



## Full wwPDB EM Validation Report ⓘ

Jun 10, 2024 – 07:21 AM EDT

PDB ID : 8FIX  
EMDB ID : EMD-29212  
Title : Cryo-EM structure of E. coli RNA polymerase backtracked elongation complex harboring a terminal mismatch  
Authors : Florez Ariza, A.; Wee, L.; Tong, A.; Canari, C.; Grob, P.; Nogales, E.; Bustamante, C.  
Deposited on : 2022-12-17  
Resolution : 3.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

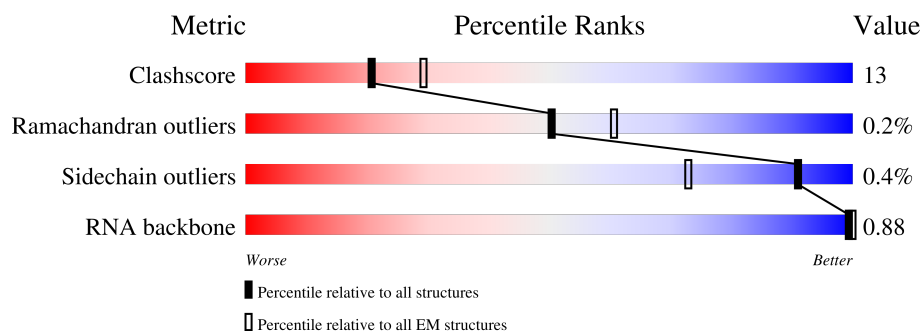
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	N	15	73% 27%
2	T	23	57% 43%
3	A	329	52% 18% 31%
3	B	329	49% 21% 30%
4	C	1342	70% 28% .
5	D	1407	64% 31% 5%
6	R	11	9% 82% 9% 9%

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Mol	Chain	Length	Quality of chain
7	E	91	<div><div></div><div>27%</div><div>53%</div><div>26%</div><div>•</div><div>20%</div></div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 25943 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 Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	15	Total	C	N	O	P	0	0
			304	144	60	85	15		

- Molecule 2 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	T	23	Total	C	N	O	P	0	0
			478	227	85	143	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	228	Total	C	N	O	S	0	0
			1768	1102	312	348	6		
3	B	229	Total	C	N	O	S	0	0
			1772	1104	313	349	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	1319	Total	C	N	O	S	0	0
			10407	6530	1814	2020	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	1336	Total	C	N	O	S	0	0
			10397	6533	1854	1960	50		

- Molecule 6 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	11	Total	C	N	O	P	0	0
			232	104	40	77	11		

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	73	Total	C	N	O	S	0	0
			582	355	111	115	1		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
8	D	2	Total	Zn	0
			2	2	

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
9	D	1	Total	Mg	0
			1	1	

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Non-template DNA

Chain N: 



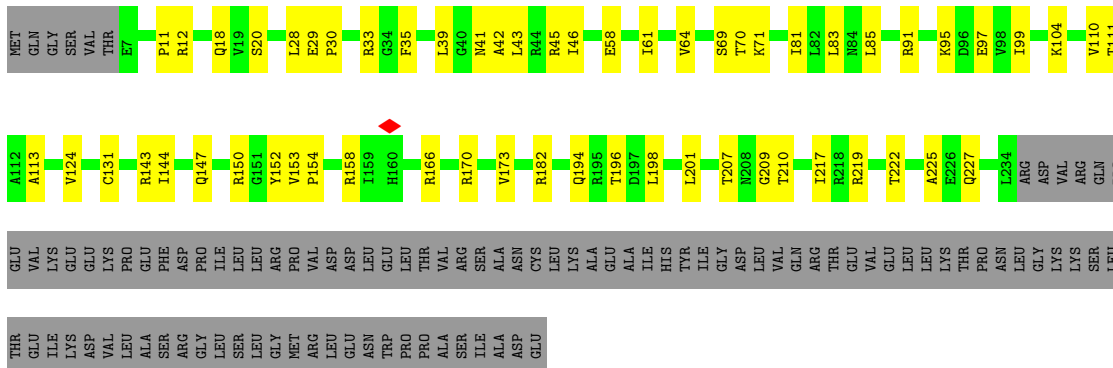
- Molecule 2: Template DNA

Chain T: 



- Molecule 3: DNA-directed RNA polymerase subunit alpha

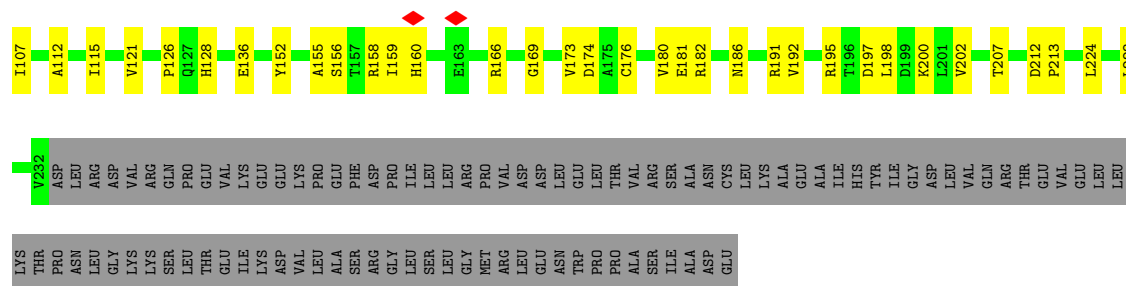
Chain A: 



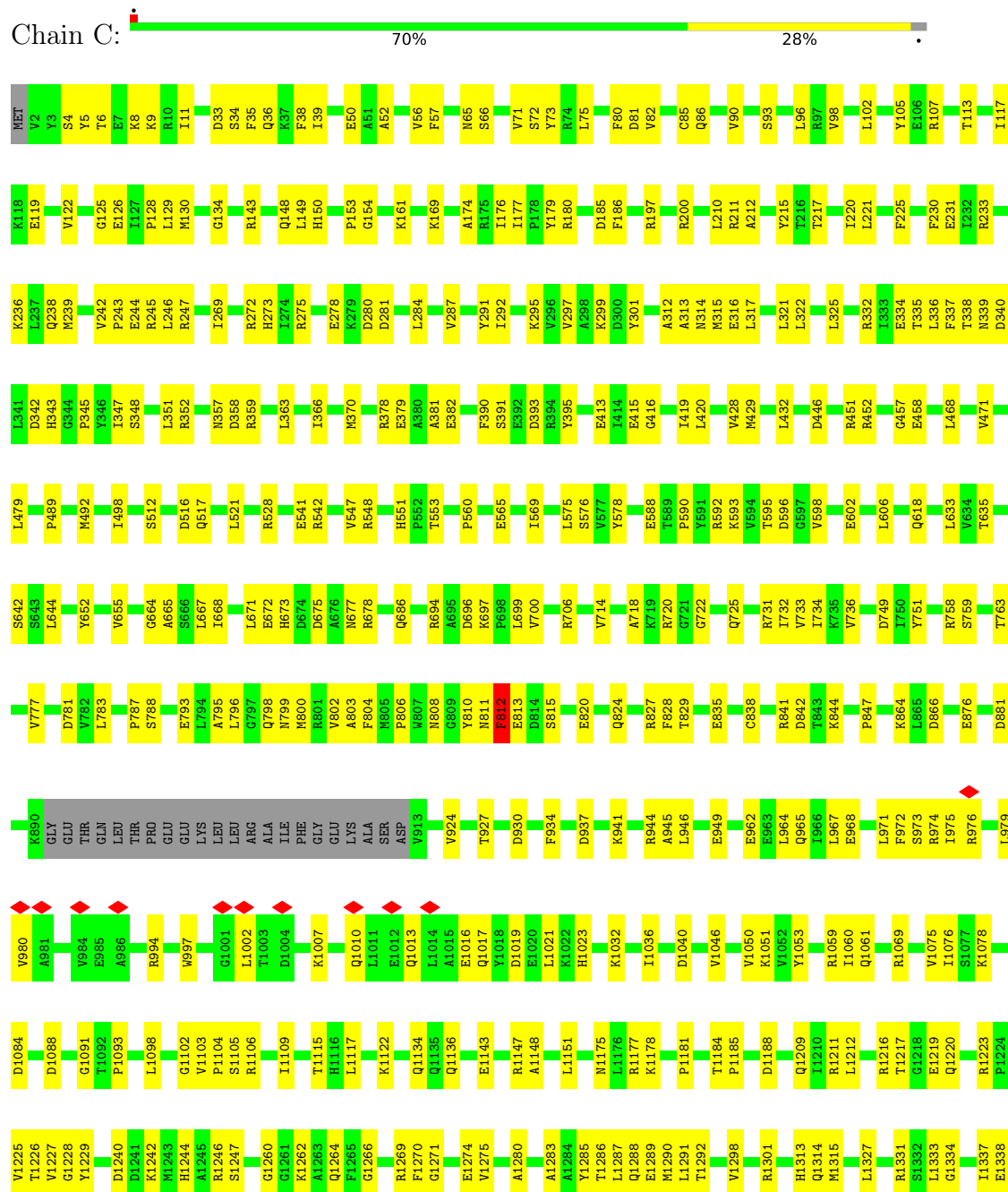
- Molecule 3: DNA-directed RNA polymerase subunit alpha

Chain B: 





• Molecule 4: DNA-directed RNA polymerase subunit beta





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

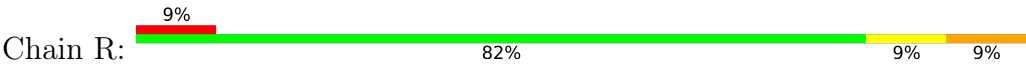
Chain D:  64% 31% 5%

Q1259	D1143	Q1044	A845	R744	T617	Q504	L412	S319	L189	R77	◆	MET
M1260	F1145	T1045	L849	M747	D622	V507	D413	N320	M192	L78	◆	LYS
L1261			K850	K748	D623		I416	K325		K79		ASP
K1262	R1148	E1052	P851	P750	A633	L510	R417	K326	Q196	H80		LEU
K1263			G852	D751			E418	L327	E197			LEU
												LYS
S1271	K1151	L1056	D855	G752	D636	T514	V421	M330	C198	V83		PHE
R1284	E1152	S1057	K955	R754	M644	V518	L423	E199	E197	I84		LEU
V1285	P1153	S1058	G956	I754			L423	Q200	Q200	C95		LEU
K1286			S957	I755		T528	N424	K332	L201	E86		ALA
	G1161	T1067	H865	E755	K650	G529	G425	G336	E204	K87		GLN
N1289	V1163	A1069	E866	T757		P530	A426	R337		E91		THR
	S1164	G1070	Q867	P759	I653	E531	P427			V92		LYS
G1296	T1177	K1072	L872		E663	E532	T428	L342	S210	T93		THR
K1297	I1178	D1073	V880	R764		E533	L429					
V1298	P1179	L1074	K881	E765	E666	E534	H430	K345	K213	V97		E16
	V1180	R1075	R882	G766		E535	R431	R346	K214	R98		F17
I1309	D1181		V883	L767	V673	L536		V347	K215	R99		D18
K1311	T1310	A1083	R884	L770	T674	R538	E438	G347	K216	E100		A19
S1312	A1312	Q1084	S883	Q771	A675	R551	P439	Y349	L217	R101		
S1313	P1185	G1085	V885	Q772	G676	L552	V440	R352	K219	M102		I22
L1314	E1186	G1085	R886	W772	R678	T553	L441	I355	R220	A112		A23
A1315	E1187	N1086	S887				I442	T356	I221	H113		L24
	E1188	D1087	C888	T776	V679			V357	L224	I114		A25
A1322	M1189	V1088	E981		N680	L563	L449			W15		S26
	R1194	D1084	G893	L783	K681	L569	H450	K363	N232	F116		M29
F1325	E1200	Y1089	V894	G794	T685	V574	P451	G365	E235			I30
Q1326								C366				
E1327								G367	I238	I124		G36
T1328	R1206	T1106	H897	L800	W686	A577	D460	L368				E42
R1330	A1216	Y1107	C998	A804	R692	L578	P461	P369	V244	R133		
V1331	A1216	Y1107	Y899	Q805		L579	Q465	K370	L245			
L1332		Q1108	R901	Q905	◆	W580	M466		P246	Y144		F49
	D1219	E993	D902	D812	◆	M581	A467		P247	V145		K50
G1339	I1220	S994	L903	D813	◆	H697	V468	A373	P247	V146		P51
	L1221	Y995		D813	◆	V583	H469		D248	I147		E52
L1344	L1222			C814	◆	P684	V470	F377	L249	E148		R53
	L1223			G815	◆							D54
K1348	L1223	D1119	N910	H817	Q702	L537	L474	I351	L252	L154		G55
E1349	V1229	V1002	N910				E475		V953	E155		L56
N1350	T1230	L1003	T918	T823	W708	L591	A476	K384	P254	R156		F57
V1351				P824	R709		Q477			E155		
I1352	T1233	Q1010	E925	W825		Q584	L478	L387	R259	Q157		
V1353		V1011	P926	I826	S721	A595	E479		F260	Q157		R60
	GLN					L596	A480	L390		I159		I61
Y1241	Y1241		L930	K832	A730	K599	R481		D264	L160		F62
R1242	L1243	SER			R731		A482	K398		T161		V65
Q1244	Q1244	GLY	F935	L835	G732	A600	L483		Y269	E162		K66
G1245	G1245	GLY	HIS	R836	S733	I601		V401		D167		D67
R1246	T1246	THR	ILE	D837	A734		I490		L285			Y68
K1247	K1247	LYS	LYS	R838	A736	Y609		E404		E170		E69
		ASP	GLY	V839	Q736		P493		D304			
ALA	H1252	ILE	GLY	G411	I737	L612	A494	V407	R311	G181		C70
ALA			ALA	G441	R738	◆	M495	V408				L71
GLY	T1256	G1136	ALA	R842	Q739	L614		W409	R311	I185		K74
GLY	V1257	G1137	SER	R942	L740	P615	I499	D410	T317	I185		K74
ALA			ARG	W843				I411	G318			K76
PRO	L1138	L1138	ALA	T844								

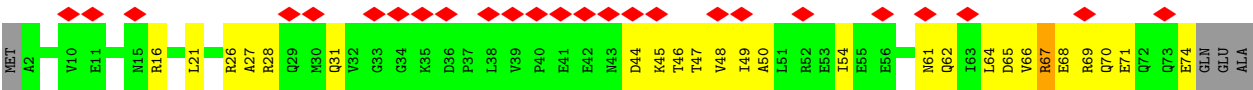


ALA  
ALA  
PRO  
GLN  
VAL  
THR  
ALA  
GLU  
ASP  
SER  
ALA  
SER  
LEU  
ALA  
GLU  
LEU  
LEU  
ASN  
ALA  
GLY  
LEU  
GLY  
GLY  
SER  
SER  
ASP  
ASN  
GLU

● Molecule 6: RNA



● Molecule 7: DNA-directed RNA polymerase subunit omega



ALA  
GLU  
LEU  
GLN  
VAL  
THR  
ALA  
ILE  
ALA  
GLU  
GLY  
ARG  
ARG

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	118450	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.748	Depositor
Minimum map value	-0.393	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	347.28, 347.28, 347.28	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.447, 1.447, 1.447	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	N	0.45	0/341	0.74	0/522
2	T	0.46	0/535	0.90	0/826
3	A	0.24	0/1790	0.55	0/2426
3	B	0.25	0/1794	0.59	0/2432
4	C	0.25	0/10573	0.54	0/14265
5	D	0.25	0/10554	0.56	0/14248
6	R	0.11	0/258	0.65	0/399
7	E	0.24	0/584	0.61	0/786
All	All	0.26	0/26429	0.57	0/35904

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	304	0	167	5	0
2	T	478	0	262	9	0
3	A	1768	0	1793	43	0
3	B	1772	0	1799	66	0
4	C	10407	0	10420	284	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	10397	0	10619	350	0
6	R	232	0	119	3	0
7	E	582	0	593	24	0
8	D	2	0	0	0	0
9	D	1	0	0	0	0
All	All	25943	0	25772	693	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (693) 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:C:812:PHE:CE2	5:D:451:PRO:HB3	1.56	1.40
4:C:812:PHE:CE2	5:D:451:PRO:CB	2.04	1.38
4:C:812:PHE:HE2	5:D:451:PRO:CA	1.64	1.10
4:C:812:PHE:CD2	5:D:451:PRO:HB3	1.91	1.05
5:D:1313:SER:OG	5:D:1325:PHE:CE2	2.16	0.98
4:C:812:PHE:HE2	5:D:451:PRO:CB	1.59	0.96
5:D:356:THR:O	5:D:461:PHE:CE1	2.21	0.94
4:C:812:PHE:CE2	5:D:451:PRO:HB2	2.05	0.91
3:B:182:ARG:HG3	5:D:531:LYS:HG3	1.51	0.90
5:D:1313:SER:OG	5:D:1325:PHE:HE2	1.56	0.86
5:D:583:VAL:HG22	5:D:587:LEU:HD13	1.59	0.83
5:D:93:THR:HB	5:D:97:VAL:HG21	1.60	0.83
4:C:297:VAL:HA	4:C:335:THR:HG22	1.60	0.82
4:C:1075:VAL:CG2	5:D:461:PHE:O	2.29	0.80
5:D:416:ILE:HD11	5:D:439:PRO:HB2	1.63	0.80
4:C:221:LEU:HB3	4:C:336:LEU:HD21	1.65	0.78
4:C:812:PHE:HE2	5:D:451:PRO:HA	1.48	0.78
4:C:1260:GLY:O	4:C:1264:GLN:NE2	2.16	0.78
5:D:365:GLN:HA	5:D:438:GLU:H	1.49	0.77
5:D:514:THR:HG21	5:D:596:LEU:HD12	1.67	0.77
5:D:708:ASN:OD1	5:D:709:ARG:N	2.17	0.76
3:B:83:LEU:HD11	5:D:528:THR:HA	1.66	0.76
3:A:207:THR:HG22	3:A:209:GLY:H	1.49	0.75
3:A:227:GLN:HE22	3:B:35:PHE:HB3	1.51	0.75
5:D:1313:SER:HG	5:D:1325:PHE:HE2	0.81	0.75
3:A:158:ARG:NH2	3:A:173:VAL:O	2.20	0.75
5:D:490:ILE:HD13	5:D:614:LEU:HD11	1.69	0.74
5:D:930:LEU:HD13	5:D:1244:GLN:HG3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:850:LYS:HD2	5:D:852:GLY:H	1.52	0.74
3:A:41:ASN:ND2	4:C:1217:THR:O	2.20	0.73
4:C:677:ASN:HB3	5:D:783:LEU:HD11	1.70	0.73
4:C:812:PHE:CE2	5:D:451:PRO:CA	2.54	0.72
4:C:808:ASN:H	5:D:633:ALA:HB2	1.53	0.72
5:D:370:LYS:HE2	5:D:441:LEU:HB3	1.71	0.72
3:B:41:ASN:HB2	4:C:1216:ARG:HH22	1.55	0.72
4:C:1075:VAL:HG23	5:D:461:PHE:O	1.90	0.72
5:D:1027:VAL:HB	5:D:1122:ALA:HB3	1.71	0.71
4:C:759:SER:HG	4:C:763:THR:HG1	1.30	0.71
5:D:425:ARG:HG2	5:D:427:PRO:HD2	1.73	0.70
5:D:477:GLN:O	5:D:481:ARG:HG3	1.91	0.70
4:C:81:ASP:O	4:C:85:CYS:HB2	1.91	0.69
5:D:910:ASN:OD1	7:E:16:ARG:NH2	2.25	0.69
3:B:191:ARG:HH12	5:D:409:TRP:HB3	1.57	0.69
4:C:332:ARG:NH1	4:C:334:GLU:HG3	2.08	0.69
5:D:97:VAL:HA	5:D:100:GLU:HG3	1.74	0.68
3:B:176:CYS:SG	5:D:535:ARG:NH2	2.67	0.68
4:C:1269:ARG:HA	5:D:346:ARG:HA	1.76	0.68
5:D:1313:SER:HB2	5:D:1325:PHE:CD2	2.29	0.67
3:A:30:PRO:HB3	3:A:198:LEU:HB3	1.76	0.67
5:D:836:ARG:O	5:D:840:LEU:HB2	1.94	0.67
4:C:799:ASN:O	4:C:800:MET:HE2	1.95	0.67
4:C:1115:THR:HG23	4:C:1228:GLY:HA3	1.76	0.66
5:D:146:VAL:O	5:D:156:ARG:NH2	2.28	0.66
4:C:280:ASP:OD1	4:C:281:ASP:N	2.28	0.66
3:B:100:LEU:HD11	3:B:121:VAL:HG21	1.77	0.66
4:C:1314:GLN:OE1	7:E:28:ARG:NH1	2.29	0.66
4:C:65:ASN:HD21	4:C:107:ARG:HH21	1.42	0.66
4:C:1013:GLN:OE1	4:C:1017:GLN:NE2	2.29	0.66
2:T:11:DT:OP1	5:D:332:LYS:NZ	2.28	0.66
3:B:33:ARG:HH21	4:C:1081:PRO:HG3	1.61	0.66
5:D:431:ARG:HE	5:D:493:PRO:HG3	1.61	0.66
5:D:154:LEU:HD12	5:D:158:GLN:HB2	1.78	0.65
5:D:356:THR:O	5:D:461:PHE:CZ	2.49	0.65
5:D:984:LEU:HD23	5:D:992:LYS:HB2	1.77	0.65
3:A:166:ARG:HG3	3:A:170:ARG:NH1	2.11	0.65
4:C:806:PRO:HD2	5:D:636:GLY:HA2	1.78	0.65
3:B:35:PHE:O	3:B:38:THR:OG1	2.11	0.65
5:D:1106:ILE:HB	5:D:1123:ARG:HB2	1.79	0.65
4:C:71:VAL:HG13	4:C:72:SER:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:812:PHE:CZ	5:D:451:PRO:HB2	2.32	0.65
4:C:1017:GLN:O	4:C:1021:LEU:HG	1.97	0.65
3:B:41:ASN:HB2	4:C:1216:ARG:NH2	2.12	0.64
5:D:210:SER:HB2	5:D:213:LYS:HB2	1.78	0.64
1:N:18:DT:H4'	5:D:133:ARG:HH12	1.60	0.64
4:C:700:VAL:HG13	4:C:1117:LEU:HD23	1.79	0.64
7:E:67:ARG:NH1	7:E:68:GLU:HG3	2.13	0.64
4:C:1289:GLU:OE1	4:C:1315:MET:HE3	1.97	0.64
3:B:44:ARG:CZ	5:D:538:ARG:HE	2.09	0.64
4:C:471:VAL:HG11	4:C:498:ILE:HD11	1.79	0.64
4:C:811:ASN:ND2	4:C:1098:LEU:O	2.31	0.64
4:C:39:ILE:HD11	4:C:75:LEU:HD11	1.80	0.63
3:B:8:PHE:CD1	3:B:35:PHE:HE2	2.16	0.63
4:C:231:GLU:OE1	4:C:238:GLN:NE2	2.31	0.63
4:C:105:TYR:HA	4:C:113:THR:HA	1.80	0.63
4:C:811:ASN:HA	4:C:815:SER:HB3	1.80	0.63
5:D:968:ASN:HD21	5:D:972:LYS:HB2	1.63	0.63
4:C:1338:GLU:HG2	4:C:1339:LEU:H	1.63	0.63
5:D:872:LEU:HD11	5:D:880:VAL:HG21	1.78	0.63
5:D:755:ILE:HG22	5:D:757:THR:H	1.64	0.63
5:D:826:ILE:HB	5:D:994:SER:HB2	1.80	0.63
5:D:804:ALA:HA	5:D:1259:GLN:HG2	1.81	0.63
5:D:814:CYS:SG	5:D:883:ARG:NH2	2.72	0.62
5:D:518:VAL:HB	5:D:709:ARG:HD3	1.79	0.62
4:C:212:ALA:HA	4:C:359:ARG:HG3	1.79	0.62
5:D:1313:SER:CB	5:D:1325:PHE:CD2	2.82	0.62
5:D:218:THR:HA	5:D:221:ILE:HG12	1.80	0.62
4:C:1185:PRO:HB2	4:C:1188:ASP:OD1	2.00	0.62
5:D:80:HIS:CD2	5:D:83:VAL:HG11	2.35	0.62
5:D:26:SER:HB3	5:D:29:MET:HG3	1.80	0.62
5:D:85:CYS:SG	5:D:86:GLU:N	2.73	0.62
3:B:33:ARG:NH2	4:C:1081:PRO:HG3	2.15	0.62
5:D:955:LYS:HE3	5:D:1010:GLN:HE21	1.64	0.62
5:D:342:LEU:HD12	5:D:1352:ILE:HG23	1.81	0.62
5:D:533:ALA:HB1	5:D:574:VAL:HG13	1.81	0.62
4:C:521:LEU:HD11	4:C:664:GLY:HA2	1.81	0.61
3:B:195:ARG:HD3	3:B:198:LEU:HD13	1.82	0.61
4:C:841:ARG:HG2	4:C:1046:VAL:HG12	1.81	0.61
5:D:957:SER:N	5:D:985:ILE:O	2.26	0.61
5:D:974:VAL:HG11	5:D:1118:GLY:HA3	1.82	0.61
4:C:1075:VAL:HG21	5:D:461:PHE:O	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:81:ASP:O	4:C:85:CYS:CB	2.48	0.61
5:D:1028:ILE:HG21	5:D:1118:GLY:HA2	1.83	0.61
3:A:124:VAL:HG21	3:A:209:GLY:HA3	1.82	0.61
1:N:14:DC:OP1	5:D:1151:LYS:NZ	2.33	0.61
3:A:91:ARG:HE	3:A:210:THR:HA	1.66	0.60
4:C:1032:LYS:O	4:C:1036:ILE:HG12	2.01	0.60
2:T:11:DT:OP1	5:D:311:ARG:NH2	2.34	0.60
3:A:152:TYR:CE2	3:A:154:PRO:HG3	2.35	0.60
4:C:593:LYS:HB3	4:C:602:GLU:HG3	1.82	0.60
5:D:1058:SER:OG	5:D:1108:GLN:OE1	2.18	0.60
4:C:722:GLY:HA3	4:C:736:VAL:HA	1.83	0.60
5:D:841:GLY:HA3	5:D:901:ARG:HG2	1.82	0.60
3:B:107:ILE:HG13	3:B:136:GLU:HG2	1.83	0.60
4:C:233:ARG:NH2	4:C:236:LYS:O	2.35	0.60
5:D:54:ASP:HB3	5:D:60:ARG:HH22	1.66	0.60
4:C:292:ILE:HG21	4:C:322:LEU:HD21	1.83	0.60
5:D:355:ILE:HG22	5:D:447:ILE:HB	1.82	0.60
5:D:367:GLY:HA3	5:D:448:GLN:HB2	1.82	0.60
3:A:45:ARG:NH2	4:C:1084:ASP:OD1	2.33	0.60
3:A:153:VAL:O	3:A:158:ARG:NH1	2.35	0.60
5:D:356:THR:O	5:D:461:PHE:HE1	1.83	0.60
4:C:391:SER:OG	4:C:393:ASP:OD1	2.20	0.59
4:C:758:ARG:NH1	4:C:759:SER:O	2.35	0.59
4:C:1290:MET:HG3	5:D:347:VAL:HG11	1.83	0.59
5:D:390:LEU:HD22	5:D:407:VAL:HG11	1.84	0.59
4:C:52:ALA:O	4:C:56:VAL:HG22	2.01	0.59
4:C:972:PHE:HA	4:C:975:ILE:HG12	1.83	0.59
4:C:1081:PRO:HD2	4:C:1084:ASP:HB2	1.84	0.59
3:A:166:ARG:HG3	3:A:170:ARG:HH12	1.67	0.59
5:D:51:PRO:HD2	5:D:71:LEU:HD11	1.84	0.59
5:D:805:GLN:HE22	5:D:1348:LYS:HB2	1.67	0.59
4:C:1122:LYS:HG2	4:C:1229:TYR:CZ	2.38	0.59
5:D:144:TYR:HB2	5:D:160:LEU:HB3	1.85	0.59
4:C:838:CYS:HB3	4:C:1050:VAL:HB	1.85	0.58
4:C:1211:ARG:NE	4:C:1220:GLN:OE1	2.36	0.58
5:D:384:LYS:HD3	5:D:387:LEU:HD21	1.85	0.58
3:B:59:VAL:HG21	3:B:85:LEU:HD13	1.85	0.58
4:C:672:GLU:OE2	5:D:767:LEU:N	2.23	0.58
4:C:8:LYS:HA	4:C:11:ILE:HD11	1.85	0.58
4:C:243:PRO:HA	4:C:246:LEU:HG	1.84	0.58
5:D:367:GLY:N	5:D:448:GLN:O	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:534:GLU:HB3	5:D:578:ILE:HG12	1.85	0.58
7:E:31:GLN:HG2	7:E:46:THR:HG21	1.86	0.58
4:C:180:ARG:NH2	4:C:393:ASP:O	2.36	0.58
5:D:404:GLU:HA	5:D:408:VAL:HG21	1.84	0.58
5:D:412:LEU:HG	5:D:441:LEU:HD11	1.85	0.58
4:C:722:GLY:H	4:C:777:VAL:HG23	1.69	0.58
4:C:844:LYS:HE2	5:D:49:PHE:HE2	1.68	0.58
3:A:42:ALA:O	3:A:46:ILE:HG12	2.03	0.57
3:B:19:VAL:HG12	3:B:21:SER:H	1.69	0.57
4:C:866:ASP:OD2	4:C:944:ARG:NH1	2.36	0.57
4:C:366:ILE:O	4:C:370:MET:HG3	2.05	0.57
4:C:1271:GLY:N	4:C:1274:GLU:OE1	2.36	0.57
5:D:245:LEU:HD12	5:D:246:PRO:HD2	1.86	0.57
5:D:1153:PRO:O	5:D:1194:ARG:NH1	2.37	0.57
3:B:192:VAL:HG23	3:B:195:ARG:HH21	1.69	0.57
5:D:584:PRO:HG2	5:D:587:LEU:HD11	1.86	0.57
4:C:1313:HIS:HD2	5:D:474:LEU:HB2	1.69	0.57
2:T:3:DG:N3	2:T:4:DT:N3	2.52	0.57
4:C:38:PHE:HB2	4:C:457:GLY:HA2	1.86	0.57
4:C:803:ALA:HB2	4:C:1227:VAL:HG23	1.87	0.57
5:D:147:ILE:HA	5:D:156:ARG:HH22	1.68	0.57
4:C:301:TYR:HH	4:C:334:GLU:H	1.51	0.57
4:C:1246:ARG:HH11	4:C:1266:GLY:HA2	1.69	0.57
5:D:213:LYS:O	5:D:217:LEU:HG	2.05	0.57
2:T:18:DG:H3'	2:T:19:DT:H5''	1.87	0.57
5:D:245:LEU:HD11	5:D:249:LEU:HD23	1.87	0.57
5:D:885:VAL:HG13	5:D:894:VAL:HG11	1.85	0.57
5:D:823:THR:O	5:D:838:ARG:NH1	2.37	0.57
3:B:61:ILE:HB	3:B:64:VAL:HB	1.87	0.56
4:C:1240:ASP:O	4:C:1262:LYS:NZ	2.37	0.56
5:D:1178:THR:HA	5:D:1184:ASP:HB3	1.85	0.56
5:D:1252:HIS:O	5:D:1256:ILE:HG12	2.04	0.56
3:A:104:LYS:HG2	3:A:110:VAL:HG22	1.86	0.56
3:B:181:GLU:HB3	5:D:531:LYS:HD3	1.87	0.56
4:C:1331:ARG:HG3	5:D:33:TRP:CZ3	2.40	0.56
5:D:264:ASP:OD2	5:D:325:LYS:NZ	2.29	0.56
5:D:850:LYS:HD2	5:D:852:GLY:N	2.19	0.56
5:D:686:TRP:CG	5:D:758:PRO:HG2	2.40	0.56
5:D:737:ILE:HD13	5:D:740:LEU:HD12	1.86	0.56
5:D:986:ASP:OD1	5:D:990:ARG:N	2.39	0.56
5:D:114:ILE:HD11	5:D:304:ASP:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:357:VAL:HG22	5:D:461:PHE:CE2	2.40	0.56
5:D:481:ARG:HH22	7:E:45:LYS:HZ1	1.52	0.56
5:D:972:LYS:HB3	5:D:1002:VAL:HG13	1.88	0.56
3:B:74:VAL:HG12	3:B:76:GLU:H	1.70	0.56
5:D:686:TRP:CD2	5:D:758:PRO:HG2	2.41	0.56
4:C:66:SER:HB2	4:C:479:LEU:HD11	1.88	0.56
4:C:731:ARG:NH2	4:C:962:GLU:OE2	2.38	0.56
5:D:66:LYS:HG3	5:D:69:GLU:HB2	1.87	0.56
5:D:80:HIS:NE2	5:D:83:VAL:HG11	2.21	0.56
5:D:1313:SER:CB	5:D:1325:PHE:CE2	2.89	0.56
4:C:245:ARG:HB3	4:C:337:PHE:CZ	2.41	0.55
4:C:798:GLN:NE2	4:C:827:ARG:O	2.39	0.55
3:B:65:LEU:HA	3:B:169:GLY:HA2	1.88	0.55
4:C:230:PHE:CE2	4:C:335:THR:HG21	2.40	0.55
5:D:609:TYR:HB2	5:D:617:THR:HG21	1.88	0.55
5:D:699:ASP:OD1	5:D:702:GLN:NE2	2.37	0.55
4:C:317:LEU:HA	4:C:321:LEU:HD12	1.88	0.55
3:B:37:HIS:O	4:C:1216:ARG:NH2	2.39	0.55
4:C:413:GLU:HG3	4:C:415:GLU:H	1.70	0.55
4:C:964:LEU:HA	4:C:967:LEU:HG	1.88	0.55
4:C:672:GLU:CD	5:D:767:LEU:H	2.08	0.55
4:C:1291:LEU:HA	5:D:345:LYS:HD2	1.88	0.55
3:B:37:HIS:CE1	4:C:1216:ARG:HE	2.25	0.55
3:B:174:ASP:OD1	3:B:174:ASP:N	2.40	0.55
4:C:174:ALA:HB2	4:C:432:LEU:HD13	1.89	0.55
5:D:91:GLU:OE1	5:D:101:ARG:NH2	2.37	0.55
5:D:1263:LYS:NZ	5:D:1315:ALA:O	2.33	0.55
4:C:521:LEU:HD23	4:C:686:GLN:HG2	1.89	0.55
5:D:481:ARG:HH12	7:E:45:LYS:HZ1	1.54	0.55
4:C:802:VAL:HG23	4:C:1098:LEU:HD13	1.88	0.55
5:D:424:ASN:N	5:D:467:ALA:O	2.36	0.55
5:D:697:MET:HE1	5:D:738:ARG:HA	1.89	0.55
5:D:975:ILE:HD13	5:D:980:THR:HG21	1.89	0.55
7:E:44:ASP:HB3	7:E:48:VAL:HB	1.88	0.55
4:C:93:SER:HA	4:C:128:PRO:HA	1.89	0.54
5:D:1028:ILE:HD13	5:D:1118:GLY:HA2	1.88	0.54
5:D:1206:ARG:HH21	5:D:1223:LEU:HD23	1.71	0.54
5:D:842:ARG:HB3	5:D:882:VAL:HG21	1.89	0.54
4:C:272:ARG:O	4:C:275:ARG:HG3	2.07	0.54
5:D:69:GLU:OE1	5:D:76:LYS:HG3	2.06	0.54
4:C:93:SER:OG	4:C:126:GLU:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:510:LEU:HD22	5:D:601:ILE:HD12	1.89	0.54
4:C:143:ARG:NH2	4:C:512:SER:O	2.41	0.54
5:D:74:LYS:HE3	5:D:86:GLU:HG3	1.90	0.54
3:B:8:PHE:CG	3:B:35:PHE:HE2	2.26	0.54
4:C:1275:VAL:HG13	4:C:1287:LEU:HD11	1.89	0.54
5:D:1313:SER:OG	5:D:1325:PHE:CD2	2.52	0.54
5:D:812:ASP:O	5:D:897:HIS:ND1	2.40	0.54
7:E:65:ASP:OD1	7:E:69:ARG:NH2	2.34	0.54
4:C:33:ASP:OD1	4:C:34:SER:N	2.40	0.54
4:C:1002:LEU:HD21	4:C:1007:LYS:HG3	1.90	0.54
5:D:429:LEU:HD11	5:D:925:GLU:HA	1.90	0.54
3:B:212:ASP:OD1	3:B:213:PRO:HD2	2.08	0.53
5:D:211:GLU:O	5:D:215:LYS:HE2	2.09	0.53
5:D:615:LYS:HB2	5:D:616:PRO:HD3	1.90	0.53
5:D:591:ILE:O	5:D:594:GLN:NE2	2.42	0.53
5:D:733:SER:H	5:D:736:GLN:HB3	1.73	0.53
5:D:863:LEU:HD13	5:D:908:ILE:HG13	1.91	0.53
5:D:978:ARG:HG2	5:D:999:TYR:HB2	1.91	0.53
4:C:1102:GLY:HA2	4:C:1106:ARG:HH21	1.74	0.53
5:D:368:LEU:HD22	5:D:373:ALA:HB2	1.91	0.53
5:D:481:ARG:NH2	7:E:45:LYS:HZ1	2.07	0.53
5:D:967:VAL:HG22	5:D:973:LEU:HD21	1.89	0.53
2:T:22:DG:O6	6:R:1:C:N4	2.39	0.53
4:C:50:GLU:HG2	4:C:73:TYR:HE1	1.74	0.53
4:C:446:ASP:O	4:C:451:ARG:NH2	2.42	0.53
4:C:820:GLU:O	4:C:824:GLN:HG2	2.09	0.53
5:D:416:ILE:CD1	5:D:439:PRO:HB2	2.36	0.53
5:D:663:GLU:O	5:D:666:GLU:HG3	2.08	0.53
7:E:61:ASN:OD1	7:E:62:GLN:N	2.41	0.53
4:C:732:ILE:HG21	4:C:783:LEU:HD23	1.91	0.53
5:D:885:VAL:HG12	5:D:1258:ARG:HD2	1.90	0.52
4:C:71:VAL:HG13	4:C:72:SER:N	2.24	0.52
5:D:211:GLU:HG2	5:D:215:LYS:NZ	2.25	0.52
5:D:679:TYR:OH	5:D:754:ILE:O	2.23	0.52
5:D:1163:VAL:HG22	5:D:1177:ILE:HG12	1.92	0.52
4:C:517:GLN:HG3	4:C:759:SER:HB2	1.90	0.52
3:B:37:HIS:CD2	4:C:1216:ARG:HH21	2.27	0.52
5:D:413:ASP:O	5:D:416:ILE:HG22	2.09	0.52
5:D:582:ILE:O	5:D:582:ILE:HG13	2.09	0.52
4:C:211:ARG:NH2	4:C:217:THR:OG1	2.36	0.52
4:C:378:ARG:NH2	4:C:379:GLU:OE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:802:VAL:O	4:C:1228:GLY:N	2.41	0.52
4:C:876:GLU:OE1	4:C:927:THR:OG1	2.26	0.52
4:C:976:ARG:HA	4:C:979:LEU:HG	1.92	0.52
5:D:675:ALA:HA	5:D:678:ARG:HG2	1.91	0.52
3:A:182:ARG:HB2	4:C:1091:GLY:O	2.10	0.52
4:C:864:LYS:NZ	4:C:881:ASP:OD2	2.43	0.52
4:C:1242:LYS:HG2	5:D:465:GLN:HE21	1.75	0.52
4:C:1313:HIS:CD2	5:D:474:LEU:HB2	2.45	0.52
5:D:644:MET:O	5:D:764:ARG:NH1	2.43	0.52
5:D:1361:THR:HG23	7:E:21:LEU:HD21	1.91	0.52
7:E:64:LEU:O	7:E:67:ARG:NH1	2.43	0.52
3:A:225:ALA:HB2	3:B:228:LEU:HB3	1.91	0.52
5:D:1322:ALA:HB1	5:D:1331:VAL:HG11	1.91	0.52
3:B:87:GLY:O	3:B:128:HIS:NE2	2.43	0.51
4:C:971:LEU:HD22	4:C:974:ARG:NH1	2.25	0.51
4:C:1288:GLN:NE2	4:C:1292:THR:OG1	2.42	0.51
3:B:86:LYS:NZ	3:B:174:ASP:OD2	2.42	0.51
4:C:930:ASP:OD1	4:C:1053:TYR:HB2	2.09	0.51
5:D:65:VAL:HG12	5:D:98:ARG:NH1	2.25	0.51
5:D:1137:GLY:H	5:D:1140:ARG:HB3	1.74	0.51
3:B:8:PHE:CD1	3:B:35:PHE:CE2	2.97	0.51
4:C:102:LEU:HD23	4:C:117:ILE:HD11	1.92	0.51
5:D:1067:ARG:HH11	5:D:1072:LYS:HE2	1.76	0.51
4:C:9:LYS:O	4:C:1175:ASN:ND2	2.44	0.51
5:D:481:ARG:NH1	7:E:45:LYS:HZ1	2.09	0.51
4:C:34:SER:HG	4:C:457:GLY:H	1.59	0.51
5:D:1145:PHE:HB3	5:D:1309:ILE:HD11	1.93	0.51
4:C:33:ASP:O	4:C:36:GLN:HG3	2.10	0.51
5:D:826:ILE:HG21	5:D:993:GLU:HA	1.93	0.51
4:C:358:ASP:N	4:C:358:ASP:OD1	2.44	0.51
4:C:588:GLU:OE2	4:C:606:LEU:N	2.44	0.51
4:C:595:THR:OG1	4:C:598:VAL:O	2.23	0.51
4:C:812:PHE:CE2	5:D:451:PRO:HA	2.37	0.51
4:C:1148:ALA:HA	4:C:1151:LEU:HD23	1.92	0.51
3:B:77:ASP:OD1	3:B:78:ILE:N	2.39	0.50
4:C:225:PHE:CE2	4:C:347:ILE:HB	2.47	0.50
4:C:633:LEU:HD11	4:C:644:LEU:HD13	1.93	0.50
4:C:697:LYS:HD2	4:C:1181:PRO:HG3	1.92	0.50
5:D:530:PRO:HB2	5:D:581:MET:HE3	1.94	0.50
4:C:976:ARG:O	4:C:980:VAL:HG23	2.12	0.50
4:C:1134:GLN:NE2	4:C:1136:GLN:HB2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:64:LEU:O	7:E:67:ARG:HD3	2.11	0.50
3:A:227:GLN:NE2	3:B:35:PHE:HB3	2.23	0.50
3:B:191:ARG:HA	3:B:195:ARG:HD2	1.92	0.50
4:C:592:ARG:HG3	4:C:655:VAL:HG22	1.93	0.50
5:D:530:PRO:HB3	5:D:577:ALA:HB1	1.93	0.50
4:C:971:LEU:HD22	4:C:974:ARG:HH12	1.77	0.50
4:C:1143:GLU:OE1	4:C:1147:ARG:NH1	2.44	0.50
4:C:1283:ALA:HB1	4:C:1286:THR:HG22	1.94	0.50
5:D:474:LEU:HD21	7:E:27:ALA:HB1	1.94	0.49
2:T:23:DG:N2	6:R:1:C:O2	2.44	0.49
7:E:45:LYS:HE3	7:E:47:THR:HB	1.94	0.49
5:D:1221:LEU:HD13	5:D:1229:VAL:HG11	1.94	0.49
3:A:45:ARG:NH2	4:C:1216:ARG:HA	2.28	0.49
4:C:844:LYS:HE2	5:D:49:PHE:CE2	2.47	0.49
4:C:1298:VAL:O	4:C:1301:ARG:HG2	2.12	0.49
5:D:964:LYS:HD2	5:D:977:SER:HB3	1.94	0.49
5:D:749:LYS:HD3	5:D:753:SER:HB2	1.95	0.49
3:A:43:LEU:HD13	3:A:217:ILE:HD11	1.95	0.49
4:C:239:MET:HG3	4:C:287:VAL:HG11	1.95	0.49
5:D:612:LEU:HD21	5:D:616:PRO:HG2	1.94	0.49
5:D:1286:LYS:HA	5:D:1289:ASN:HD21	1.78	0.49
4:C:452:ARG:NH2	4:C:458:GLU:OE1	2.46	0.49
4:C:618:GLN:OE1	4:C:635:THR:OG1	2.30	0.49
5:D:188:LEU:O	5:D:192:MET:HE2	2.13	0.49
5:D:217:LEU:O	5:D:221:ILE:HG23	2.13	0.49
3:A:33:ARG:HH22	3:A:196:THR:HB	1.77	0.49
4:C:338:THR:HG22	4:C:345:PRO:HB3	1.94	0.49
5:D:86:GLU:OE2	5:D:87:LYS:HG3	2.13	0.49
4:C:247:ARG:NH2	4:C:342:ASP:OD1	2.46	0.48
5:D:413:ASP:HA	5:D:416:ILE:HG22	1.94	0.48
5:D:54:ASP:H	5:D:60:ARG:HH12	1.60	0.48
4:C:225:PHE:HB2	4:C:336:LEU:HD22	1.95	0.48
4:C:804:PHE:HE1	4:C:1098:LEU:HD22	1.78	0.48
4:C:946:LEU:O	4:C:949:GLU:HG2	2.12	0.48
5:D:317:THR:HG22	5:D:319:SER:H	1.78	0.48
5:D:552:ILE:HG22	5:D:553:THR:N	2.28	0.48
5:D:1373:ARG:HG2	5:D:1373:ARG:HH11	1.78	0.48
5:D:951:GLN:O	5:D:995:TYR:OH	2.25	0.48
5:D:1189:MET:HG3	5:D:1189:MET:O	2.13	0.48
5:D:844:THR:HA	5:D:882:VAL:HA	1.94	0.48
5:D:850:LYS:N	5:D:855:ASP:O	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:345:PRO:HB2	4:C:348:SER:HB3	1.95	0.48
4:C:521:LEU:HD22	4:C:667:LEU:HD22	1.95	0.48
4:C:528:ARG:NH2	4:C:575:LEU:O	2.47	0.48
3:B:197:ASP:OD1	3:B:197:ASP:N	2.42	0.48
4:C:1217:THR:OG1	4:C:1219:GLU:OE1	2.25	0.48
4:C:1223:ARG:NH2	5:D:721:SER:OG	2.46	0.48
4:C:314:ASN:HD22	4:C:351:LEU:HB3	1.78	0.48
5:D:886:VAL:HA	5:D:1258:ARG:HG3	1.96	0.48
4:C:154:GLY:N	4:C:177:ILE:O	2.47	0.48
5:D:22:ILE:O	5:D:1339:GLY:HA2	2.14	0.48
3:A:111:THR:HG23	3:A:113:ALA:H	1.79	0.48
3:B:92:VAL:HG13	3:B:95:LYS:HG3	1.96	0.48
4:C:1019:ASP:O	4:C:1023:HIS:ND1	2.47	0.48
5:D:68:TYR:HE1	5:D:93:THR:O	1.96	0.48
5:D:759:ILE:HD12	5:D:771:GLN:HB3	1.95	0.48
4:C:339:ASN:HB3	4:C:343:HIS:H	1.79	0.47
5:D:23:ALA:HB1	5:D:232:ASN:HD21	1.78	0.47
5:D:423:LEU:HA	5:D:468:VAL:HA	1.95	0.47
5:D:816:THR:OG1	5:D:883:ARG:NH2	2.43	0.47
3:B:29:GLU:HB2	3:B:30:PRO:HD3	1.95	0.47
5:D:42:GLU:HB2	5:D:52:GLU:HG2	1.96	0.47
5:D:650:LYS:O	5:D:653:ILE:HG22	2.14	0.47
5:D:805:GLN:OE1	5:D:1348:LYS:N	2.40	0.47
7:E:45:LYS:O	7:E:49:ILE:HD12	2.14	0.47
3:B:45:ARG:HG2	5:D:538:ARG:HH22	1.80	0.47
4:C:390:PHE:HA	4:C:419:ILE:HD12	1.96	0.47
4:C:802:VAL:N	4:C:1228:GLY:O	2.40	0.47
5:D:528:THR:OG1	5:D:532:GLU:HG3	2.15	0.47
5:D:563:LEU:HD23	5:D:563:LEU:H	1.79	0.47
4:C:275:ARG:O	4:C:278:GLU:HG3	2.14	0.47
5:D:254:PRO:HA	5:D:260:PHE:HA	1.96	0.47
3:B:83:LEU:HD12	5:D:528:THR:HG22	1.96	0.47
3:B:112:ALA:HB3	3:B:126:PRO:HA	1.96	0.47
4:C:185:ASP:OD2	4:C:200:ARG:NE	2.48	0.47
5:D:409:TRP:HA	5:D:409:TRP:CE3	2.48	0.47
5:D:993:GLU:HB3	5:D:995:TYR:HE1	1.79	0.47
5:D:25:ALA:HB1	5:D:30:ILE:HD11	1.96	0.47
5:D:220:ARG:O	5:D:224:LEU:HD23	2.14	0.47
5:D:744:ARG:NH2	5:D:767:LEU:HD11	2.29	0.47
5:D:973:LEU:HB2	5:D:1003:LEU:HB3	1.96	0.47
4:C:6:THR:HG21	4:C:781:ASP:OD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:210:LEU:HD21	4:C:429:MET:SD	2.54	0.47
4:C:714:VAL:HB	4:C:787:PRO:HD2	1.97	0.47
4:C:57:PHE:CE1	4:C:468:LEU:HD21	2.49	0.47
4:C:316:GLU:OE2	4:C:352:ARG:NH2	2.48	0.47
4:C:813:GLU:OE2	5:D:460:ASP:HA	2.14	0.47
5:D:892:PHE:HZ	5:D:1284:ARG:HH22	1.63	0.47
4:C:788:SER:HB2	4:C:796:LEU:HA	1.97	0.47
4:C:1244:HIS:NE2	4:C:1266:GLY:O	2.40	0.47
4:C:673:HIS:O	4:C:1109:ILE:HG22	2.15	0.47
3:B:156:SER:HA	3:B:159:ILE:HG22	1.97	0.46
4:C:941:LYS:HB3	4:C:945:ALA:HB3	1.97	0.46
4:C:1010:GLN:O	4:C:1013:GLN:HG3	2.14	0.46
5:D:1230:THR:HA	5:D:1233:ILE:HG22	1.97	0.46
3:A:83:LEU:HD22	4:C:694:ARG:HH22	1.79	0.46
4:C:221:LEU:HD13	4:C:336:LEU:HD11	1.96	0.46
4:C:699:LEU:HD11	4:C:799:ASN:HD22	1.79	0.46
5:D:955:LYS:HD2	5:D:1011:VAL:O	2.15	0.46
3:B:191:ARG:HH22	5:D:409:TRP:HB3	1.80	0.46
5:D:185:ILE:O	5:D:189:LEU:HD23	2.15	0.46
5:D:369:PRO:HD3	5:D:447:ILE:HD13	1.98	0.46
5:D:1327:GLU:OE2	5:D:1330:ARG:NH1	2.49	0.46
3:B:207:THR:HG23	3:B:213:PRO:HG3	1.97	0.46
4:C:119:GLU:HB2	4:C:489:PRO:HG2	1.98	0.46
4:C:415:GLU:HG3	4:C:416:GLY:H	1.81	0.46
5:D:18:ASP:N	5:D:18:ASP:OD1	2.48	0.46
5:D:849:LEU:H	5:D:849:LEU:HD23	1.80	0.46
4:C:1270:PHE:CE1	4:C:1274:GLU:HG2	2.51	0.46
4:C:1082:ILE:HG23	4:C:1093:PRO:HG2	1.98	0.46
4:C:231:GLU:HB2	4:C:238:GLN:HE21	1.79	0.46
4:C:930:ASP:OD1	4:C:930:ASP:N	2.48	0.46
5:D:493:PRO:HA	5:D:903:LEU:HB3	1.98	0.46
5:D:751:ASP:OD1	5:D:752:GLY:N	2.48	0.46
3:A:95:LYS:HD2	3:A:95:LYS:HA	1.73	0.46
3:B:29:GLU:HA	3:B:200:LYS:HG3	1.97	0.46
3:B:102:LEU:HB2	3:B:115:ILE:HG12	1.97	0.46
3:B:152:TYR:CZ	5:D:536:LEU:HD11	2.50	0.46
4:C:93:SER:HB3	4:C:126:GLU:OE1	2.16	0.46
4:C:148:GLN:OE1	4:C:150:HIS:HB3	2.16	0.46
5:D:330:MET:O	5:D:336:GLY:HA2	2.15	0.46
5:D:1109:LEU:HD23	5:D:1113:VAL:HB	1.97	0.46
7:E:67:ARG:HA	7:E:70:GLN:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:18:GLN:NE2	3:A:20:SER:O	2.48	0.46
4:C:1088:ASP:OD1	4:C:1088:ASP:N	2.49	0.46
4:C:1247:SER:HA	5:D:349:TYR:HA	1.98	0.46
5:D:407:VAL:HA	5:D:410:ASP:OD2	2.16	0.46
2:T:21:DC:H4'	2:T:22:DG:OP1	2.16	0.46
5:D:120:LEU:HD12	5:D:1330:ARG:HH21	1.80	0.46
5:D:259:ARG:HE	5:D:260:PHE:H	1.64	0.46
5:D:735:ALA:HA	5:D:738:ARG:HH11	1.81	0.46
5:D:865:HIS:CE1	5:D:867:GLN:HB3	2.51	0.46
3:A:194:GLN:OE1	3:A:194:GLN:N	2.49	0.45
4:C:593:LYS:HD2	4:C:652:TYR:HE1	1.81	0.45
5:D:201:LEU:HD11	5:D:220:ARG:NH1	2.32	0.45
5:D:285:LEU:HD23	5:D:285:LEU:H	1.80	0.45
5:D:684:ASP:OD1	5:D:685:ILE:N	2.49	0.45
1:N:17:DA:H2	2:T:7:DT:H3	1.62	0.45
3:A:28:LEU:HB2	3:A:201:LEU:HB3	1.97	0.45
3:A:45:ARG:HH21	4:C:1216:ARG:HA	1.79	0.45
4:C:516:ASP:OD1	4:C:516:ASP:N	2.48	0.45
5:D:1164:SER:HA	5:D:1200:GLU:HG2	1.98	0.45
4:C:828:PHE:HB3	4:C:1060:ILE:HD11	1.97	0.45
5:D:580:TRP:O	5:D:583:VAL:HG12	2.16	0.45
7:E:50:ALA:O	7:E:54:ILE:HG12	2.17	0.45
5:D:200:GLN:O	5:D:204:GLU:HG2	2.17	0.45
5:D:772:TYR:O	5:D:776:THR:OG1	2.27	0.45
5:D:1271:SER:OG	5:D:1298:VAL:O	2.30	0.45
4:C:153:PRO:HG2	4:C:179:TYR:HD1	1.82	0.45
4:C:706:ARG:HG3	4:C:793:GLU:HG2	1.99	0.45
4:C:1105:SER:HB2	5:D:731:ARG:HH11	1.82	0.45
3:A:152:TYR:CZ	3:A:154:PRO:HG3	2.52	0.45
4:C:395:TYR:HE2	4:C:420:LEU:H	1.64	0.45
5:D:115:TRP:CZ2	5:D:1329:THR:HG22	2.52	0.45
5:D:1044:GLN:O	5:D:1045:THR:HG22	2.17	0.45
7:E:71:GLU:HA	7:E:74:GLU:HG2	1.99	0.45
3:A:11:PRO:HA	3:A:29:GLU:HB2	1.99	0.45
5:D:370:LYS:HG2	5:D:409:TRP:CZ3	2.51	0.45
3:A:58:GLU:CD	3:A:170:ARG:HH21	2.20	0.45
4:C:1051:LYS:HD3	4:C:1053:TYR:CE1	2.52	0.45
5:D:1285:VAL:O	5:D:1289:ASN:ND2	2.50	0.45
3:B:31:LEU:O	3:B:198:LEU:HD23	2.17	0.45
4:C:82:VAL:O	4:C:86:GLN:HG3	2.17	0.45
5:D:29:MET:SD	5:D:30:ILE:HG13	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:842:ARG:HA	5:D:900:GLY:HA3	1.99	0.45
3:A:150:ARG:HB2	3:B:5:VAL:HG23	1.97	0.44
3:B:29:GLU:HG2	3:B:200:LYS:HD2	1.99	0.44
4:C:176:ILE:HD11	4:C:428:VAL:HG11	2.00	0.44
4:C:696:ASP:O	4:C:795:ALA:HB1	2.17	0.44
3:B:195:ARG:HB2	3:B:198:LEU:HD13	2.00	0.44
4:C:186:PHE:CE2	4:C:429:MET:HG2	2.52	0.44
4:C:1280:ALA:HB1	5:D:918:ILE:HD13	2.00	0.44
1:N:16:DC:H2''	1:N:17:DA:C8	2.52	0.44
4:C:675:ASP:HB3	4:C:678:ARG:HG2	2.00	0.44
4:C:359:ARG:NH1	4:C:382:GLU:OE1	2.51	0.44
4:C:560:PRO:HB2	5:D:776:THR:HG21	2.00	0.44
4:C:578:TYR:HB3	4:C:590:PRO:HG2	2.00	0.44
4:C:937:ASP:OD1	4:C:937:ASP:N	2.50	0.44
5:D:551:ARG:HG2	5:D:569:LEU:HB3	1.99	0.44
5:D:116:PHE:HB3	5:D:124:ILE:HG13	1.98	0.44
3:A:219:ARG:HA	3:A:222:THR:HG22	1.98	0.44
4:C:642:SER:HB2	5:D:770:LEU:HD11	1.98	0.44
4:C:1331:ARG:HG2	5:D:102:MET:HE1	1.99	0.44
5:D:1350:ASN:HA	5:D:1353:VAL:HG22	2.00	0.44
4:C:803:ALA:HA	4:C:1227:VAL:HA	2.00	0.44
4:C:1270:PHE:HA	4:C:1274:GLU:OE1	2.16	0.44
5:D:319:SER:OG	5:D:320:ASN:N	2.48	0.44
4:C:521:LEU:HD12	4:C:521:LEU:HA	1.85	0.44
3:B:158:ARG:NH1	3:B:173:VAL:O	2.51	0.44
4:C:225:PHE:CZ	4:C:345:PRO:HA	2.53	0.44
4:C:269:ILE:HG23	4:C:273:HIS:HB2	2.00	0.44
4:C:314:ASN:ND2	4:C:351:LEU:HB3	2.33	0.44
5:D:36:GLY:HA3	5:D:61:ILE:HG12	1.99	0.44
5:D:167:ASP:O	5:D:170:GLU:HG3	2.17	0.44
3:A:61:ILE:HB	3:A:64:VAL:HB	2.00	0.43
3:B:156:SER:O	3:B:160:HIS:ND1	2.43	0.43
3:B:191:ARG:NH1	5:D:409:TRP:HB3	2.30	0.43
4:C:65:ASN:ND2	4:C:107:ARG:HH21	2.12	0.43
4:C:565:GLU:HA	4:C:569:ILE:HG12	1.98	0.43
4:C:1333:LEU:HG	4:C:1334:GLY:H	1.83	0.43
5:D:112:ALA:HA	5:D:238:ILE:HD11	2.00	0.43
5:D:673:VAL:HB	5:D:677:GLU:HG3	2.00	0.43
5:D:692:ARG:O	5:D:695:LYS:HG3	2.17	0.43
4:C:291:TYR:HE1	4:C:295:LYS:HE2	1.83	0.43
4:C:994:ARG:HG3	4:C:997:TRP:CH2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:18:DT:H4'	5:D:133:ARG:NH1	2.29	0.43
4:C:275:ARG:HA	4:C:278:GLU:HG3	2.00	0.43
5:D:1216:ALA:HB3	5:D:1219:ASP:HB2	2.00	0.43
4:C:829:THR:HG23	4:C:1059:ARG:HG2	2.00	0.43
5:D:449:LEU:H	5:D:449:LEU:HD23	1.83	0.43
3:A:182:ARG:HD2	3:A:182:ARG:O	2.18	0.43
5:D:192:MET:HB2	5:D:197:GLU:OE2	2.19	0.43
5:D:528:THR:OG1	5:D:529:GLY:N	2.51	0.43
3:A:35:PHE:O	3:A:39:LEU:HD23	2.19	0.43
3:B:19:VAL:HB	3:B:23:HIS:HB3	2.01	0.43
3:B:224:LEU:O	3:B:228:LEU:HD23	2.19	0.43
4:C:231:GLU:CB	4:C:238:GLN:HE21	2.31	0.43
4:C:489:PRO:HA	4:C:492:MET:HG3	2.00	0.43
4:C:1184:THR:HG23	4:C:1184:THR:O	2.19	0.43
3:A:12:ARG:H	3:A:29:GLU:HB2	1.84	0.43
5:D:363:LEU:HD23	5:D:622:ASP:HB2	2.00	0.43
5:D:805:GLN:NE2	5:D:1348:LYS:HB2	2.34	0.43
5:D:902:ASP:HB2	5:D:909:ILE:HA	2.01	0.43
3:A:85:LEU:HD21	3:A:144:ILE:HD12	2.00	0.43
4:C:842:ASP:HA	4:C:847:PRO:HA	2.01	0.43
5:D:211:GLU:HG2	5:D:215:LYS:HZ1	1.82	0.43
5:D:235:GLU:HA	5:D:238:ILE:HG22	2.01	0.43
5:D:530:PRO:HB2	5:D:581:MET:CE	2.48	0.43
5:D:986:ASP:HB3	5:D:992:LYS:HD2	2.01	0.43
5:D:1074:LEU:HG	5:D:1075:ARG:H	1.83	0.43
5:D:1138:LEU:HB3	5:D:1139:PRO:HD3	2.01	0.43
5:D:1356:LEU:HD23	5:D:1362:GLY:HA2	2.01	0.43
4:C:339:ASN:OD1	4:C:340:ASP:N	2.51	0.43
4:C:1103:VAL:HB	4:C:1104:PRO:HD3	2.00	0.43
5:D:181:GLY:O	5:D:185:ILE:HG12	2.19	0.43
2:T:14:DA:H1'	5:D:794:GLY:HA3	2.00	0.43
3:B:180:VAL:O	5:D:535:ARG:NH1	2.52	0.43
4:C:547:VAL:HG23	4:C:548:ARG:HD2	2.00	0.43
4:C:734:ILE:HB	4:C:749:ASP:HB2	2.00	0.43
3:B:32:GLU:OE2	3:B:35:PHE:CD2	2.72	0.42
4:C:994:ARG:HA	4:C:997:TRP:CE2	2.54	0.42
4:C:1177:ARG:HG3	4:C:1178:LYS:HG3	2.00	0.42
5:D:50:LYS:NZ	5:D:71:LEU:HG	2.34	0.42
5:D:57:PHE:HD1	5:D:247:PRO:HB3	1.83	0.42
5:D:327:LEU:O	5:D:330:MET:HG3	2.19	0.42
5:D:800:LEU:HD11	5:D:1145:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:800:LEU:HD23	5:D:800:LEU:HA	1.81	0.42
5:D:1028:ILE:HD13	5:D:1118:GLY:CA	2.48	0.42
5:D:1328:THR:O	5:D:1332:LEU:HD13	2.18	0.42
3:A:69:SER:OG	3:A:70:THR:N	2.51	0.42
3:B:65:LEU:HD23	3:B:65:LEU:H	1.84	0.42
5:D:355:ILE:HG13	5:D:461:PHE:CD1	2.53	0.42
5:D:1311:LYS:HB3	5:D:1311:LYS:HE3	1.82	0.42
4:C:1109:ILE:HD12	4:C:1109:ILE:HA	1.93	0.42
4:C:299:LYS:HG3	4:C:301:TYR:CE2	2.55	0.42
4:C:1333:LEU:HD21	5:D:115:TRP:CH2	2.55	0.42
5:D:531:LYS:O	5:D:534:GLU:HG3	2.19	0.42
5:D:926:PRO:HB2	5:D:1241:TYR:HE1	1.84	0.42
5:D:1148:ARG:HH12	5:D:1151:LYS:HD2	1.83	0.42
3:A:71:LYS:HB3	3:A:71:LYS:HE2	1.85	0.42
4:C:149:LEU:HD21	4:C:451:ARG:HH11	1.84	0.42
4:C:686:GLN:HE21	4:C:796:LEU:HD13	1.85	0.42
5:D:1108:GLN:HB2	5:D:1123:ARG:NH2	2.35	0.42
3:A:99:ILE:HD11	3:A:143:ARG:HB3	2.01	0.42
4:C:924:VAL:HG13	4:C:924:VAL:O	2.19	0.42
5:D:196:GLN:O	5:D:199:GLU:HG3	2.19	0.42
5:D:377:PHE:O	5:D:381:ILE:HG12	2.19	0.42
5:D:490:ILE:O	5:D:499:ILE:HG22	2.20	0.42
3:A:81:ILE:HG12	3:A:131:CYS:HB3	2.01	0.42
3:B:48:LEU:HD23	5:D:538:ARG:HD2	2.01	0.42
4:C:217:THR:HG21	4:C:313:ALA:HB1	2.02	0.42
4:C:1061:GLN:O	4:C:1076:ILE:HD11	2.19	0.42
5:D:355:ILE:HG21	5:D:466:MET:HG3	2.01	0.42
5:D:1034:PHE:HD2	5:D:1083:ALA:HA	1.84	0.42
4:C:98:VAL:O	4:C:122:VAL:HG12	2.19	0.42
5:D:418:GLU:HG3	7:E:45:LYS:HB3	2.01	0.42
5:D:681:LYS:HA	5:D:684:ASP:OD2	2.20	0.42
5:D:747:MET:SD	5:D:747:MET:N	2.92	0.42
3:A:227:GLN:HE22	3:B:35:PHE:CB	2.26	0.42
4:C:528:ARG:NH1	4:C:576:SER:O	2.47	0.42
4:C:934:PHE:HB3	4:C:1040:ASP:OD2	2.20	0.42
4:C:1109:ILE:HD11	5:D:644:MET:SD	2.60	0.42
5:D:440:VAL:O	5:D:442:ILE:HG12	2.20	0.42
5:D:532:GLU:H	5:D:532:GLU:HG2	1.67	0.42
4:C:80:PHE:CD2	4:C:90:VAL:HG11	2.54	0.42
4:C:551:HIS:CE1	4:C:553:THR:HG23	2.55	0.42
4:C:813:GLU:HA	5:D:504:GLN:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:888:CYS:HB2	5:D:898:CYS:SG	2.60	0.42
3:A:97:GLU:HB3	3:A:147:GLN:NE2	2.35	0.41
4:C:758:ARG:CD	4:C:835:GLU:HG3	2.50	0.41
5:D:57:PHE:HE2	5:D:252:LEU:HD22	1.85	0.41
5:D:148:GLU:H	5:D:156:ARG:HH12	1.67	0.41
5:D:368:LEU:HD23	5:D:369:PRO:O	2.20	0.41
5:D:817:HIS:HA	5:D:845:ALA:HB1	2.02	0.41
5:D:973:LEU:HD23	5:D:973:LEU:HA	1.92	0.41
4:C:35:PHE:CZ	4:C:129:LEU:HA	2.55	0.41
4:C:718:ALA:HA	4:C:751:TYR:CZ	2.55	0.41
5:D:154:LEU:HD23	5:D:154:LEU:H	1.84	0.41
5:D:993:GLU:HB3	5:D:995:TYR:CE1	2.55	0.41
5:D:1119:ASP:OD1	5:D:1119:ASP:N	2.53	0.41
4:C:810:TYR:HE2	4:C:1078:LYS:HD3	1.85	0.41
5:D:832:LYS:HB3	5:D:1242:ARG:HD2	2.01	0.41
5:D:925:GLU:HB3	5:D:926:PRO:HD3	2.03	0.41
7:E:26:ARG:HB3	7:E:26:ARG:CZ	2.50	0.41
4:C:130:MET:SD	4:C:134:GLY:HA2	2.59	0.41
4:C:725:GLN:NE2	4:C:733:VAL:HG12	2.36	0.41
4:C:1327:LEU:HD22	4:C:1337:ILE:HG21	2.03	0.41
5:D:1030:GLU:HG2	5:D:1099:TYR:OH	2.20	0.41
5:D:1161:GLY:HA3	5:D:1179:PRO:HA	2.02	0.41
5:D:1373:ARG:HG2	5:D:1373:ARG:NH1	2.34	0.41
4:C:161:LYS:HD2	4:C:161:LYS:HA	1.81	0.41
4:C:244:GLU:O	4:C:247:ARG:HG2	2.20	0.41
5:D:56:LEU:HD21	5:D:269:TYR:HB2	2.02	0.41
5:D:114:ILE:HD12	5:D:114:ILE:H	1.85	0.41
5:D:352:ARG:NE	5:D:465:GLN:HB3	2.35	0.41
5:D:460:ASP:OD1	5:D:460:ASP:N	2.53	0.41
4:C:169:LYS:HA	4:C:169:LYS:HD2	1.86	0.41
4:C:835:GLU:HG2	4:C:1053:TYR:HE1	1.85	0.41
5:D:62:PHE:O	5:D:98:ARG:HA	2.20	0.41
5:D:582:ILE:HG12	5:D:623:GLN:HB3	2.01	0.41
5:D:749:LYS:HG3	5:D:751:ASP:OD1	2.21	0.41
5:D:824:PRO:HB3	5:D:835:LEU:HD21	2.02	0.41
5:D:1331:VAL:HG23	5:D:1332:LEU:HD12	2.03	0.41
4:C:211:ARG:NH1	4:C:357:ASN:O	2.53	0.41
4:C:321:LEU:O	4:C:325:LEU:HG	2.21	0.41
4:C:1269:ARG:HB2	5:D:346:ARG:NH1	2.35	0.41
5:D:421:VAL:HG12	5:D:470:VAL:HG12	2.03	0.41
5:D:835:LEU:O	5:D:839:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:238:GLN:CD	4:C:284:LEU:HD22	2.41	0.41
4:C:242:VAL:HG12	4:C:244:GLU:H	1.86	0.41
4:C:363:LEU:HB3	4:C:381:ALA:HB1	2.02	0.41
4:C:1209:GLN:HG2	4:C:1226:THR:HG22	2.03	0.41
5:D:950:ILE:HG21	5:D:982:LEU:HD23	2.01	0.41
5:D:957:SER:HA	5:D:1010:GLN:HA	2.03	0.41
5:D:1143:ASP:OD1	5:D:1148:ARG:HB3	2.21	0.41
3:B:31:LEU:HD13	3:B:36:GLY:HA3	2.03	0.41
3:B:82:LEU:O	3:B:86:LYS:HG3	2.20	0.41
3:B:192:VAL:HG23	3:B:195:ARG:NH2	2.34	0.41
4:C:215:TYR:HB3	4:C:220:ILE:HG13	2.03	0.41
4:C:541:GLU:HG2	4:C:542:ARG:HG3	2.03	0.41
4:C:596:ASP:OD1	4:C:596:ASP:N	2.54	0.41
4:C:668:ILE:HG23	4:C:1069:ARG:O	2.21	0.41
4:C:720:ARG:HG3	4:C:736:VAL:HG11	2.03	0.41
4:C:1013:GLN:HA	4:C:1016:GLU:HG2	2.03	0.41
4:C:1212:LEU:HD12	4:C:1225:VAL:HG21	2.03	0.41
5:D:120:LEU:HB2	5:D:121:PRO:HD3	2.03	0.41
5:D:161:THR:OG1	5:D:162:GLU:N	2.54	0.41
5:D:495:ASN:HD21	5:D:1247:LYS:C	2.24	0.41
5:D:1296:GLY:O	5:D:1297:LYS:HG3	2.21	0.41
4:C:4:SER:OG	4:C:5:TYR:N	2.54	0.41
4:C:238:GLN:OE1	4:C:284:LEU:HB3	2.21	0.41
4:C:965:GLN:O	4:C:968:GLU:HG3	2.20	0.41
5:D:1044:GLN:HA	5:D:1071:GLY:HA2	2.03	0.41
5:D:1261:LEU:HD12	5:D:1261:LEU:O	2.20	0.41
4:C:185:ASP:OD1	4:C:197:ARG:HB3	2.20	0.40
4:C:808:ASN:N	5:D:633:ALA:HB2	2.27	0.40
5:D:479:GLU:OE2	5:D:483:LEU:HB2	2.20	0.40
5:D:1181:ASP:OD1	5:D:1181:ASP:N	2.46	0.40
7:E:66:VAL:HA	7:E:69:ARG:HE	1.86	0.40
4:C:1242:LYS:CG	5:D:465:GLN:HE21	2.34	0.40
5:D:744:ARG:HD2	5:D:759:ILE:HG13	2.04	0.40
7:E:26:ARG:HH12	7:E:50:ALA:HB1	1.85	0.40
4:C:973:SER:O	4:C:976:ARG:HG2	2.22	0.40
4:C:1117:LEU:HD12	4:C:1117:LEU:HA	1.81	0.40
4:C:1285:TYR:CG	5:D:475:GLU:HG3	2.57	0.40
3:B:155:ALA:O	3:B:159:ILE:HG22	2.22	0.40
4:C:96:LEU:HB3	4:C:125:GLY:O	2.20	0.40
4:C:312:ALA:HB3	4:C:315:MET:HG2	2.02	0.40
5:D:504:GLN:HA	5:D:507:VAL:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:675:ALA:O	5:D:678:ARG:HG2	2.22	0.40
5:D:1186:TYR:HE2	5:D:1188:GLU:HG3	1.85	0.40
5:D:1344:LEU:HD13	5:D:1350:ASN:OD1	2.21	0.40
3:B:186:ASN:HB3	3:B:202:VAL:HG23	2.04	0.40
4:C:665:ALA:O	4:C:671:LEU:HD11	2.22	0.40
5:D:244:VAL:HG12	5:D:269:TYR:HE2	1.86	0.40
5:D:398:LYS:HA	5:D:401:VAL:HG12	2.02	0.40
5:D:504:GLN:HB2	5:D:730:ALA:HB1	2.03	0.40
6:R:11:U:H3'	6:R:11:U:H6	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	226/329 (69%)	203 (90%)	23 (10%)	0	100	100
3	B	227/329 (69%)	198 (87%)	29 (13%)	0	100	100
4	C	1315/1342 (98%)	1152 (88%)	162 (12%)	1 (0%)	51	84
5	D	1330/1407 (94%)	1146 (86%)	180 (14%)	4 (0%)	41	75
7	E	71/91 (78%)	60 (84%)	11 (16%)	0	100	100
All	All	3169/3498 (91%)	2759 (87%)	405 (13%)	5 (0%)	50	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	812	PHE
5	D	584	PRO
5	D	765	GLU
5	D	19	ALA
5	D	1245	GLY

### 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	A	196/286 (68%)	196 (100%)	0	100	100
3	B	197/286 (69%)	195 (99%)	2 (1%)	76	86
4	C	1138/1157 (98%)	1137 (100%)	1 (0%)	93	97
5	D	1121/1168 (96%)	1115 (100%)	6 (0%)	88	93
7	E	63/75 (84%)	62 (98%)	1 (2%)	62	79
All	All	2715/2972 (91%)	2705 (100%)	10 (0%)	91	94

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

Mol	Chain	Res	Type
3	B	95	LYS
3	B	166	ARG
4	C	812	PHE
5	D	337	ARG
5	D	460	ASP
5	D	599	LYS
5	D	695	LYS
5	D	1123	ARG
5	D	1326	GLN
7	E	67	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	41	ASN
3	A	227	GLN
4	C	1013	GLN
4	C	1017	GLN
5	D	1010	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	R	10/11 (90%)	1 (10%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	R	11	U

There are no RNA pucker outliers to report.

## 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 3 ligands modelled in this entry, 3 are 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.

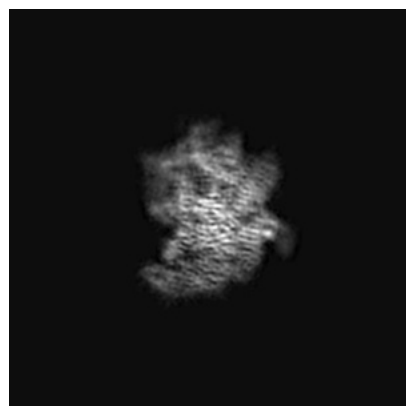
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29212. These allow visual inspection of the internal detail of the map and identification of artifacts.

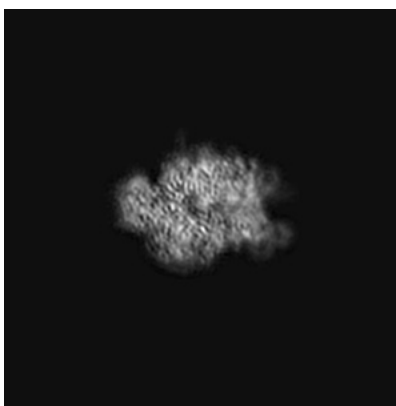
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

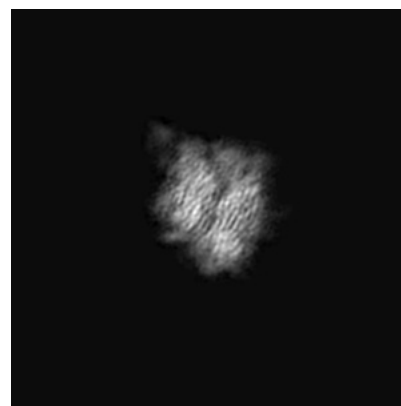
#### 6.1.1 Primary map



X

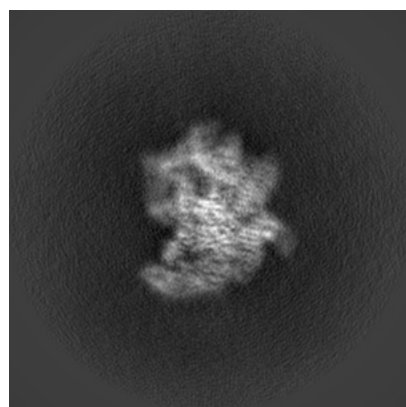


Y

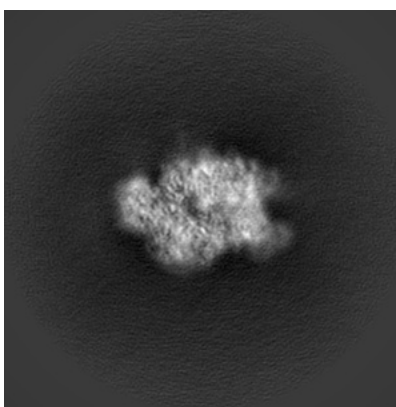


Z

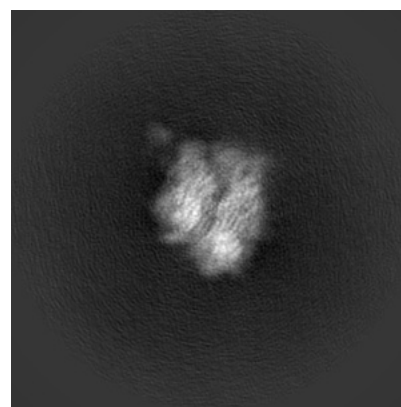
#### 6.1.2 Raw map



X



Y



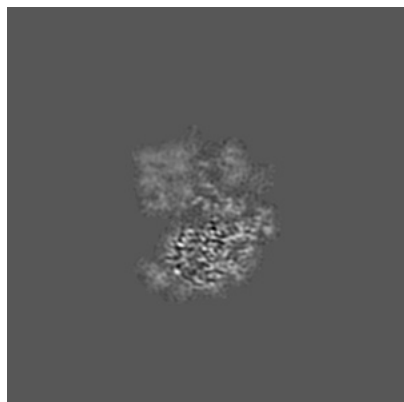
Z

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

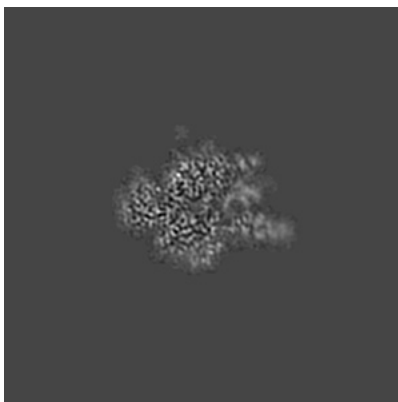


## 6.2 Central slices [i](#)

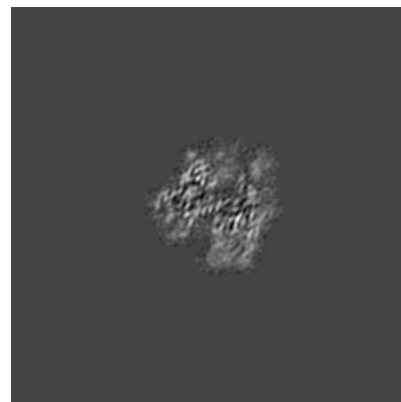
### 6.2.1 Primary map



X Index: 120

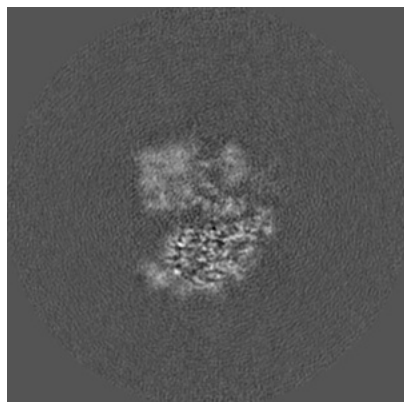


Y Index: 120

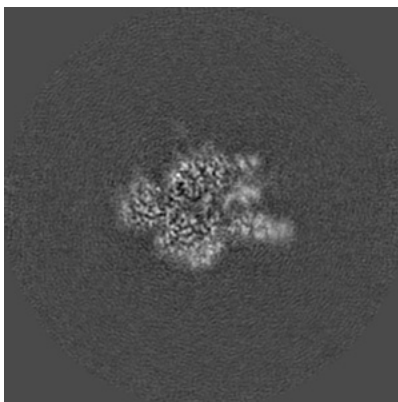


Z Index: 120

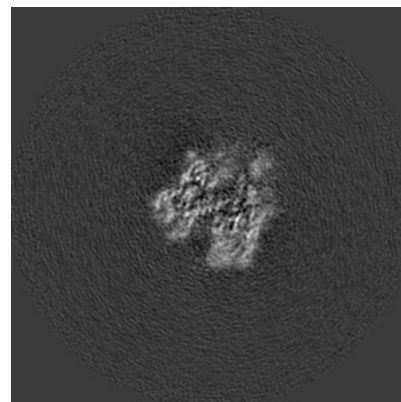
### 6.2.2 Raw map



X Index: 120



Y Index: 120

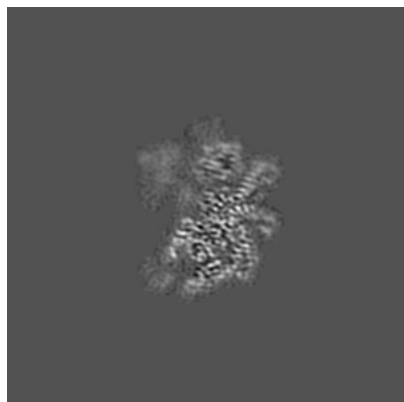


Z Index: 120

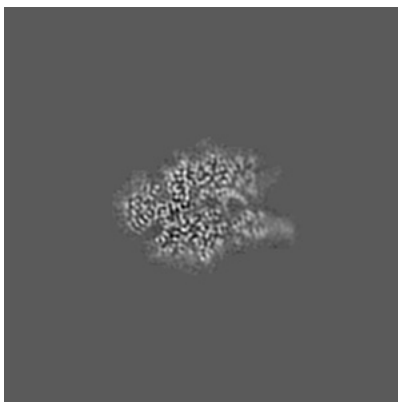
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

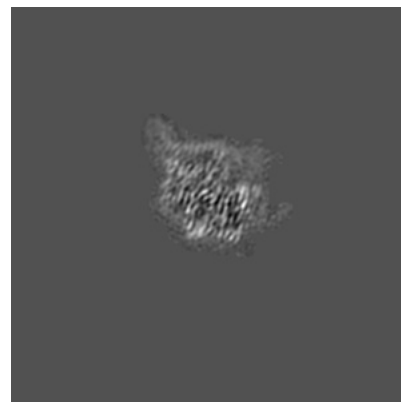
### 6.3.1 Primary map



X Index: 113

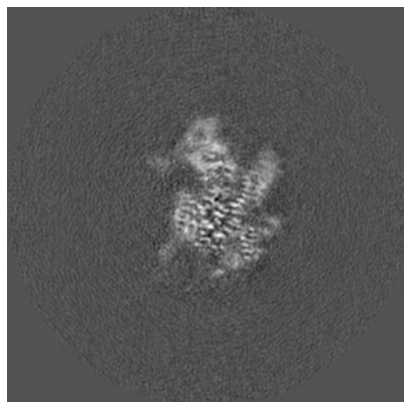


Y Index: 123

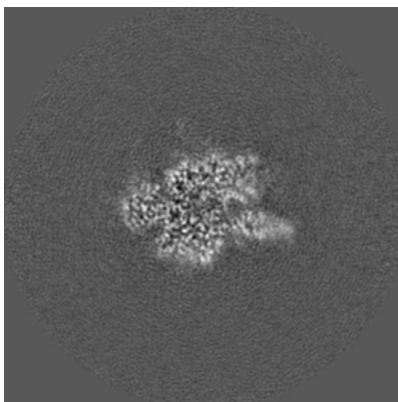


Z Index: 104

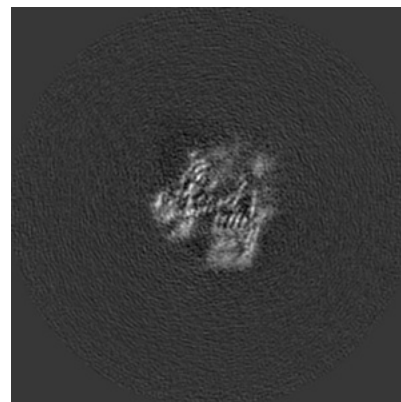
### 6.3.2 Raw map



X Index: 105



Y Index: 122

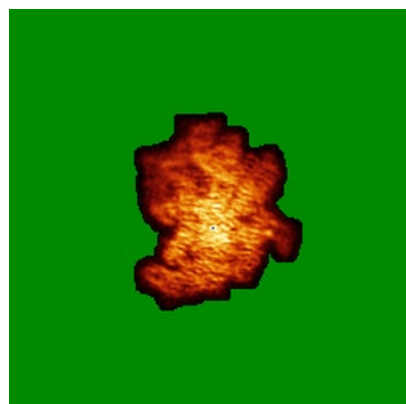


Z Index: 119

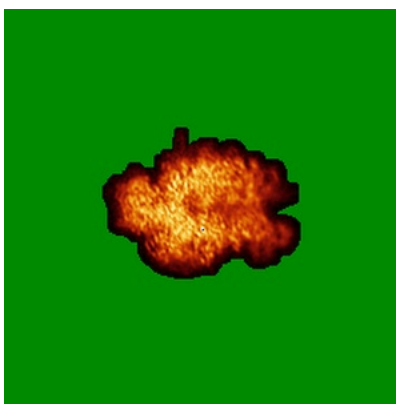
The images above show the largest variance slices of the map in three orthogonal directions.

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

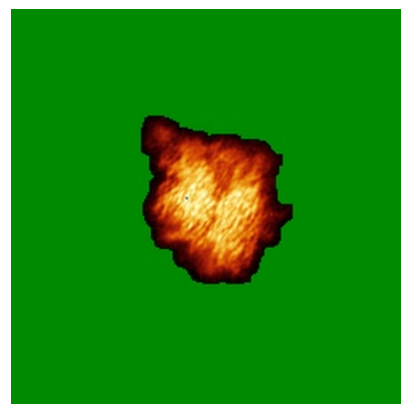
### 6.4.1 Primary map



X

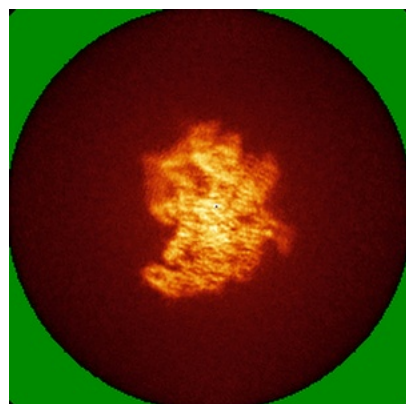


Y

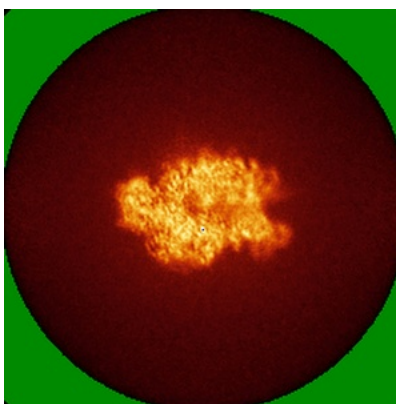


Z

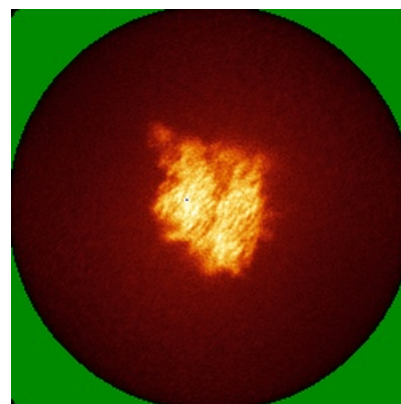
### 6.4.2 Raw map



X



Y

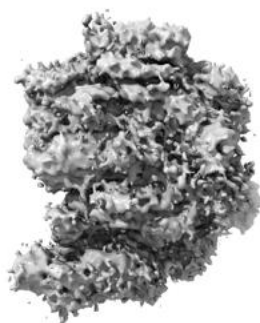


Z

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

## 6.5 Orthogonal surface views [i](#)

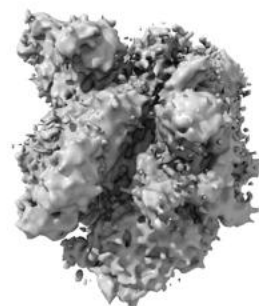
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.

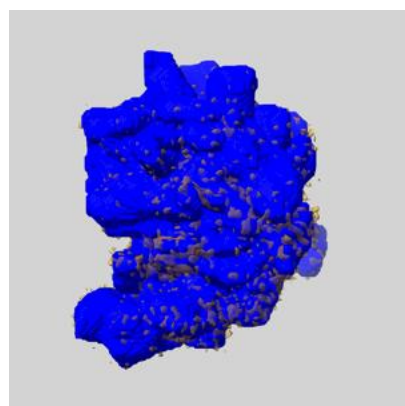
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

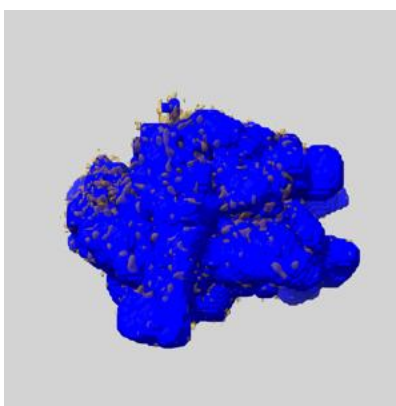
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

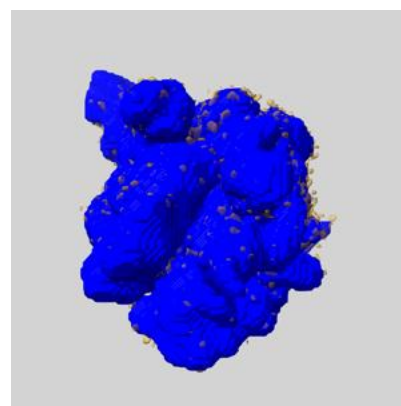
### 6.6.1 emd\_29212\_msk\_1.map [i](#)



X



Y

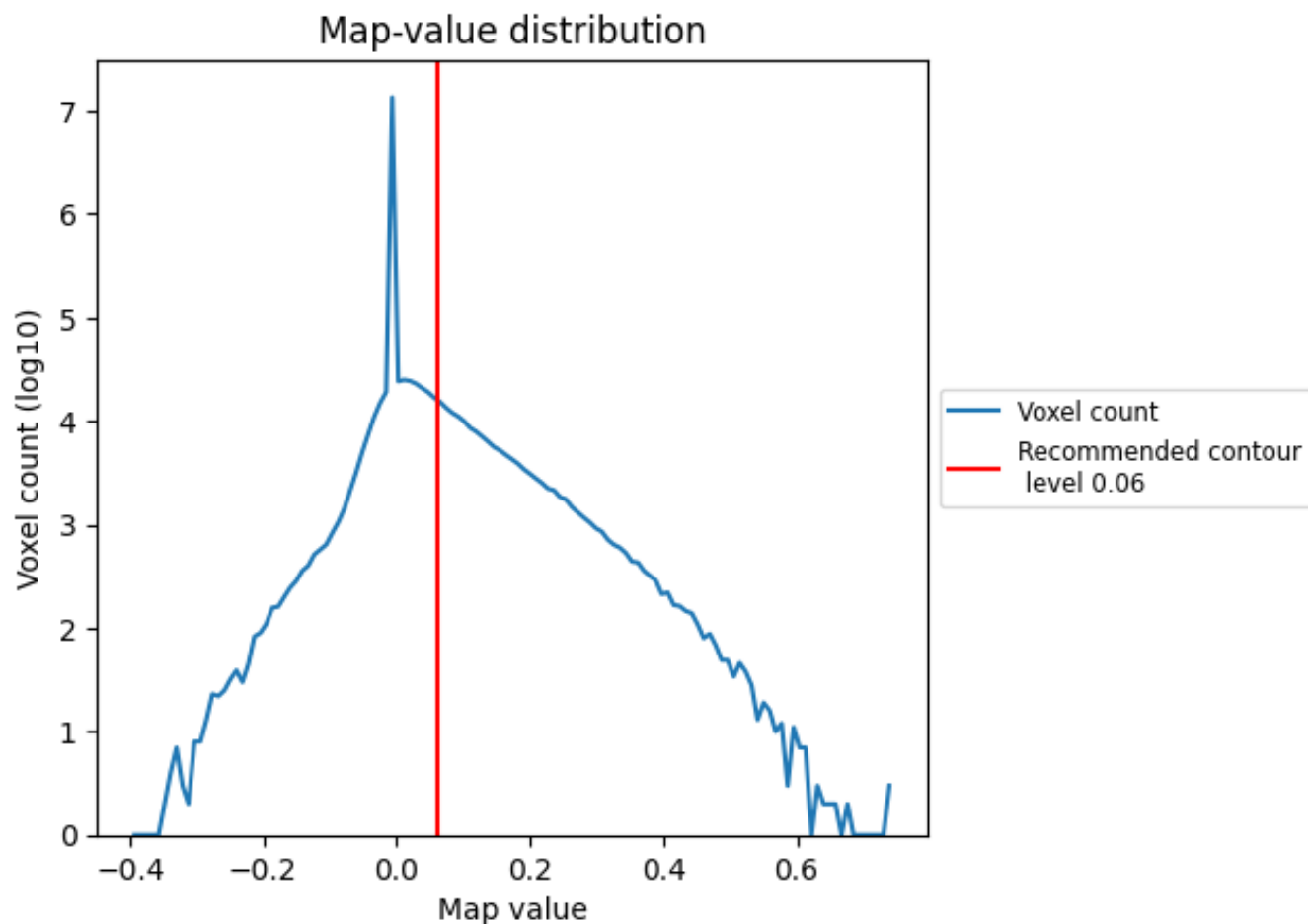


Z

## 7 Map analysis [i](#)

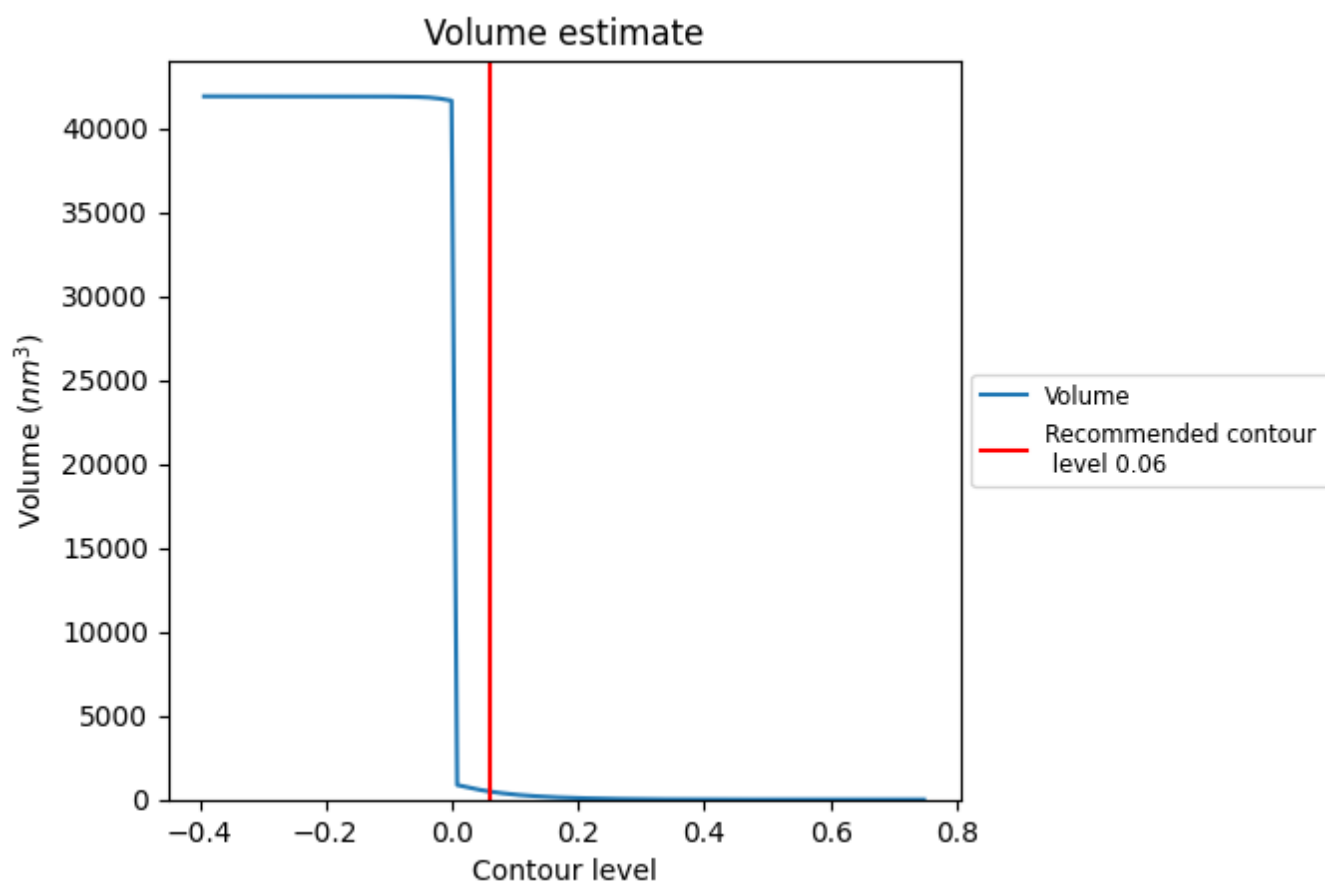
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

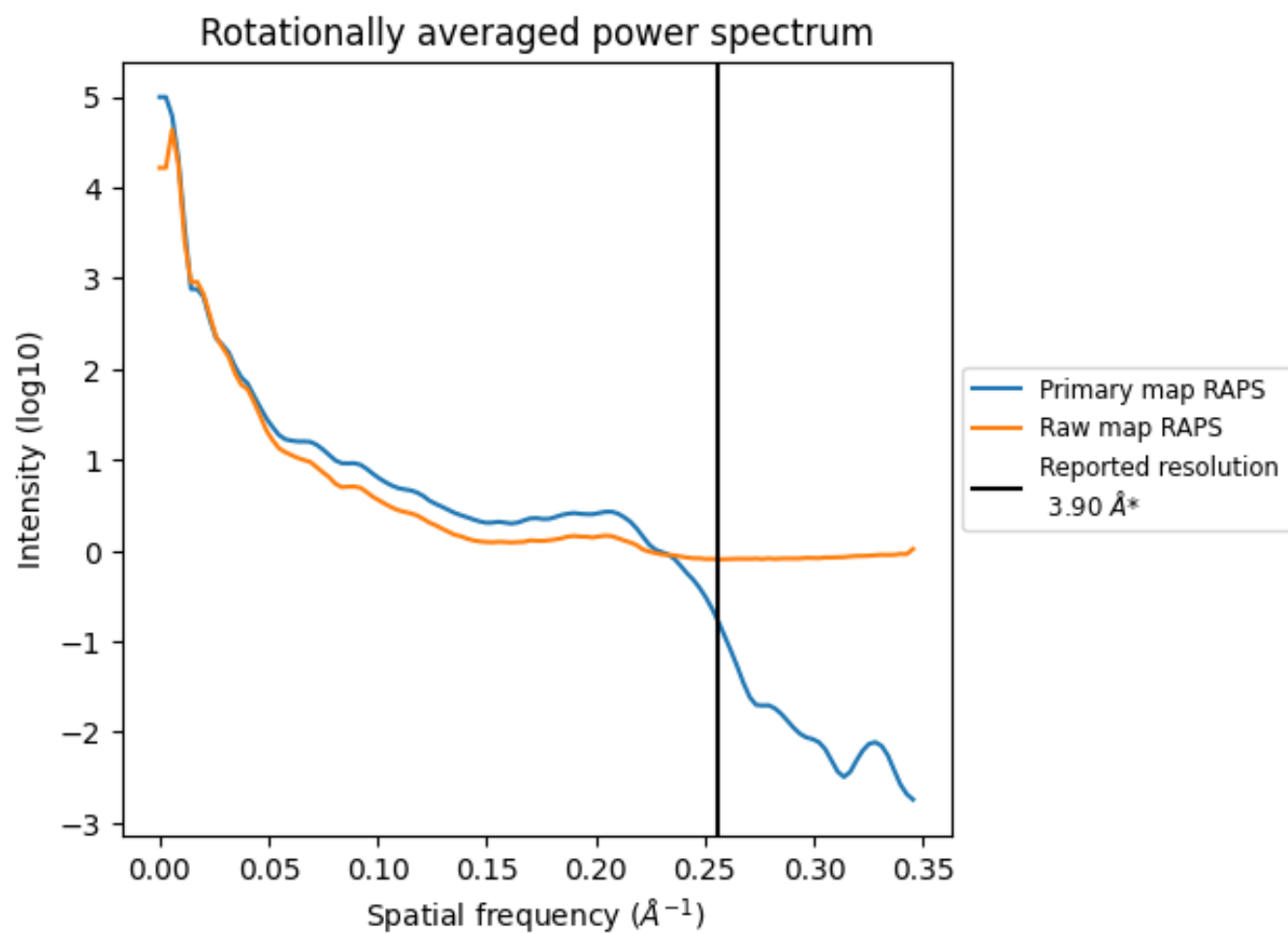
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 479 nm<sup>3</sup>; this corresponds to an approximate mass of 432 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 ⓘ



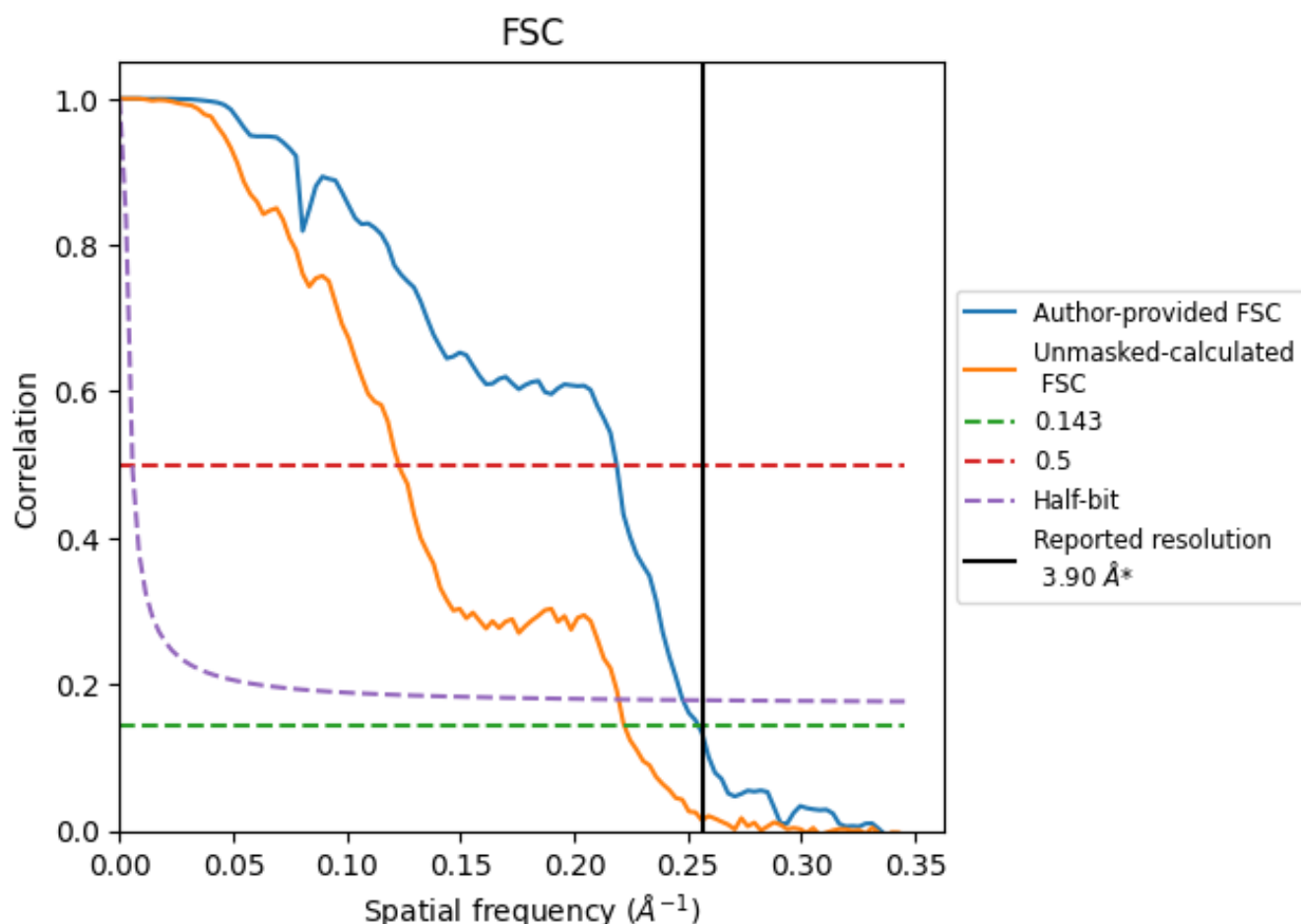
\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

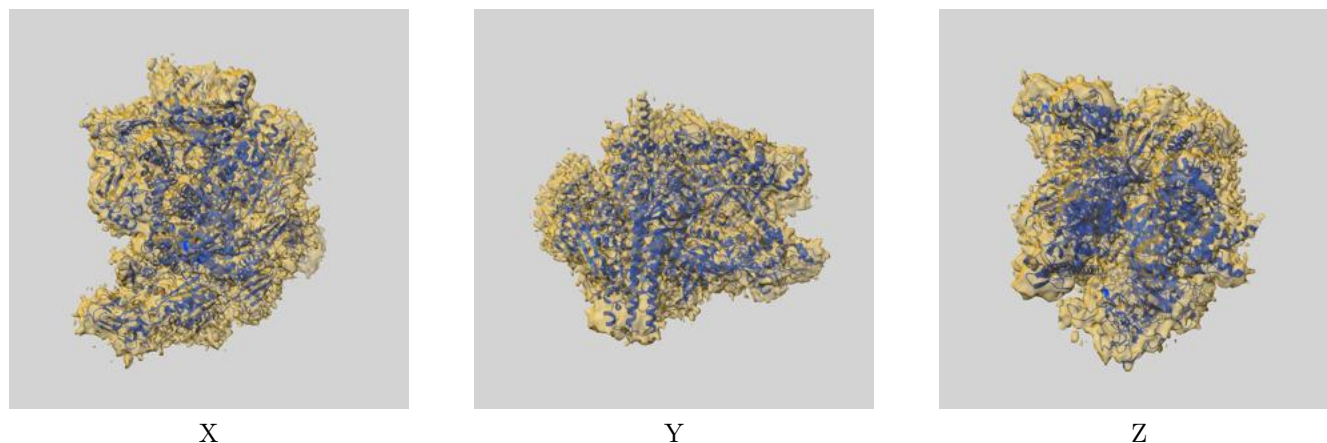
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.93	4.57	4.03
Unmasked-calculated*	4.50	8.13	4.55

\*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 4.50 differs from the reported value 3.9 by more than 10 %

## 9 Map-model fit [i](#)

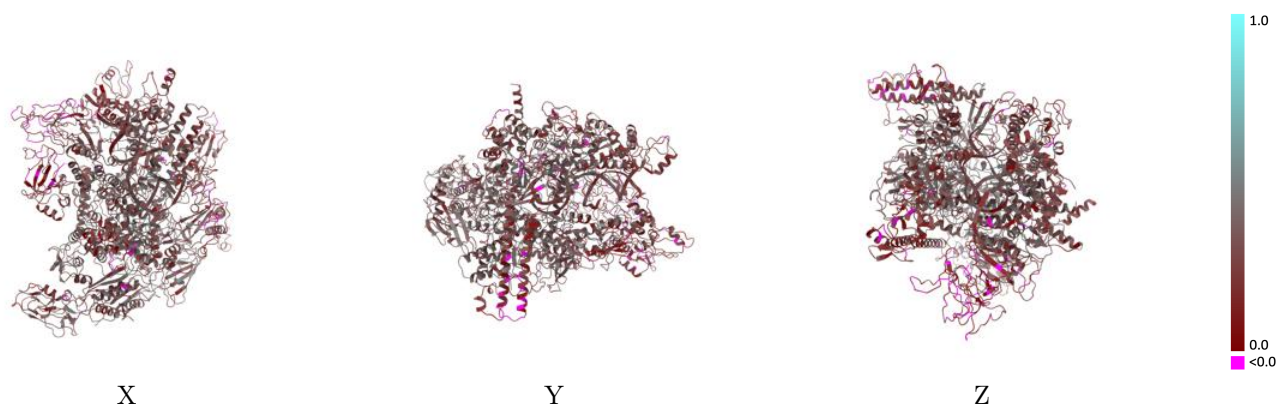
This section contains information regarding the fit between EMDB map EMD-29212 and PDB model 8FIX. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

### 9.1 Map-model overlay [i](#)



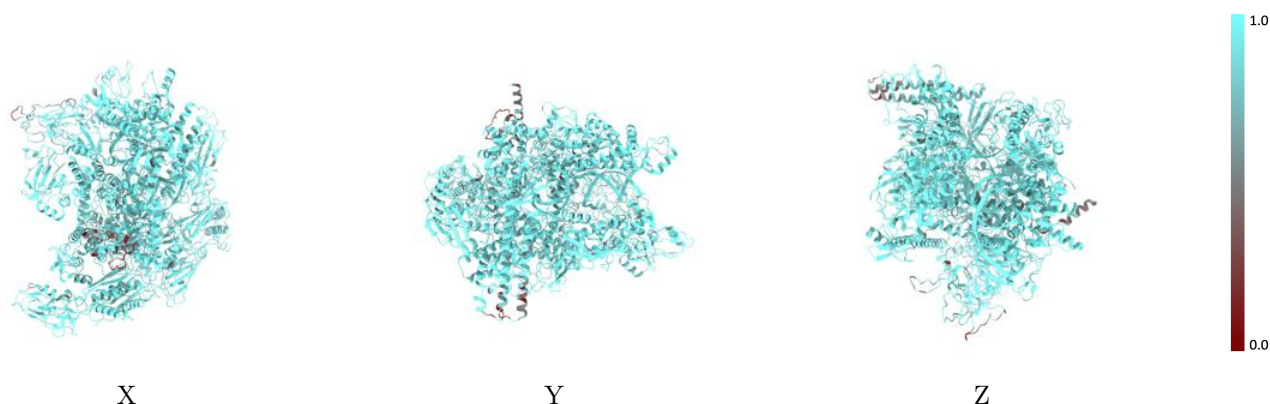
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



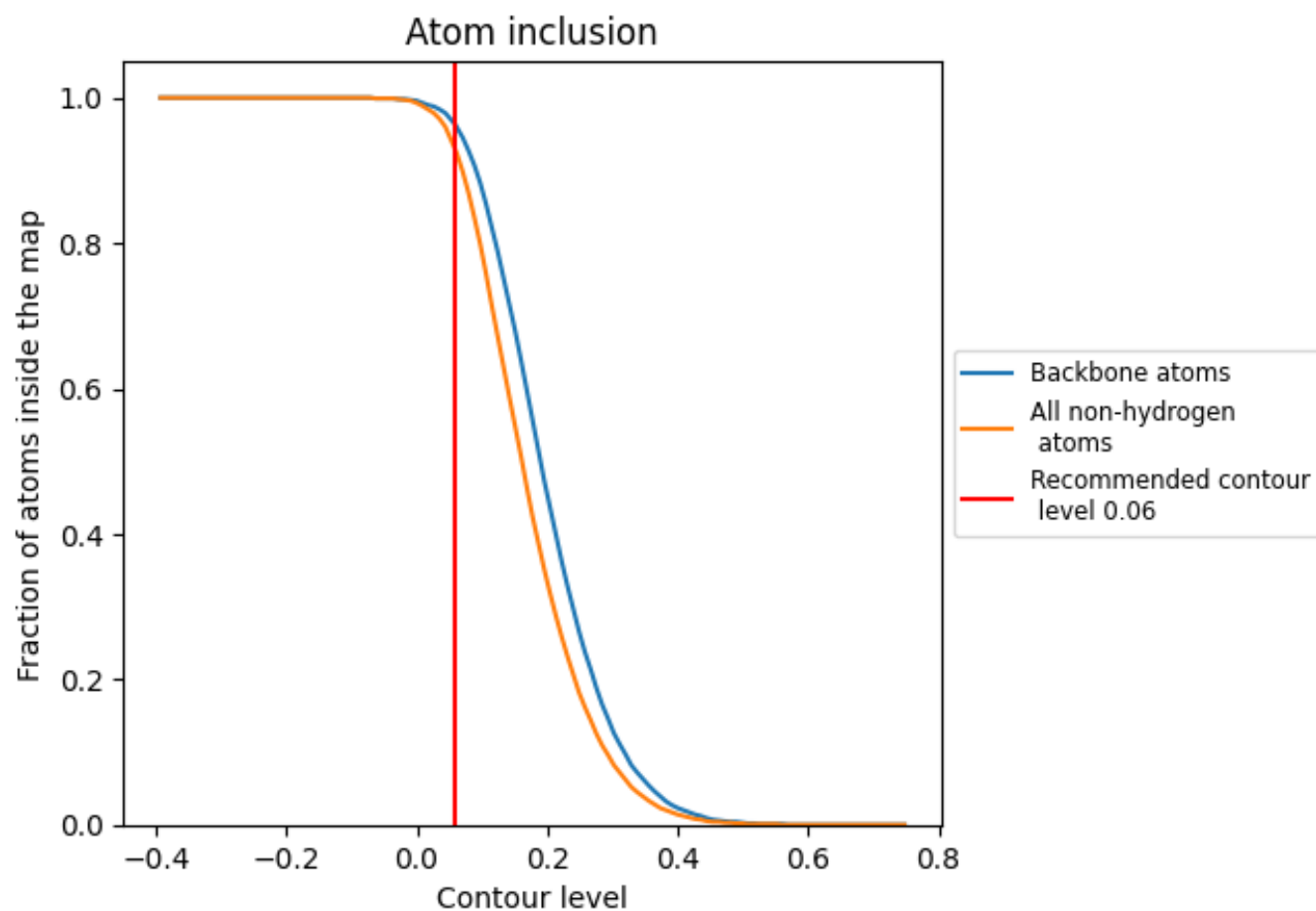
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 93% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9270	<div></div> 0.3000
A	<div></div> 0.9450	<div></div> 0.3420
B	<div></div> 0.9290	<div></div> 0.3040
C	<div></div> 0.9370	<div></div> 0.3100
D	<div></div> 0.9360	<div></div> 0.2890
E	<div></div> 0.5300	<div></div> 0.1960
N	<div></div> 0.9470	<div></div> 0.2410
R	<div></div> 0.8450	<div></div> 0.3110
T	<div></div> 0.9850	<div></div> 0.3060

1.0

0.0

<0.0