W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB EM Validation Report (i)

Jul 19, 2023 – 02:48 PM EDT

PDB ID	:	8F3C
EMDB ID	:	EMD-28845
Title	:	Cryo-EM consensus structure of Escherichia coli que-PEC (paused elongation complex) RNA Polymerase minus preQ1 ligand
Authors	:	Porta, J.C.; Chauvier, A.; Deb, I.; Ellinger, E.; Frank, A.T.; Meze, K.; Ohi, M.D.; Walter, N.G.
Deposited on	:	2022-11-09
Resolution	:	3.40 Å(reported)
Based on initial model	:	6ALF

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 3.40 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	Percentile Ranks	Value
Clashscore		12
Ramachandran outliers		0.1%
Sidechain outliers		1.7%
RNA backbone		0.39

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures
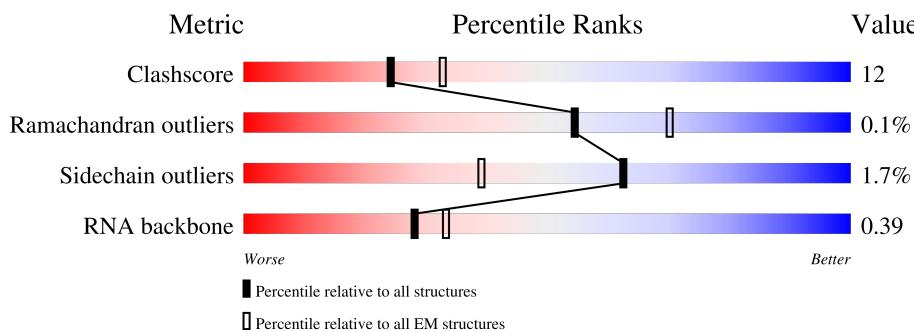
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	39	8% — 18% / 31% / 51%
2	B	39	13% — 36% / 44% / 21%
3	G	328	· — 45% / 21% · 33%
3	H	328	6% — 46% / 21% / 33%
4	I	1342	15% — 72% / 26% ··
5	J	1434	17% — 64% / 28% · 7%
6	K	102	16% — 47% / 30% / 23%
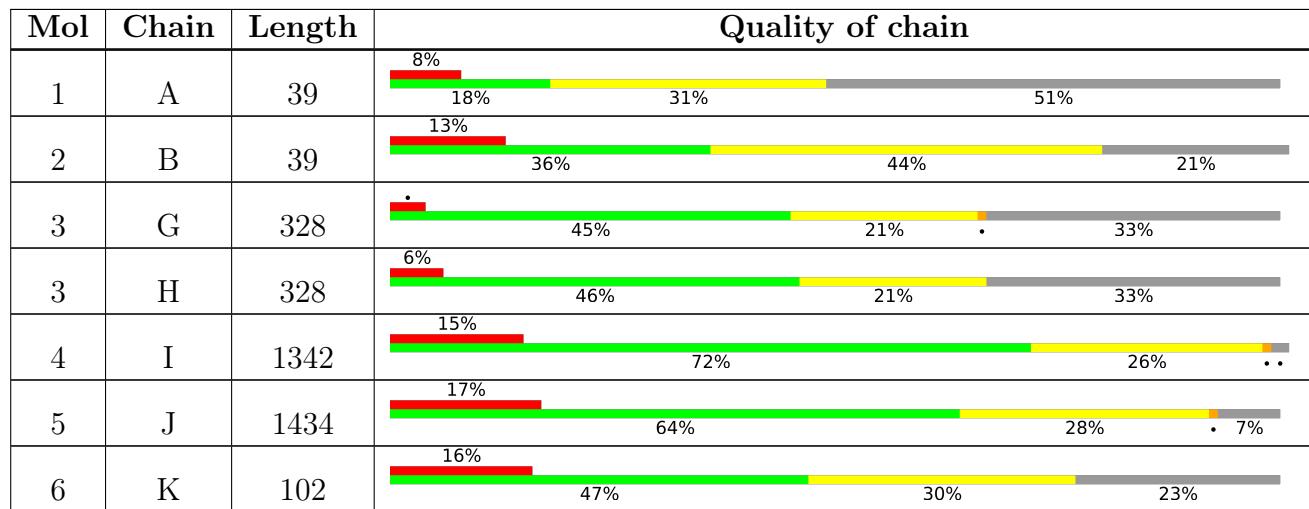
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Mol	Chain	Length	Quality of chain
7	R	47	79% / 45% / 49% / 6%

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 26819 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 DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	19	Total 388	C 186	N 78	O 107	P 17	0	0

- Molecule 2 is a DNA chain called DNA (39-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	31	Total 631	C 301	N 107	O 192	P 31	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	221	Total 1702	C 1066	N 300	O 330	S 6	0	0
3	H	219	Total 1689	C 1056	N 298	O 329	S 6	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	1316	Total 10381	C 6514	N 1810	O 2014	S 43	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	1337	Total 10403	C 6536	N 1856	O 1961	S 50	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1408	LEU	-	expression tag	UNP C3SIA2

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1409	ASP	-	expression tag	UNP C3SIA2
J	1410	ARG	-	expression tag	UNP C3SIA2
J	1411	ARG	-	expression tag	UNP C3SIA2
J	1412	ALA	-	expression tag	UNP C3SIA2
J	1413	SER	-	expression tag	UNP C3SIA2
J	1414	GLU	-	expression tag	UNP C3SIA2
J	1415	ASN	-	expression tag	UNP C3SIA2
J	1416	LEU	-	expression tag	UNP C3SIA2
J	1417	TYR	-	expression tag	UNP C3SIA2
J	1418	PHE	-	expression tag	UNP C3SIA2
J	1419	GLN	-	expression tag	UNP C3SIA2
J	1420	GLY	-	expression tag	UNP C3SIA2
J	1421	GLY	-	expression tag	UNP C3SIA2
J	1422	LEU	-	expression tag	UNP C3SIA2
J	1423	ASN	-	expression tag	UNP C3SIA2
J	1424	ASP	-	expression tag	UNP C3SIA2
J	1425	ILE	-	expression tag	UNP C3SIA2
J	1426	PHE	-	expression tag	UNP C3SIA2
J	1427	GLU	-	expression tag	UNP C3SIA2
J	1428	ALA	-	expression tag	UNP C3SIA2
J	1429	GLN	-	expression tag	UNP C3SIA2
J	1430	LYS	-	expression tag	UNP C3SIA2
J	1431	ILE	-	expression tag	UNP C3SIA2
J	1432	GLU	-	expression tag	UNP C3SIA2
J	1433	TRP	-	expression tag	UNP C3SIA2
J	1434	HIS	-	expression tag	UNP C3SIA2

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	K	79	627	382	118	126	1	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	92	ALA	-	expression tag	UNP A1AHI0
K	93	ALA	-	expression tag	UNP A1AHI0
K	94	ALA	-	expression tag	UNP A1AHI0
K	95	VAL	-	expression tag	UNP A1AHI0
K	96	GLU	-	expression tag	UNP A1AHI0
K	97	HIS	-	expression tag	UNP A1AHI0

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Chain	Residue	Modelled	Actual	Comment	Reference
K	98	HIS	-	expression tag	UNP A1AHI0
K	99	HIS	-	expression tag	UNP A1AHI0
K	100	HIS	-	expression tag	UNP A1AHI0
K	101	HIS	-	expression tag	UNP A1AHI0
K	102	HIS	-	expression tag	UNP A1AHI0

- Molecule 7 is a RNA chain called RNA (47-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	R	47	997	449	185	317	46	0	0

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
8	J	1	1	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: DNA (38-MER)


- Molecule 2: DNA (39-MER)

- Molecule 3: DNA-directed RNA polymerase subunit alpha

- Molecule 3: DNA-directed RNA polymerase subunit alpha

MET GLN GLY SER V5 T6 E7 F8 L9 K10 P11 R12 L13 V14 D15 V19 S20 T27 L28 E29 P30 L31 L43 R44 R45 I46 L47 L48 M51 V56 I61 D62 G63 V64 L65 H66 E67 Y68 E72 I78 L79 E80 I81 L82 L83 K86 A89 V90 R91

G94 V98 I99 L100 S105 G106 I107 A112 D118 G119 D120 V121 V124 H128 C131 T134 D135 E136 N137 I140 R143 I144 K145 V146 Y152 R158 ILE HIS SER GLU GLU ASP GLU ARG PRO ILE GLY R170 P179 V180 E181 R182 I183 A190 R191 V192

E193 Q194 R195 T196 D197 K200 L201 V202 M205 E206 T207 N208 G209 T210 I211 E215 A216 I217 R218 R219 A220 E226 Q227 L228 E229 V232 D233 L234 ARG ASP VAL ARG GLN PRO GLU VAL LYS GLU GLU LYS PRO GLU PHE ASP PRO ILE LEU LEU ARG PRO VAL ASP ASP LEU GLU

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

PRO PRO ALA SER ILE ALA ASP

• Molecule 4: DNA-directed RNA polymerase subunit beta

15%

Chain I:　72%　　　26%

MET V2 Y5 K8 K9 R10 I11 D14 F15 V21 L27 D33 Q36 I39 E40 Q41 E44 L49 E50 R54 S55 V56 F57 P58 I59 Q60 S61 Y62 S63 G64 N65 S66 E67 S93 R97 V98 K99 V103 E106 R107 E108 A109 P110 E111 G112

T113 V114 K115 D116 I117 K118 E119 Q120 Y123 P128 D132 T135 T141 E142 R143 V144 D160 K163 T164 H165 S166 S167 G168 L171 I176 R180 G181 S182 D185 F188 D189 N193 I198 D199 R200 T207 I208 L213 K227 F230 E231 I232

R233 D234 N235 K236 L237 Q238 M239 E240 L241 V242 P243 E244 R245 L246 R247 G248 E249 T250 A251 S252 F253 D254 I255 E256 A257 N258 G259 K260 V261 Y262 K265 G266 R267 R268 I269 T270 A271 R272 H273 I274 R275 Q276 L277 E278 K279 D280 D281 V282 K283 L284 I285 E286 E290 Y291 I292 A293 G294

V297 D300 Y301 I302 D303 E304 S305 T306 G307 E308 L309 I310 C311 A312 A313 N314 M315 E316 L317 S318 L319 D320 L321 L322 A323 Q327 S328 G329 H330 K331 R332 I333 D340 L341 S348 E349 T350 L351 R352 V353 D354 E365 I366 Y367 R371 P372 G373 E374 P375 R378 E382

E386 N387 L388 D393 M403 K404 R407 S408 L409 L420 S421 K422 D423 D424 I425 I426 D427 V428 R436 D444 L448 G449 N450 Q463 F464 E477 S480 L481 G482 D483 L484 D485 T486 L487 M488 P489 Q490 D491 M492 K496 P497 I498 F505 Q510 Q513 F514

M515 D516 N519 P520 L521 H526 K527 R528 L533 G534 P535 L538 T539 R540 E541 R542 F545 E546 V547 R548 D549 T553 R557 V558 C559 P560 I561 I572 L575 S576 L587 Y591 R592 K593 V594 T595 D596 G597 V598 E602 L606 S607 A608 I609 E610 Q618

A619 N620 D624 E625 E626 F629 V630 E631 D632 L633 V634 L644 V661 S662 V663 G664 L667 I668 P669 F670 I671 E672 H673 D674 D675 R678 A679 L680 M681 M685 Q686 R687 Q688 A689 V690 L693 K697 P698 L699 V700 E705 V714 R720 Y726 V727 D728 A729

V736 M741 G744 E745 A746 R758 Q761 Q767 L773 V777 E778 D781 V782 L783 A784 D785 D790 E793 L794 Q797 Q798 N799 M800 A803 N808 G809 Y810 N811 F812 E813 D814 S815 E820 R821 V822 V823 Q824 E825 D826 R827 F828 T829 T830 I831

This is a graphical residue validation chart. The following residue labels appear in the chart rows:

Row 1: E835 R841 D842 L845 G846 T851 A852 D853 I854 P855 N856 E867 I870 G874 L883 V884 G885 K890 GLY GLU THR GLN LEU THR PRO GLU GLU LYS LEU LEU ARG ALA ILE PHE GLY GLU LYS ALA SER ASP VAL LYS D915 S925 V928 F934 T935 R936 D937

Row 2: G938 V939 E940 K941 D942 K943 R944 A945 K958 D959 L960 S961 E962 E963 L964 Q965 E968 S973 R974 I975 R976 A977 V978 L979 V980 A981 G982 G983 V984 E985 A986 E987 K988 L989 D990 K991 L992 P993 R994 D995 R996 W997 L998 E999 L1000 G1001 L1002 T1003 D1004 E1005 E1006 K1007 Q1008 N1009 Q1010 L1011 E1012

Row 3: Q1013 L1014 A1015 E1016 Q1017 Y1018 D1019 E1020 L1021 K1022 H1023 E1024 F1025 E1026 K1027 L1028 L1029 R1034 G1039 D1040 D1041 L1042 A1043 V1046 K1051 V1052 V1056 R1057 R1058 R1059 I1060 Q1061 P1062 K1065 M1066 A1067 G1068 R1069 H1070 K1073 G1074 V1075 I1076 S1077 P1081 I1082 E1083 D1084 M1085 P1086 Y1087 D1088

Row 4: E1089 N1090 G1091 V1094 N1099 P1100 L1101 G1102 V1103 P1104 S1105 R1106 M1107 N1108 I1109 G1110 Q1111 I1112 L1113 E1114 M1119 A1120 A1121 K1122 G1123 I1124 Q1134 Q1135 G1136 E1137 K1140 L1141 R1142 E1143 L1151 G1152 A1153 L1161 F1164 S1165 D1166 E1167 E1168 L1172 L1176 M1180 P1181 I1182 A1183

Row 5: T1184 P1185 G1189 A1190 L1198 L1199 D1203 L1204 L1212 Y1213 D1214 G1215 R1216 T1217 Q1220 R1223 P1224 V1225 Y1229 M1230 Y1231 M1232 L1233 K1234 L1235 R1246 S1247 Y1251 S1252 L1253 V1254 T1255 Q1256 Q1257 P1258 L1259 G1260 G1261 K1262 A1263 Q1264 F1265 G1266 G1267 Q1268 R1269 F1270 G1271 E1272 M1273 E1274

Row 6: V1275 W1276 A1277 L1278 G1282 T1286 L1287 Q1288 E1289 M1290 L1291 T1292 D1296 D1297 K1303 M1315 E1316 M1319 P1320 E1321 S1322 V1325 E1329 E1338 D1341 GLU

• Molecule 5: DNA-directed RNA polymerase subunit beta'

Chain J:
17% | 64% | 28% | 7%

Row (Chain J) 1: MET LYS ASP LEU LEU LYS PHE LEU LYS ALA GLN THR LYS THR GLU E16 I20 K21 P27 R31 G36 K40 I44 N45 Y46 R47 T48 F49 R53 D54 F57 C58 A59 R60 I61 P64 D67 Y68 E69 C70 L71 C72 R81 G82 C85 E86 K87 C88

Row 2: G89 V90 T93 Q94 T95 K96 V97 R101 L107 T111 A112 H113 F116 L117 K118 S119 L120 D129 R133 D134 L139 Y140 F141 I142 S143 Y144 I147 E148 G149 G150 M151 T152 N153 L154 E155 R156 I159 L160 T161 E162 E163 Q164 D167 A168 L169 E170 E171 F172 G173

Row 3: D174 E175 F176 D177 A178 K179 M180 L188 L189 K190 L194 E199 Q200 L201 R202 E203 T208 N209 S210 R214 K215 K216 L217 R220 I221 E225 A226 F227 V228 P234 T240 V241 L242 P243 V244 L245 P246 P247 R250 P251 L252 V253 P254 L255 D256 G257 G258 R259 F260 A261

Row 4: T262 S263 D264 L265 L268 Y269 R270 R271 R275 D284 R293 N294 E295 K296 Q300 V303 L306 G313 R314 S319 N320 K321 R322 P323 L324 K325 S326 L327 A328 D329 M330 I331 K332 L343 G344 K345 R346 V347 D348 Y349 S350 G351 R352 I355 T356 V357 L363

Row 5: G367 L368 P369 K370 L374 E375 K378 I381 R388 T393 I394 K395 K399 R403 E404 E405 L412 D413 E414 V415 I416 R417 E418 H419 P420 L423 N424 R425 A426 P427 T428 L429 H430 R431 L432 G433 I434 Q435 P439 I442 E443 I447 Q448 D460 F461 D462 G463

Row 6: D464 P471 L472 T473 L474 E475 A476 Q477 L478 E479 L483 M484 M485 N488 L491 N495 I499 P502 S503 Q504 D505 V506 V507 L508 G509 L510 Y511 V512 M513 T514 R515 D516 C517 V518 N519 A520 E523 G524 M525 V526 L527 E532 A533 E534 R535 L536 Y537 L541 L544

• Molecule 6: DNA-directed RNA polymerase subunit omega

Chain K:

• Molecule 7: RNA (47-MER)

Chain R:

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	142410	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 $(e^-/\text{Å}^2)$	62.00	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.525	Depositor
Minimum map value	-1.446	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.078	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	300.0, 300.0, 300.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	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	0.62	0/436	0.91	0/670
2	B	0.53	0/704	0.94	0/1084
3	G	0.28	0/1722	0.53	0/2334
3	H	0.30	0/1708	0.52	0/2315
4	I	0.28	0/10547	0.52	0/14232
5	J	0.29	0/10560	0.54	0/14257
6	K	0.25	0/629	0.54	0/847
7	R	0.25	0/1116	0.82	0/1736
All	All	0.30	0/27422	0.57	0/37475

There are no bond length outliers.

There are no bond angle outliers.

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	388	0	216	12	0
2	B	631	0	352	17	0
3	G	1702	0	1741	47	0
3	H	1689	0	1725	42	0
4	I	10381	0	10392	257	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	10403	0	10636	295	0
6	K	627	0	634	23	0
7	R	997	0	511	14	0
8	J	1	0	0	0	0
All	All	26819	0	26207	631	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 (631) 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:I:595:THR:CG2	4:I:598:VAL:HB	1.90	1.00
4:I:1108:ASN:OD1	4:I:1111:GLN:NE2	2.03	0.91
5:J:460:ASP:HB2	5:J:464:ASP:OD2	1.74	0.88
4:I:1253:LEU:HD22	5:J:251:PRO:HG2	1.56	0.88
5:J:245:LEU:HD11	5:J:327:LEU:HD21	1.56	0.86
5:J:370:LYS:HD2	5:J:443:GLU:HG2	1.61	0.82
5:J:134:ASP:HB3	5:J:159:ILE:HD11	1.60	0.82
4:I:1258:PRO:HB3	4:I:1267:GLY:H	1.45	0.82
4:I:595:THR:HG21	4:I:598:VAL:HB	1.63	0.80
5:J:703:THR:HG23	5:J:715:LYS:HD3	1.65	0.79
3:G:11:PRO:HA	3:G:30:PRO:HD2	1.65	0.79
4:I:1274:GLU:HG2	5:J:424:ASN:HD21	1.46	0.78
5:J:536:LEU:HD22	5:J:541:LEU:HD11	1.64	0.77
4:I:513:GLN:OE1	7:R:44:A:H5'	1.85	0.76
4:I:808:ASN:H	5:J:633:ALA:HB2	1.50	0.76
4:I:403:MET:O	4:I:407:ARG:HG2	1.87	0.75
6:K:3:ARG:HH22	6:K:6:VAL:HA	1.52	0.75
4:I:292:ILE:HD13	4:I:322:LEU:HD11	1.69	0.75
5:J:363:LEU:HD21	5:J:618:VAL:HG13	1.68	0.75
4:I:595:THR:HG22	4:I:598:VAL:O	1.87	0.74
5:J:31:ARG:HE	5:J:241:VAL:HG11	1.51	0.74
5:J:1221:LEU:HD13	5:J:1306:LEU:HB2	1.69	0.74
4:I:1120:ALA:HB2	4:I:1199:LEU:HD22	1.70	0.74
5:J:506:VAL:HG23	5:J:628:GLY:HA3	1.70	0.74
5:J:93:THR:HG22	5:J:94:GLN:H	1.53	0.73
4:I:595:THR:HG22	4:I:598:VAL:HB	1.69	0.73
3:G:39:LEU:HD11	3:H:228:LEU:HD21	1.69	0.73
5:J:111:THR:HG23	5:J:300:GLN:HG2	1.70	0.72
4:I:538:LEU:HA	4:I:542:ARG:HH21	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:825:GLU:HG3	4:I:827:ARG:HG3	1.69	0.71
3:G:58:GLU:OE2	3:G:170:ARG:NH1	2.24	0.71
4:I:618:GLN:HE22	5:J:770:LEU:H	1.39	0.70
4:I:1246:ARG:HH22	4:I:1257:GLN:HG3	1.56	0.70
4:I:1315:MET:HB2	5:J:473:THR:HG21	1.73	0.69
2:B:27:DG:O6	5:J:46:TYR:HB2	1.91	0.69
4:I:1213:TYR:HA	4:I:1220:GLN:HA	1.75	0.69
1:A:12:DC:C2	1:A:13:DC:C5	2.80	0.69
4:I:144:VAL:HG21	4:I:527:LYS:HG2	1.74	0.69
5:J:814:CYS:SG	5:J:890:THR:OG1	2.50	0.69
5:J:517:CYS:HB2	5:J:520:ALA:HB2	1.75	0.69
5:J:926:PRO:HG2	5:J:1248:ILE:HD11	1.75	0.69
5:J:144:TYR:CD1	5:J:180:MET:HG3	2.28	0.68
2:B:25:DC:H4'	2:B:26:DA:H5'	1.75	0.68
5:J:1108:GLN:H	5:J:1123:ARG:HH12	1.39	0.68
5:J:343:LEU:HD21	5:J:1324:SER:HB2	1.74	0.68
5:J:478:LEU:HD21	6:K:23:ALA:HB3	1.75	0.68
5:J:442:ILE:HD13	5:J:448:GLN:HG3	1.76	0.68
5:J:1215:GLU:HG3	5:J:1220:ILE:HD11	1.76	0.67
3:G:195:ARG:HD3	3:G:198:LEU:HD11	1.76	0.67
4:I:103:VAL:HB	4:I:114:VAL:HG11	1.76	0.67
5:J:1067:ARG:HE	5:J:1072:LYS:HG3	1.59	0.67
5:J:117:LEU:HD11	5:J:139:LEU:HG	1.75	0.67
5:J:836:ARG:HG2	5:J:869:CYS:HB3	1.77	0.67
5:J:1048:ARG:HH11	5:J:1059:LEU:HG	1.60	0.66
4:I:1338:GLU:HG2	5:J:21:LYS:HE3	1.76	0.66
5:J:820:ILE:HG12	5:J:884:SER:HB2	1.78	0.66
5:J:1191:PRO:HG2	5:J:1194:ARG:HG3	1.76	0.66
3:H:182:ARG:NH1	5:J:581:MET:SD	2.69	0.65
2:B:19:DT:H2'	2:B:20:DG:H8	1.62	0.65
5:J:502:PRO:HB3	5:J:506:VAL:HG13	1.79	0.65
5:J:804:ALA:O	5:J:805:GLN:HG3	1.96	0.65
4:I:528:ARG:NH2	4:I:576:SER:O	2.30	0.65
4:I:314:ASN:HD21	4:I:348:SER:HA	1.61	0.64
5:J:1221:LEU:HD12	5:J:1229:VAL:HG11	1.78	0.64
6:K:3:ARG:HH12	6:K:6:VAL:HG12	1.63	0.64
4:I:811:ASN:O	4:I:1099:ASN:ND2	2.31	0.64
3:G:82:LEU:HD11	3:G:171:LEU:HD23	1.79	0.64
4:I:14:ASP:HA	4:I:1183:ALA:HB3	1.80	0.64
5:J:743:MET:HG3	5:J:760:THR:HA	1.80	0.64
4:I:1105:SER:HB2	5:J:731:ARG:HG2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:799:ARG:HG2	5:J:1325:PHE:HZ	1.63	0.63
4:I:678:ARG:HD2	4:I:1108:ASN:HD22	1.63	0.63
5:J:741:ALA:O	5:J:762:ASN:ND2	2.31	0.63
5:J:514:THR:HG21	5:J:596:LEU:HD12	1.81	0.63
4:I:1274:GLU:HG2	5:J:424:ASN:ND2	2.14	0.62
5:J:506:VAL:HG21	5:J:625:MET:HA	1.80	0.62
5:J:1207:GLY:O	5:J:1224:ARG:NH1	2.32	0.62
3:G:231:PHE:O	3:H:218:ARG:NH1	2.31	0.62
4:I:821:ARG:HB2	4:I:1082:ILE:HD12	1.81	0.62
5:J:1135:THR:HG23	5:J:1140:ARG:HB2	1.81	0.62
4:I:746:ALA:H	4:I:974:ARG:HH12	1.48	0.62
4:I:1124:ILE:HD11	4:I:1198:LEU:HD11	1.82	0.62
5:J:1166:GLY:HA3	5:J:1174:ARG:HE	1.63	0.62
5:J:58:CYS:SG	5:J:60:ARG:HG2	2.38	0.62
5:J:255:LEU:HB3	5:J:258:GLY:H	1.64	0.62
5:J:849:LEU:HD23	5:J:855:ASP:H	1.64	0.62
5:J:973:LEU:HB3	5:J:1003:LEU:HB3	1.82	0.62
5:J:759:ILE:HG23	5:J:771:GLN:HB3	1.82	0.61
3:H:27:THR:HB	3:H:202:VAL:HG23	1.82	0.61
5:J:1000:GLY:HA3	5:J:1026:PRO:HG2	1.82	0.61
3:G:74:VAL:HG11	3:G:81:ILE:HD11	1.81	0.61
4:I:813:GLU:OE2	5:J:461:PHE:N	2.33	0.61
2:B:17:DC:H1'	5:J:426:ALA:HB1	1.83	0.61
3:G:182:ARG:NH1	4:I:1090:ASN:O	2.31	0.61
4:I:1142:ARG:NH1	4:I:1161:LEU:O	2.33	0.61
4:I:510:GLN:HB3	4:I:535:PRO:HD3	1.82	0.61
2:B:4:DT:H2"	2:B:5:DG:C8	2.36	0.60
4:I:1101:LEU:HD13	5:J:504:GLN:HG2	1.83	0.60
4:I:1287:LEU:HD23	5:J:1357:ILE:HG13	1.82	0.60
2:B:26:DA:H61	5:J:319:SER:HA	1.65	0.60
3:H:47:LEU:HD11	3:H:183:ILE:HG13	1.84	0.60
4:I:538:LEU:HD11	4:I:547:VAL:HG11	1.84	0.60
1:A:34:DC:H2"	1:A:35:DA:N7	2.16	0.59
4:I:678:ARG:NH2	4:I:681:MET:SD	2.75	0.59
5:J:60:ARG:HB3	5:J:90:VAL:HG12	1.84	0.59
5:J:503:SER:HA	5:J:598:LYS:HE3	1.83	0.59
4:I:519:ASN:HD21	4:I:689:ALA:HB3	1.67	0.59
4:I:714:VAL:O	4:I:767:GLN:NE2	2.34	0.59
5:J:460:ASP:CB	5:J:464:ASP:OD2	2.48	0.59
4:I:1246:ARG:NH1	5:J:348:ASP:OD1	2.33	0.59
5:J:64:PRO:HG3	5:J:93:THR:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:851:THR:HG23	4:I:853:ASP:H	1.67	0.59
4:I:1061:GLN:HG2	4:I:1062:PRO:HD2	1.85	0.59
5:J:70:CYS:SG	5:J:71:LEU:N	2.76	0.58
5:J:85:CYS:SG	5:J:86:GLU:N	2.76	0.58
5:J:381:ILE:HD11	5:J:412:LEU:HD13	1.85	0.58
4:I:160:ASP:OD2	4:I:164:THR:OG1	2.21	0.58
5:J:388:ARG:HH22	5:J:414:GLU:HG3	1.67	0.58
4:I:1268:GLN:HG3	5:J:352:ARG:HG3	1.84	0.58
4:I:233:ARG:HG3	4:I:238:GLN:HB3	1.85	0.58
5:J:606:ASN:OD1	5:J:610:ARG:NH1	2.37	0.58
3:H:48:LEU:HD11	5:J:535:ARG:HG3	1.84	0.58
4:I:985:GLU:HB3	4:I:988:LYS:HB2	1.85	0.58
3:H:182:ARG:NH1	5:J:534:GLU:OE1	2.36	0.58
5:J:160:LEU:HD12	5:J:164:GLN:HB3	1.85	0.58
1:A:35:DA:H2"	1:A:36:DG:N7	2.19	0.58
3:G:18:GLN:NE2	3:G:20:SER:O	2.36	0.58
5:J:639:VAL:HG23	5:J:722:ILE:HD11	1.86	0.58
4:I:448:LEU:H	4:I:553:THR:HG21	1.68	0.57
4:I:1260:GLY:O	4:I:1264:GLN:NE2	2.36	0.57
2:B:19:DT:H2'	2:B:20:DG:C8	2.38	0.57
4:I:93:SER:HA	4:I:128:PRO:HA	1.86	0.57
4:I:633:LEU:HB3	4:I:644:LEU:HD22	1.86	0.57
4:I:777:VAL:HG21	4:I:783:LEU:HD21	1.87	0.57
4:I:841:ARG:HA	4:I:1046:VAL:HA	1.85	0.57
3:G:180:VAL:HB	3:G:183:ILE:HD11	1.85	0.57
4:I:1025:PHE:HD1	4:I:1028:LYS:HE2	1.70	0.57
5:J:194:LEU:HD11	5:J:234:PRO:HD3	1.86	0.57
5:J:151:MET:HG2	5:J:151:MET:O	2.05	0.57
5:J:367:GLY:HA3	5:J:448:GLN:HB2	1.87	0.57
5:J:485:MET:HB2	5:J:488:ASN:HD22	1.70	0.57
3:G:150:ARG:NH1	3:H:7:GLU:O	2.37	0.56
4:I:11:ILE:HG22	4:I:1172:LEU:HD11	1.87	0.56
5:J:972:LYS:HD2	5:J:1004:ALA:HA	1.87	0.56
3:H:91:ARG:NH2	3:H:210:THR:O	2.38	0.56
4:I:97:ARG:HH21	4:I:123:TYR:HB2	1.69	0.56
7:R:7:G:N3	7:R:30:A:N6	2.53	0.56
4:I:135:THR:HG23	4:I:144:VAL:HB	1.85	0.56
4:I:348:SER:O	4:I:352:ARG:HG2	2.05	0.56
5:J:271:ARG:O	5:J:275:ARG:HG2	2.06	0.56
5:J:527:LEU:HB2	5:J:550:VAL:HG12	1.88	0.56
5:J:903:LEU:HD11	5:J:1249:ASN:HD22	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:317:LEU:HA	4:I:321:LEU:HD12	1.88	0.56
4:I:1142:ARG:NH2	4:I:1166:ASP:OD1	2.38	0.56
4:I:180:ARG:NH1	4:I:393:ASP:O	2.38	0.56
5:J:460:ASP:N	5:J:464:ASP:OD2	2.38	0.56
4:I:1261:GLY:O	4:I:1262:LYS:HG3	2.04	0.56
5:J:951:GLN:HA	5:J:1016:THR:HA	1.87	0.56
4:I:1065:LYS:HE3	4:I:1235:LEU:HD12	1.87	0.56
4:I:538:LEU:HD23	4:I:538:LEU:H	1.71	0.56
5:J:957:SER:N	5:J:985:ILE:O	2.39	0.56
2:B:12:DT:H4'	5:J:1327:GLU:HG2	1.89	0.55
4:I:521:LEU:HD23	4:I:686:GLN:HB3	1.88	0.55
5:J:504:GLN:NE2	5:J:731:ARG:HE	2.05	0.55
3:H:152:TYR:OH	5:J:532:GLU:OE2	2.23	0.55
4:I:5:TYR:N	4:I:778:GLU:OE2	2.34	0.55
5:J:507:VAL:HG23	5:J:601:ILE:HD12	1.87	0.55
2:B:18:DG:H3'	2:B:19:DT:H71	1.88	0.55
5:J:428:THR:HG23	5:J:433:GLY:HA3	1.89	0.55
7:R:41:C:H2'	7:R:42:A:C8	2.40	0.55
4:I:297:VAL:HB	4:I:317:LEU:HD11	1.89	0.55
5:J:808:VAL:HG12	5:J:914:ALA:HA	1.88	0.55
4:I:1068:GLY:HA2	4:I:1232:MET:HA	1.88	0.55
4:I:629:PHE:C	4:I:631:GLU:H	2.09	0.55
5:J:194:LEU:HD21	5:J:234:PRO:HG3	1.88	0.55
5:J:511:TYR:OH	5:J:515:ARG:NH1	2.40	0.55
7:R:41:C:H2'	7:R:42:A:H8	1.70	0.55
4:I:521:LEU:HD22	4:I:667:LEU:HD12	1.89	0.55
3:G:60:GLU:OE2	3:G:170:ARG:NH1	2.40	0.54
4:I:1101:LEU:HD21	5:J:508:LEU:HD22	1.89	0.54
5:J:1344:LEU:HD13	5:J:1349:GLU:HB3	1.90	0.54
4:I:996:ARG:HH21	4:I:999:GLU:HG3	1.72	0.54
5:J:527:LEU:HG	5:J:532:GLU:HG2	1.89	0.54
3:G:104:LYS:HG2	3:G:110:VAL:HG22	1.88	0.54
5:J:524:GLY:H	5:J:548:VAL:HG12	1.73	0.54
5:J:952:VAL:HG13	5:J:1013:GLY:HA2	1.89	0.54
4:I:57:PHE:N	4:I:58:PRO:HD3	2.23	0.54
5:J:1080:ILE:HG21	5:J:1097:ALA:HB3	1.89	0.54
4:I:241:LEU:HB3	4:I:285:ILE:HD13	1.90	0.54
4:I:521:LEU:HB2	4:I:794:LEU:HD21	1.89	0.54
4:I:533:LEU:HD12	4:I:572:ILE:HD11	1.90	0.54
4:I:925:SER:O	4:I:1056:VAL:HG22	2.08	0.54
5:J:807:LEU:HD11	5:J:1258:ARG:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:959:LYS:HE2	5:J:985:ILE:HG13	1.89	0.54
5:J:1181:ASP:OD1	5:J:1182:GLY:N	2.41	0.54
3:G:167:PRO:HD2	3:G:170:ARG:HE	1.72	0.54
5:J:515:ARG:HH22	5:J:717:VAL:HG22	1.73	0.54
4:I:1119:MET:HG2	4:I:1204:LEU:HD13	1.90	0.53
4:I:808:ASN:OD1	4:I:1216:ARG:NH2	2.40	0.53
5:J:225:GLU:HA	5:J:228:VAL:HG22	1.89	0.53
5:J:584:PRO:HG2	5:J:587:LEU:HD13	1.90	0.53
3:G:135:ASP:HB3	3:G:138:ALA:HB2	1.89	0.53
3:G:184:ALA:HB2	4:I:1091:GLY:HA3	1.88	0.53
5:J:189:LEU:HD22	5:J:234:PRO:HB2	1.90	0.53
4:I:1258:PRO:HB3	4:I:1267:GLY:N	2.18	0.53
5:J:395:LYS:NZ	5:J:399:LYS:HD3	2.23	0.53
5:J:842:ARG:NH2	5:J:1254:GLU:OE1	2.38	0.53
5:J:1093:THR:HG22	5:J:1095:MET:H	1.73	0.53
4:I:595:THR:HG22	4:I:598:VAL:CB	2.38	0.53
5:J:978:ARG:HH22	5:J:1199:PHE:H	1.56	0.53
6:K:7:GLN:NE2	6:K:11:GLU:OE2	2.42	0.53
4:I:176:ILE:HD11	4:I:428:VAL:HG11	1.91	0.53
3:G:28:LEU:HD12	3:G:201:LEU:HD23	1.89	0.53
3:G:44:ARG:HG3	3:G:183:ILE:HB	1.90	0.53
5:J:368:LEU:HD13	5:J:439:PRO:HB3	1.91	0.53
5:J:510:LEU:HD11	5:J:624:ILE:HG12	1.91	0.53
3:H:64:VAL:HG11	3:H:78:ILE:HD13	1.90	0.52
4:I:1291:LEU:HD12	5:J:345:LYS:HE3	1.90	0.52
5:J:516:ASP:HB3	5:J:573:THR:HG21	1.92	0.52
5:J:844:THR:HA	5:J:882:VAL:HA	1.91	0.52
4:I:799:ASN:HB3	4:I:1231:TYR:HD1	1.74	0.52
5:J:516:ASP:OD1	5:J:516:ASP:N	2.43	0.52
5:J:72:CYS:HB3	5:J:87:LYS:HE2	1.90	0.52
5:J:242:LEU:HD21	5:J:306:LEU:HD22	1.92	0.52
5:J:268:LEU:HD13	5:J:306:LEU:HA	1.91	0.52
5:J:328:ALA:O	5:J:332:LYS:HG2	2.10	0.52
6:K:9:ALA:HB1	6:K:19:LEU:HD11	1.92	0.52
4:I:741:MET:HB2	4:I:746:ALA:HB1	1.91	0.52
5:J:959:LYS:HE3	5:J:983:LYS:HE2	1.91	0.52
2:B:16:DT:H4'	4:I:1273:MET:HG3	1.90	0.52
5:J:252:LEU:O	5:J:253:VAL:HB	2.10	0.52
5:J:646:ILE:HD12	5:J:762:ASN:HD21	1.74	0.52
5:J:1327:GLU:OE1	5:J:1330:ARG:NE	2.43	0.52
7:R:4:G:H2'	7:R:5:A:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:207:THR:HG21	4:I:351:LEU:HG	1.92	0.51
4:I:727:VAL:HG12	4:I:773:LEU:HG	1.92	0.51
4:I:1251:TYR:HB3	4:I:1257:GLN:OE1	2.10	0.51
5:J:1153:PRO:O	5:J:1194:ARG:NH2	2.43	0.51
3:G:222:THR:HG22	3:H:232:VAL:HA	1.92	0.51
7:R:40:C:H2'	7:R:41:C:C6	2.45	0.51
1:A:12:DC:C2	1:A:13:DC:C4	2.98	0.51
3:G:100:LEU:HD21	3:G:121:VAL:HG21	1.92	0.51
4:I:699:LEU:HD21	4:I:1122:LYS:HE2	1.92	0.51
4:I:1261:GLY:HA2	4:I:1266:GLY:HA3	1.92	0.51
5:J:770:LEU:O	5:J:774:ILE:HG13	2.10	0.51
5:J:1266:ILE:HD11	5:J:1280:VAL:HG12	1.91	0.51
6:K:46:THR:HA	6:K:49:ILE:HG22	1.92	0.51
4:I:1066:MET:HG3	4:I:1233:LEU:O	2.10	0.51
4:I:823:VAL:HG22	4:I:1060:ILE:CG2	2.41	0.51
5:J:747:MET:HB3	5:J:774:ILE:HG22	1.91	0.51
4:I:618:GLN:HG3	4:I:620:ASN:H	1.76	0.50
5:J:57:PHE:CZ	5:J:252:LEU:HD22	2.47	0.50
5:J:425:ARG:HG2	5:J:427:PRO:HD2	1.93	0.50
3:H:83:LEU:HD12	3:H:86:LYS:HD3	1.91	0.50
5:J:1290:ARG:HA	5:J:1293:GLU:HG2	1.92	0.50
4:I:378:ARG:NH1	4:I:382:GLU:OE1	2.45	0.50
5:J:537:TYR:CZ	5:J:544:LEU:HD12	2.45	0.50
6:K:67:ARG:O	6:K:71:GLU:HG2	2.12	0.50
5:J:244:VAL:HG12	5:J:269:TYR:CE1	2.47	0.50
6:K:29:GLN:HB3	6:K:35:LYS:HG3	1.93	0.50
3:G:81:ILE:HG12	3:G:131:CYS:HB3	1.94	0.50
4:I:549:ASP:OD2	5:J:750:PRO:HB3	2.12	0.50
4:I:728:ASP:OD1	4:I:729:ALA:N	2.44	0.50
4:I:1185:PRO:HD2	4:I:1189:GLY:HA2	1.94	0.50
5:J:1184:ASP:N	5:J:1184:ASP:OD1	2.44	0.50
4:I:803:ALA:HB2	4:I:1094:VAL:HG11	1.93	0.50
3:G:102:LEU:HD21	3:G:110:VAL:HG11	1.94	0.49
4:I:812:PHE:O	4:I:1099:ASN:ND2	2.45	0.49
4:I:27:LEU:HD13	4:I:663:VAL:HG11	1.94	0.49
4:I:668:ILE:HB	4:I:671:LEU:HD13	1.93	0.49
2:B:28:DG:H2"	2:B:29:DA:OP2	2.11	0.49
4:I:516:ASP:HA	4:I:761:GLN:HE22	1.78	0.49
4:I:936:ARG:NE	4:I:1046:VAL:O	2.37	0.49
5:J:841:GLY:O	5:J:901:ARG:N	2.41	0.49
5:J:911:LYS:NZ	5:J:1363:TYR:OH	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:1297:ASP:OD2	4:I:1319:MET:N	2.45	0.49
3:G:61:ILE:HB	3:G:64:VAL:HB	1.94	0.49
5:J:850:LYS:NZ	5:J:855:ASP:OD2	2.29	0.49
4:I:960:LEU:O	4:I:963:GLU:HG3	2.11	0.49
5:J:1364:ALA:HA	5:J:1367:GLN:HG2	1.95	0.49
3:H:100:LEU:HB2	3:H:144:ILE:HB	1.95	0.49
4:I:10:ARG:NH2	4:I:793:GLU:OE1	2.35	0.49
4:I:540:ARG:HH22	7:R:43:C:P	2.36	0.49
2:B:17:DC:OP2	4:I:1269:ARG:NH1	2.46	0.49
3:H:47:LEU:HA	3:H:51:MET:HG3	1.94	0.49
4:I:667:LEU:HD22	4:I:705:GLU:HG3	1.93	0.49
2:B:25:DC:H5'	5:J:261:ALA:HB1	1.95	0.49
3:H:14:VAL:HG23	3:H:15:ASP:OD1	2.13	0.49
4:I:1086:PRO:HB2	4:I:1212:LEU:HD23	1.95	0.49
5:J:690:ASN:HD21	5:J:738:ARG:NH2	2.10	0.49
5:J:741:ALA:C	5:J:762:ASN:HD22	2.16	0.49
4:I:1022:LYS:HA	4:I:1025:PHE:CD2	2.48	0.49
4:I:1106:ARG:O	4:I:1108:ASN:N	2.45	0.49
5:J:107:LEU:HB2	5:J:240:THR:O	2.12	0.49
5:J:412:LEU:O	5:J:416:ILE:HG12	2.13	0.49
1:A:28:DG:H5"	5:J:1148:ARG:HD3	1.95	0.48
1:A:34:DC:H2"	1:A:35:DA:C8	2.48	0.48
4:I:700:VAL:HG11	4:I:1114:GLU:HG3	1.94	0.48
5:J:998:PRO:HG3	5:J:1020:TRP:CE2	2.48	0.48
3:G:211:ILE:HG12	3:G:216:ALA:HB2	1.96	0.48
4:I:198:ILE:HD11	4:I:388:LEU:HD21	1.94	0.48
6:K:10:VAL:HG11	6:K:16:ARG:HD3	1.95	0.48
7:R:6:G:O2'	7:R:27:A:O2'	2.21	0.48
1:A:11:DT:H2"	1:A:12:DC:C5	2.49	0.48
3:H:56:VAL:HA	3:H:146:VAL:HG12	1.94	0.48
6:K:15:ASN:ND2	6:K:18:ASP:OD2	2.46	0.48
4:I:1103:VAL:HG21	5:J:639:VAL:HG11	1.96	0.48
4:I:1256:GLN:HE22	5:J:345:LYS:HD3	1.78	0.48
5:J:144:TYR:HD1	5:J:180:MET:HG3	1.78	0.48
3:G:76:GLU:HG3	3:G:80:GLU:HB2	1.96	0.48
4:I:188:PHE:HE2	4:I:436:ARG:HB2	1.79	0.48
5:J:395:LYS:O	5:J:399:LYS:HG2	2.13	0.48
5:J:802:ASP:OD2	5:J:1325:PHE:HB2	2.14	0.48
5:J:836:ARG:NH2	5:J:837:ASP:OD1	2.46	0.48
4:I:118:LYS:HZ1	4:I:488:MET:HG3	1.78	0.48
4:I:164:THR:HG21	4:I:171:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:1088:ASP:OD1	4:I:1088:ASP:N	2.45	0.48
4:I:1282:GLY:HA3	6:K:17:PHE:CE1	2.49	0.48
5:J:495:ASN:HD22	5:J:1247:LYS:HG3	1.79	0.48
6:K:58:LEU:HG	6:K:59:ILE:HG12	1.95	0.48
5:J:201:LEU:CB	5:J:221:ILE:HD11	2.44	0.47
5:J:227:PHE:HE2	5:J:234:PRO:HA	1.79	0.47
3:G:100:LEU:HB2	3:G:144:ILE:HB	1.96	0.47
3:H:215:GLU:HG2	3:H:219:ARG:HH12	1.78	0.47
4:I:182:SER:HB2	4:I:199:ASP:OD1	2.15	0.47
4:I:575:LEU:HD23	4:I:576:SER:O	2.14	0.47
4:I:141:THR:OG1	4:I:143:ARG:NH2	2.47	0.47
4:I:303:ASP:OD2	4:I:306:THR:OG1	2.33	0.47
4:I:561:ILE:HD12	4:I:661:VAL:HG12	1.95	0.47
3:G:100:LEU:O	3:G:144:ILE:N	2.39	0.47
4:I:678:ARG:HD2	4:I:1106:ARG:HB3	1.97	0.47
4:I:781:ASP:OD1	4:I:782:VAL:N	2.47	0.47
5:J:860:ARG:NH1	5:J:861:ASN:OD1	2.48	0.47
3:G:29:GLU:HB3	3:G:30:PRO:HD3	1.95	0.47
4:I:404:LYS:HA	4:I:404:LYS:HD2	1.67	0.47
4:I:607:SER:OG	4:I:608:ALA:N	2.47	0.47
4:I:874:GLY:H	4:I:928:VAL:HG23	1.78	0.47
4:I:1269:ARG:HA	5:J:346:ARG:HA	1.95	0.47
5:J:268:LEU:HG	5:J:324:LEU:HD11	1.97	0.47
4:I:350:THR:O	4:I:354:ASP:N	2.39	0.47
7:R:40:C:O2'	7:R:41:C:OP1	2.28	0.47
4:I:176:ILE:HG21	4:I:420:LEU:HD21	1.97	0.47
5:J:1200:GLU:OE1	5:J:1200:GLU:N	2.48	0.47
5:J:464:ASP:OD1	7:R:47:A:H4'	2.15	0.47
4:I:423:ASP:OD1	4:I:424:ASP:N	2.47	0.47
4:I:673:HIS:HB3	4:I:1109:ILE:HG23	1.96	0.47
4:I:1184:THR:HG23	4:I:1189:GLY:HA3	1.97	0.47
4:I:1272:GLU:HG2	4:I:1276:TRP:CE2	2.49	0.47
5:J:20:ILE:HG23	5:J:1342:ASP:HB3	1.96	0.47
5:J:430:HIS:HA	5:J:921:GLN:HB3	1.97	0.47
5:J:479:GLU:HB3	6:K:20:VAL:HG11	1.97	0.46
5:J:582:ILE:HG23	5:J:623:GLN:HB3	1.95	0.46
5:J:978:ARG:HH12	5:J:1198:VAL:HG23	1.81	0.46
5:J:1261:LEU:HD13	5:J:1304:ARG:HD3	1.98	0.46
3:G:26:VAL:HG21	3:G:217:ILE:HG13	1.97	0.46
4:I:1122:LYS:HG2	4:I:1229:TYR:CZ	2.50	0.46
5:J:491:LEU:HB2	5:J:904:ALA:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:107:ILE:HG23	3:H:134:THR:HA	1.97	0.46
4:I:1109:ILE:HG21	5:J:763:PHE:HB3	1.98	0.46
4:I:1278:LEU:HD12	4:I:1287:LEU:HD13	1.98	0.46
4:I:1278:LEU:HD22	5:J:484:MET:HE1	1.97	0.46
4:I:1286:THR:N	5:J:479:GLU:OE2	2.32	0.46
6:K:26:ARG:HG3	6:K:30:MET:HE3	1.96	0.46
3:G:33:ARG:H	3:G:33:ARG:HG3	1.47	0.46
5:J:141:PHE:CZ	5:J:296:LYS:HB3	2.50	0.46
5:J:215:LYS:HB3	5:J:215:LYS:HE2	1.67	0.46
5:J:1090:ILE:HB	5:J:1093:THR:HB	1.97	0.46
3:G:17:GLU:HB3	3:G:25:LYS:HB3	1.96	0.46
4:I:463:GLN:HG3	4:I:505:PHE:CG	2.51	0.46
4:I:1247:SER:HB3	5:J:375:GLU:O	2.15	0.46
4:I:1255:THR:HG22	4:I:1255:THR:O	2.15	0.46
4:I:1258:PRO:HG2	5:J:347:VAL:N	2.31	0.46
5:J:217:LEU:O	5:J:221:ILE:HG12	2.15	0.46
5:J:265:LEU:HD13	5:J:265:LEU:HA	1.75	0.46
3:H:190:ALA:HB2	3:H:200:LYS:HB2	1.97	0.46
4:I:36:GLN:O	4:I:40:GLU:HB2	2.15	0.46
5:J:1344:LEU:HD11	5:J:1353:VAL:HG21	1.97	0.46
4:I:230:PHE:HB2	4:I:333:ILE:HB	1.96	0.46
4:I:595:THR:CG2	4:I:598:VAL:CB	2.80	0.46
4:I:797:GLY:N	4:I:1231:TYR:OH	2.49	0.46
5:J:821:MET:HA	5:J:881:LYS:HA	1.97	0.46
4:I:189:ASP:HB3	4:I:193:ASN:HB2	1.98	0.46
4:I:1041:ASP:OD1	4:I:1041:ASP:N	2.48	0.46
5:J:858:VAL:HG22	5:J:868:TRP:CE3	2.51	0.46
5:J:930:LEU:HA	5:J:1244:GLN:HG3	1.97	0.46
6:K:12:LYS:HB2	6:K:12:LYS:HE2	1.65	0.46
2:B:6:DA:H2"	2:B:7:DA:C8	2.51	0.46
4:I:883:LEU:HD13	4:I:1052:VAL:HG11	1.98	0.46
5:J:423:LEU:HD11	5:J:447:ILE:HG21	1.98	0.46
5:J:574:VAL:O	5:J:578:ILE:HG12	2.16	0.46
5:J:141:PHE:HB3	5:J:293:ARG:HG3	1.98	0.45
5:J:647:PRO:HG3	5:J:697:MET:HA	1.97	0.45
5:J:850:LYS:HB2	5:J:851:PRO:HD2	1.98	0.45
3:G:68:TYR:HE2	4:I:831:ILE:HG12	1.80	0.45
4:I:1223:ARG:NH2	5:J:721:SER:OG	2.40	0.45
4:I:273:HIS:O	4:I:276:GLN:HG3	2.15	0.45
5:J:554:GLU:HA	5:J:580:TRP:HZ2	1.81	0.45
5:J:665:GLN:OE1	5:J:678:ARG:NH1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:850:LYS:HG2	5:J:855:ASP:OD2	2.16	0.45
5:J:1060:VAL:HG22	5:J:1106:ILE:HG23	1.98	0.45
4:I:39:ILE:HA	4:I:49:LEU:HD12	1.97	0.45
5:J:36:GLY:HA3	5:J:61:ILE:HG23	1.97	0.45
5:J:1229:VAL:O	5:J:1233:ILE:HG22	2.17	0.45
1:A:12:DC:N3	1:A:13:DC:N4	2.65	0.45
4:I:671:LEU:HD11	4:I:679:ALA:HB1	1.99	0.45
5:J:1346:GLY:O	5:J:1350:ASN:ND2	2.47	0.45
4:I:675:ASP:HB2	4:I:1107:MET:HB2	1.99	0.45
4:I:1151:LEU:HD22	4:I:1198:LEU:HD13	1.98	0.45
4:I:1292:THR:HG23	4:I:1320:PRO:HD3	1.98	0.45
5:J:68:TYR:HE1	5:J:81:ARG:HB3	1.81	0.45
5:J:208:THR:HG22	5:J:210:SER:H	1.81	0.45
6:K:7:GLN:O	6:K:10:VAL:HG22	2.16	0.45
6:K:66:VAL:O	6:K:70:GLN:HG2	2.16	0.45
3:G:45:ARG:O	3:G:49:SER:OG	2.20	0.45
3:G:212:ASP:HB3	3:G:215:GLU:HG2	1.97	0.45
3:H:89:ALA:HB2	3:H:208:ASN:HB2	1.99	0.45
4:I:618:GLN:NE2	5:J:770:LEU:HD23	2.32	0.45
3:G:85:LEU:O	3:G:88:LEU:HG	2.17	0.45
5:J:615:LYS:HB2	6:K:5:THR:HG21	1.98	0.45
3:G:188:GLU:OE2	3:G:200:LYS:NZ	2.40	0.45
4:I:448:LEU:HD23	4:I:553:THR:HG23	1.99	0.45
5:J:964:LYS:HB2	5:J:976:THR:HB	1.97	0.45
4:I:233:ARG:H	4:I:237:LEU:HA	1.82	0.44
5:J:355:ILE:HD11	5:J:460:ASP:O	2.17	0.44
3:H:98:VAL:HG11	3:H:121:VAL:HG21	1.98	0.44
4:I:208:ILE:HD11	4:I:365:GLU:HB3	1.98	0.44
4:I:595:THR:HG22	4:I:598:VAL:CA	2.48	0.44
4:I:690:VAL:HG13	4:I:830:THR:HG21	2.00	0.44
5:J:160:LEU:CD1	5:J:164:GLN:HB3	2.47	0.44
5:J:515:ARG:NH2	5:J:718:SER:O	2.50	0.44
5:J:537:TYR:OH	5:J:634:ARG:NE	2.50	0.44
5:J:1025:MET:HB3	5:J:1124:ILE:HB	1.99	0.44
4:I:120:GLN:HE21	4:I:489:PRO:HG2	1.83	0.44
4:I:606:LEU:HD22	4:I:610:GLU:HG3	1.99	0.44
4:I:915:ASP:OD1	4:I:915:ASP:N	2.50	0.44
4:I:557:ARG:HB3	4:I:587:LEU:HD13	2.00	0.44
4:I:870:ILE:HG12	4:I:884:VAL:HG23	1.98	0.44
3:G:15:ASP:OD1	3:G:16:ILE:N	2.51	0.44
4:I:303:ASP:OD1	4:I:303:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:1140:LYS:O	4:I:1143:GLU:HG3	2.17	0.44
5:J:519:ASN:HB2	5:J:709:ARG:HA	1.99	0.44
4:I:10:ARG:NH1	4:I:790:ASP:OD2	2.49	0.44
4:I:521:LEU:HD11	4:I:664:GLY:HA2	1.98	0.44
5:J:849:LEU:HD23	5:J:855:ASP:N	2.31	0.44
1:A:12:DC:N3	1:A:13:DC:C4	2.86	0.44
4:I:591:TYR:HD2	4:I:606:LEU:HB2	1.82	0.44
7:R:40:C:H2'	7:R:41:C:H6	1.82	0.44
3:G:31:LEU:HD22	3:G:35:PHE:HB3	2.00	0.44
5:J:321:LYS:HA	5:J:321:LYS:HD3	1.78	0.44
3:G:101:THR:O	3:G:116:THR:OG1	2.27	0.44
4:I:464:PHE:CE1	4:I:498:ILE:HD11	2.53	0.44
5:J:968:ASN:HD21	5:J:972:LYS:HB2	1.81	0.44
4:I:686:GLN:HG2	4:I:1233:LEU:HD11	2.00	0.43
5:J:147:ILE:HG22	5:J:188:LEU:HD12	2.00	0.43
5:J:432:LEU:HB3	5:J:435:GLN:HE21	1.83	0.43
5:J:907:HIS:ND1	5:J:908:ILE:O	2.45	0.43
4:I:8:LYS:HD2	4:I:1164:PHE:CE2	2.53	0.43
4:I:1073:LYS:HG3	5:J:462:ASP:HB2	2.00	0.43
1:A:31:DA:H1'	1:A:32:DT:H5'	2.00	0.43
3:H:180:VAL:HG21	3:H:183:ILE:HG12	2.01	0.43
4:I:1303:LYS:HD2	4:I:1303:LYS:HA	1.70	0.43
3:H:47:LEU:HB3	3:H:220:ALA:HB2	1.99	0.43
4:I:1108:ASN:CG	4:I:1111:GLN:HE21	2.13	0.43
4:I:1276:TRP:CH2	5:J:798:ARG:HG3	2.53	0.43
5:J:578:ILE:HG21	5:J:631:TYR:CE2	2.53	0.43
3:H:43:LEU:HA	3:H:46:ILE:HG22	2.00	0.43
4:I:1225:VAL:HA	5:J:638:SER:HB3	2.01	0.43
5:J:483:LEU:HD21	6:K:17:PHE:HE1	1.84	0.43
5:J:833:GLU:OE2	5:J:1242:ARG:NE	2.35	0.43
6:K:65:ASP:O	6:K:68:GLU:HG3	2.18	0.43
3:G:45:ARG:NH1	4:I:1084:ASP:OD1	2.50	0.43
3:H:112:ALA:N	3:H:128:HIS:O	2.51	0.43
4:I:99:LYS:HE3	4:I:99:LYS:HB3	1.80	0.43
4:I:516:ASP:HA	4:I:761:GLN:NE2	2.33	0.43
5:J:691:ASP:OD1	5:J:695:LYS:HE3	2.19	0.43
5:J:802:ASP:OD2	5:J:1348:LYS:NZ	2.50	0.43
3:H:9:LEU:HD21	3:H:192:VAL:HG11	2.01	0.43
3:H:66:HIS:CE1	3:H:68:TYR:HB2	2.54	0.43
4:I:1258:PRO:HG2	5:J:346:ARG:HB2	2.00	0.43
5:J:1089:LEU:HA	5:J:1096:PRO:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:179:PRO:HG2	3:H:211:ILE:HD11	2.00	0.43
4:I:492:MET:SD	4:I:492:MET:N	2.90	0.43
4:I:1075:VAL:HG22	5:J:461:PHE:O	2.18	0.43
5:J:44:ILE:HG12	5:J:252:LEU:HD11	2.01	0.43
5:J:57:PHE:CD2	5:J:247:PRO:HB3	2.54	0.42
3:H:181:GLU:HB2	3:H:206:GLU:HG2	2.00	0.42
4:I:815:SER:OG	4:I:1077:SER:HB3	2.19	0.42
5:J:420:PRO:O	5:J:471:PRO:HD2	2.19	0.42
5:J:925:GLU:HB3	5:J:926:PRO:HD3	2.01	0.42
5:J:1199:PHE:HB2	5:J:1202:GLU:OE1	2.20	0.42
3:H:78:ILE:HA	3:H:81:ILE:HB	2.00	0.42
4:I:1296:ASP:N	4:I:1296:ASP:OD1	2.51	0.42
5:J:460:ASP:CA	5:J:464:ASP:OD2	2.67	0.42
5:J:582:ILE:HG13	5:J:627:THR:HG21	2.01	0.42
3:H:124:VAL:HG21	3:H:209:GLY:O	2.19	0.42
4:I:629:PHE:CD2	4:I:634:VAL:HG11	2.54	0.42
4:I:1121:ALA:HB1	4:I:1180:MET:O	2.19	0.42
4:I:118:LYS:NZ	4:I:488:MET:HG3	2.35	0.42
4:I:188:PHE:CE2	4:I:436:ARG:HB2	2.55	0.42
4:I:1021:LEU:HB3	4:I:1025:PHE:CZ	2.55	0.42
4:I:1176:LEU:HD22	4:I:1181:PRO:HD3	2.01	0.42
5:J:865:HIS:CE1	5:J:867:GLN:HB2	2.54	0.42
5:J:1046:ILE:HG12	5:J:1061:VAL:HG22	2.01	0.42
5:J:1150:PRO:HG2	5:J:1153:PRO:HA	2.01	0.42
3:G:31:LEU:HD13	3:G:36:GLY:HA2	2.01	0.42
4:I:1276:TRP:HH2	5:J:798:ARG:HG3	1.85	0.42
5:J:93:THR:HG22	5:J:94:GLN:N	2.27	0.42
5:J:141:PHE:HA	5:J:180:MET:SD	2.60	0.42
5:J:464:ASP:OD1	7:R:47:A:O3'	2.22	0.42
5:J:473:THR:O	5:J:477:GLN:HG3	2.19	0.42
4:I:867:GLU:OE2	4:I:943:LYS:NZ	2.36	0.42
5:J:97:VAL:HG12	5:J:101:ARG:HD2	2.01	0.42
5:J:612:LEU:HB3	5:J:616:PRO:HB2	2.02	0.42
5:J:697:MET:SD	5:J:741:ALA:HB3	2.59	0.42
1:A:28:DG:H2"	1:A:29:DA:C8	2.54	0.42
4:I:409:LEU:HD13	4:I:427:ASP:HB3	2.01	0.42
4:I:720:ARG:HH21	4:I:736:VAL:HG21	1.85	0.42
4:I:978:VAL:HG21	4:I:1010:GLN:HE22	1.84	0.42
5:J:255:LEU:O	5:J:259:ARG:N	2.53	0.42
5:J:418:GLU:HG3	6:K:48:VAL:HG11	2.01	0.42
5:J:1032:SER:HB3	5:J:1117:SER:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:44:ARG:NH2	4:I:1217:THR:HG23	2.35	0.42
4:I:515:MET:HA	4:I:526:HIS:CD2	2.55	0.42
4:I:1121:ALA:HB2	4:I:1182:ILE:HD12	2.02	0.42
4:I:1122:LYS:HD3	4:I:1122:LYS:HA	1.81	0.42
5:J:432:LEU:HD13	5:J:499:ILE:HG21	2.01	0.42
5:J:1167:LYS:HA	5:J:1167:LYS:HD2	1.93	0.42
3:H:131:CYS:SG	3:H:140:ILE:HD13	2.60	0.42
4:I:557:ARG:HG2	4:I:587:LEU:HB3	2.02	0.42
4:I:687:ARG:HH22	7:R:45:C:H5"	1.84	0.42
4:I:936:ARG:HH21	4:I:1046:VAL:HG12	1.85	0.42
4:I:1268:GLN:HG2	5:J:350:SER:OG	2.20	0.42
4:I:1325:VAL:O	4:I:1329:GLU:HG3	2.19	0.42
5:J:475:GLU:HG3	6:K:24:ALA:HB1	2.02	0.42
3:H:83:LEU:O	3:H:86:LYS:HG2	2.20	0.41
4:I:820:GLU:HB2	4:I:1081:PRO:HA	2.01	0.41
2:B:26:DA:N6	5:J:319:SER:HA	2.33	0.41
4:I:21:VAL:HG11	4:I:592:ARG:HD2	2.02	0.41
2:B:2:DT:H2"	2:B:3:DC:C6	2.56	0.41
5:J:743:MET:HG2	5:J:745:GLY:H	1.84	0.41
5:J:842:ARG:HB2	5:J:882:VAL:HG21	2.02	0.41
5:J:1344:LEU:O	5:J:1345:ARG:HG2	2.19	0.41
4:I:1056:VAL:HG12	4:I:1058:ARG:HG2	2.02	0.41
5:J:510:LEU:HD23	5:J:513:MET:HE3	2.02	0.41
4:I:116:ASP:OD1	4:I:116:ASP:N	2.54	0.41
4:I:255:ILE:HG23	4:I:285:ILE:HG21	2.01	0.41
4:I:559:CYS:HB2	4:I:662:SER:HB3	2.03	0.41
4:I:669:PRO:O	4:I:1070:HIS:NE2	2.54	0.41
4:I:800:MET:HE2	4:I:800:MET:HB3	1.87	0.41
5:J:374:LEU:O	5:J:378:LYS:HG3	2.20	0.41
5:J:954:ASN:OD1	5:J:954:ASN:N	2.53	0.41
5:J:1259:GLN:HE22	5:J:1262:ARG:NH1	2.18	0.41
3:G:10:LYS:HE2	3:H:226:GLU:OE2	2.20	0.41
4:I:213:LEU:HB3	4:I:422:LYS:HG2	2.02	0.41
4:I:423:ASP:HA	4:I:426:ILE:HG12	2.03	0.41
4:I:726:TYR:OH	4:I:728:ASP:OD2	2.37	0.41
4:I:854:ILE:HD11	4:I:885:GLY:HA3	2.01	0.41
4:I:960:LEU:HD13	4:I:1029:LEU:HD12	2.02	0.41
4:I:1077:SER:HA	5:J:356:THR:HG23	2.01	0.41
4:I:1113:LEU:HD22	5:J:641:ILE:HD11	2.02	0.41
4:I:1270:PHE:CZ	4:I:1274:GLU:HB3	2.55	0.41
5:J:20:ILE:O	5:J:1342:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:641:ILE:HD13	5:J:641:ILE:HA	1.89	0.41
7:R:40:C:HO2'	7:R:41:C:P	2.43	0.41
4:I:444:ASP:O	4:I:450:ASN:ND2	2.51	0.41
4:I:758:ARG:HD2	4:I:835:GLU:HB2	2.03	0.41
4:I:141:THR:HB	4:I:514:PHE:HE1	1.84	0.41
4:I:1289:GLU:HA	4:I:1315:MET:HE3	2.03	0.41
5:J:513:MET:HG3	5:J:544:LEU:HD21	2.03	0.41
5:J:1289:ASN:OD1	5:J:1290:ARG:N	2.54	0.41
1:A:26:DA:H4'	1:A:27:DA:OP1	2.20	0.41
3:G:67:GLU:HG2	3:G:79:LEU:HD13	2.03	0.41
3:H:10:LYS:HB3	3:H:10:LYS:HE2	1.76	0.41
3:H:15:ASP:OD1	3:H:15:ASP:N	2.53	0.41
3:H:79:LEU:HD21	5:J:526:VAL:HG11	2.03	0.41
4:I:593:LYS:HB3	4:I:602:GLU:HG3	2.02	0.41
4:I:1164:PHE:HD2	4:I:1168:GLU:HG3	1.84	0.41
5:J:143:SER:HA	5:J:161:THR:HA	2.03	0.41
5:J:144:TYR:OH	5:J:293:ARG:NH2	2.54	0.41
5:J:557:LYS:HD3	5:J:611:ILE:HG23	2.02	0.41
5:J:610:ARG:HG3	5:J:866:GLU:HG3	2.02	0.41
5:J:699:ASP:O	5:J:703:THR:HB	2.21	0.41
5:J:960:LEU:HD13	5:J:963:VAL:HG21	2.03	0.41
5:J:1178:THR:HA	5:J:1184:ASP:HB3	2.02	0.41
4:I:809:GLY:O	5:J:357:VAL:HG11	2.21	0.41
5:J:111:THR:HG21	5:J:303:VAL:HB	2.01	0.41
5:J:403:ARG:HB3	5:J:405:GLU:HG2	2.02	0.41
5:J:587:LEU:HD11	5:J:608:CYS:HA	2.01	0.41
5:J:802:ASP:OD1	5:J:1348:LYS:NZ	2.52	0.41
5:J:1358:PRO:HB3	5:J:1366:HIS:ND1	2.36	0.41
6:K:26:ARG:HD2	6:K:26:ARG:HA	1.85	0.41
4:I:690:VAL:HG12	4:I:1234:LYS:O	2.21	0.40
4:I:934:PHE:HE2	4:I:1051:LYS:HD2	1.86	0.40
4:I:1256:GLN:NE2	4:I:1322:SER:OG	2.47	0.40
5:J:326:SER:O	5:J:330:MET:HG2	2.21	0.40
5:J:591:ILE:HG23	5:J:604:MET:HE2	2.03	0.40
3:H:61:ILE:HB	3:H:64:VAL:HB	2.03	0.40
4:I:367:TYR:OH	4:I:371:ARG:NH2	2.47	0.40
4:I:693:LEU:HB2	4:I:829:THR:O	2.21	0.40
4:I:1007:LYS:O	4:I:1011:LEU:HD23	2.21	0.40
4:I:1134:GLN:HG3	4:I:1136:GLN:HG3	2.03	0.40
5:J:147:ILE:HG12	5:J:179:LYS:H	1.85	0.40
5:J:201:LEU:HB2	5:J:221:ILE:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:523:GLU:HB2	5:J:546:ALA:HB1	2.03	0.40
3:G:89:ALA:HB1	3:G:210:THR:HG23	2.03	0.40
3:G:175:ALA:HB1	3:G:177:TYR:CZ	2.56	0.40
3:G:192:VAL:HG21	3:G:198:LEU:HD12	2.04	0.40
3:H:19:VAL:HG12	3:H:20:SER:N	2.36	0.40
4:I:595:THR:HG22	4:I:598:VAL:C	2.42	0.40
4:I:1278:LEU:HD22	5:J:484:MET:CE	2.52	0.40
5:J:27:PRO:O	5:J:31:ARG:HG2	2.22	0.40
5:J:57:PHE:CE2	5:J:252:LEU:HD22	2.56	0.40
5:J:393:THR:HG22	5:J:395:LYS:H	1.85	0.40
5:J:824:PRO:HD3	5:J:835:LEU:HB2	2.01	0.40
5:J:1173:ARG:HH21	5:J:1192:LYS:HA	1.86	0.40
5:J:1268:ASN:HB3	5:J:1301:THR:HG22	2.03	0.40
5:J:1323:ALA:O	5:J:1328:THR:OG1	2.30	0.40
3:G:109:PRO:HA	3:G:132:HIS:HA	2.03	0.40
3:H:205:MET:SD	3:H:217:ILE:HG13	2.61	0.40
4:I:941:LYS:HE2	4:I:945:ALA:HB1	2.04	0.40
4:I:1113:LEU:CD2	5:J:641:ILE:HD11	2.52	0.40
4:I:1276:TRP:CE2	5:J:801:VAL:HG11	2.56	0.40
5:J:71:LEU:HD23	5:J:71:LEU:HA	1.92	0.40
5:J:513:MET:SD	5:J:579:LEU:HG	2.61	0.40
5:J:1143:ASP:HA	5:J:1148:ARG:HE	1.87	0.40
2:B:17:DC:OP1	4:I:1271:GLY:HA3	2.21	0.40
4:I:15:PHE:CD2	4:I:1190:ALA:HB2	2.57	0.40
4:I:685:MET:SD	4:I:1073:LYS:HB3	2.61	0.40
4:I:1142:ARG:HH22	4:I:1166:ASP:HA	1.86	0.40
5:J:113:HIS:HB3	5:J:116:PHE:HD2	1.87	0.40
5:J:981:GLU:HG2	5:J:996:LYS:HA	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	
3	G	217/328 (66%)	208 (96%)	9 (4%)	0	100	100
3	H	215/328 (66%)	202 (94%)	12 (6%)	1 (0%)	29	61
4	I	1312/1342 (98%)	1254 (96%)	57 (4%)	1 (0%)	51	82
5	J	1331/1434 (93%)	1280 (96%)	51 (4%)	0	100	100
6	K	77/102 (76%)	74 (96%)	3 (4%)	0	100	100
All	All	3152/3534 (89%)	3018 (96%)	132 (4%)	2 (0%)	54	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	30	PRO
4	I	58	PRO

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	
3	G	188/285 (66%)	186 (99%)	2 (1%)	73	86
3	H	187/285 (66%)	180 (96%)	7 (4%)	34	62
4	I	1135/1157 (98%)	1119 (99%)	16 (1%)	67	83
5	J	1122/1191 (94%)	1102 (98%)	20 (2%)	59	79
6	K	67/83 (81%)	67 (100%)	0	100	100
All	All	2699/3001 (90%)	2654 (98%)	45 (2%)	62	80

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	29	GLU
3	G	33	ARG
3	H	29	GLU
3	H	31	LEU
3	H	143	ARG
3	H	192	VAL

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Mol	Chain	Res	Type
3	H	194	GLN
3	H	195	ARG
3	H	197	ASP
4	I	41	GLN
4	I	50	GLU
4	I	54	ARG
4	I	56	VAL
4	I	57	PHE
4	I	59	ILE
4	I	60	GLN
4	I	67	GLU
4	I	107	ARG
4	I	378	ARG
4	I	697	LYS
4	I	758	ARG
4	I	841	ARG
4	I	1106	ARG
4	I	1216	ARG
4	I	1291	LEU
5	J	21	LYS
5	J	47	ARG
5	J	53	ARG
5	J	54	ASP
5	J	87	LYS
5	J	118	LYS
5	J	120	LEU
5	J	148	GLU
5	J	154	LEU
5	J	214	ARG
5	J	220	ARG
5	J	227	PHE
5	J	250	ARG
5	J	260	PHE
5	J	265	LEU
5	J	321	LYS
5	J	322	ARG
5	J	346	ARG
5	J	403	ARG
5	J	1123	ARG

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

Mol	Chain	Res	Type
4	I	36	GLN
4	I	41	GLN
4	I	519	ASN
4	I	618	GLN
4	I	620	ASN
5	J	504	GLN
5	J	1249	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	R	46/47 (97%)	15 (32%)	4 (8%)

All (15) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	R	3	A
7	R	16	A
7	R	18	A
7	R	25	A
7	R	26	U
7	R	27	A
7	R	31	A
7	R	33	C
7	R	35	A
7	R	36	A
7	R	37	G
7	R	38	G
7	R	39	A
7	R	40	C
7	R	41	C

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	R	2	C
7	R	35	A
7	R	37	G
7	R	40	C

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 monosaccharides 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-28845. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections (i)

6.1.1 Primary map
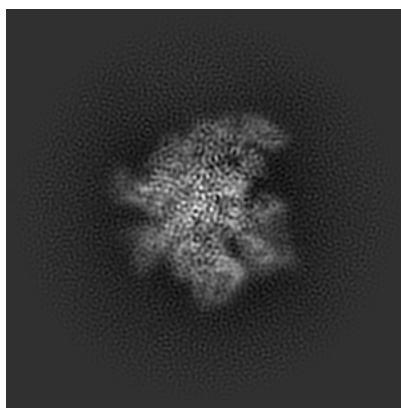
X
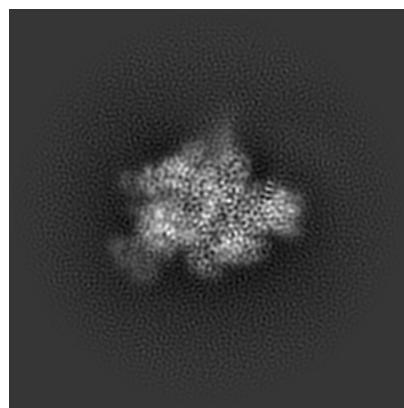
Y
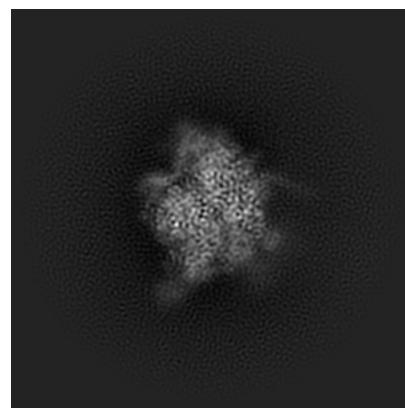
Z

6.1.2 Raw map

X

Y

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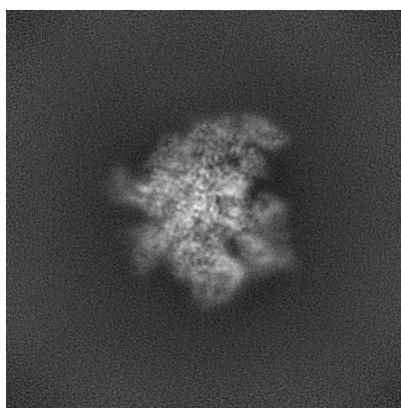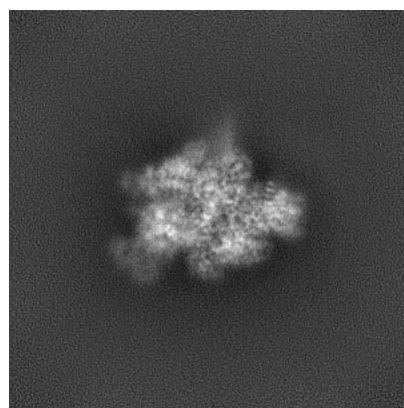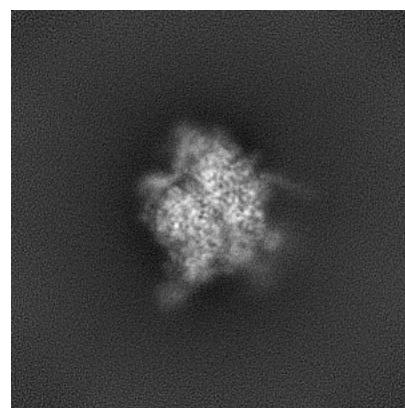
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
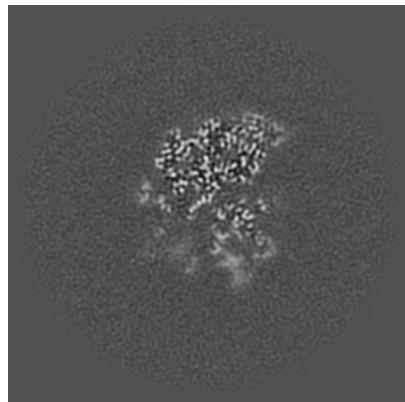
6.2.1 Primary map
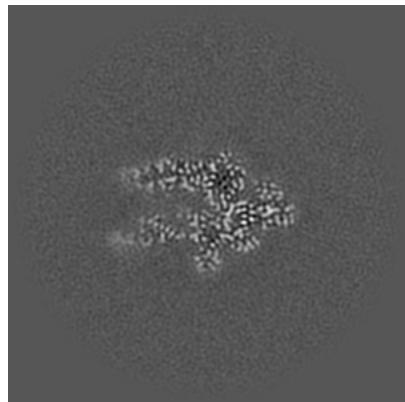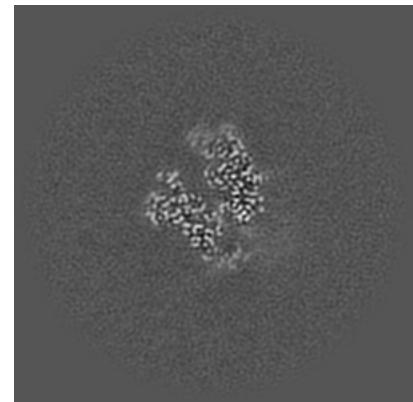
| X Index: 150 | Y Index: 150 | Z Index: 150 |

6.2.2 Raw map
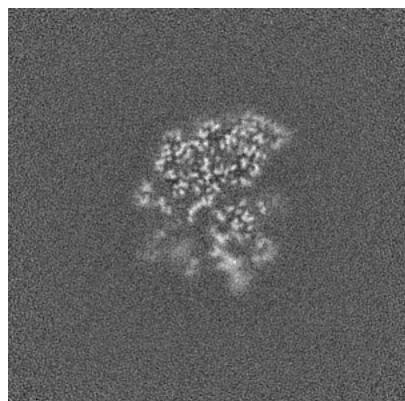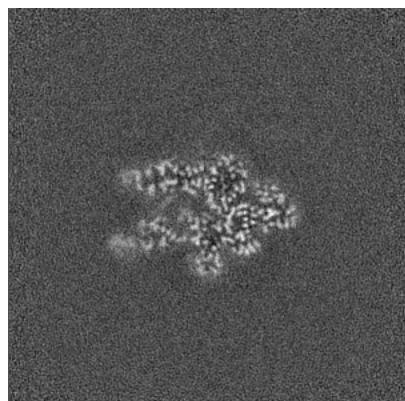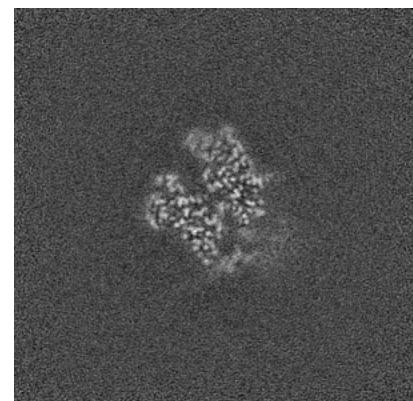
| X Index: 150 | Y Index: 150 | Z Index: 150 |

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

6.3 Largest variance slices ⓘ
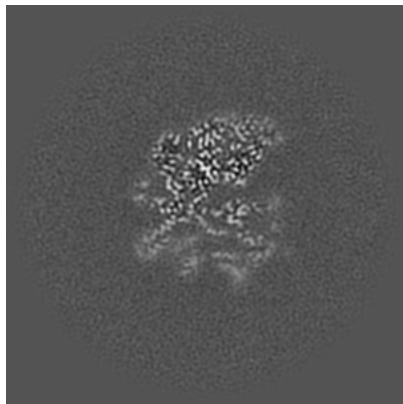
6.3.1 Primary map
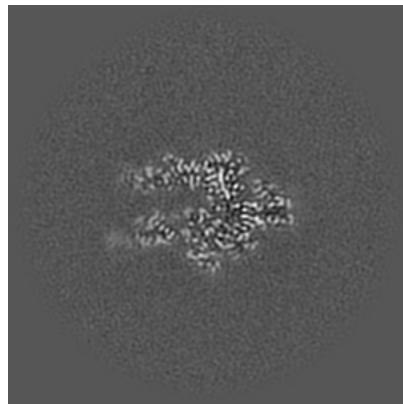
X Index: 146	Y Index: 148	Z Index: 165
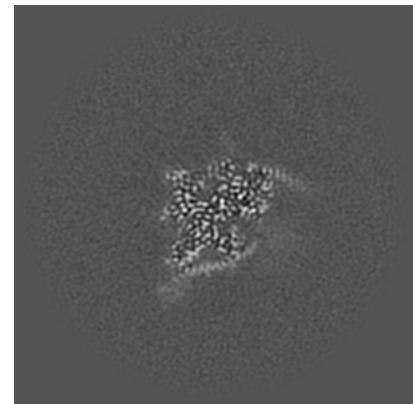
6.3.2 Raw map
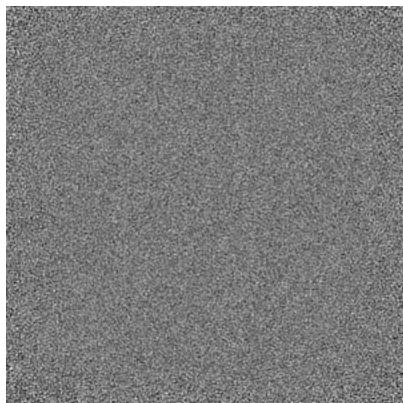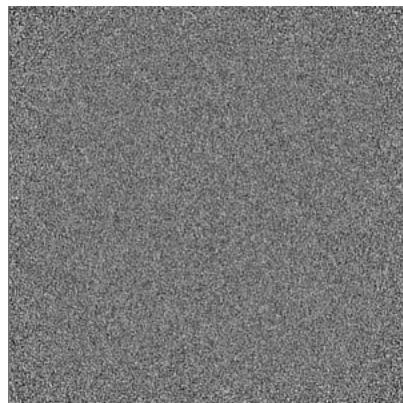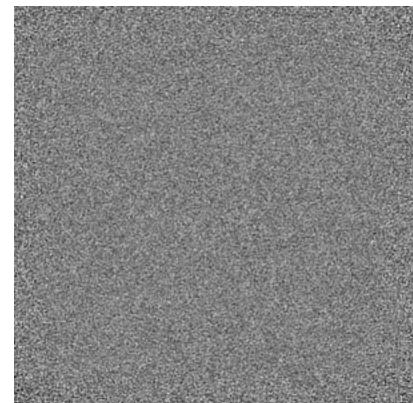
X Index: 0	Y Index: 0	Z Index: 1

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 |

6.4.2　Raw map

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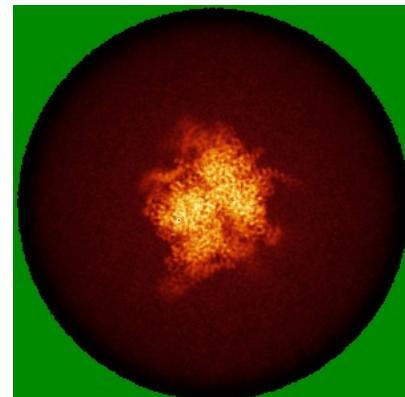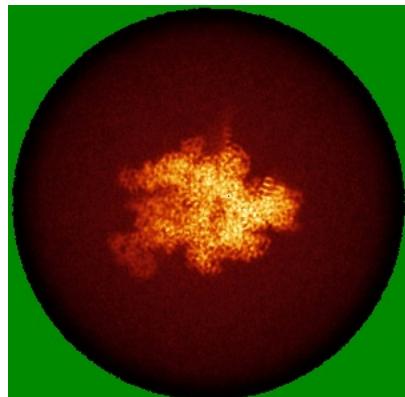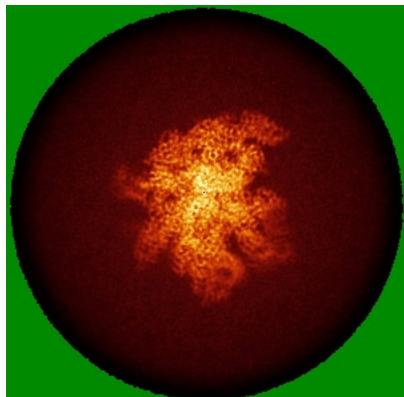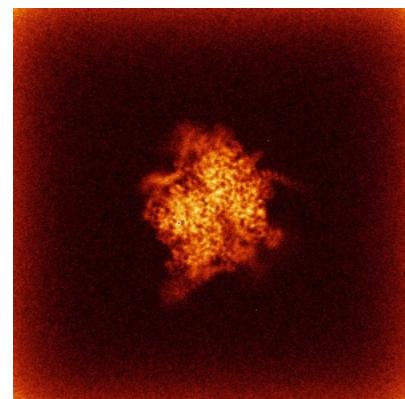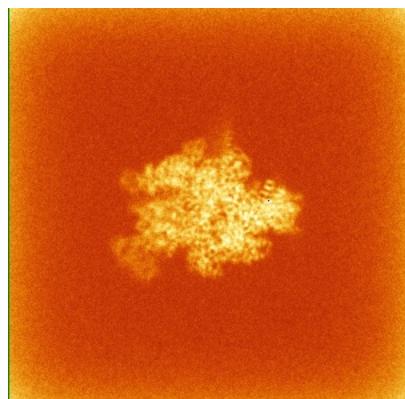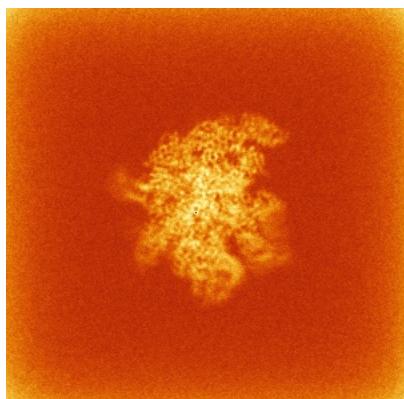
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X   Y   Z
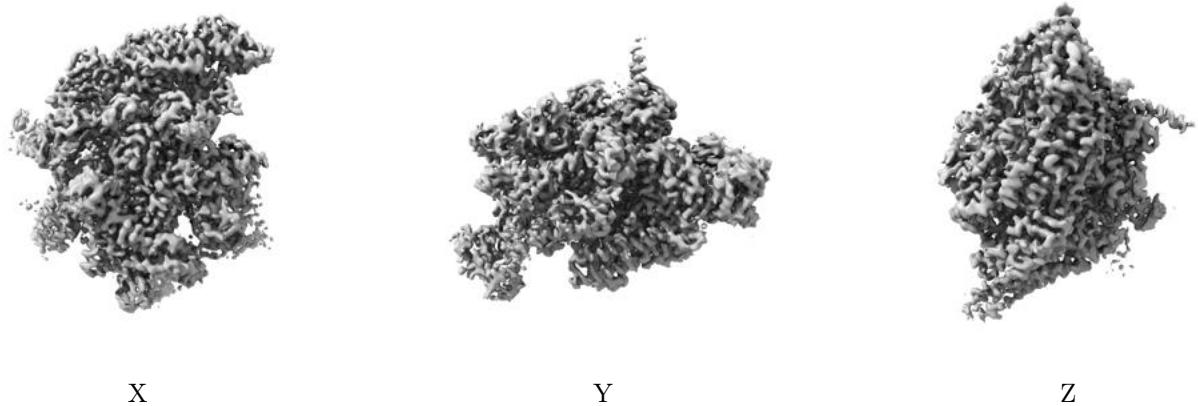
The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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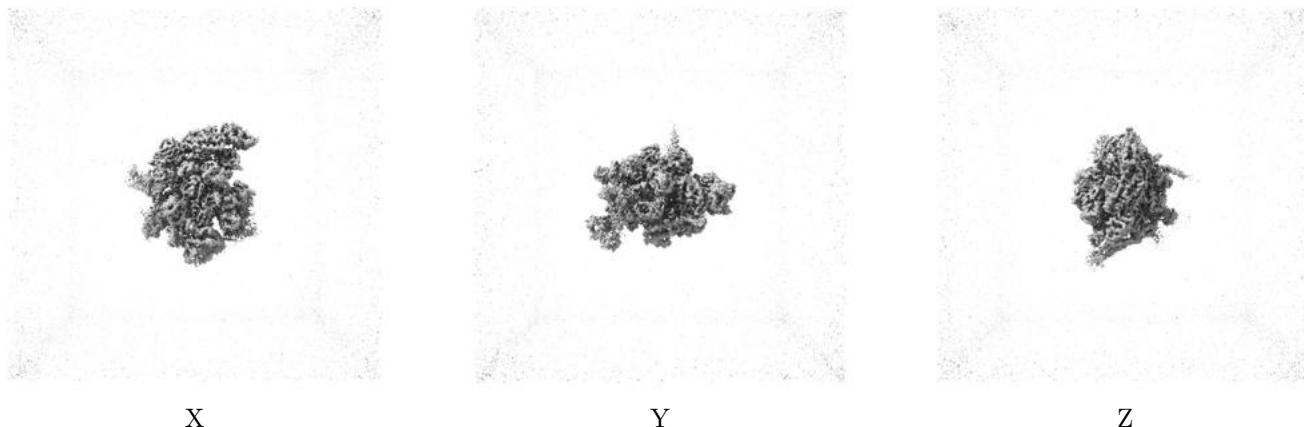
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

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

7   Map analysis ⓘ

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

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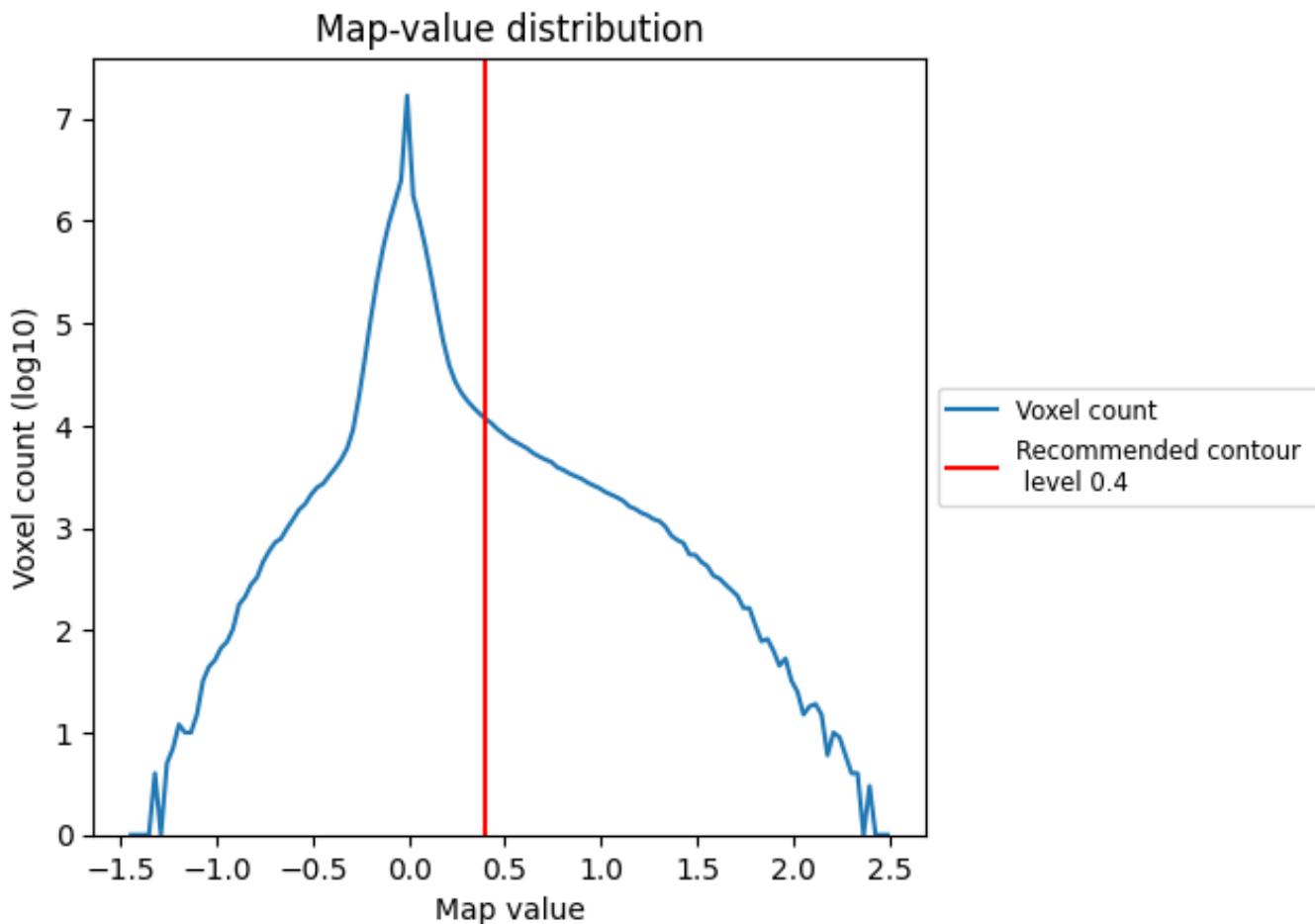
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
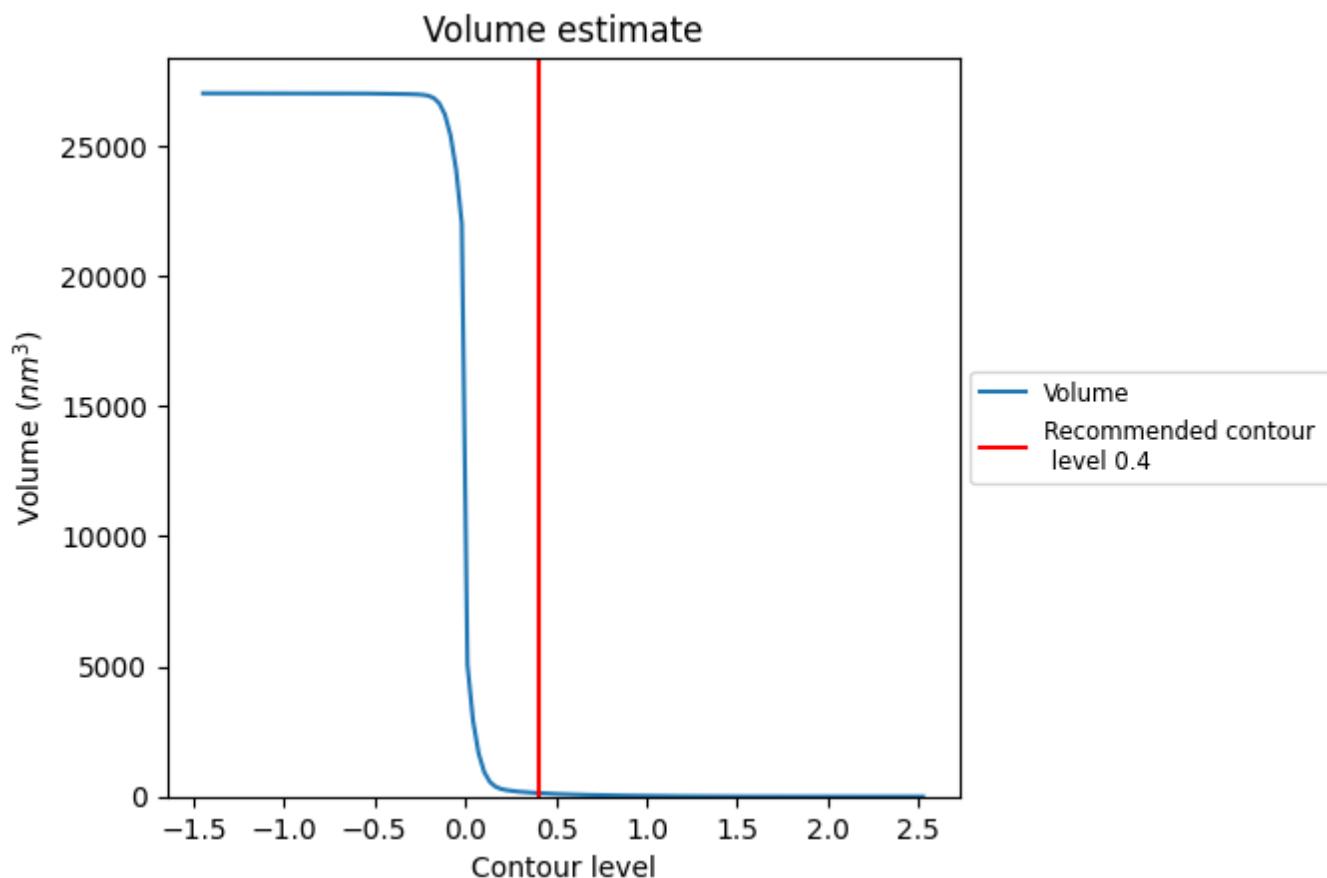
The volume at the recommended contour level is 135 nm^3; this corresponds to an approximate mass of 122 kDa.

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 ⓘ
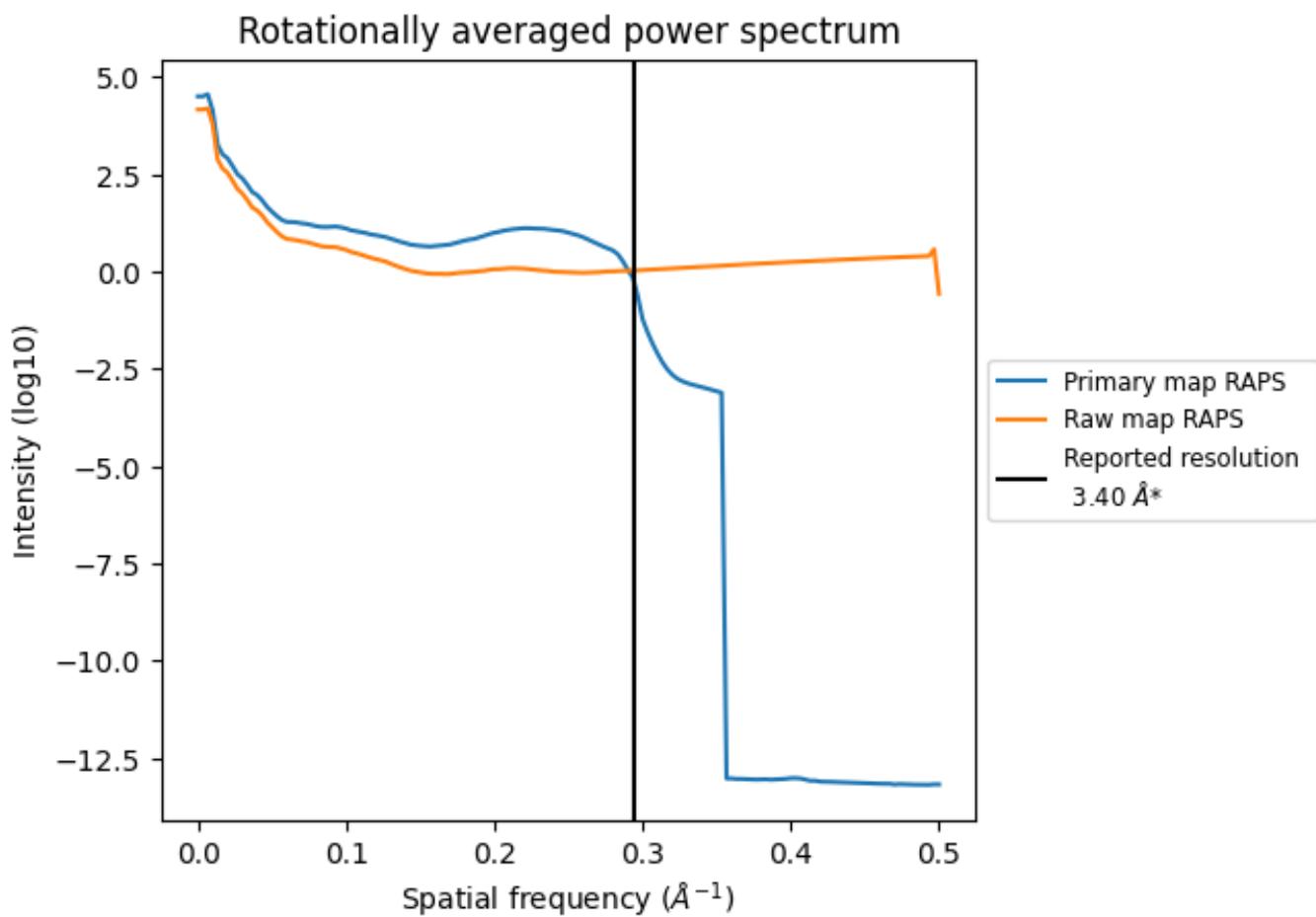
*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8　Fourier-Shell correlation ⓘ

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

8.1　FSC ⓘ
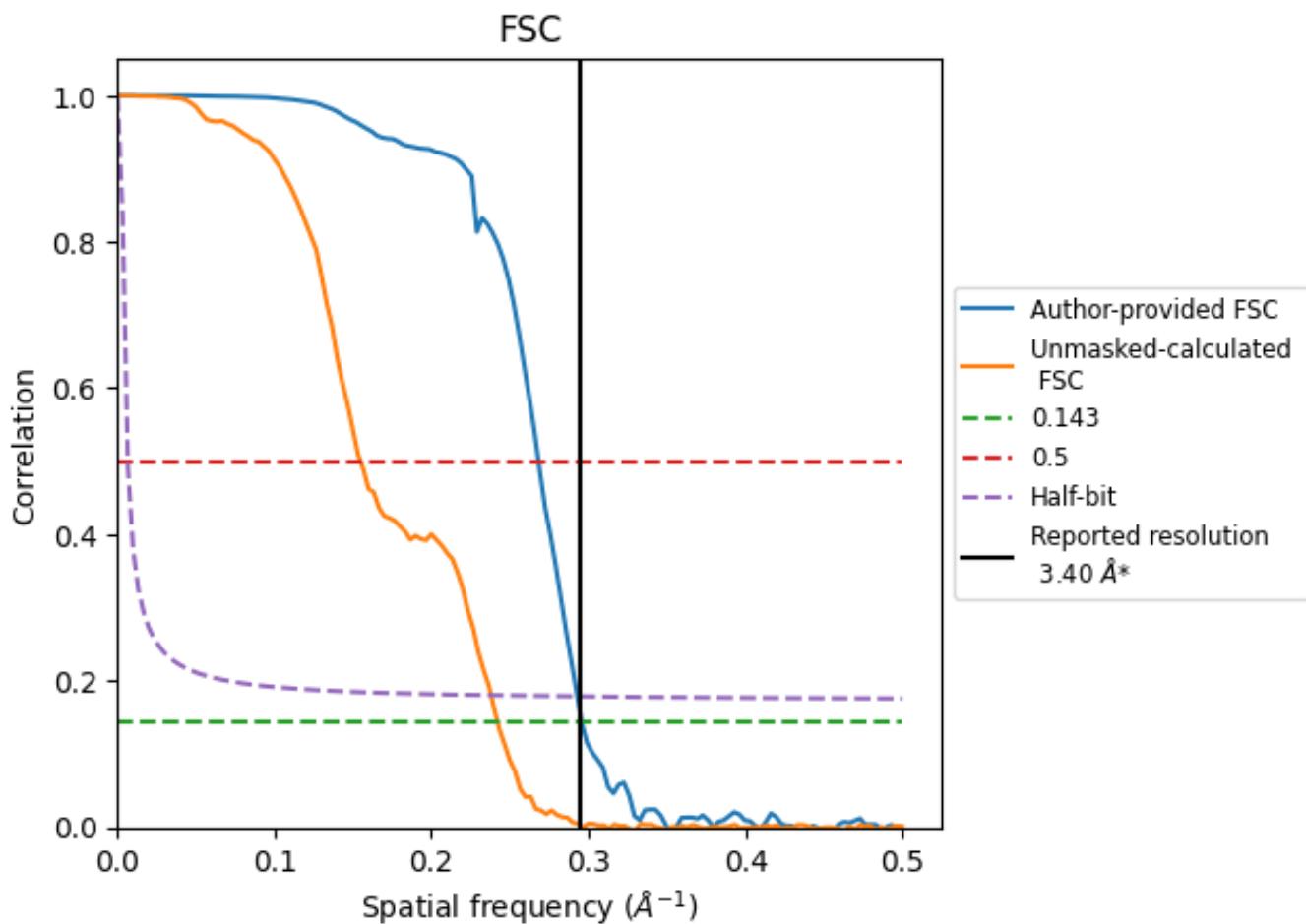
*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2   Resolution estimates   (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.38	3.73	3.41
Unmasked-calculated*	4.13	6.46	4.20

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.13 differs from the reported value 3.4 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-28845 and PDB model 8F3C. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay ⓘ

X	Y	Z
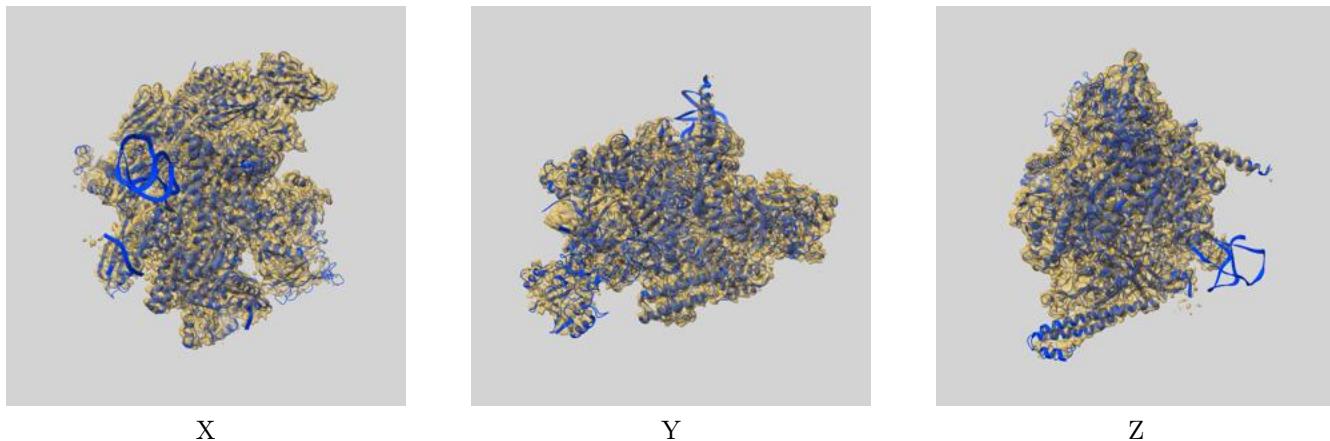
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

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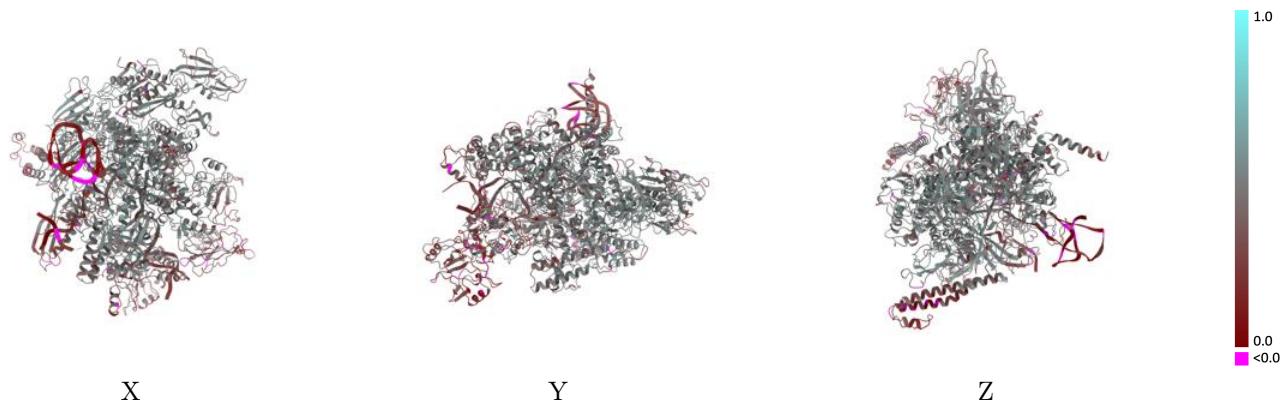
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)

X Y Z
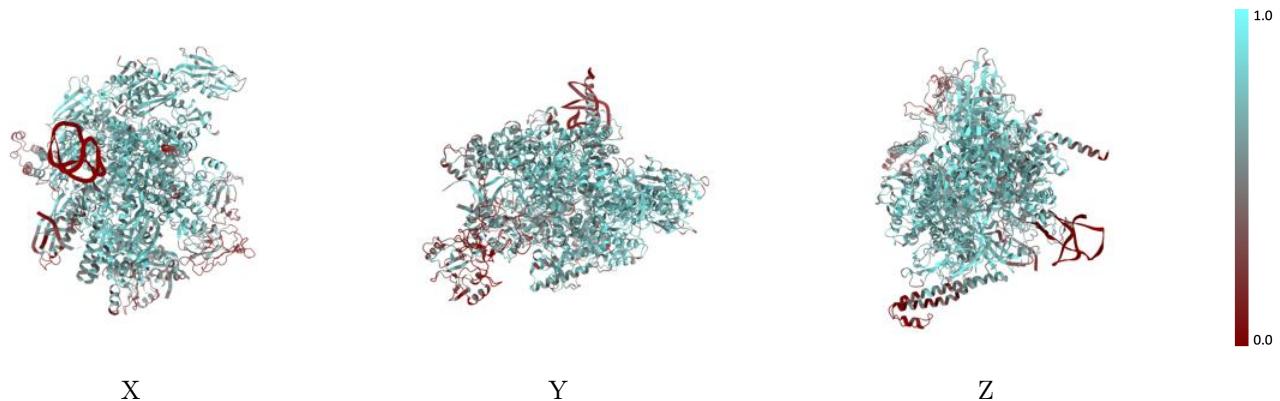
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion ⓘ
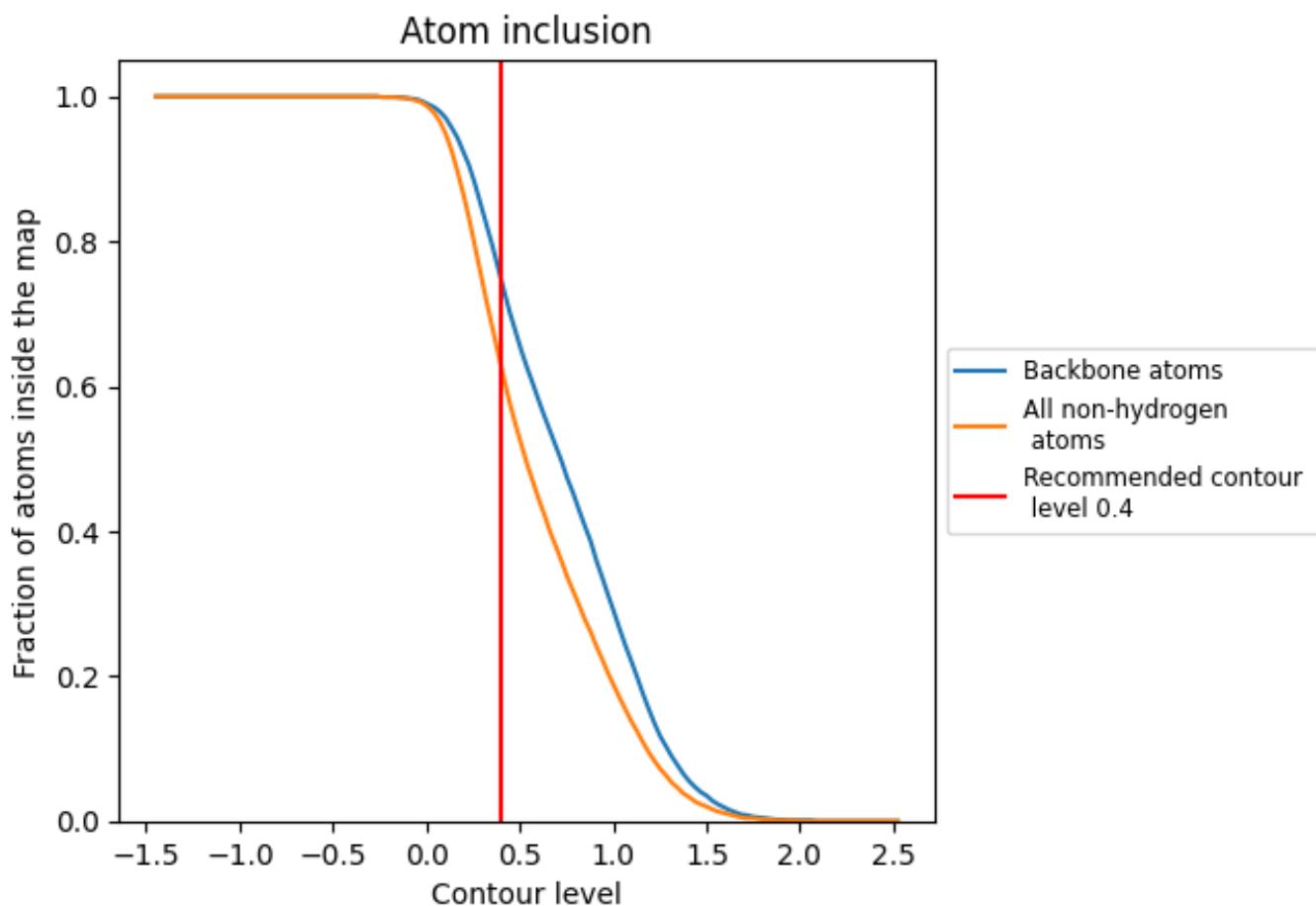
At the recommended contour level, 75% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6280	0.4190
A	0.6210	0.2550
B	0.6310	0.3030
G	0.7250	0.4710
H	0.6750	0.4380
I	0.6490	0.4330
J	0.6280	0.4320
K	0.6170	0.4410
R	0.1780	0.1490

1.0

0.0
<0.0