43:DT:H2"	3:E:44:DC:O5'	1.92	0.69
1:A:779:HIS:HD1	1:A:779:HIS:H	1.39	0.69
1:C:111:ASP:HA	1:C:114:ARG:HB2	1.73	0.69
1:A:826:LEU:HB3	5:F:18:DG:C2	2.28	0.69
1:C:91:ARG:NH2	1:C:211:GLU:O	2.26	0.69
1:C:339:MET:CE	1:C:377:LEU:HD12	2.23	0.69
1:A:474:ARG:NH2	1:A:968:GLU:O	2.26	0.69
1:A:584:ASP:OD2	2:B:522:ARG:NH2	2.25	0.68
1:C:339:MET:HE2	1:C:377:LEU:HD12	1.75	0.68
3:E:27:DT:H2"	3:E:28:DA:H8	1.58	0.68
2:B:648:PRO:HD3	5:F:15:DA:N6	2.08	0.68
1:A:420:LEU:HD12	1:A:421:SER:H	1.59	0.68
2:B:142:GLN:NE2	2:B:201:ASN:OD1	2.27	0.67
2:B:505:ARG:NH1	2:B:629:GLU:OE1	2.27	0.67
1:A:786:PRO:HD2	1:A:788:ARG:NH2	2.10	0.67
2:B:31:LYS:HB2	2:B:82:GLU:HB2	1.77	0.66
2:B:171:TRP:HB2	3:E:30:DT:C5	2.30	0.66
3:E:36:DA:H2"	3:E:37:DG:H5"	1.75	0.66
2:B:449:SER:HG	2:B:464:TYR:HH	1.42	0.66
1:A:1139:THR:HG21	1:A:1164:LEU:HB2	1.77	0.66
1:C:201:GLN:HG3	1:C:202:PRO:HD3	1.76	0.66
1:A:93:LEU:HD23	1:A:147:TRP:NE1	2.11	0.66
1:A:46:ILE:HD13	1:A:76:SER:HA	1.77	0.65
5:F:17:DT:O2	5:F:17:DT:C2'	2.44	0.65
1:A:624:ARG:CG	1:A:624:ARG:O	2.43	0.65
1:A:144:LYS:HA	5:F:28:DG:C6	2.32	0.65
1:C:474:ARG:HG2	1:C:801:GLU:OE1	1.96	0.65
1:A:1129:ILE:HG23	1:A:1150:LEU:HB3	1.79	0.65
3:E:50:DT:H71	5:F:10:DA:C6	2.32	0.65
5:F:16:DC:O2	5:F:16:DC:C2'	2.45	0.64
1:A:624:ARG:O	1:A:624:ARG:HG2	1.96	0.64
2:B:665:ASP:O	2:B:668:ILE:HG12	1.98	0.64
1:A:54:PHE:HB2	1:A:257:VAL:HG12	1.79	0.63
5:F:11:DT:H2"	5:F:12:DA:C8	2.33	0.63
1:A:823:HIS:CD2	1:A:825:ARG:HH22	2.16	0.63
1:A:752:ILE:N	1:A:855:PHE:O	2.28	0.63
1:A:820:GLY:HA2	1:A:825:ARG:NH1	2.13	0.63
3:E:48:DT:H2"	3:E:49:DA:C8	2.34	0.63
1:A:365:ASN:CB	1:A:383:ASN:HB3	2.23	0.62
2:B:303:GLN:HA	2:B:306:ARG:HG2	1.82	0.62
1:C:491:HIS:O	1:C:491:HIS:ND1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:GLN:O	2:B:289:GLN:NE2	2.33	0.62
1:A:298:VAL:HG12	1:A:303:LEU:HG	1.82	0.62
1:C:475:PHE:HD2	1:C:801:GLU:CB	2.12	0.61
1:C:278:LEU:HD21	1:C:794:LEU:HD13	1.80	0.61
1:A:137:LYS:CE	1:A:143:LEU:HB2	2.24	0.61
2:B:648:PRO:HD3	5:F:15:DA:C6	2.35	0.61
2:B:355:ASN:ND2	4:D:2:DG:OP1	2.31	0.61
1:A:1011:LEU:HD13	1:A:1052:LEU:HD21	1.81	0.61
2:B:421:TYR:HB2	2:B:700:LEU:HD13	1.81	0.61
1:C:185:LYS:O	1:C:190:SER:OG	2.18	0.61
5:F:22:DA:C8	5:F:22:DA:H5'	2.36	0.61
1:C:383:ASN:ND2	1:C:383:ASN:O	2.32	0.61
3:E:45:DA:N6	5:F:15:DA:H62	1.88	0.61
5:F:10:DA:H2'	5:F:11:DT:C6	2.36	0.61
2:B:584:LYS:HE3	5:F:14:DG:C2'	2.26	0.60
3:E:37:DG:H2"	3:E:38:DA:C8	2.36	0.60
1:A:114:ARG:O	1:A:120:LYS:NZ	2.31	0.60
1:A:362:LYS:NZ	1:A:363:PRO:O	2.31	0.60
1:A:628:LYS:O	1:A:632:ARG:HG2	2.02	0.60
1:A:946:VAL:HG21	1:A:1051:LEU:HD22	1.83	0.60
3:E:31:DA:H2"	3:E:32:DG:O5'	2.02	0.60
2:B:286:ARG:NH2	2:B:364:LYS:O	2.34	0.60
1:A:136:MET:HE3	1:A:136:MET:HA	1.83	0.60
1:C:259:LEU:HD22	1:C:265:THR:HG21	1.83	0.60
3:E:40:DC:H2'	3:E:41:DC:C6	2.37	0.60
2:B:139:MET:SD	2:B:139:MET:N	2.75	0.60
2:B:604:LYS:HZ2	5:F:14:DG:H5'	1.65	0.60
1:C:205:ASP:N	1:C:205:ASP:OD1	2.34	0.60
1:A:820:GLY:HA2	1:A:825:ARG:HH11	1.67	0.59
2:B:329:ASP:O	2:B:333:ARG:NH1	2.34	0.59
1:C:455:HIS:O	1:C:455:HIS:ND1	2.34	0.59
4:D:2:DG:H2'	4:D:3:DA:C8	2.37	0.59
3:E:50:DT:C7	5:F:10:DA:H62	2.14	0.59
1:A:825:ARG:HH11	1:A:825:ARG:CG	2.14	0.59
2:B:689:GLN:HE22	3:E:44:DC:P	2.24	0.59
1:A:355:THR:HA	1:A:919:ARG:HH21	1.67	0.59
2:B:383:VAL:HG21	3:E:44:DC:C5	2.38	0.59
2:B:407:GLU:HG2	2:B:408:PRO:HD2	1.84	0.59
2:B:545:GLY:HA3	2:B:549:TYR:HD2	1.68	0.59
2:B:162:THR:OG1	4:D:9:DC:OP2	2.21	0.59
2:B:643:ASP:OD1	2:B:643:ASP:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:701:ARG:NH1	4:D:4:DC:OP1	2.36	0.58
1:A:72:TRP:O	1:A:76:SER:CB	2.51	0.58
2:B:171:TRP:HB2	3:E:30:DT:C6	2.38	0.58
3:E:35:DT:H2"	3:E:36:DA:C8	2.39	0.58
2:B:496:LYS:HD3	2:B:668:ILE:HD12	1.84	0.58
2:B:580:GLY:O	2:B:585:ARG:NH1	2.33	0.58
1:C:280:ILE:HD13	1:C:448:LYS:HD3	1.86	0.58
2:B:51:GLU:HB3	2:B:108:GLN:HE22	1.68	0.58
2:B:317:LYS:O	2:B:319:GLN:NE2	2.36	0.58
1:C:91:ARG:O	1:C:230:LYS:NZ	2.36	0.58
5:F:30:DT:H2'	5:F:31:DA:O4'	2.04	0.58
1:A:1008:ALA:O	1:A:1049:ARG:NH2	2.37	0.58
1:C:386:ASN:OD1	1:C:389:ARG:N	2.37	0.58
1:C:475:PHE:CE2	1:C:801:GLU:HB3	2.39	0.58
1:C:19:GLU:O	1:C:547:ARG:NH1	2.36	0.58
1:A:823:HIS:CD2	1:A:825:ARG:NH2	2.67	0.57
2:B:530:ASP:OD1	2:B:530:ASP:N	2.35	0.57
1:C:86:ARG:O	1:C:222:GLN:N	2.33	0.57
1:C:83:PHE:O	1:C:85:GLU:N	2.38	0.57
1:C:103:ASP:HA	1:C:108:GLN:HB2	1.85	0.57
1:A:576:VAL:HG22	1:A:861:ILE:HB	1.87	0.57
1:C:262:PHE:HB3	1:C:523:SER:HB3	1.86	0.57
1:C:278:LEU:HD21	1:C:794:LEU:HD12	1.86	0.57
1:A:731:ILE:O	1:A:850:ARG:NH1	2.36	0.57
2:B:438:LEU:HB2	2:B:700:LEU:HD21	1.87	0.57
1:C:278:LEU:CD2	1:C:794:LEU:CD1	2.82	0.57
1:A:624:ARG:HB3	1:A:624:ARG:CZ	2.33	0.57
2:B:360:GLN:N	2:B:360:GLN:OE1	2.38	0.56
2:B:427:LYS:NZ	2:B:712:PRO:O	2.36	0.56
1:A:490:GLN:OE1	1:C:444:LYS:NZ	2.33	0.56
1:C:191:LYS:HG3	1:C:239:PHE:HE2	1.70	0.56
3:E:38:DA:H2"	3:E:39:DG:O4'	2.05	0.56
1:A:660:LEU:HD22	1:A:697:SER:HB2	1.88	0.56
1:C:104:TRP:HZ2	1:C:120:LYS:HD3	1.70	0.56
3:E:50:DT:H73	5:F:10:DA:N7	2.20	0.56
1:A:186:LEU:HD13	1:A:239:PHE:CD2	2.35	0.56
2:B:636:THR:HG21	2:B:669:ILE:HG21	1.86	0.56
1:C:158:ARG:O	1:C:162:ILE:HD12	2.05	0.56
1:C:277:ALA:O	1:C:281:GLN:NE2	2.37	0.56
1:C:376:VAL:HG12	1:C:378:GLY:H	1.71	0.56
1:A:903:LYS:HB2	1:A:904:PRO:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1016:ARG:HD2	1:A:1159:GLN:HA	1.88	0.56
1:A:950:THR:HG22	1:A:1039:ILE:HG13	1.86	0.55
1:A:1173:TRP:O	1:A:1177:ASN:ND2	2.39	0.55
2:B:507:ILE:HB	2:B:654:VAL:HG23	1.88	0.55
1:C:367:TYR:CD1	1:C:367:TYR:N	2.72	0.55
1:C:39:ARG:O	1:C:39:ARG:NH1	2.38	0.55
1:C:173:LEU:HG	1:C:173:LEU:O	2.05	0.55
1:C:473:ARG:CB	1:C:805:ASP:HB3	2.37	0.55
2:B:268:ILE:HG12	2:B:390:GLN:HG3	1.87	0.55
1:A:696:VAL:HG23	1:A:726:SER:HB2	1.88	0.55
2:B:15:LYS:HG2	2:B:244:LEU:HD12	1.87	0.55
3:E:42:DG:H1	4:D:4:DC:H42	1.55	0.55
2:B:252:SER:OG	2:B:625:THR:OG1	2.20	0.55
2:B:288:SER:OG	2:B:289:GLN:NE2	2.39	0.55
1:A:186:LEU:HD13	1:A:239:PHE:CE2	2.39	0.55
1:A:852:ASN:HA	1:A:857:LYS:HZ1	1.70	0.55
2:B:20:GLN:NE2	2:B:24:ASP:OD2	2.39	0.55
3:E:51:DC:H2"	3:E:52:DA:H8	1.71	0.55
2:B:385:ILE:HA	2:B:388:LEU:HD12	1.88	0.55
1:A:1014:MET:HE2	1:A:1133:ILE:HG21	1.89	0.55
1:A:157:VAL:O	1:A:161:MET:HG2	2.07	0.54
1:A:741:MET:SD	1:A:746:ARG:HG3	2.46	0.54
1:C:191:LYS:HG3	1:C:239:PHE:CE2	2.41	0.54
3:E:45:DA:OP2	3:E:45:DA:H2'	2.07	0.54
3:E:50:DT:H72	5:F:9:DG:N1	2.20	0.54
2:B:525:LYS:NZ	2:B:600:THR:O	2.41	0.54
1:C:324:ALA:HB2	1:C:397:PHE:CZ	2.42	0.54
2:B:407:GLU:HG2	2:B:408:PRO:HD3	1.88	0.54
1:A:907:GLU:O	1:A:911:GLN:HG3	2.07	0.54
1:C:338:LYS:O	1:C:376:VAL:O	2.26	0.54
3:E:47:DG:O5'	3:E:47:DG:H2'	2.08	0.54
5:F:29:DA:C2'	5:F:30:DT:H4'	2.32	0.54
1:A:136:MET:CE	1:A:136:MET:CA	2.85	0.54
2:B:279:ILE:HD13	2:B:324:ILE:HB	1.90	0.54
1:C:365:ASN:HB3	1:C:384:ASP:CG	2.28	0.54
1:A:597:LYS:H	1:A:597:LYS:HD2	1.72	0.54
2:B:383:VAL:HG11	3:E:44:DC:H2'	1.90	0.53
1:C:415:SER:O	1:C:419:LYS:HG2	2.08	0.53
1:A:186:LEU:HD21	1:A:239:PHE:CB	2.27	0.53
1:C:39:ARG:HH12	1:C:43:ARG:HB2	1.72	0.53
1:C:319:GLU:HA	1:C:322:ASN:HD21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:657:ARG:NH1	4:D:6:DG:OP1	2.32	0.53
1:C:399:LYS:O	1:C:403:LYS:HG2	2.08	0.53
1:A:112:LEU:HD11	1:A:168:LYS:HG3	1.89	0.53
1:A:367:TYR:CD2	1:A:382:ARG:HG2	2.43	0.53
1:C:318:LYS:O	1:C:322:ASN:ND2	2.41	0.53
1:C:428:THR:O	1:C:429:ILE:HG22	2.09	0.53
1:A:474:ARG:NH1	1:A:920:ASP:OD1	2.40	0.53
1:A:624:ARG:O	1:A:624:ARG:HD2	2.08	0.53
1:C:491:HIS:CE1	1:C:496:LYS:HG2	2.43	0.53
1:C:82:ALA:HB3	1:C:85:GLU:HB3	1.91	0.53
2:B:173:LYS:HD2	2:B:198:VAL:HG21	1.91	0.52
2:B:354:GLU:OE1	2:B:354:GLU:N	2.42	0.52
5:F:13:DC:H2"	5:F:14:DG:H8	1.73	0.52
1:C:110:PRO:HG3	1:C:205:ASP:HA	1.91	0.52
3:E:49:DA:H2"	3:E:50:DT:O2	2.09	0.52
1:C:41:LEU:HD11	1:C:258:VAL:HG21	1.91	0.52
1:C:473:ARG:HE	1:C:473:ARG:HA	1.75	0.52
1:A:826:LEU:CD2	5:F:18:DG:N2	2.69	0.52
2:B:627:ILE:HB	2:B:637:PHE:HE1	1.75	0.52
1:A:557:ASP:N	1:A:557:ASP:OD1	2.42	0.52
2:B:131:GLU:OE1	2:B:131:GLU:N	2.31	0.52
1:A:190:SER:HA	1:A:193:LYS:HG3	1.90	0.52
1:C:74:GLU:N	1:C:74:GLU:OE1	2.42	0.51
1:A:579:GLU:HB2	1:A:864:VAL:HG12	1.92	0.51
1:A:942:ARG:HB3	1:A:1051:LEU:HD12	1.92	0.51
2:B:544:SER:O	2:B:544:SER:OG	2.23	0.51
1:A:768:ASP:OD2	1:A:853:ARG:N	2.42	0.51
5:F:17:DT:C6	5:F:17:DT:OP1	2.64	0.51
1:A:1061:PHE:HE1	1:A:1067:LEU:HD11	1.75	0.51
1:A:921:TYR:HA	1:A:924:VAL:HG12	1.93	0.51
2:B:233:ASP:OD2	2:B:515:ARG:NH1	2.41	0.51
1:A:362:LYS:HZ2	1:A:379:ARG:HA	1.76	0.51
2:B:550:VAL:O	2:B:554:GLU:HG2	2.10	0.51
1:A:87:VAL:HG22	1:A:223:ILE:HB	1.92	0.51
1:A:726:SER:OG	1:A:727:ALA:N	2.44	0.51
1:C:309:LYS:O	1:C:310:SER:C	2.50	0.51
1:A:624:ARG:O	1:A:624:ARG:CD	2.59	0.51
2:B:168:GLU:OE2	2:B:170:GLN:NE2	2.44	0.51
1:C:190:SER:HA	1:C:193:LYS:HG3	1.92	0.51
2:B:319:GLN:O	2:B:323:ASN:ND2	2.44	0.50
2:B:164:THR:OG1	2:B:200:GLY:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:27:DT:H2"	3:E:28:DA:C8	2.42	0.50
1:A:1141:PRO:HA	1:A:1151:GLU:O	2.11	0.50
1:C:201:GLN:N	1:C:202:PRO:HD2	2.26	0.50
3:E:26:DC:H2"	3:E:27:DT:C2	2.46	0.50
3:E:39:DG:H2"	3:E:40:DC:H6	1.76	0.50
1:A:476:GLN:O	1:A:508:ARG:NH2	2.35	0.50
1:A:784:ASN:HD22	1:A:792:ALA:HB1	1.75	0.50
1:A:1106:ALA:O	1:A:1110:LYS:HG3	2.12	0.50
1:A:133:PHE:CD1	1:A:133:PHE:C	2.85	0.50
1:A:387:PHE:O	1:A:390:MET:HG3	2.11	0.50
1:C:22:LEU:HD22	1:C:544:LEU:HD22	1.93	0.50
1:C:326:GLN:O	1:C:330:GLU:HG2	2.12	0.50
4:D:14:DC:H2"	4:D:15:DT:C6	2.46	0.50
1:A:858:MET:HG3	1:A:859:PRO:HD2	1.94	0.50
2:B:695:TYR:N	2:B:696:PRO:HD2	2.27	0.49
1:C:331:PHE:CD1	1:C:390:MET:HG2	2.47	0.49
5:F:11:DT:H2"	5:F:12:DA:H8	1.76	0.49
1:C:201:GLN:N	1:C:202:PRO:CD	2.75	0.49
1:A:93:LEU:HD23	1:A:147:TRP:CD1	2.47	0.49
1:A:103:ASP:OD1	1:A:106:ARG:NH2	2.45	0.49
2:B:712:PRO:HA	2:B:715:ARG:HG3	1.94	0.49
1:A:800:GLN:HG3	1:A:817:TYR:CE2	2.47	0.49
1:A:610:LEU:O	1:A:614:VAL:HG22	2.12	0.49
1:A:494:GLN:HE22	1:C:438:ALA:HB1	1.77	0.49
1:A:752:ILE:HG22	1:A:855:PHE:HA	1.94	0.49
2:B:460:SER:HB3	2:B:465:THR:HG21	1.94	0.49
1:C:85:GLU:HG2	1:C:86:ARG:HD2	1.94	0.49
1:C:302:GLN:O	1:C:303:LEU:HB2	2.12	0.49
1:A:825:ARG:NH1	1:A:825:ARG:CG	2.73	0.49
1:A:910:LYS:O	1:A:914:THR:HG23	2.12	0.49
1:A:89:VAL:HG22	1:A:225:ILE:HB	1.95	0.49
2:B:342:ALA:HB2	2:B:348:VAL:HG12	1.94	0.49
1:C:250:PRO:HB2	1:C:424:ASP:OD1	2.12	0.49
1:A:604:TRP:CD1	2:B:114:LYS:HE3	2.48	0.49
2:B:291:LEU:HA	2:B:366:ILE:HD13	1.93	0.49
1:C:319:GLU:HA	1:C:322:ASN:ND2	2.27	0.49
1:A:579:GLU:OE2	1:A:862:ARG:NH1	2.45	0.48
2:B:402:LYS:NZ	2:B:443:GLU:O	2.42	0.48
3:E:25:DA:H2"	3:E:26:DC:H5"	1.95	0.48
1:A:1098:ASP:N	1:A:1098:ASP:OD1	2.43	0.48
2:B:586:ARG:CZ	3:E:51:DC:H5'	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:GLU:HG3	1:C:424:ASP:CB	2.43	0.48
1:C:364:TRP:N	1:C:364:TRP:CD1	2.80	0.48
1:A:57:THR:O	1:A:228:THR:N	2.46	0.48
1:A:953:ASP:O	1:A:957:LYS:HG2	2.13	0.48
1:A:19:GLU:O	1:A:547:ARG:NH1	2.46	0.48
1:A:875:ASP:HB3	1:A:891:LEU:HD13	1.96	0.48
1:C:228:THR:O	1:C:232:ILE:HG12	2.13	0.48
2:B:351:LEU:HD13	2:B:356:PHE:CD2	2.48	0.48
1:C:86:ARG:NH1	1:C:220:LYS:O	2.47	0.48
2:B:540:ARG:O	2:B:540:ARG:NH1	2.35	0.48
3:E:44:DC:H5"	3:E:44:DC:C6	2.49	0.48
1:A:287:LEU:HD11	1:A:450:LEU:HG	1.95	0.48
1:A:527:THR:HA	1:A:537:LEU:HD11	1.96	0.48
2:B:402:LYS:HD2	2:B:445:GLU:HG3	1.94	0.48
2:B:573:ASP:HA	2:B:603:LEU:HD23	1.96	0.48
1:A:136:MET:HE3	1:A:136:MET:CA	2.44	0.48
1:A:412:TYR:HE1	1:A:427:MET:HE2	1.79	0.48
1:C:119:PHE:HE1	1:C:161:MET:HG3	1.79	0.48
1:C:158:ARG:HG2	1:C:238:PHE:CE1	2.48	0.48
1:A:93:LEU:CD2	1:A:147:TRP:NE1	2.76	0.48
1:A:541:ARG:HG3	1:A:548:LEU:HD23	1.96	0.48
1:A:945:TYR:CZ	1:A:1044:GLN:HG2	2.49	0.48
1:A:186:LEU:HD11	1:A:239:PHE:CG	2.40	0.47
1:A:910:LYS:HG2	1:A:974:LEU:HD22	1.96	0.47
2:B:214:LEU:HD11	2:B:616:LEU:HD11	1.95	0.47
1:C:335:PHE:HE2	1:C:368:PHE:CZ	2.31	0.47
5:F:27:DA:H2"	5:F:28:DG:C8	2.48	0.47
1:C:109:ILE:HD11	1:C:113:TYR:HB2	1.95	0.47
1:A:281:GLN:HG2	1:A:500:CYS:HB3	1.95	0.47
1:A:811:ILE:HG12	1:A:915:PHE:CE2	2.50	0.47
1:C:278:LEU:HD11	1:C:790:ASP:HB3	1.96	0.47
1:C:454:GLY:O	1:C:456:ASP:N	2.45	0.47
1:C:482:LEU:HG	1:C:500:CYS:HB3	1.95	0.47
3:E:39:DG:H2"	3:E:40:DC:C6	2.49	0.47
3:E:46:DC:H2"	3:E:47:DG:C8	2.49	0.47
2:B:286:ARG:O	2:B:290:GLU:HG2	2.15	0.47
5:F:14:DG:H4'	5:F:14:DG:OP1	2.14	0.47
1:A:101:ILE:HD12	1:A:130:PHE:HD2	1.79	0.47
1:A:129:ALA:O	1:A:132:SER:OG	2.27	0.47
1:A:263:ASP:OD2	1:A:525:THR:OG1	2.32	0.47
1:A:1150:LEU:HD23	1:A:1175:PHE:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:349:GLN:NE2	2:B:350:HIS:O	2.45	0.47
1:C:333:LEU:HD12	1:C:333:LEU:H	1.79	0.47
1:A:1004:VAL:HG13	1:A:1045:PHE:CG	2.49	0.47
1:A:133:PHE:CE1	1:A:137:LYS:HG2	2.49	0.47
1:A:755:LYS:HB2	1:A:755:LYS:HE3	1.79	0.47
1:A:965:ARG:HD2	1:A:965:ARG:HA	1.64	0.47
1:A:1131:ILE:HG13	1:A:1152:ILE:HD13	1.96	0.47
1:A:1131:ILE:CG1	1:A:1152:ILE:HD13	2.45	0.47
1:A:1165:THR:OG1	1:A:1166:PRO:HD3	2.14	0.47
1:C:144:LYS:NZ	5:F:32:DA:O4'	2.36	0.47
3:E:50:DT:C7	5:F:9:DG:H1	2.25	0.47
3:E:50:DT:C7	5:F:9:DG:N1	2.77	0.47
1:A:226:LEU:HD12	1:A:230:LYS:HG3	1.97	0.47
1:A:885:GLN:NE2	1:A:889:CYS:SG	2.88	0.47
2:B:65:TYR:OH	3:E:33:DA:OP1	2.33	0.47
1:C:415:SER:O	1:C:418:GLN:HG3	2.14	0.47
1:A:987:PRO:HD3	1:A:1002:MET:HB3	1.96	0.47
1:A:1017:TYR:CE2	1:A:1060:ILE:HG12	2.50	0.47
2:B:406:VAL:HG21	2:B:695:TYR:CZ	2.50	0.47
1:A:647:ASP:OD2	1:A:862:ARG:NH2	2.48	0.47
1:C:99:LYS:NZ	1:C:211:GLU:HG2	2.27	0.47
3:E:44:DC:OP1	3:E:44:DC:O4'	2.32	0.47
1:A:352:VAL:HG23	1:A:355:THR:H	1.79	0.46
1:A:1085:TRP:O	1:A:1086:GLU:HG2	2.14	0.46
2:B:107:ASN:O	2:B:184:ARG:NH1	2.49	0.46
3:E:42:DG:H1	4:D:4:DC:N4	2.13	0.46
1:A:247:ARG:NH2	1:A:504:GLU:OE2	2.41	0.46
1:A:474:ARG:NH2	1:A:920:ASP:OD2	2.38	0.46
1:C:21:ALA:HB1	1:C:547:ARG:HB2	1.97	0.46
1:A:825:ARG:NH1	1:A:825:ARG:HG2	2.30	0.46
1:C:118:ILE:HG13	1:C:121:LYS:HE3	1.97	0.46
1:A:491:HIS:O	1:A:491:HIS:ND1	2.45	0.46
2:B:115:SER:OG	2:B:116:LEU:N	2.49	0.46
2:B:461:ASP:O	2:B:466:GLN:NE2	2.49	0.46
2:B:613:ASP:OD1	2:B:613:ASP:N	2.48	0.46
1:C:401:ALA:O	1:C:405:ILE:HG12	2.16	0.46
3:E:28:DA:H2"	3:E:29:DA:H5'	1.97	0.46
1:A:898:GLU:O	2:B:564:ARG:NH2	2.48	0.46
1:C:339:MET:HE2	1:C:377:LEU:CD1	2.42	0.46
1:A:144:LYS:NZ	5:F:28:DG:H2'	2.30	0.46
1:A:778:THR:OG1	1:A:779:HIS:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:ALA:O	1:C:164:ILE:HG13	2.15	0.46
1:A:187:ASP:O	1:A:190:SER:OG	2.29	0.46
1:A:412:TYR:CE1	1:A:427:MET:HE2	2.51	0.46
4:D:7:DC:H2"	4:D:8:DT:C7	2.46	0.46
1:A:598:ILE:HG23	1:A:682:LEU:HD11	1.98	0.46
2:B:383:VAL:CG1	3:E:44:DC:H2'	2.45	0.46
3:E:44:DC:H5'	3:E:45:DA:H5'	1.97	0.46
1:A:428:THR:O	1:A:429:ILE:HG22	2.17	0.45
2:B:97:TYR:O	2:B:99:ASN:N	2.46	0.45
2:B:627:ILE:HB	2:B:637:PHE:CE1	2.51	0.45
1:A:429:ILE:O	1:A:429:ILE:HG12	2.17	0.45
1:A:1090:VAL:N	1:A:1127:ARG:O	2.40	0.45
1:C:196:GLU:HG2	1:C:200:LYS:HZ3	1.80	0.45
3:E:47:DG:C2	5:F:14:DG:N2	2.84	0.45
2:B:604:LYS:NZ	5:F:14:DG:H5'	2.32	0.45
1:C:168:LYS:HE2	1:C:168:LYS:HB2	1.77	0.45
1:C:203:LYS:O	1:C:203:LYS:NZ	2.41	0.45
1:C:323:ASP:O	1:C:327:LEU:HG	2.17	0.45
2:B:683:GLU:OE1	2:B:683:GLU:N	2.50	0.45
1:C:125:ASN:ND2	1:C:156:GLN:OE1	2.39	0.45
1:A:26:ASN:OD1	1:A:26:ASN:N	2.44	0.45
1:C:305:ALA:C	1:C:308:GLY:H	2.20	0.45
1:C:316:ALA:O	1:C:319:GLU:HG2	2.17	0.45
3:E:50:DT:C7	5:F:10:DA:N7	2.80	0.45
1:A:128:ASN:HA	1:A:131:LYS:HE3	1.99	0.45
1:A:533:ASP:OD2	1:A:839:SER:OG	2.31	0.45
1:A:621:GLU:H	1:A:621:GLU:HG3	1.57	0.45
1:A:655:GLY:N	1:A:724:ILE:O	2.48	0.45
2:B:64:ASP:O	2:B:65:TYR:CG	2.67	0.45
2:B:174:GLN:NE2	3:E:33:DA:OP2	2.50	0.45
1:A:143:LEU:HG	5:F:28:DG:O6	2.16	0.45
1:A:1139:THR:HA	1:A:1153:SER:HB2	1.99	0.45
1:C:536:ASP:O	1:C:539:TYR:N	2.50	0.45
1:A:337:TYR:O	1:A:495:THR:N	2.41	0.45
1:A:449:ILE:HD11	1:A:501:PHE:HD1	1.82	0.45
1:A:611:ALA:O	1:A:615:ASN:ND2	2.48	0.45
1:A:1088:LYS:HE2	1:A:1127:ARG:NE	2.32	0.45
1:C:307:LEU:HD21	1:C:311:PHE:HE1	1.81	0.45
1:A:598:ILE:HD12	1:A:598:ILE:H	1.82	0.45
1:A:651:THR:OG1	1:A:652:SER:N	2.49	0.45
1:A:945:TYR:OH	1:A:970:GLY:O	2.22	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1065:TRP:CZ2	1:A:1169:LYS:HA	2.51	0.44
1:C:307:LEU:HD22	1:C:307:LEU:O	2.16	0.44
1:C:473:ARG:HA	1:C:473:ARG:NE	2.31	0.44
1:C:505:THR:OG1	1:C:508:ARG:HG3	2.17	0.44
1:C:538:GLY:O	1:C:542:GLU:HG3	2.16	0.44
1:A:194:ILE:O	1:A:198:VAL:HG13	2.18	0.44
1:A:523:SER:HB3	1:A:526:ALA:HB2	1.99	0.44
1:A:712:LEU:HB3	1:A:739:HIS:HB3	1.99	0.44
2:B:546:ASP:O	2:B:550:VAL:HG22	2.18	0.44
2:B:689:GLN:HE21	3:E:44:DC:P	2.38	0.44
1:C:796:SER:O	1:C:800:GLN:HG3	2.18	0.44
1:A:593:LYS:HA	1:A:593:LYS:HD2	1.81	0.44
1:A:658:SER:OG	1:A:778:THR:HB	2.17	0.44
1:A:1128:VAL:O	1:A:1149:ILE:HA	2.18	0.44
2:B:165:GLN:HG3	2:B:195:ILE:HD11	1.98	0.44
2:B:680:MET:HG2	2:B:691:THR:O	2.16	0.44
1:C:91:ARG:HB3	1:C:95:ASP:OD1	2.17	0.44
4:D:14:DC:H2"	4:D:15:DT:H6	1.83	0.44
1:A:420:LEU:HD12	1:A:421:SER:N	2.31	0.44
2:B:398:LEU:HD11	2:B:702:GLU:HB3	2.00	0.44
1:C:262:PHE:HA	1:C:265:THR:HG23	2.00	0.44
1:C:367:TYR:HB2	1:C:368:PHE:H	1.54	0.44
1:C:25:LEU:HA	1:C:521:GLY:O	2.18	0.44
1:C:339:MET:HE1	1:C:377:LEU:HD12	2.00	0.44
1:A:268:GLN:O	1:A:271:GLU:HG3	2.17	0.44
1:C:166:ALA:HA	1:C:194:ILE:HD11	1.99	0.44
1:C:240:GLU:OE1	1:C:240:GLU:N	2.42	0.44
1:A:387:PHE:O	1:A:390:MET:N	2.51	0.44
1:A:1096:TRP:CD1	1:A:1099:ALA:HA	2.52	0.44
1:C:67:ASP:HA	1:C:70:VAL:HG12	1.99	0.44
1:A:35:TYR:CZ	1:A:39:ARG:HD3	2.53	0.44
1:C:37:ILE:HD12	1:C:37:ILE:HA	1.87	0.44
1:C:202:PRO:HB2	1:C:206:SER:HB2	2.00	0.44
1:A:355:THR:HA	1:A:919:ARG:NH2	2.32	0.43
1:A:779:HIS:HB2	5:F:21:DG:C6	2.52	0.43
4:D:8:DT:H2"	4:D:9:DC:C6	2.53	0.43
1:A:136:MET:HA	1:A:136:MET:CE	2.47	0.43
1:A:137:LYS:HA	1:A:137:LYS:HD3	1.36	0.43
1:A:903:LYS:N	1:A:903:LYS:HD3	2.32	0.43
1:A:946:VAL:HG21	1:A:1051:LEU:HB3	2.00	0.43
3:E:42:DG:H2"	3:E:43:DT:H72	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:MET:HG2	1:A:745:GLU:HG2	2.00	0.43
2:B:18:MET:HB3	2:B:19:MET:HE3	1.99	0.43
1:C:290:ASP:HB3	1:C:442:LEU:HD23	2.00	0.43
1:A:1074:LYS:O	1:A:1078:TYR:N	2.51	0.43
1:C:309:LYS:O	1:C:311:PHE:N	2.51	0.43
1:A:197:PHE:O	1:A:201:GLN:HG3	2.19	0.43
1:A:810:ASN:OD1	1:A:810:ASN:N	2.52	0.43
1:A:945:TYR:OH	1:A:1044:GLN:HG2	2.18	0.43
2:B:581:LEU:HD23	2:B:581:LEU:HA	1.84	0.43
2:B:643:ASP:HB3	2:B:690:TYR:CE2	2.53	0.43
1:C:87:VAL:HG22	1:C:223:ILE:HD13	1.99	0.43
1:C:305:ALA:O	1:C:308:GLY:N	2.52	0.43
2:B:175:ILE:HG23	2:B:196:TYR:HB3	2.00	0.43
2:B:427:LYS:HE3	2:B:427:LYS:HB2	1.81	0.43
2:B:564:ARG:H	2:B:564:ARG:HG2	1.52	0.43
2:B:285:ASP:O	2:B:289:GLN:HG2	2.19	0.43
1:A:51:PHE:CZ	1:A:53:ALA:HB2	2.53	0.43
1:A:266:LYS:NZ	1:A:531:VAL:O	2.51	0.43
2:B:26:LYS:HD2	2:B:72:LEU:HB2	2.01	0.43
2:B:461:ASP:OD1	2:B:466:GLN:NE2	2.49	0.43
1:C:475:PHE:CE2	1:C:798:ILE:HA	2.53	0.43
5:F:30:DT:H2'	5:F:30:DT:O2	2.18	0.43
1:A:37:ILE:HD12	1:A:522:LEU:HD11	1.99	0.43
1:A:159:ARG:HA	1:A:162:ILE:HG12	2.00	0.43
1:A:187:ASP:OD1	1:A:188:SER:N	2.52	0.43
1:A:224:ILE:HG22	1:A:226:LEU:HD22	2.01	0.42
1:A:492:ASP:OD1	1:A:492:ASP:N	2.52	0.42
1:A:557:ASP:HB2	1:A:561:LYS:NZ	2.34	0.42
1:A:774:LEU:HD13	1:A:844:ILE:HD11	2.01	0.42
1:C:47:LYS:HB2	1:C:47:LYS:HE2	1.84	0.42
1:A:454:GLY:O	1:A:455:HIS:C	2.58	0.42
2:B:493:SER:O	2:B:493:SER:OG	2.30	0.42
4:D:9:DC:H2"	4:D:10:DT:C6	2.53	0.42
1:A:679:LEU:O	1:A:683:VAL:HG12	2.19	0.42
1:C:118:ILE:HA	1:C:121:LYS:HE2	2.02	0.42
1:C:453:LEU:HD12	1:C:503:ASN:ND2	2.34	0.42
5:F:17:DT:O4'	5:F:17:DT:P	2.78	0.42
1:A:13:LEU:HD23	1:A:13:LEU:HA	1.84	0.42
1:A:186:LEU:CD1	1:A:239:PHE:HD2	2.22	0.42
1:A:257:VAL:HG21	1:A:513:LEU:HD21	2.00	0.42
1:A:429:ILE:O	1:A:429:ILE:CG1	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1052:LEU:HD12	1:A:1052:LEU:HA	1.85	0.42
2:B:51:GLU:HB3	2:B:108:GLN:NE2	2.31	0.42
2:B:616:LEU:HD13	2:B:646:LEU:HD22	2.01	0.42
1:A:657:GLN:O	1:A:727:ALA:HA	2.18	0.42
1:A:807:ASN:HA	1:A:912:ASN:HD22	1.83	0.42
1:A:817:TYR:CE2	1:A:821:LEU:HD11	2.54	0.42
1:A:1092:ASP:OD1	1:A:1092:ASP:N	2.50	0.42
2:B:689:GLN:NE2	3:E:44:DC:OP2	2.51	0.42
1:C:258:VAL:HG22	1:C:520:LEU:HD23	2.00	0.42
1:A:147:TRP:CE3	5:F:28:DG:C8	3.07	0.42
1:A:622:GLN:NE2	1:A:622:GLN:C	2.73	0.42
2:B:383:VAL:HG11	3:E:44:DC:C6	2.55	0.42
2:B:430:ASP:OD2	2:B:456:ASN:ND2	2.53	0.42
2:B:587:ASP:OD1	2:B:588:MET:N	2.52	0.42
1:C:160:ALA:HA	1:C:163:THR:HG22	2.00	0.42
1:C:369:ASP:OD1	1:C:369:ASP:N	2.51	0.42
2:B:56:ILE:HD11	2:B:66:LEU:HD12	2.02	0.42
2:B:134:ARG:NH2	2:B:205:ASN:OD1	2.52	0.42
1:A:27:ALA:HB3	1:A:33:LYS:HE2	2.02	0.42
1:A:57:THR:OG1	1:A:58:ASP:N	2.53	0.42
1:A:86:ARG:NH1	1:A:220:LYS:O	2.51	0.42
1:A:306:LYS:H	1:A:306:LYS:HG3	1.73	0.42
2:B:106:LEU:HD12	2:B:106:LEU:HA	1.92	0.42
2:B:212:LEU:HD13	2:B:509:PRO:HG3	2.02	0.42
2:B:352:THR:HG23	4:D:1:DT:O3'	2.19	0.42
1:A:187:ASP:O	1:A:188:SER:C	2.57	0.42
1:A:917:THR:HG21	1:A:1044:GLN:HG3	2.02	0.42
2:B:44:LEU:HA	2:B:44:LEU:HD23	1.87	0.42
2:B:176:TYR:O	2:B:197:PHE:N	2.50	0.42
1:A:784:ASN:N	1:A:784:ASN:OD1	2.53	0.42
1:A:790:ASP:OD1	1:A:790:ASP:N	2.52	0.42
2:B:64:ASP:C	2:B:65:TYR:CD1	2.92	0.42
2:B:25:PHE:HE1	2:B:51:GLU:HG3	1.85	0.41
1:C:404:PHE:O	1:C:408:ARG:HG2	2.20	0.41
1:C:405:ILE:HG23	1:C:436:ILE:HG21	2.01	0.41
1:A:406:LEU:HD21	1:A:456:ASP:HA	2.02	0.41
1:C:198:VAL:HG11	1:C:216:PHE:CE2	2.55	0.41
1:A:1061:PHE:CD1	1:A:1069:LEU:HD11	2.55	0.41
1:A:1072:PHE:CD2	1:A:1084:HIS:HD2	2.38	0.41
1:A:128:ASN:O	1:A:131:LYS:HG2	2.20	0.41
1:A:828:ARG:NH2	5:F:18:DG:H5'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1020:LEU:HD12	1:A:1020:LEU:HA	1.81	0.41
2:B:163:PHE:CE1	2:B:199:GLN:HG2	2.55	0.41
1:A:106:ARG:HB2	1:A:108:GLN:OE1	2.20	0.41
1:A:116:SER:HB2	1:A:164:ILE:HD12	2.03	0.41
1:A:338:LYS:HB2	1:A:493:LEU:O	2.20	0.41
1:A:626:ASP:C	1:A:628:LYS:H	2.24	0.41
1:A:668:ASP:HB3	1:A:671:TYR:HB3	2.01	0.41
1:A:891:LEU:HD23	1:A:891:LEU:HA	1.91	0.41
1:A:1104:THR:O	1:A:1108:ARG:HG2	2.19	0.41
1:C:274:ILE:HD12	1:C:274:ILE:HA	1.96	0.41
5:F:18:DG:O4'	5:F:18:DG:P	2.78	0.41
1:A:9:MET:HG2	1:A:23:MET:SD	2.61	0.41
1:A:142:ASP:O	1:A:144:LYS:N	2.54	0.41
1:A:1132:ASN:O	1:A:1154:GLY:HA2	2.21	0.41
2:B:54:THR:HG21	2:B:100:HIS:HB3	2.02	0.41
2:B:134:ARG:NH1	2:B:205:ASN:HD21	2.19	0.41
2:B:692:VAL:HG22	4:D:5:DG:OP1	2.20	0.41
1:C:306:LYS:HB2	1:C:306:LYS:NZ	2.35	0.41
1:A:369:ASP:OD2	1:A:372:LEU:HB3	2.21	0.41
1:A:484:GLN:O	1:A:498:ASN:N	2.53	0.41
1:A:973:TYR:HB2	1:A:1038:ARG:HH11	1.86	0.41
1:A:1134:LEU:HD23	1:A:1135:ALA:N	2.35	0.41
2:B:640:VAL:HG21	2:B:692:VAL:HA	2.02	0.41
1:C:126:LEU:HD12	1:C:157:VAL:HG11	2.02	0.41
1:C:423:LEU:O	1:C:424:ASP:C	2.59	0.41
1:C:549:LEU:O	1:C:550:ASP:CB	2.68	0.41
1:A:26:ASN:HA	1:A:523:SER:O	2.20	0.41
1:A:1040:LEU:HD22	1:A:1044:GLN:HB3	2.03	0.41
2:B:49:SER:HA	2:B:121:LYS:HE2	2.01	0.41
2:B:221:TYR:OH	2:B:515:ARG:NE	2.54	0.41
2:B:531:LYS:HE3	2:B:531:LYS:HB2	1.91	0.41
1:C:391:LEU:HD23	1:C:483:PHE:CD1	2.55	0.41
5:F:10:DA:H2"	5:F:11:DT:OP1	2.21	0.41
1:A:136:MET:HB3	1:A:136:MET:HE2	1.83	0.41
1:A:507:GLU:OE1	1:A:802:TYR:OH	2.22	0.41
1:A:752:ILE:HD12	1:A:752:ILE:HA	1.82	0.41
1:A:816:LYS:HB3	1:A:827:GLU:OE2	2.21	0.41
2:B:705:TYR:O	2:B:709:ARG:HG2	2.21	0.41
1:C:304:PRO:O	1:C:305:ALA:HB3	2.19	0.41
1:C:305:ALA:O	1:C:306:LYS:C	2.57	0.41
1:C:520:LEU:HD12	1:C:521:GLY:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:41:DC:H2"	3:E:42:DG:C8	2.56	0.41
3:E:50:DT:H71	5:F:10:DA:C5	2.56	0.41
1:A:487:ASN:OD1	1:A:487:ASN:N	2.54	0.41
1:A:841:SER:HA	1:A:844:ILE:HG22	2.03	0.41
1:A:1085:TRP:CD1	1:A:1176:LEU:HD21	2.56	0.41
1:A:1137:ASN:OD1	1:A:1138:GLN:N	2.53	0.41
2:B:271:GLN:OE1	2:B:271:GLN:N	2.54	0.41
1:A:537:LEU:HD23	1:A:537:LEU:HA	1.90	0.40
1:A:1072:PHE:CE1	1:A:1074:LYS:HB3	2.56	0.40
2:B:482:SER:CB	3:E:37:DG:H21	2.34	0.40
1:C:248:TYR:HB3	1:C:429:ILE:HG22	2.02	0.40
1:C:368:PHE:O	1:C:368:PHE:CG	2.74	0.40
1:C:403:LYS:HZ2	1:C:454:GLY:HA2	1.86	0.40
1:C:449:ILE:HD13	1:C:449:ILE:HA	1.90	0.40
1:A:272:SER:O	1:A:276:GLU:HG2	2.21	0.40
1:C:502:PHE:CE2	1:C:798:ILE:HD11	2.55	0.40
1:A:474:ARG:HA	1:A:474:ARG:HD3	1.77	0.40
1:A:534:ASN:OD1	1:A:535:TYR:N	2.52	0.40
1:A:565:PHE:H	1:A:568:ARG:HH21	1.68	0.40
2:B:220:PHE:O	2:B:226:GLY:HA3	2.22	0.40
2:B:394:ILE:HG12	2:B:699:TYR:HE1	1.87	0.40
3:E:37:DG:H2"	3:E:38:DA:N7	2.37	0.40
3:E:47:DG:O5'	3:E:47:DG:C2'	2.70	0.40
1:A:613:LEU:HG	1:A:671:TYR:CD2	2.56	0.40
1:A:625:ILE:H	1:A:625:ILE:CD1	2.13	0.40
2:B:529:ARG:HB3	2:B:565:PRO:HA	2.03	0.40
1:C:85:GLU:HG3	1:C:220:LYS:NZ	2.36	0.40
1:C:88:ALA:HB1	1:C:214:PRO:HB2	2.04	0.40
1:C:405:ILE:HG21	1:C:437:TYR:CE1	2.56	0.40
5:F:29:DA:N3	5:F:30:DT:H1'	2.35	0.40
1:A:141:PHE:C	1:A:143:LEU:N	2.75	0.40
1:A:664:ASP:OD1	1:A:664:ASP:N	2.51	0.40
2:B:13:ASP:OD2	2:B:250:HIS:HA	2.21	0.40
2:B:212:LEU:HD23	2:B:650:VAL:HB	2.04	0.40
1:C:258:VAL:HA	1:C:520:LEU:HB3	2.02	0.40
1:C:423:LEU:HD22	1:C:423:LEU:N	2.35	0.40
5:F:16:DC:H2"	5:F:17:DT:H5'	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1161/1192 (97%)	1108 (95%)	49 (4%)	4 (0%)	37	66
1	C	505/1192 (42%)	450 (89%)	45 (9%)	10 (2%)	6	27
2	B	711/715 (99%)	693 (98%)	16 (2%)	2 (0%)	37	66
All	All	2377/3099 (77%)	2251 (95%)	110 (5%)	16 (1%)	21	49

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	460	PRO
2	B	407	GLU
1	C	28	PRO
1	C	84	SER
1	C	550	ASP
1	A	143	LEU
1	C	173	LEU
2	B	408	PRO
1	C	368	PHE
1	C	172	LYS
1	C	310	SER
1	A	459	SER
1	C	17	SER
1	C	171	VAL
1	C	429	ILE
1	A	429	ILE

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	1022/1054 (97%)	991 (97%)	31 (3%)	36	60
1	C	413/1054 (39%)	386 (94%)	27 (6%)	14	39
2	B	642/644 (100%)	630 (98%)	12 (2%)	52	71
All	All	2077/2752 (76%)	2007 (97%)	70 (3%)	34	57

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	MET
1	A	136	MET
1	A	137	LYS
1	A	140	GLU
1	A	143	LEU
1	A	186	LEU
1	A	303	LEU
1	A	314	ARG
1	A	344	ARG
1	A	350	MET
1	A	385	LEU
1	A	427	MET
1	A	430	GLU
1	A	455	HIS
1	A	486	THR
1	A	621	GLU
1	A	622	GLN
1	A	624	ARG
1	A	625	ILE
1	A	626	ASP
1	A	633	ARG
1	A	779	HIS
1	A	825	ARG
1	A	865	MET
1	A	953	ASP
1	A	954	LYS
1	A	1025	GLU
1	A	1065	TRP
1	A	1072	PHE
1	A	1127	ARG
1	A	1150	LEU
2	B	60	TYR

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Mol	Chain	Res	Type
2	B	99	ASN
2	B	252	SER
2	B	259	ARG
2	B	314	ARG
2	B	333	ARG
2	B	407	GLU
2	B	481	TYR
2	B	548	ASP
2	B	564	ARG
2	B	633	HIS
2	B	689	GLN
1	C	12	LYS
1	C	44	TYR
1	C	51	PHE
1	C	54	PHE
1	C	72	TRP
1	C	95	ASP
1	C	141	PHE
1	C	149	MET
1	C	173	LEU
1	C	201	GLN
1	C	264	SER
1	C	272	SER
1	C	313	PHE
1	C	365	ASN
1	C	367	TYR
1	C	369	ASP
1	C	375	VAL
1	C	377	LEU
1	C	445	SER
1	C	473	ARG
1	C	475	PHE
1	C	509	TYR
1	C	790	ASP
1	C	794	LEU
1	C	795	ARG
1	C	799	GLU
1	C	802	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	622	GLN
1	A	823	HIS
1	A	885	GLN
1	A	1084	HIS
2	B	289	GLN
1	C	322	ASN
1	C	374	GLN

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 ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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-60973. 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 |
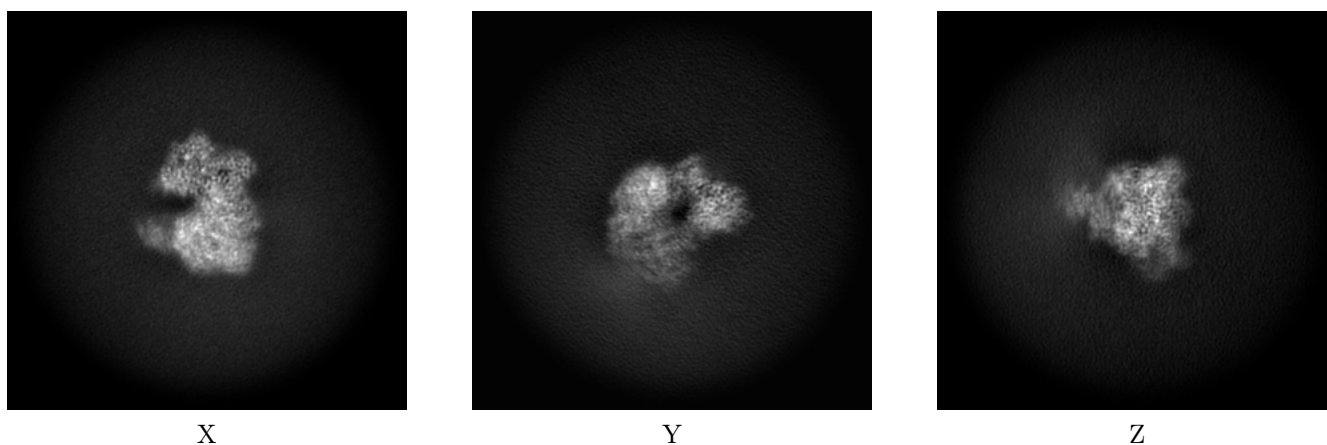
The images above show the map projected in three orthogonal directions.

6.2　Central slices (i)

6.2.1　Primary map

| X Index: 192 | Y Index: 192 | Z Index: 192 |
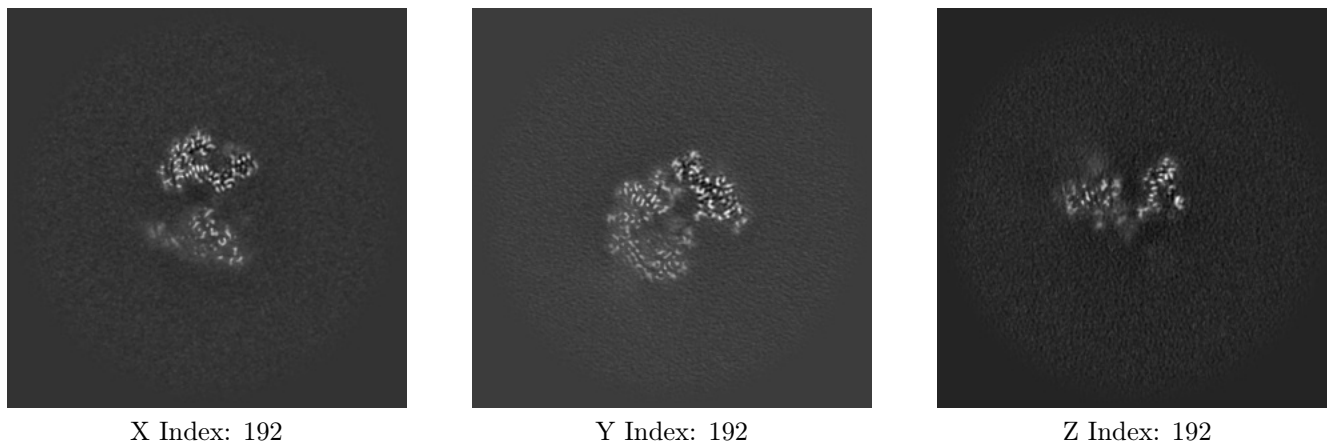
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
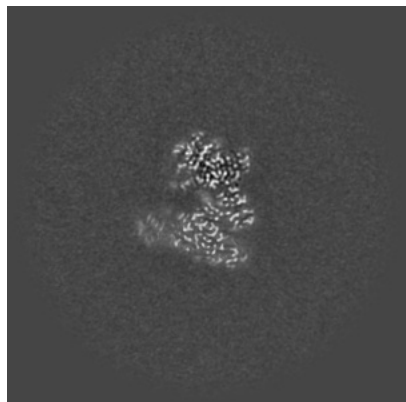
6.3.1 Primary map
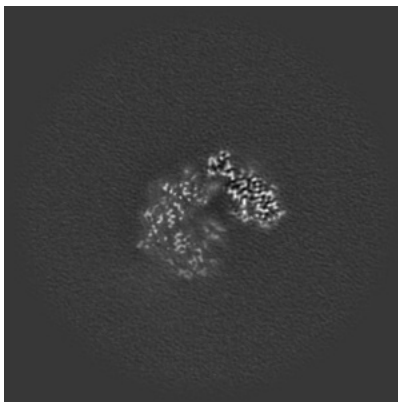
| X Index: 208 | Y Index: 188 | Z Index: 222 |
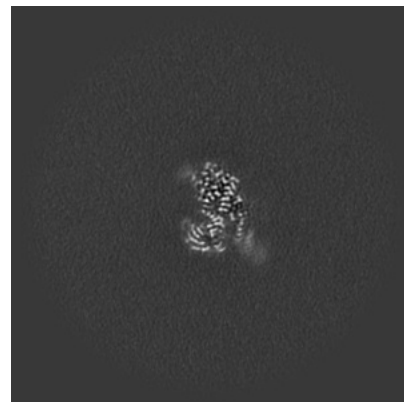
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map

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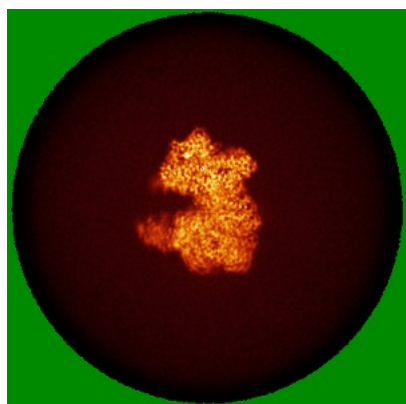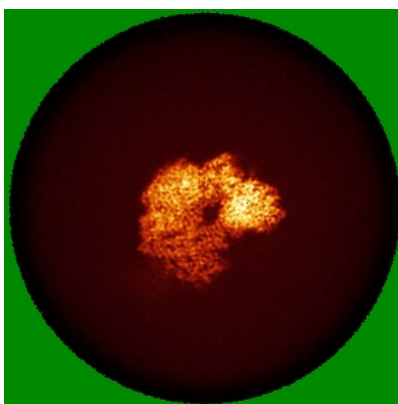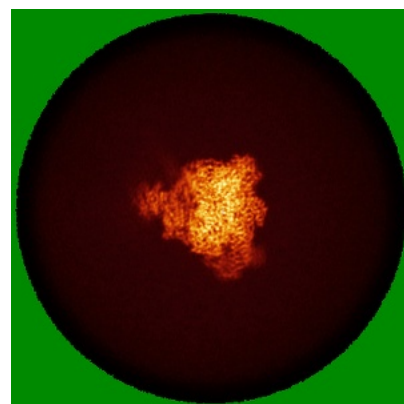
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5　Orthogonal surface views　ⓘ

6.5.1　Primary map

X　　　　　　　　　　Y　　　　　　　　　　Z
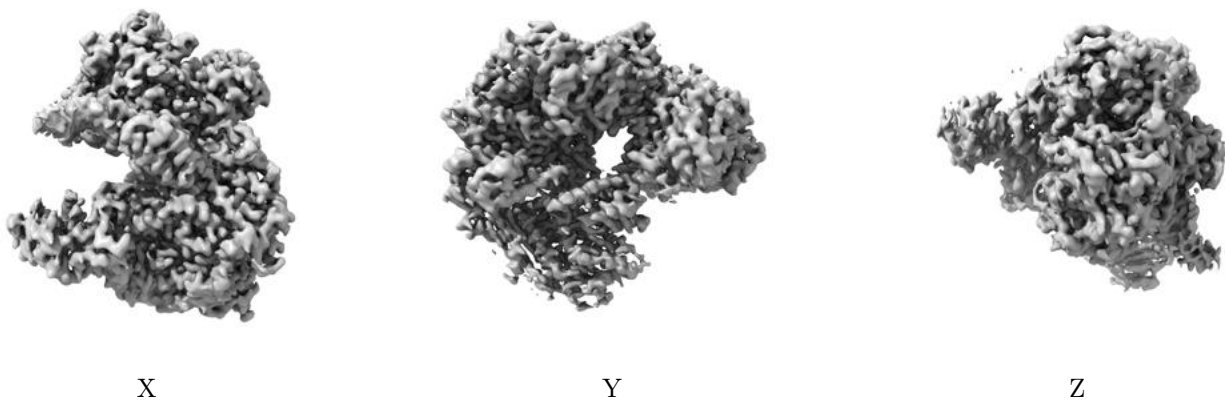
The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6　Mask visualisation　ⓘ

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

7 Map analysis ⓘ

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

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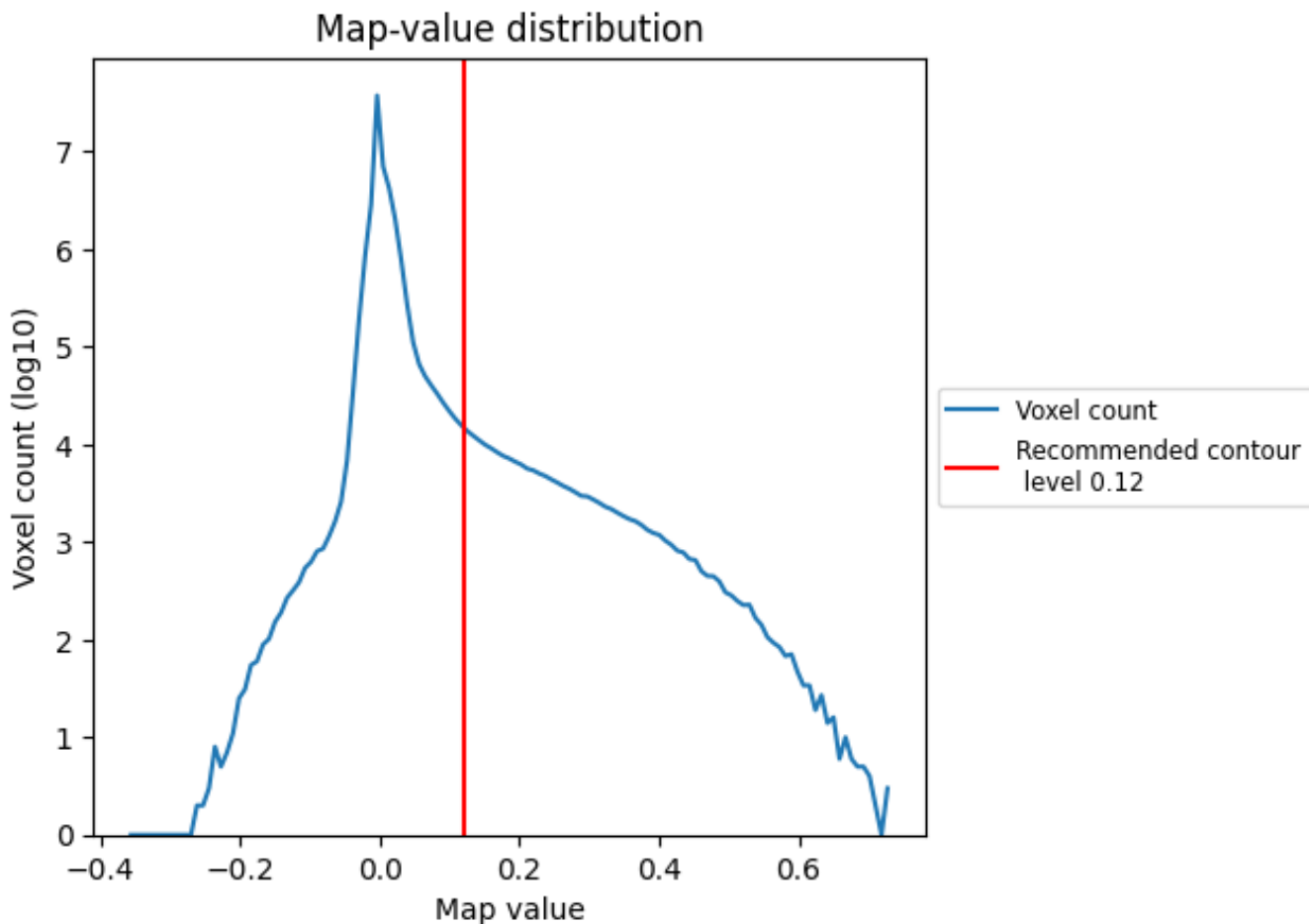
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
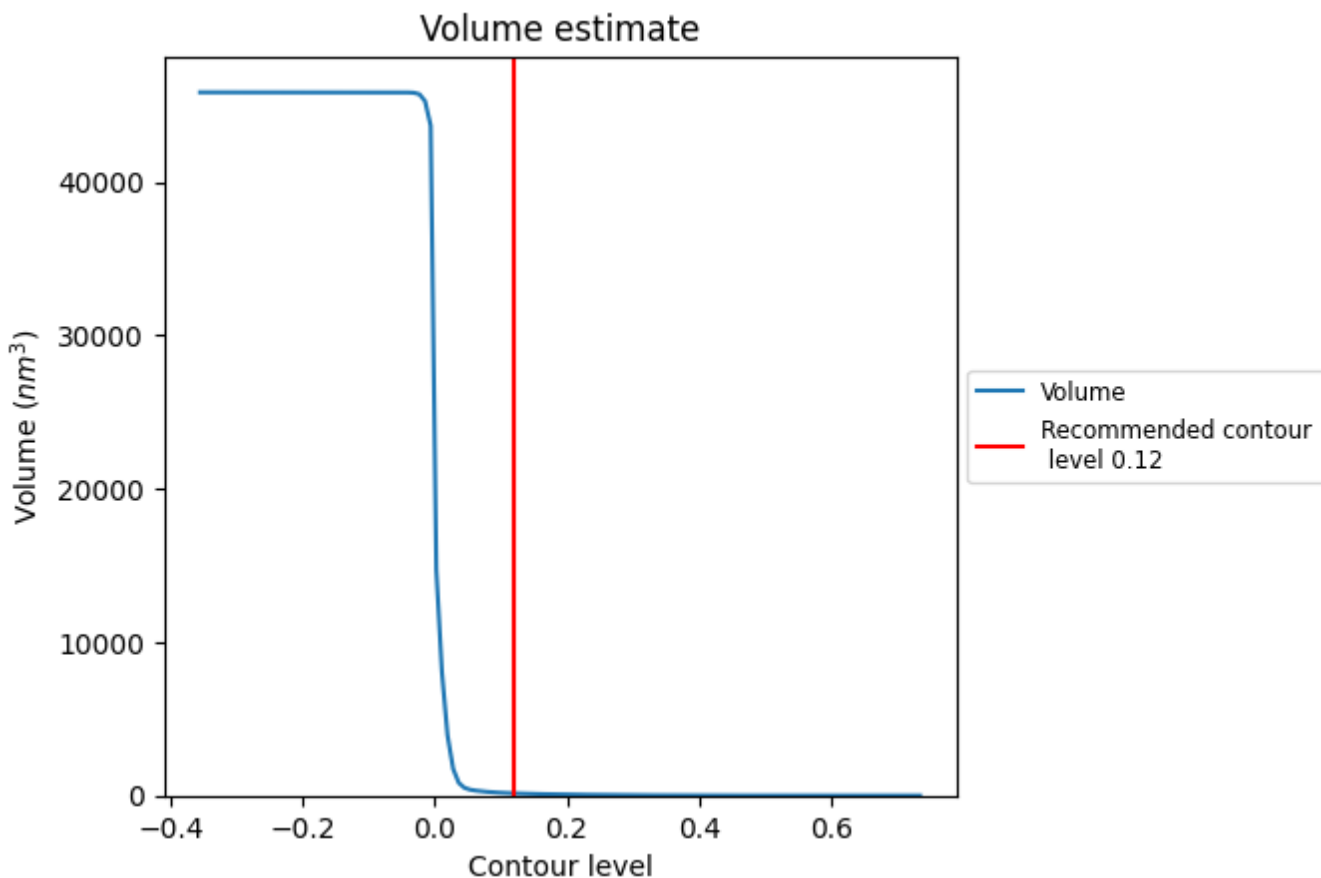
The volume at the recommended contour level is 145 nm^3; this corresponds to an approximate mass of 131 kDa.

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 ⓘ
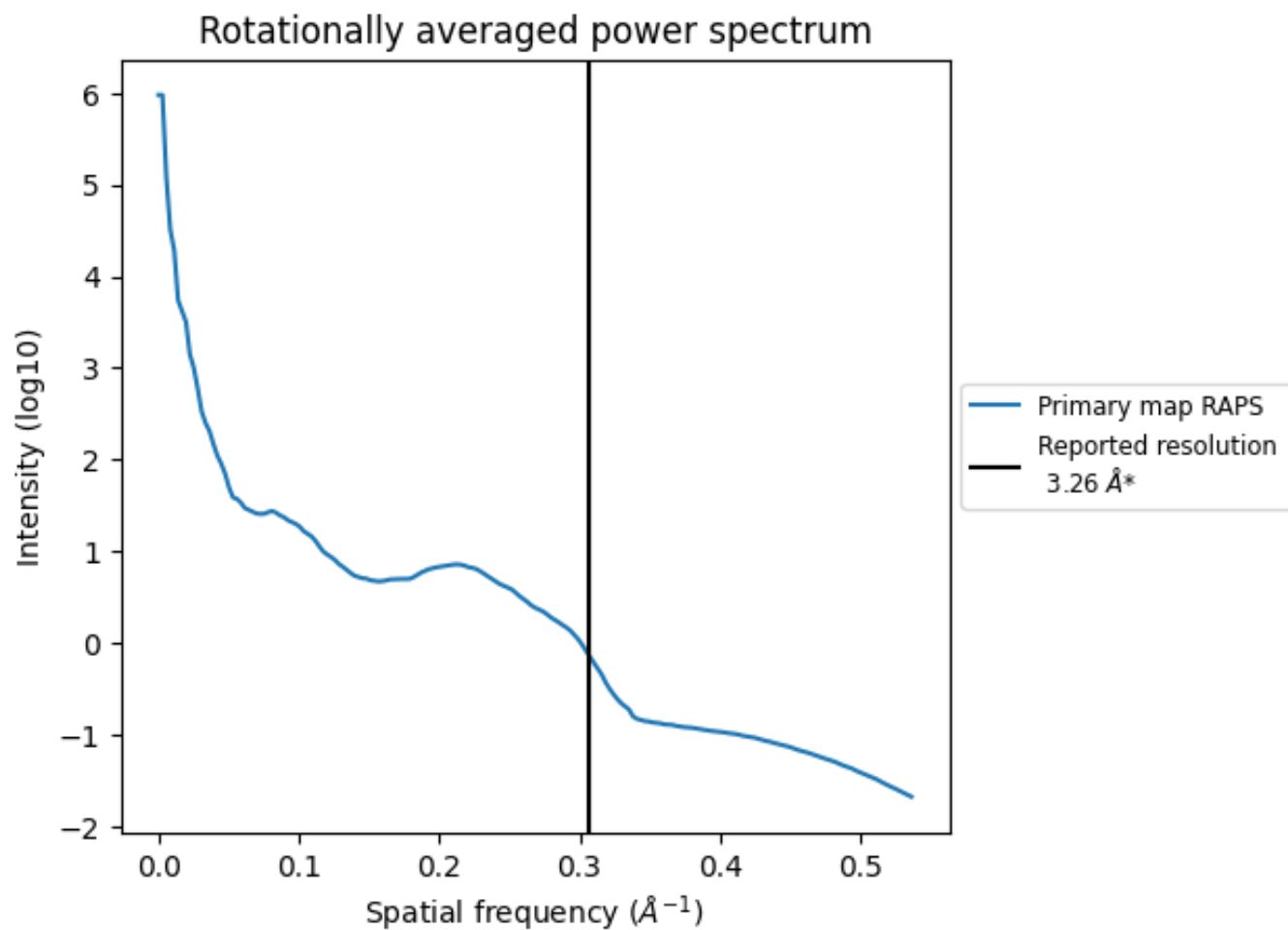
*Reported resolution corresponds to spatial frequency of 0.307 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-60973 and PDB model 9IXM. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay ⓘ

| X | Y | Z |
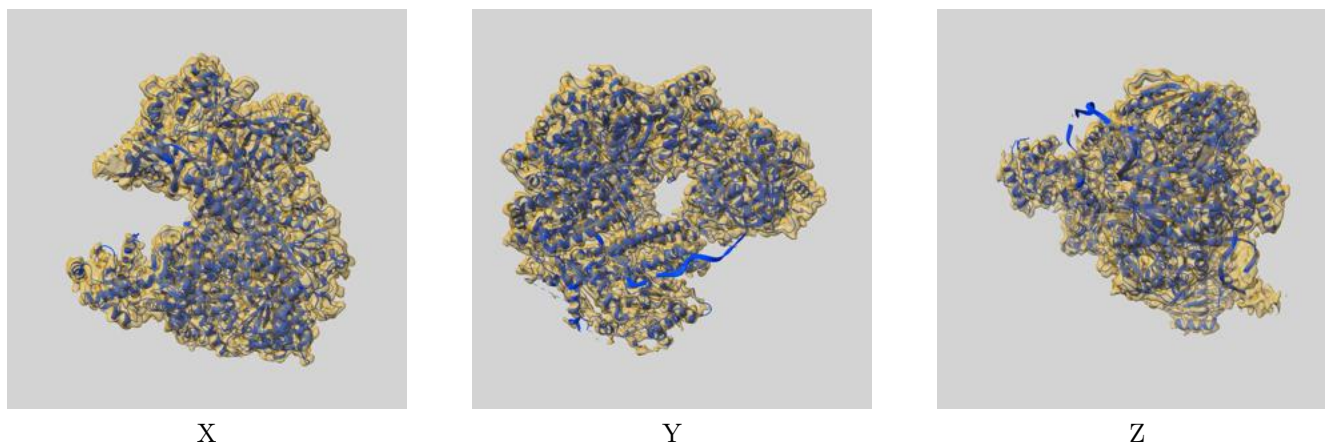
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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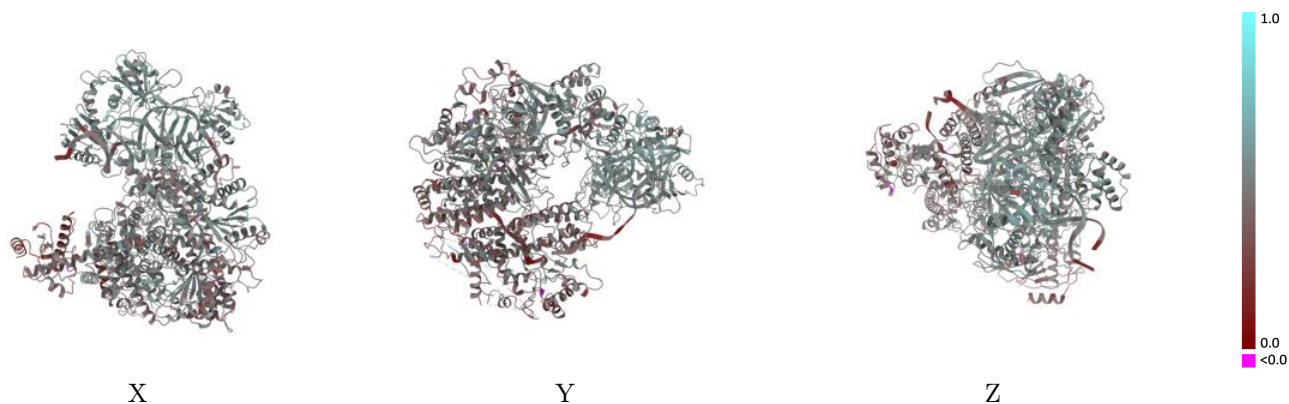
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3   Atom inclusion mapped to coordinate model ⓘ
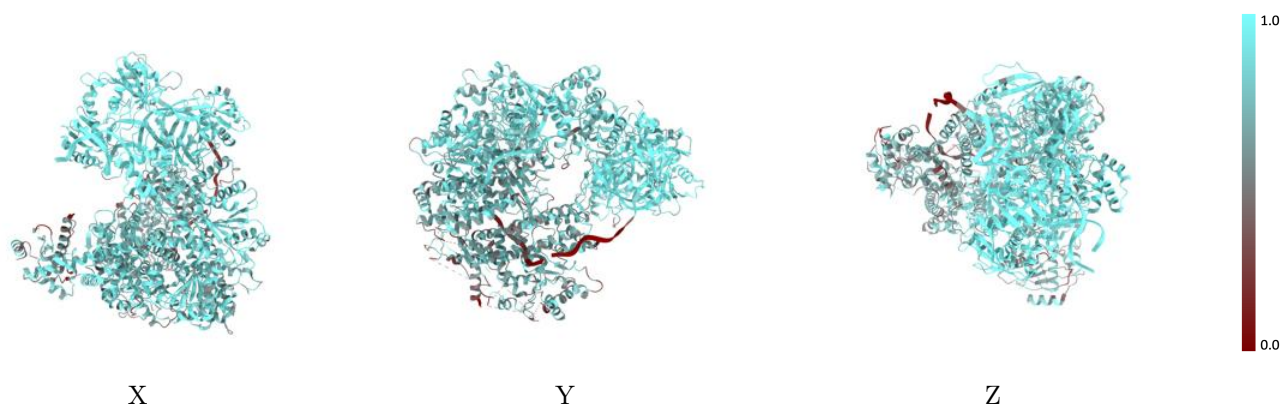
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion ⓘ
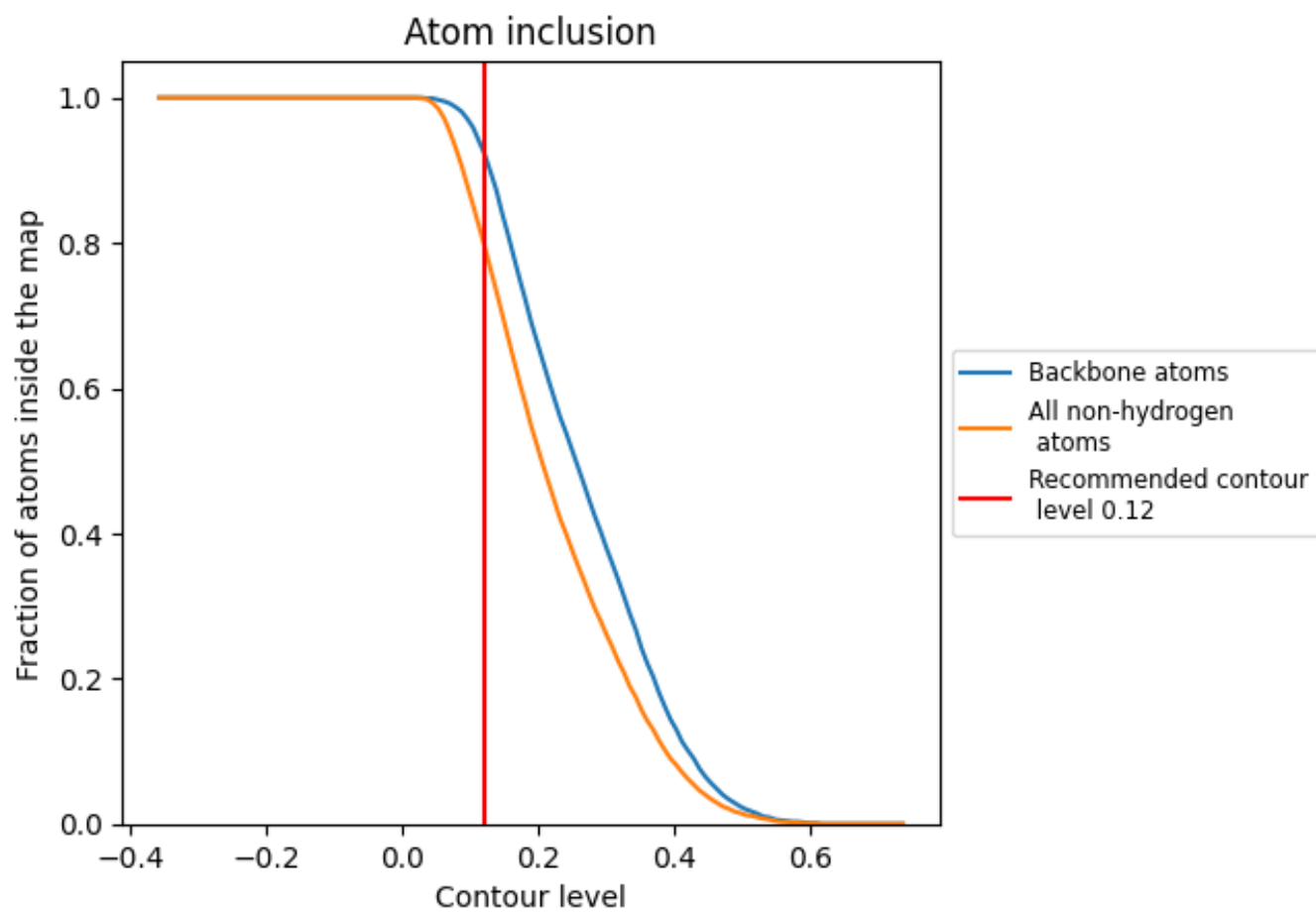
At the recommended contour level, 93% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8000	0.4640
A	0.7920	0.4510
B	0.9050	0.5240
C	0.6820	0.4190
D	0.9870	0.5540
E	0.7350	0.4210
F	0.7010	0.3860

1.0

0.0
<0.0