



## Full wwPDB EM Validation Report ⓘ

May 14, 2026 – 01:57 pm BST

PDB ID : 9HZG / pdb\_00009hgz  
EMDB ID : EMD-52524  
Title : Ku70/80 bound to WRN-exo  
Authors : Hardwick, S.W.; Zahid, S.; Chaplin, A.K.; Ropars, R.; Charbonnier, J.B.  
Deposited on : 2025-01-13  
Resolution : 3.33 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.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

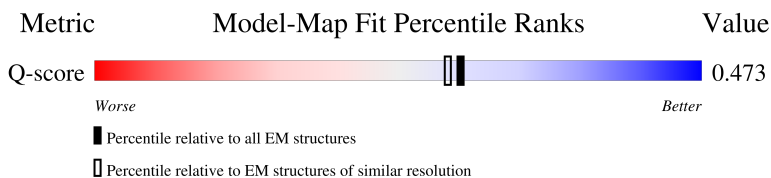
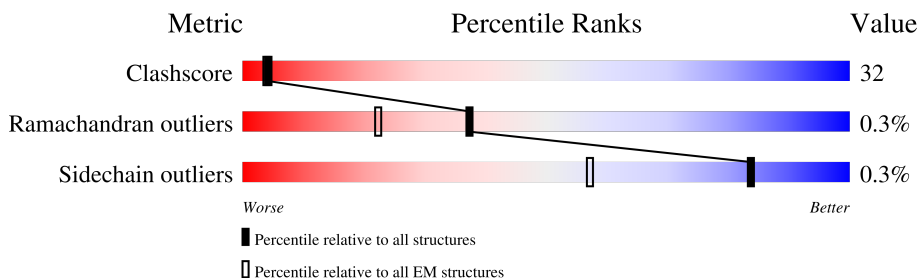
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.33 Å.

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



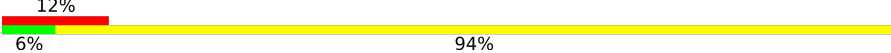
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14484 ( 2.83 - 3.83 )

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	A	609	50% 41% 9%
2	E	1432	8% 7% 85%
3	B	732	41% 31% 28%
4	O	17	12% 12% 88%

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Mol	Chain	Length	Quality of chain
5	P	17	 A horizontal bar chart showing the quality of chain P. The bar is divided into three segments: a green segment on the left labeled '6%', a red segment in the middle labeled '12%', and a yellow segment on the right labeled '94%'. The segments are stacked horizontally, with the green segment starting from the left, followed by the red segment, and then the yellow segment.

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10567 atoms, of which 6 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	554	Total	C	N	O	S	0	0
			4136	2665	702	751	18		

- Molecule 2 is a protein called Bifunctional 3'-5' exonuclease/ATP-dependent helicase WRN.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	218	Total	C	N	O	S	0	0
			1603	1044	262	286	11		

- Molecule 3 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	530	Total	C	N	O	S	0	0
			4085	2627	688	748	22		

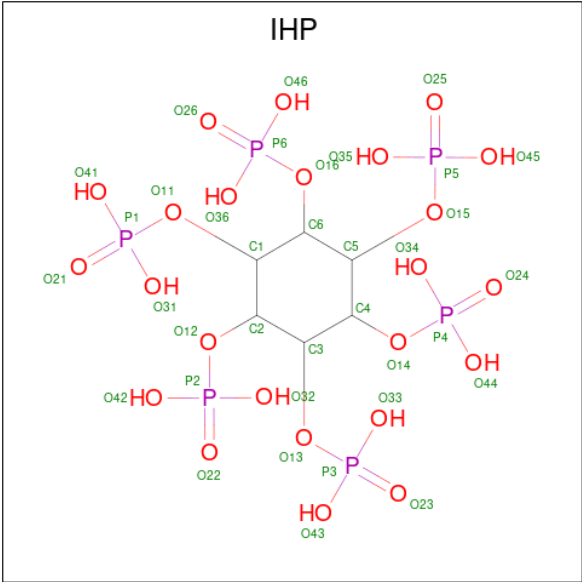
- Molecule 4 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	17	Total	C	N	O	P	0	0
			351	170	55	109	17		

- Molecule 5 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	17	Total	C	N	O	P	0	0
			349	168	69	95	17		

- Molecule 6 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C<sub>6</sub>H<sub>18</sub>O<sub>24</sub>P<sub>6</sub>).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	H	O	P	0
			42	6	6	24	6	

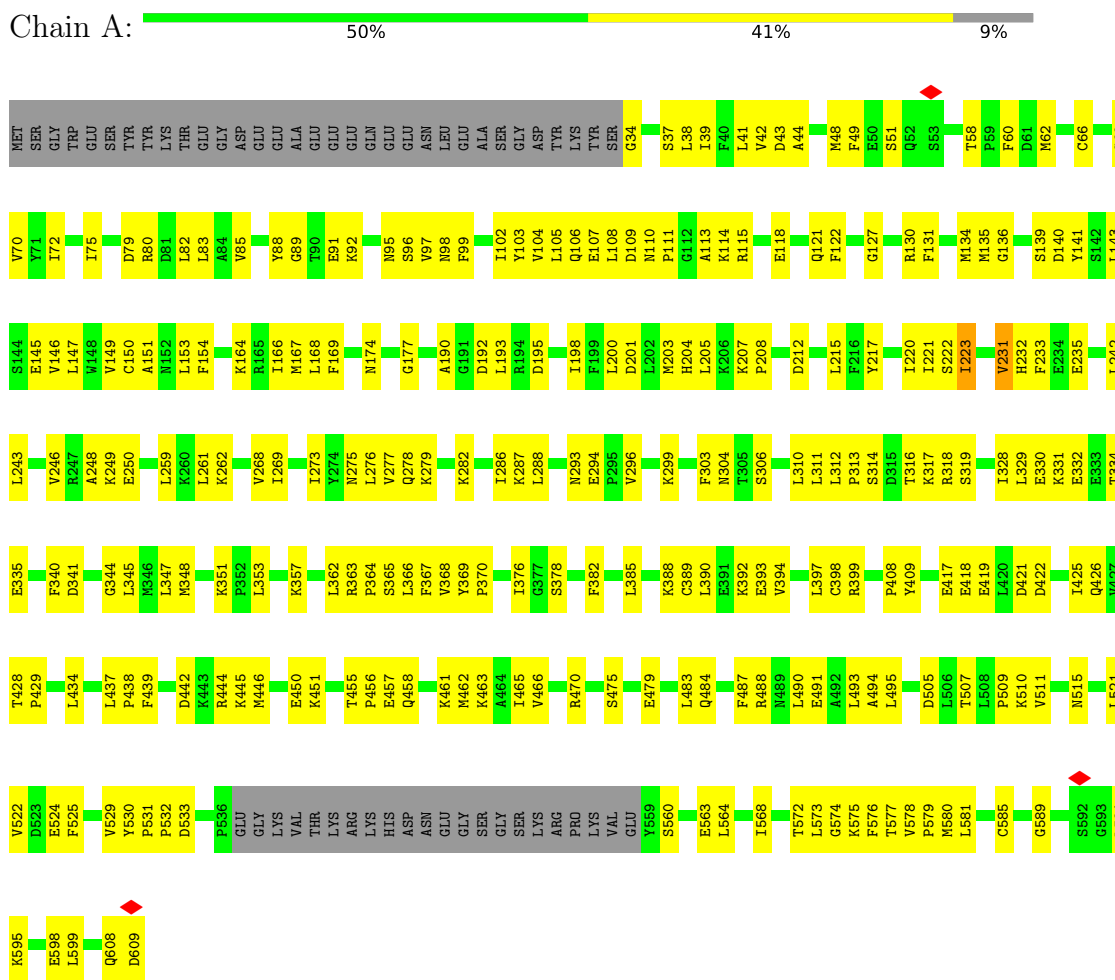
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
7	E	1	Total	Mg	0
			1	1	

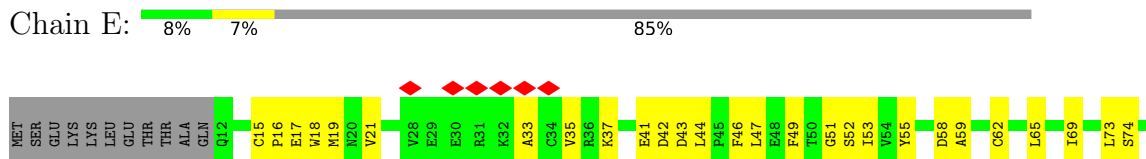
### 3 Residue-property plots

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: X-ray repair cross-complementing protein 6



- Molecule 2: Bifunctional 3'-5' exonuclease/ATP-dependent helicase WRN





VAL	ILE	ARG	ASN	PRO	PRO	VAL	ASN	SER	ARG	ASP	MET	SER	GLY	LYS	ILE	SER	ILE	ASN	THR	GLY	THR	LEU	VAL	GLU	ALA	GLU	ASN	ILE	ASP	THR	ARG	TYR	LEU	ILE	HIS	MET	TRP	PHE	ALA	ILE	LYS	GLY	ILE	SER	LEU	LYS	HIS	GLY	PRO	LYS	ASP	LEU	GLY	LEU	GLN	ASP	THR	LYS	ARG	CYS	VAL	VAL	GLY	LEU	PHE	SER
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• Molecule 3: X-ray repair cross-complementing protein 5

Chain B:  41% 31% 28%

ALA	ASN	ASN	L536	E417	V342	I253	G170	P86	MET
VAL	PHE	PHE	F537			G254	LYS		VAL
PHE	LEU	ARG	P538	V420	L343	S255	GLU	L91	ARG
GLU	LYS	VAL	L539	Y421	G344	N256	ASP	E92	S4
GLU	ALA	LEU	I540	V422	F345	L257	GLY	D93	G5
GLY	LEU	VAL		Q423	C346	S258	SER	I94	N6
GLN	GLN	LYS	K543	L424	K347	I259	GLY	E95	K7
ASP	GLN	ASP	LYS	P425		K260	ASP	S96	A8
VAL	LYS	LYS	LYS	M427	Q350	L261	ARG	K97	A9
ASP	GLU	ALA	ASP	E428	V351		GLY		V10
LEU	ILE	SER	GLN	D429	Q352	Y264	ASP	D106	V11
LEU	LYS	PHE	THR	L430	R353	K265	G181	F107	L12
ASP	GLN	GLU	ALA	R431	R354	L268	P182	L108	C13
MET	LEU	GLU	GLN	Q432	F355		F183		M14
ILE	ASN	ALA	GLU	Y433	F356	R271	R184	L111	D15
HIS	ASN	ALA	GLU	M334	M357			I112	V16
ASN	ASN	SER	ILE	Y435			P190	V113	
PHE	ASN	ASN	PHE	F435	V361	T275	S191	S114	M20
THR	GLN	GLN	GLN		L362		S192	S115	
GLU	GLU	LEU	ASP	Y444	K363	V279	P193	M115	S23
ILE	ILE	ILE	ASN			D280		I118	I24
VAL	ASN	HIS	ASN	T447	A366	A281	T198	Q119	P25
VAL	VAL	HIS	GLU				E199	H118	G26
GLN	ILE	ILE	ASP	Q450	A372	L284	K202	E121	I27
ASP	GLU	GLY	GLY		A373	K285	E203	I122	E28
GLY	GLN	THR	PHE	L457	A374	K286	G204	I123	S29
ILE	PHE	ILE	THR			E287	E204	G124	P30
THR	LEU	THR	ALA	D475	L377	D288	L205	K125	F31
LEU	ASP	LYS	LYS			L289		K126	
ILE	THR	LYS	LYS	T479	L380		M210	F127	K36
THR	ASN	LEU	LEU		L381	V294	V211		V37
LYS	GLU	LYS	LYS	I482	H382	Y295	M212	H131	I38
GLU	THR	THR	THR	P483	A383	Y295	I213	I132	T39
GLU	PRO	GLU	GLU	M484	L384	L306	S214	E133	N40
ALA	ALA	GLN	GLN	R485		K307		I134	F41
SER	THR	PHE	GLY	R486	L387	E308	L221		V42
GLY	GLY	MET	GLY	F487	D388	D309	D222	D137	Q43
SER	LYS	LYS	ALA	Q488	M389	I310	E223	L138	R44
SER	SER	SER	HIS	R489		I311		S139	Q45
VAL	ILE	ILE	PHE	L490	V393	Q312	S226		V46
THR	ASP	SER	SER			G313	F227	L147	
ALA	CYS	VAL	VAL	L494	Y387	F314	S228	D148	D52
GLU	ILE	SER	SER	L495	D398	R315	E229	E53	
GLU	ARG	GLU	ARG	H496	K399	K399	S230	I149	I54
ALA	ALA	ALA	LEU	R497	R400	D319	L231	I151	
LYS	PHE	ALA	ALA	A401	A401	I320	R232		F59
ARG	ARG	GLU	GLU	N402	N402	V321	K233		
GLU	GLU	GLY	GLY	F403	F403	F322		L154	
LEU	SER	SER	SER	Q404	Q404	F323	F237		T64
ALA	ALA	VAL	VAL	V405	V405		K238	D158	D65
THR	THR	THR	THR	G406	G406	D327	K239	I159	N66
LYS	LYS	LYS	SER	E521	V407	E328	L240	S160	
PHE	PHE	LYS	LYS		A408	E329		L161	S69
ASP	ASP	THR	VAL	VAL	F409			Q162	
LYS	SER	SER	GLY			Q330	I245	F163	N76
PRO	GLU	GLU	SER			M331	H246	F164	
GLU	GLU	VAL	VAL	I412	I412	K332	W247	L165	I77
GLN	GLN	ASN	ASN	P529	K413		P248	P166	H82
ARG	ARG	ASN	PRO		H414	E536	C249	F167	L83
PHE	PHE	ALA	ALA	I533	N415	G337	R250	S168	M84
ASN	ASN	GLU	GLU		Y416	V228		L169	L95

• Molecule 4: DNA

Chain O:  12% 12% 88%

T3	T6	A7	G8	T9	T10	T11	A12	T13	T14	G15	G16	G17	T18	A19
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• Molecule 5: DNA

Chain P:  12% 6% 94%

A17	T18	C19	T20	A21	A22	T23	A24	A25	A26	C27	T28	A29	A30	A31	A32	A33
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	83379	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	47.24	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.344	Depositor
Minimum map value	-0.195	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.0397	Depositor
Map size (Å)	260.80002, 260.80002, 260.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.65200007, 0.65200007, 0.65200007	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: IHP, 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	0.13	0/4217	0.27	0/5728
2	E	0.19	0/1636	0.32	0/2227
3	B	0.13	0/4171	0.24	0/5651
4	O	0.22	0/391	0.46	0/603
5	P	0.24	0/393	0.42	0/603
All	All	0.15	0/10808	0.28	0/14812

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	A	4136	0	3963	294	0
2	E	1603	0	1484	115	0
3	B	4085	0	3998	244	0
4	O	351	0	198	31	0
5	P	349	0	192	49	0
6	A	36	6	6	2	0
7	E	1	0	0	0	0
All	All	10561	6	9841	657	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 32.

All (657) 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:O:13:DT:H1'	4:O:14:DT:H73	1.35	1.08
5:P:24:DA:H2'	5:P:25:DA:C8	2.05	0.91
1:A:167:MET:HE1	1:A:250:GLU:HB3	1.51	0.90
1:A:203:MET:HE1	1:A:246:VAL:HA	1.54	0.89
1:A:446:MET:HA	1:A:446:MET:HE2	1.52	0.89
1:A:34:GLY:HA3	4:O:3:DT:H1'	1.54	0.89
5:P:25:DA:H2'	5:P:26:DA:H5'	1.53	0.87
2:E:99:LEU:HD21	2:E:111:LEU:HD12	1.55	0.87
1:A:465:ILE:HD11	1:A:521:LEU:HB3	1.57	0.87
5:P:21:DA:OP2	5:P:21:DA:H3'	1.74	0.87
2:E:65:LEU:O	2:E:69:ILE:HG12	1.75	0.86
3:B:112:ILE:HD11	3:B:150:ILE:HD11	1.56	0.86
5:P:20:DT:H2''	5:P:21:DA:O5'	1.74	0.86
5:P:19:DC:H4'	5:P:20:DT:OP1	1.76	0.85
1:A:390:LEU:HD11	1:A:417:GLU:HB2	1.57	0.83
3:B:24:ILE:HD12	3:B:25:PRO:HD2	1.60	0.83
1:A:573:LEU:O	1:A:573:LEU:HD23	1.79	0.83
3:B:39:THR:O	3:B:43:GLN:HG3	1.78	0.83
1:A:462:MET:HG2	3:B:380:LEU:HA	1.60	0.82
4:O:3:DT:H2'	4:O:3:DT:O2	1.79	0.81
1:A:103:TYR:CD1	1:A:135:MET:HE1	2.16	0.81
1:A:39:ILE:HD12	1:A:154:PHE:CE2	2.17	0.80
1:A:316:THR:HG23	1:A:318:ARG:HH12	1.45	0.80
1:A:312:LEU:HD12	1:A:313:PRO:HD2	1.64	0.79
1:A:576:PHE:HB3	1:A:580:MET:SD	2.22	0.79
2:E:88:LEU:HD23	2:E:89:TYR:H	1.46	0.79
1:A:286:ILE:HD13	3:B:315:ARG:HG2	1.64	0.79
2:E:47:LEU:HB3	2:E:189:LEU:HD23	1.64	0.79
4:O:17:DG:H1	5:P:18:DT:H72	1.46	0.79
3:B:428:GLU:OE1	3:B:428:GLU:N	2.17	0.78
1:A:304:ASN:HB2	1:A:311:LEU:HD21	1.64	0.78
5:P:25:DA:C2'	5:P:26:DA:H5'	2.13	0.78
1:A:203:MET:HE1	1:A:246:VAL:CA	2.13	0.77
1:A:222:SER:O	1:A:223:ILE:HG22	1.81	0.77
1:A:353:LEU:HD12	1:A:393:GLU:HB2	1.65	0.77
1:A:220:ILE:HD12	1:A:220:ILE:H	1.50	0.77
3:B:286:LYS:O	3:B:286:LYS:NZ	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:197:CYS:SG	4:O:19:DA:N6	2.57	0.76
1:A:479:GLU:HB3	3:B:427:MET:HE2	1.65	0.76
1:A:522:VAL:HG13	3:B:257:LEU:CD2	2.17	0.75
3:B:11:VAL:HG23	3:B:118:ILE:HD11	1.67	0.75
3:B:24:ILE:HG23	3:B:27:ILE:HD13	1.67	0.75
1:A:329:LEU:HD21	3:B:497:ARG:HG2	1.68	0.75
5:P:22:DA:H2''	5:P:23:DT:H71	1.69	0.75
3:B:213:ILE:HG13	3:B:221:LEU:HD21	1.68	0.75
3:B:14:MET:HE2	3:B:16:VAL:HG12	1.69	0.74
2:E:141:GLU:O	2:E:144:GLN:HG3	1.87	0.74
1:A:426:GLN:NE2	3:B:435:PHE:O	2.20	0.74
1:A:34:GLY:CA	4:O:3:DT:H1'	2.16	0.74
1:A:312:LEU:HG	1:A:314:SER:H	1.52	0.73
1:A:106:GLN:HE22	1:A:115:ARG:HB3	1.53	0.73
2:E:83:MET:SD	2:E:143:ASP:HB3	2.28	0.73
1:A:121:GLN:HE22	1:A:130:ARG:HD3	1.54	0.73
1:A:174:ASN:HD21	1:A:177:GLY:HA3	1.54	0.73
3:B:15:ASP:HB3	3:B:20:MET:HE3	1.69	0.73
1:A:328:ILE:O	1:A:329:LEU:HD23	1.89	0.72
1:A:121:GLN:NE2	1:A:130:ARG:HD3	2.04	0.72
4:O:16:DG:N3	4:O:16:DG:H2'	2.02	0.72
4:O:13:DT:H1'	4:O:14:DT:C7	2.18	0.72
1:A:113:ALA:HB1	1:A:495:LEU:HD11	1.72	0.72
1:A:462:MET:HE2	1:A:462:MET:HA	1.70	0.72
2:E:138:VAL:HG11	2:E:177:LEU:HG	1.71	0.72
1:A:102:ILE:HD13	1:A:149:VAL:HG21	1.72	0.72
3:B:93:ASP:HA	3:B:97:LYS:CB	2.19	0.72
3:B:323:PHE:CE2	3:B:328:GLU:HB2	2.25	0.72
4:O:10:DT:H2''	4:O:11:DT:OP1	1.89	0.72
3:B:138:LEU:HD11	3:B:165:LEU:HD22	1.71	0.71
3:B:426:PHE:N	3:B:429:ASP:OD2	2.23	0.71
3:B:450:GLN:HB3	3:B:537:PHE:CZ	2.25	0.71
2:E:161:LEU:HD13	2:E:223:ILE:HG22	1.72	0.71
1:A:122:PHE:HD2	1:A:131:PHE:HB2	1.56	0.71
1:A:269:ILE:HB	1:A:378:SER:OG	1.91	0.71
4:O:7:DA:N6	5:P:27:DC:O2	2.24	0.71
2:E:83:MET:HB3	2:E:100:ILE:HD13	1.72	0.70
3:B:24:ILE:HG23	3:B:27:ILE:HB	1.74	0.70
2:E:18:TRP:CH2	3:B:119:GLN:HG3	2.25	0.70
1:A:103:TYR:CG	1:A:135:MET:HE1	2.25	0.70
1:A:465:ILE:CD1	1:A:521:LEU:HB3	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:177:LEU:O	2:E:181:VAL:HG23	1.91	0.70
1:A:578:VAL:CG1	1:A:579:PRO:HD3	2.21	0.70
5:P:24:DA:H2'	5:P:25:DA:H8	1.54	0.69
1:A:207:LYS:NZ	1:A:208:PRO:O	2.25	0.69
1:A:41:LEU:HD11	1:A:146:VAL:HG22	1.73	0.69
3:B:246:HIS:NE2	3:B:248:PRO:HG3	2.07	0.69
3:B:27:ILE:HG23	3:B:183:PHE:CD2	2.26	0.69
1:A:457:GLU:OE1	1:A:457:GLU:N	2.18	0.69
2:E:58:ASP:C	2:E:117:MET:HE1	2.16	0.69
2:E:212:TYR:O	2:E:215:THR:HG22	1.93	0.69
2:E:177:LEU:HD13	2:E:216:ASP:OD1	1.94	0.68
1:A:363:ARG:HB2	1:A:364:PRO:HD2	1.74	0.68
1:A:577:THR:OG1	1:A:579:PRO:HD2	1.92	0.68
3:B:167:PHE:HE2	3:B:205:LEU:HD22	1.57	0.68
4:O:8:DG:OP2	4:O:8:DG:H4'	1.93	0.68
3:B:306:LEU:HD12	3:B:307:LYS:N	2.08	0.68
2:E:53:ILE:HG23	2:E:111:LEU:HD23	1.74	0.68
3:B:10:VAL:HG22	3:B:131:HIS:HB3	1.75	0.68
2:E:88:LEU:HG	2:E:89:TYR:CD2	2.28	0.68
1:A:577:THR:O	1:A:581:LEU:HD23	1.94	0.67
1:A:369:TYR:CD1	1:A:370:PRO:HD2	2.29	0.67
3:B:198:THR:O	3:B:202:LYS:HG2	1.94	0.67
2:E:114:VAL:O	2:E:117:MET:HB2	1.94	0.67
3:B:245:ILE:HD12	3:B:246:HIS:H	1.60	0.67
3:B:265:LYS:HZ1	5:P:24:DA:P	2.16	0.67
1:A:299:LYS:N	3:B:294:VAL:O	2.27	0.67
2:E:134:LYS:HD3	2:E:159:VAL:HG11	1.77	0.67
3:B:38:ILE:HG22	3:B:94:ILE:HD13	1.76	0.67
3:B:521:GLU:N	3:B:521:GLU:OE1	2.27	0.67
1:A:578:VAL:HG13	1:A:579:PRO:HD3	1.77	0.67
2:E:46:PHE:HD2	2:E:190:LEU:HG	1.60	0.67
1:A:217:TYR:HA	1:A:220:ILE:CD1	2.25	0.66
1:A:595:LYS:O	1:A:598:GLU:N	2.27	0.66
2:E:178:ASN:OD1	2:E:189:LEU:HB2	1.96	0.66
5:P:22:DA:N3	5:P:22:DA:H2'	2.10	0.66
1:A:97:VAL:HG23	1:A:99:PHE:CD1	2.31	0.66
3:B:323:PHE:HE2	3:B:328:GLU:HB2	1.60	0.66
1:A:261:LEU:HB3	1:A:269:ILE:HG13	1.77	0.66
3:B:118:ILE:O	3:B:122:THR:HG23	1.95	0.66
1:A:560:SER:CB	1:A:563:GLU:HB3	2.26	0.65
1:A:351:LYS:HE2	3:B:475:ASP:OD2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:73:LEU:HD11	2:E:77:ASP:HB2	1.77	0.65
1:A:231:VAL:HG23	1:A:232:HIS:H	1.62	0.65
1:A:43:ASP:HA	1:A:88:TYR:CE1	2.32	0.65
1:A:43:ASP:OD1	1:A:44:ALA:N	2.29	0.65
1:A:455:THR:HG23	1:A:458:GLN:H	1.62	0.65
2:E:15:CYS:SG	2:E:16:PRO:HD2	2.36	0.65
3:B:255:SER:OG	3:B:256:ASN:OD1	2.13	0.64
3:B:382:HIS:NE2	3:B:417:GLU:OE2	2.29	0.64
2:E:78:VAL:HG21	2:E:224:TYR:CD1	2.32	0.64
1:A:143:LEU:O	1:A:147:LEU:HD23	1.97	0.64
2:E:78:VAL:HG21	2:E:224:TYR:CE1	2.32	0.64
2:E:84:GLU:OE1	4:O:19:DA:H2'	1.97	0.64
3:B:66:ASN:OD1	3:B:69:SER:N	2.30	0.64
1:A:515:ASN:HD21	3:B:255:SER:HB3	1.62	0.64
3:B:408:ALA:HA	3:B:420:VAL:O	1.98	0.64
1:A:95:ASN:OD1	1:A:98:ASN:N	2.29	0.64
1:A:273:ILE:CD1	1:A:368:VAL:HG22	2.27	0.64
3:B:23:SER:HB2	3:B:29:SER:CA	2.28	0.64
1:A:335:GLU:HA	1:A:335:GLU:OE1	1.98	0.63
2:E:165:ALA:HB2	2:E:227:LEU:HD11	1.80	0.63
1:A:109:ASP:OD1	1:A:110:ASN:N	2.31	0.63
2:E:173:GLU:OE1	3:B:7:LYS:NZ	2.24	0.63
5:P:33:DA:OP2	5:P:33:DA:H2'	1.98	0.63
2:E:78:VAL:HG11	2:E:224:TYR:CZ	2.34	0.63
1:A:131:PHE:O	1:A:135:MET:HB2	1.97	0.63
3:B:203:GLU:OE1	3:B:203:GLU:HA	1.98	0.63
1:A:39:ILE:HD12	1:A:154:PHE:CD2	2.33	0.63
1:A:286:ILE:CD1	3:B:315:ARG:HG2	2.29	0.63
1:A:511:VAL:O	1:A:515:ASN:ND2	2.32	0.63
2:E:53:ILE:CD1	2:E:109:CYS:HB3	2.29	0.62
4:O:17:DG:H2''	4:O:18:DT:OP1	1.98	0.62
5:P:25:DA:C3'	5:P:26:DA:H5'	2.29	0.62
1:A:490:LEU:HD22	3:B:321:VAL:HG21	1.81	0.62
2:E:46:PHE:CD2	2:E:190:LEU:HG	2.34	0.62
1:A:608:GLN:HG3	1:A:609:ASP:OD2	2.00	0.62
2:E:101:GLN:N	2:E:101:GLN:OE1	2.31	0.62
1:A:79:ASP:OD1	1:A:80:ARG:N	2.33	0.62
1:A:479:GLU:HB3	3:B:427:MET:CE	2.28	0.62
1:A:580:MET:O	1:A:580:MET:HE2	2.00	0.62
1:A:317:LYS:HG2	1:A:330:GLU:OE1	1.99	0.62
1:A:455:THR:OG1	1:A:456:PRO:HD2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:ASP:OD1	1:A:507:THR:N	2.32	0.62
1:A:463:LYS:O	1:A:466:VAL:HG12	1.99	0.62
5:P:30:DA:H3'	5:P:31:DA:C2	2.35	0.62
1:A:362:LEU:HD21	1:A:409:TYR:OH	1.99	0.62
1:A:146:VAL:HG13	1:A:147:LEU:HD22	1.82	0.62
1:A:91:GLU:H	1:A:136:GLY:HA3	1.65	0.62
2:E:37:LYS:HD3	2:E:41:GLU:CB	2.30	0.61
3:B:20:MET:HG3	3:B:31:PHE:HB2	1.82	0.61
5:P:30:DA:H3'	5:P:31:DA:H2	1.63	0.61
1:A:329:LEU:CD2	3:B:497:ARG:HG2	2.29	0.61
3:B:286:LYS:HZ3	3:B:289:ILE:HB	1.64	0.61
3:B:23:SER:HB2	3:B:29:SER:HA	1.83	0.61
2:E:183:HIS:NE2	3:B:125:LYS:HE3	2.15	0.61
1:A:511:VAL:HG22	1:A:515:ASN:HD21	1.66	0.61
3:B:265:LYS:HE3	5:P:23:DT:H5''	1.82	0.61
2:E:47:LEU:HB3	2:E:189:LEU:CD2	2.31	0.61
2:E:147:LEU:HD21	2:E:153:ILE:CG1	2.31	0.61
1:A:192:ASP:HA	1:A:195:ASP:OD2	2.01	0.61
1:A:462:MET:SD	3:B:380:LEU:HD13	2.41	0.60
2:E:73:LEU:HD12	2:E:74:SER:N	2.16	0.60
1:A:347:LEU:HA	1:A:398:CYS:SG	2.41	0.60
2:E:99:LEU:HD21	2:E:111:LEU:CD1	2.29	0.60
3:B:24:ILE:CG2	3:B:27:ILE:HD13	2.31	0.60
3:B:199:GLU:HA	3:B:202:LYS:HD2	1.83	0.60
2:E:82:ASP:HB3	2:E:101:GLN:NE2	2.16	0.60
1:A:217:TYR:O	1:A:221:ILE:HG22	2.01	0.60
1:A:455:THR:HG22	1:A:458:GLN:HB2	1.84	0.60
2:E:84:GLU:OE1	2:E:84:GLU:HA	2.02	0.60
2:E:161:LEU:HD13	2:E:223:ILE:CG2	2.32	0.60
5:P:27:DC:H2''	5:P:28:DT:H71	1.84	0.60
1:A:217:TYR:HA	1:A:220:ILE:HD13	1.82	0.60
1:A:69:SER:O	1:A:72:ILE:HG22	2.02	0.59
2:E:43:ASP:OD1	2:E:43:ASP:O	2.20	0.59
2:E:52:SER:O	2:E:53:ILE:HD13	2.02	0.59
3:B:356:PHE:CG	3:B:422:VAL:HG11	2.37	0.59
2:E:180:LEU:HD23	2:E:223:ILE:HG21	1.84	0.59
1:A:190:ALA:HB2	1:A:220:ILE:HG23	1.84	0.59
3:B:259:ILE:O	3:B:261:ILE:HG23	2.03	0.59
5:P:21:DA:H2''	5:P:22:DA:C6	2.38	0.59
1:A:376:ILE:HB	3:B:540:ILE:HG23	1.85	0.59
3:B:95:GLU:HG3	3:B:96:SER:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:GLU:O	1:A:334:THR:HG22	2.02	0.59
1:A:522:VAL:HG13	3:B:257:LEU:HD23	1.84	0.59
5:P:17:DA:H2''	5:P:18:DT:OP2	2.01	0.59
1:A:313:PRO:O	1:A:316:THR:HG22	2.02	0.59
1:A:347:LEU:HD12	1:A:398:CYS:SG	2.43	0.59
1:A:419:GLU:HB2	1:A:428:THR:OG1	2.03	0.59
5:P:21:DA:H4'	5:P:22:DA:OP1	1.99	0.59
1:A:89:GLY:HA2	1:A:140:ASP:O	2.03	0.59
1:A:418:GLU:HA	1:A:428:THR:O	2.03	0.59
1:A:428:THR:HG22	3:B:354:ARG:NH2	2.18	0.58
3:B:27:ILE:HG23	3:B:183:PHE:CE2	2.38	0.58
3:B:199:GLU:HA	3:B:202:LYS:CG	2.33	0.58
3:B:249:CYS:SG	3:B:250:ARG:N	2.75	0.58
3:B:412:ILE:HG22	3:B:417:GLU:HG2	1.84	0.58
1:A:475:SER:HB2	3:B:430:LEU:HD21	1.85	0.58
3:B:226:SER:N	3:B:229:GLU:OE2	2.36	0.58
2:E:125:LYS:NZ	2:E:153:ILE:HG22	2.19	0.58
2:E:196:ARG:HG3	2:E:212:TYR:OH	2.04	0.58
1:A:204:HIS:CD2	1:A:235:GLU:HA	2.39	0.58
1:A:131:PHE:CE2	1:A:135:MET:HG3	2.39	0.58
1:A:37:SER:C	1:A:38:LEU:HD12	2.29	0.57
2:E:101:GLN:HB3	2:E:111:LEU:HD13	1.85	0.57
2:E:134:LYS:HA	2:E:157:ASN:OD1	2.04	0.57
3:B:309:ASP:C	3:B:310:ILE:HD13	2.29	0.57
1:A:261:LEU:HD13	1:A:345:LEU:HB2	1.87	0.57
1:A:580:MET:HE2	1:A:580:MET:C	2.29	0.57
1:A:577:THR:CB	1:A:579:PRO:HD2	2.35	0.57
2:E:59:ALA:HA	2:E:62:CYS:SG	2.45	0.57
1:A:106:GLN:NE2	1:A:115:ARG:HB3	2.19	0.57
1:A:370:PRO:HD3	1:A:382:PHE:CE2	2.40	0.57
1:A:488:ARG:O	1:A:491:GLU:HG2	2.05	0.57
1:A:365:SER:HB3	1:A:434:LEU:O	2.05	0.56
2:E:33:ALA:O	2:E:35:VAL:HG13	2.05	0.56
1:A:118:GLU:O	1:A:121:GLN:HB3	2.04	0.56
1:A:212:ASP:CB	1:A:215:LEU:HD23	2.35	0.56
1:A:317:LYS:O	3:B:279:VAL:HG22	2.06	0.56
3:B:24:ILE:CD1	3:B:25:PRO:HD2	2.33	0.56
3:B:137:ASP:C	3:B:137:ASP:OD1	2.49	0.56
1:A:286:ILE:HD13	3:B:315:ARG:CG	2.35	0.56
1:A:203:MET:HE1	1:A:246:VAL:N	2.21	0.56
1:A:392:LYS:O	1:A:393:GLU:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:124:LEU:O	2:E:128:LEU:HD23	2.06	0.56
3:B:13:CYS:SG	3:B:114:SER:HB2	2.46	0.56
1:A:66:CYS:SG	1:A:246:VAL:HG21	2.44	0.56
1:A:296:VAL:CG1	3:B:295:TYR:HB3	2.36	0.56
1:A:484:GLN:O	1:A:488:ARG:HG2	2.06	0.56
3:B:336:GLU:N	3:B:336:GLU:OE1	2.39	0.56
2:E:195:ILE:HD12	2:E:195:ILE:H	1.71	0.56
3:B:53:GLU:HB2	3:B:83:LEU:HD22	1.87	0.56
1:A:95:ASN:OD1	1:A:97:VAL:N	2.36	0.56
1:A:304:ASN:CA	1:A:311:LEU:HD11	2.36	0.56
3:B:315:ARG:NH1	3:B:320:ILE:HD11	2.19	0.56
1:A:304:ASN:CB	1:A:311:LEU:HD21	2.32	0.55
3:B:351:VAL:HG12	3:B:351:VAL:O	2.06	0.55
1:A:82:LEU:HB2	1:A:108:LEU:HD22	1.88	0.55
1:A:150:CYS:HB3	1:A:166:ILE:HD11	1.88	0.55
2:E:18:TRP:CZ3	3:B:119:GLN:HG3	2.41	0.55
3:B:154:LEU:CD2	3:B:159:ILE:HB	2.35	0.55
1:A:422:ASP:OD1	1:A:422:ASP:N	2.35	0.55
3:B:366:ALA:HB1	3:B:373:ALA:O	2.07	0.55
1:A:107:GLU:O	1:A:115:ARG:NH1	2.35	0.55
1:A:190:ALA:CB	1:A:220:ILE:HG23	2.37	0.55
2:E:44:LEU:HD21	3:B:123:ILE:HD11	1.86	0.55
2:E:206:THR:O	2:E:207:GLU:C	2.48	0.55
3:B:41:PHE:CE2	3:B:54:ILE:HD12	2.42	0.55
3:B:319:ASP:O	3:B:320:ILE:HD13	2.06	0.55
4:O:6:DT:H2''	4:O:7:DA:C8	2.42	0.55
1:A:85:VAL:H	1:A:106:GLN:HB2	1.71	0.55
3:B:327:ASP:O	3:B:331:MET:HB3	2.07	0.55
1:A:525:PHE:CE2	3:B:257:LEU:HD11	2.42	0.54
5:P:25:DA:H2'	5:P:26:DA:C5'	2.30	0.54
3:B:11:VAL:CG2	3:B:118:ILE:HD11	2.37	0.54
2:E:17:GLU:OE1	2:E:17:GLU:HA	2.08	0.54
3:B:76:ASN:C	3:B:77:ILE:HD12	2.33	0.54
4:O:6:DT:H5''	4:O:6:DT:O2	2.06	0.54
1:A:428:THR:HG22	3:B:354:ARG:HH21	1.72	0.54
4:O:7:DA:H4'	4:O:8:DG:OP1	2.07	0.54
1:A:341:ASP:N	1:A:341:ASP:OD1	2.37	0.54
2:E:83:MET:HE1	2:E:143:ASP:HB3	1.90	0.54
2:E:97:VAL:HG12	2:E:146:LYS:HE3	1.89	0.54
3:B:447:THR:N	3:B:450:GLN:OE1	2.25	0.54
3:B:147:LEU:O	3:B:151:ILE:HD12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:520:ALA:O	3:B:524:THR:HG23	2.08	0.54
1:A:167:MET:CE	1:A:250:GLU:HB3	2.32	0.54
3:B:338:LYS:HG2	3:B:397:TYR:O	2.08	0.54
1:A:83:LEU:HD13	1:A:111:PRO:HG3	1.90	0.54
2:E:15:CYS:SG	2:E:19:MET:HE2	2.48	0.53
3:B:245:ILE:HD12	3:B:246:HIS:N	2.23	0.53
1:A:275:ASN:ND2	1:A:278:GLN:OE1	2.42	0.53
1:A:41:LEU:HD11	1:A:146:VAL:CG2	2.38	0.53
1:A:304:ASN:OD1	1:A:306:SER:N	2.42	0.53
2:E:178:ASN:O	2:E:182:LYS:HG3	2.09	0.53
3:B:23:SER:HB2	3:B:29:SER:CB	2.38	0.53
5:P:22:DA:C2'	5:P:23:DT:H71	2.38	0.53
2:E:190:LEU:HD12	2:E:190:LEU:H	1.73	0.53
1:A:286:ILE:HG12	3:B:313:GLY:O	2.09	0.53
1:A:515:ASN:ND2	3:B:255:SER:HB3	2.23	0.53
3:B:24:ILE:HD12	3:B:25:PRO:CD	2.34	0.53
2:E:168:LYS:HE2	2:E:230:LEU:HD23	1.91	0.53
5:P:24:DA:H2''	5:P:25:DA:OP1	2.09	0.53
5:P:26:DA:H8	5:P:26:DA:OP2	1.91	0.53
3:B:309:ASP:O	3:B:310:ILE:HD13	2.09	0.53
3:B:329:GLU:HA	3:B:332:LYS:NZ	2.24	0.53
5:P:21:DA:H3'	5:P:21:DA:P	2.49	0.53
1:A:493:LEU:HD12	3:B:323:PHE:CD1	2.44	0.52
2:E:44:LEU:HD11	3:B:123:ILE:HD11	1.91	0.52
3:B:131:HIS:ND1	3:B:160:SER:HB2	2.25	0.52
1:A:507:THR:O	3:B:343:LEU:HD21	2.09	0.52
5:P:23:DT:H2''	5:P:24:DA:C8	2.44	0.52
3:B:223:GLU:OE2	3:B:239:LYS:HE2	2.10	0.52
1:A:287:LYS:O	1:A:288:LEU:HD22	2.10	0.52
1:A:304:ASN:HA	1:A:311:LEU:HD11	1.90	0.52
3:B:239:LYS:C	3:B:240:ILE:HD13	2.35	0.52
2:E:78:VAL:HG11	2:E:224:TYR:CE1	2.45	0.52
2:E:161:LEU:HA	2:E:164:VAL:HG12	1.91	0.52
2:E:128:LEU:HD12	2:E:155:LEU:CD1	2.40	0.52
3:B:164:PHE:O	3:B:165:LEU:HD23	2.09	0.52
1:A:288:LEU:HB2	3:B:311:ILE:O	2.10	0.52
1:A:390:LEU:CD1	1:A:417:GLU:HB2	2.36	0.52
1:A:445:LYS:O	1:A:446:MET:HE2	2.10	0.52
2:E:83:MET:CE	2:E:143:ASP:HB3	2.40	0.52
3:B:137:ASP:C	3:B:138:LEU:HD12	2.35	0.52
1:A:85:VAL:H	1:A:106:GLN:CB	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:147:LEU:HD21	2:E:153:ILE:HG13	1.91	0.52
3:B:331:MET:HG3	3:B:331:MET:O	2.09	0.52
3:B:271:ARG:HB2	3:B:271:ARG:CZ	2.39	0.52
4:O:17:DG:H1	5:P:18:DT:C7	2.21	0.52
5:P:29:DA:H2''	5:P:30:DA:H8	1.74	0.52
1:A:43:ASP:HB3	1:A:48:MET:HG3	1.92	0.51
3:B:538:PRO:O	3:B:539:LEU:HD23	2.09	0.51
1:A:370:PRO:HD3	1:A:382:PHE:CD2	2.45	0.51
2:E:203:PHE:HB3	2:E:204:PRO:HD3	1.92	0.51
5:P:21:DA:H2''	5:P:22:DA:C5	2.45	0.51
3:B:106:ASP:OD1	3:B:108:LEU:HB2	2.09	0.51
1:A:594:LEU:N	1:A:599:LEU:HD21	2.26	0.51
3:B:486:ARG:HG3	3:B:487:PHE:N	2.25	0.51
3:B:82:HIS:ND1	3:B:121:GLU:OE2	2.42	0.51
3:B:284:LEU:N	3:B:284:LEU:HD12	2.26	0.51
1:A:319:SER:HB2	1:A:328:ILE:HD13	1.92	0.51
1:A:426:GLN:OE1	1:A:429:PRO:HA	2.11	0.51
1:A:608:GLN:HG3	1:A:609:ASP:CG	2.36	0.51
3:B:23:SER:HB2	3:B:29:SER:HB3	1.92	0.51
3:B:137:ASP:OD1	3:B:139:SER:N	2.44	0.51
1:A:331:LYS:HA	1:A:334:THR:HG22	1.92	0.51
1:A:392:LYS:O	1:A:394:VAL:HG13	2.11	0.51
3:B:353:ARG:HG2	3:B:353:ARG:HH11	1.76	0.51
1:A:75:ILE:HG13	1:A:111:PRO:HB2	1.92	0.50
2:E:69:ILE:O	2:E:73:LEU:HB3	2.11	0.50
1:A:104:VAL:O	1:A:106:GLN:N	2.39	0.50
3:B:41:PHE:HE2	3:B:54:ILE:HD12	1.75	0.50
1:A:578:VAL:HA	1:A:581:LEU:HB2	1.93	0.50
3:B:28:GLU:OE2	3:B:36:LYS:HE3	2.11	0.50
3:B:148:ASP:OD1	3:B:149:ILE:N	2.44	0.50
5:P:25:DA:H3'	5:P:26:DA:C8	2.46	0.50
1:A:455:THR:HG22	1:A:458:GLN:CD	2.36	0.50
1:A:580:MET:SD	1:A:581:LEU:HD22	2.52	0.50
1:A:114:LYS:HE2	1:A:114:LYS:HA	1.94	0.50
1:A:446:MET:HE2	1:A:446:MET:CA	2.33	0.50
2:E:101:GLN:O	2:E:102:LEU:HD23	2.12	0.50
3:B:91:LEU:HD13	3:B:495:LEU:HD13	1.94	0.50
2:E:18:TRP:CZ3	2:E:19:MET:HG2	2.47	0.50
3:B:402:ASN:HB2	5:P:25:DA:OP2	2.12	0.50
3:B:46:VAL:CG2	3:B:86:PRO:HB2	2.41	0.50
3:B:482:ILE:HG23	3:B:515:MET:HE3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:17:DA:H4'	5:P:18:DT:O5'	2.11	0.50
5:P:27:DC:H2''	5:P:28:DT:C7	2.41	0.50
1:A:51:SER:HB3	1:A:58:THR:HG22	1.94	0.49
1:A:259:LEU:HB3	1:A:344:GLY:HA2	1.94	0.49
1:A:311:LEU:HD12	3:B:289:ILE:CD1	2.42	0.49
3:B:147:LEU:HD21	3:B:210:MET:HE2	1.93	0.49
2:E:88:LEU:HD23	2:E:89:TYR:N	2.22	0.49
3:B:122:THR:HB	3:B:127:PHE:CD2	2.48	0.49
1:A:140:ASP:OD1	1:A:141:TYR:N	2.38	0.49
3:B:306:LEU:HD12	3:B:307:LYS:H	1.75	0.49
1:A:261:LEU:HB3	1:A:269:ILE:CG1	2.42	0.49
2:E:128:LEU:HD12	2:E:155:LEU:HD11	1.94	0.49
3:B:356:PHE:CD2	3:B:422:VAL:HG11	2.47	0.49
3:B:361:VAL:HG22	3:B:422:VAL:HG22	1.93	0.49
3:B:64:THR:CG2	3:B:69:SER:HB2	2.42	0.49
1:A:461:LYS:NZ	1:A:524:GLU:HB3	2.28	0.49
1:A:105:LEU:O	1:A:106:GLN:HG2	2.11	0.49
1:A:470:ARG:HD2	3:B:389:MET:HE1	1.95	0.49
1:A:578:VAL:HG12	1:A:579:PRO:HD3	1.95	0.49
4:O:3:DT:O2	4:O:3:DT:C2'	2.58	0.49
1:A:299:LYS:O	3:B:294:VAL:N	2.33	0.48
1:A:340:PHE:HB2	1:A:408:PRO:HD3	1.95	0.48
3:B:199:GLU:HA	3:B:202:LYS:CD	2.44	0.48
1:A:331:LYS:HA	1:A:334:THR:CG2	2.43	0.48
4:O:12:DA:H4'	4:O:13:DT:OP1	2.12	0.48
3:B:154:LEU:HD22	3:B:159:ILE:HB	1.95	0.48
2:E:148:LEU:HD12	2:E:152:ASP:HA	1.94	0.48
3:B:285:LYS:HB2	3:B:288:ASP:OD2	2.13	0.48
1:A:233:PHE:HE1	1:A:425:ILE:HA	1.78	0.48
3:B:457:LEU:HD22	3:B:533:ILE:HD12	1.94	0.48
1:A:278:GLN:HG2	3:B:431:ARG:HH21	1.79	0.48
1:A:564:LEU:O	1:A:568:ILE:HG13	2.14	0.48
3:B:164:PHE:C	3:B:165:LEU:HD23	2.38	0.48
1:A:89:GLY:O	1:A:139:SER:N	2.46	0.48
1:A:288:LEU:HD13	1:A:294:GLU:O	2.14	0.48
2:E:134:LYS:HD3	2:E:159:VAL:CG1	2.43	0.48
1:A:70:VAL:HG21	1:A:246:VAL:HG11	1.96	0.48
1:A:369:TYR:CG	1:A:370:PRO:HD2	2.49	0.48
3:B:192:PHE:CD1	3:B:193:PRO:HD2	2.49	0.48
1:A:122:PHE:C	1:A:127:GLY:HA3	2.39	0.47
2:E:138:VAL:CG1	2:E:177:LEU:HG	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:169:LEU:HD11	3:B:205:LEU:HD11	1.95	0.47
3:B:479:THR:HA	3:B:482:ILE:HD12	1.97	0.47
1:A:106:GLN:HE22	1:A:115:ARG:CB	2.25	0.47
1:A:168:LEU:HD23	1:A:169:PHE:N	2.28	0.47
1:A:357:LYS:HD3	6:A:701:IHP:P5	2.54	0.47
1:A:362:LEU:HD22	1:A:438:PRO:HA	1.97	0.47
2:E:42:ASP:OD1	2:E:42:ASP:O	2.31	0.47
2:E:44:LEU:HD21	3:B:123:ILE:CD1	2.45	0.47
2:E:160:GLU:OE1	2:E:160:GLU:N	2.44	0.47
1:A:296:VAL:HG11	3:B:295:TYR:HB3	1.95	0.47
3:B:115:MET:SD	3:B:154:LEU:HG	2.54	0.47
3:B:319:ASP:C	3:B:320:ILE:HD13	2.40	0.47
3:B:406:GLY:HA3	3:B:421:TYR:CE2	2.49	0.47
1:A:198:ILE:HG22	1:A:200:LEU:HD12	1.96	0.47
1:A:312:LEU:HD12	1:A:313:PRO:CD	2.40	0.47
2:E:196:ARG:HH22	4:O:18:DT:H3'	1.79	0.47
3:B:528:ILE:HB	3:B:529:PRO:HD3	1.97	0.47
2:E:41:GLU:O	2:E:44:LEU:HD12	2.15	0.47
2:E:172:THR:HG23	3:B:85:LEU:HD11	1.97	0.47
1:A:311:LEU:HD12	3:B:289:ILE:HD11	1.96	0.47
1:A:389:CYS:O	1:A:393:GLU:N	2.48	0.47
2:E:53:ILE:HD12	2:E:109:CYS:HB3	1.96	0.47
3:B:14:MET:SD	3:B:38:ILE:HD12	2.55	0.47
5:P:23:DT:C2'	5:P:24:DA:C8	2.97	0.47
1:A:278:GLN:HG2	3:B:431:ARG:NH2	2.29	0.47
1:A:461:LYS:O	1:A:465:ILE:HG12	2.14	0.47
3:B:246:HIS:HB3	3:B:264:TYR:CE2	2.49	0.47
3:B:425:PRO:HB2	3:B:430:LEU:CD1	2.45	0.47
1:A:446:MET:HA	1:A:446:MET:CE	2.25	0.47
3:B:14:MET:HE2	3:B:16:VAL:CG1	2.43	0.47
1:A:332:GLU:OE1	1:A:332:GLU:N	2.35	0.47
3:B:232:ARG:O	3:B:233:LYS:HG3	2.15	0.47
4:O:11:DT:H2''	4:O:12:DA:OP1	2.09	0.47
4:O:12:DA:H2''	4:O:13:DT:C2	2.50	0.47
3:B:25:PRO:O	3:B:27:ILE:HD12	2.14	0.46
3:B:223:GLU:HA	3:B:223:GLU:OE1	2.14	0.46
2:E:116:SER:O	2:E:116:SER:OG	2.29	0.46
1:A:276:LEU:HD23	1:A:367:PHE:HB2	1.96	0.46
4:O:14:DT:H4'	4:O:15:DG:OP2	2.11	0.46
1:A:143:LEU:HA	1:A:146:VAL:HG12	1.98	0.46
1:A:92:LYS:O	1:A:103:TYR:HD2	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:ARG:HH12	3:B:268:LEU:CD2	2.28	0.46
1:A:490:LEU:HD22	3:B:321:VAL:CG2	2.46	0.46
3:B:8:ALA:N	3:B:52:ASP:OD1	2.46	0.46
1:A:151:ALA:HB2	1:A:193:LEU:HD11	1.97	0.46
1:A:578:VAL:HG13	1:A:579:PRO:CD	2.44	0.46
2:E:62:CYS:SG	2:E:121:PRO:HG3	2.56	0.46
3:B:239:LYS:O	3:B:240:ILE:HD13	2.16	0.46
3:B:342:VAL:HG22	3:B:393:VAL:HG12	1.98	0.46
3:B:434:MET:O	3:B:434:MET:HG3	2.14	0.46
1:A:444:ARG:HH12	3:B:268:LEU:HD23	1.81	0.46
1:A:585:CYS:O	1:A:589:GLY:HA2	2.16	0.46
3:B:444:TYR:CD1	3:B:444:TYR:N	2.83	0.46
4:O:9:DT:H72	5:P:26:DA:H1'	1.98	0.46
1:A:154:PHE:HE2	1:A:166:ILE:CG1	2.29	0.46
3:B:15:ASP:HB2	3:B:59:PHE:CZ	2.51	0.45
3:B:488:GLN:OE1	3:B:488:GLN:HA	2.15	0.45
5:P:29:DA:H2''	5:P:30:DA:C8	2.51	0.45
1:A:99:PHE:HD2	1:A:145:GLU:CB	2.28	0.45
1:A:242:LEU:HD12	1:A:242:LEU:O	2.16	0.45
2:E:101:GLN:CB	2:E:111:LEU:HD13	2.45	0.45
3:B:240:ILE:HG22	3:B:240:ILE:O	2.17	0.45
3:B:280:ASP:OD1	3:B:281:ALA:N	2.49	0.45
1:A:174:ASN:HD21	1:A:177:GLY:CA	2.24	0.45
3:B:161:LEU:HD23	3:B:163:PHE:HE1	1.81	0.45
1:A:95:ASN:OD1	1:A:96:SER:N	2.49	0.45
3:B:323:PHE:CD2	3:B:328:GLU:HB2	2.51	0.45
1:A:37:SER:HB2	1:A:154:PHE:HE1	1.82	0.45
3:B:151:ILE:HD11	3:B:211:VAL:HG22	1.98	0.45
4:O:9:DT:O2	4:O:9:DT:O4'	2.34	0.45
1:A:463:LYS:HD3	3:B:387:LEU:HG	1.99	0.45
1:A:578:VAL:N	1:A:579:PRO:CD	2.79	0.45
2:E:62:CYS:SG	2:E:117:MET:HE3	2.57	0.45
3:B:447:THR:OG1	3:B:450:GLN:OE1	2.35	0.45
1:A:303:PHE:HA	1:A:311:LEU:HG	1.99	0.45
3:B:85:LEU:CD2	3:B:86:PRO:HD2	2.47	0.45
1:A:243:LEU:HD12	1:A:243:LEU:O	2.17	0.45
2:E:49:PHE:CZ	2:E:51:GLY:HA3	2.52	0.45
3:B:347:LYS:HB2	3:B:350:GLN:HG3	1.98	0.45
5:P:21:DA:H4'	5:P:22:DA:O5'	2.14	0.45
3:B:404:GLN:OE1	3:B:423:GLN:HG3	2.17	0.45
3:B:409:PHE:CE1	3:B:420:VAL:HB	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:ALA:HB2	3:B:321:VAL:HG11	1.99	0.45
1:A:529:VAL:HG12	1:A:530:TYR:HD1	1.81	0.45
6:A:701:IHP:O44	3:B:363:LYS:NZ	2.49	0.45
1:A:82:LEU:CB	1:A:108:LEU:HD22	2.47	0.44
1:A:328:ILE:C	1:A:329:LEU:HD23	2.42	0.44
1:A:576:PHE:HB2	1:A:581:LEU:HD21	2.00	0.44
2:E:42:ASP:OD1	2:E:42:ASP:C	2.60	0.44
2:E:98:ALA:CB	2:E:115:SER:HB3	2.47	0.44
3:B:132:ILE:HB	3:B:161:LEU:HD12	1.98	0.44
1:A:348:MET:HE2	1:A:399:ARG:HB2	2.00	0.44
3:B:210:MET:SD	3:B:210:MET:C	3.00	0.44
1:A:149:VAL:O	1:A:153:LEU:HD23	2.17	0.44
3:B:213:ILE:HG13	3:B:221:LEU:CD2	2.43	0.44
3:B:213:ILE:HG22	3:B:214:SER:N	2.31	0.44
1:A:104:VAL:O	1:A:104:VAL:HG22	2.17	0.44
1:A:207:LYS:HG2	1:A:208:PRO:N	2.32	0.44
1:A:316:THR:HG23	1:A:318:ARG:NH1	2.22	0.44
1:A:462:MET:HE2	1:A:462:MET:CA	2.40	0.44
1:A:462:MET:CG	3:B:380:LEU:HA	2.41	0.44
1:A:510:LYS:H	1:A:510:LYS:HD2	1.83	0.44
2:E:18:TRP:CE2	2:E:19:MET:HG3	2.52	0.44
3:B:20:MET:HG3	3:B:20:MET:O	2.17	0.44
3:B:321:VAL:HG23	3:B:321:VAL:O	2.17	0.44
1:A:38:LEU:HD12	1:A:38:LEU:N	2.32	0.44
1:A:286:ILE:O	1:A:288:LEU:HD23	2.18	0.44
2:E:52:SER:C	2:E:53:ILE:HD13	2.43	0.44
3:B:165:LEU:O	3:B:226:SER:HA	2.17	0.44
2:E:168:LYS:HE2	2:E:230:LEU:CD2	2.48	0.44
3:B:184:ARG:HH12	3:B:520:ALA:HB2	1.82	0.44
3:B:199:GLU:HA	3:B:202:LYS:HG2	1.99	0.44
1:A:198:ILE:HG22	1:A:200:LEU:CD1	2.47	0.44
1:A:248:ALA:HA	3:B:432:GLN:HG2	2.00	0.44
1:A:303:PHE:HB3	1:A:310:LEU:HA	2.00	0.44
1:A:450:GLU:OE1	1:A:451:LYS:N	2.51	0.44
1:A:463:LYS:HE2	1:A:463:LYS:HB2	1.79	0.44
3:B:227:PHE:HA	3:B:230:SER:OG	2.17	0.44
3:B:372:ALA:C	3:B:374:ALA:H	2.25	0.44
4:O:11:DT:H2''	4:O:12:DA:O5'	2.18	0.44
1:A:49:PHE:HE1	1:A:60:PHE:CD2	2.36	0.43
1:A:110:ASN:N	1:A:110:ASN:OD1	2.51	0.43
2:E:148:LEU:HD12	2:E:148:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:398:ASP:OD1	3:B:400:ARG:N	2.51	0.43
1:A:49:PHE:HE1	1:A:60:PHE:CG	2.36	0.43
1:A:134:MET:SD	1:A:135:MET:HG2	2.59	0.43
3:B:44:ARG:HG2	3:B:237:PHE:CE1	2.52	0.43
1:A:122:PHE:CD2	1:A:131:PHE:HB2	2.45	0.43
1:A:318:ARG:HE	1:A:331:LYS:HZ1	1.66	0.43
1:A:522:VAL:HG11	3:B:256:ASN:HB2	2.00	0.43
1:A:41:LEU:HD21	1:A:146:VAL:HG21	1.99	0.43
1:A:97:VAL:HG23	1:A:99:PHE:HD1	1.82	0.43
2:E:69:ILE:HD12	2:E:110:TYR:CE2	2.54	0.43
2:E:81:PHE:HD2	2:E:102:LEU:HD21	1.83	0.43
3:B:65:ASP:OD1	3:B:65:ASP:O	2.36	0.43
3:B:158:ASP:O	3:B:158:ASP:CG	2.61	0.43
1:A:231:VAL:HG23	1:A:232:HIS:N	2.32	0.43
3:B:247:TRP:CZ2	3:B:338:LYS:HD2	2.54	0.43
3:B:538:PRO:C	3:B:539:LEU:HD23	2.43	0.43
1:A:279:LYS:HG2	3:B:357:MET:CE	2.48	0.43
3:B:400:ARG:NH2	5:P:24:DA:H1'	2.34	0.43
3:B:536:LEU:HD23	3:B:536:LEU:HA	1.82	0.43
1:A:531:PRO:CB	1:A:532:PRO:HD2	2.48	0.43
3:B:154:LEU:HD23	3:B:154:LEU:HA	1.90	0.43
1:A:421:ASP:OD1	1:A:425:ILE:N	2.40	0.43
1:A:439:PHE:N	1:A:442:ASP:OD2	2.46	0.43
3:B:213:ILE:CG1	3:B:221:LEU:HD21	2.43	0.43
5:P:20:DT:O2	5:P:20:DT:C2'	2.67	0.43
1:A:102:ILE:HD11	1:A:149:VAL:HG11	1.99	0.43
1:A:113:ALA:HB1	1:A:495:LEU:CD1	2.43	0.42
1:A:262:LYS:HA	1:A:268:VAL:HG23	2.01	0.42
1:A:385:LEU:HD12	1:A:385:LEU:HA	1.82	0.42
1:A:483:LEU:HD22	1:A:487:PHE:HE2	1.83	0.42
2:E:17:GLU:OE1	2:E:17:GLU:CA	2.67	0.42
3:B:214:SER:O	3:B:214:SER:OG	2.33	0.42
3:B:226:SER:OG	3:B:229:GLU:OE2	2.30	0.42
3:B:377:LEU:HD12	3:B:377:LEU:HA	1.76	0.42
1:A:154:PHE:CE1	1:A:164:LYS:HB3	2.54	0.42
1:A:388:LYS:HA	1:A:388:LYS:HD3	1.66	0.42
3:B:275:THR:HG23	4:O:9:DT:OP1	2.19	0.42
2:E:65:LEU:HD12	2:E:110:TYR:CE1	2.54	0.42
3:B:111:LEU:HD13	3:B:134:ILE:HD11	2.00	0.42
3:B:361:VAL:HG22	3:B:422:VAL:CG2	2.49	0.42
5:P:24:DA:C2'	5:P:25:DA:H8	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:VAL:HG22	1:A:169:PHE:HB2	1.99	0.42
1:A:466:VAL:HG23	3:B:345:PHE:CG	2.55	0.42
3:B:85:LEU:HD22	3:B:86:PRO:HD2	2.01	0.42
2:E:17:GLU:OE2	2:E:21:VAL:HG23	2.20	0.42
5:P:25:DA:H3'	5:P:26:DA:H8	1.84	0.42
1:A:168:LEU:C	1:A:169:PHE:HD1	2.27	0.42
2:E:226:ASN:OD1	2:E:226:ASN:C	2.62	0.42
2:E:176:SER:O	2:E:179:SER:N	2.52	0.42
2:E:182:LYS:O	2:E:186:GLY:HA2	2.19	0.42
2:E:195:ILE:HD12	2:E:195:ILE:N	2.35	0.42
3:B:246:HIS:HE2	3:B:248:PRO:HG3	1.83	0.42
4:O:6:DT:H5''	4:O:6:DT:C2	2.54	0.42
5:P:27:DC:H6	5:P:27:DC:H2'	1.63	0.42
1:A:304:ASN:HB2	1:A:311:LEU:CD2	2.42	0.42
3:B:11:VAL:HG21	3:B:118:ILE:HG12	2.02	0.42
3:B:286:LYS:NZ	3:B:289:ILE:O	2.48	0.42
3:B:484:ASN:OD1	3:B:485:PRO:HD2	2.20	0.42
3:B:202:LYS:HB3	3:B:202:LYS:HE2	1.75	0.42
4:O:13:DT:C1'	4:O:14:DT:H73	2.27	0.42
5:P:21:DA:H2''	5:P:22:DA:C2	2.55	0.42
1:A:286:ILE:HG13	1:A:288:LEU:CD2	2.50	0.41
1:A:399:ARG:HG2	1:A:408:PRO:HB2	2.02	0.41
1:A:608:GLN:O	1:A:608:GLN:OE1	2.38	0.41
3:B:38:ILE:O	3:B:42:VAL:HG23	2.20	0.41
3:B:489:ARG:HD2	3:B:508:ILE:HG12	2.02	0.41
1:A:150:CYS:HB3	1:A:166:ILE:CD1	2.50	0.41
2:E:47:LEU:N	2:E:188:GLN:O	2.53	0.41
2:E:55:TYR:HE2	2:E:205:LEU:CB	2.33	0.41
2:E:78:VAL:HG12	2:E:134:LYS:HB3	2.02	0.41
1:A:62:MET:HE2	1:A:62:MET:HB2	1.82	0.41
2:E:229:ILE:HG13	2:E:230:LEU:N	2.34	0.41
2:E:230:LEU:HD23	2:E:230:LEU:O	2.20	0.41
3:B:6:ASN:OD1	3:B:6:ASN:N	2.41	0.41
3:B:161:LEU:O	3:B:162:GLN:HG3	2.20	0.41
3:B:490:LEU:HD12	3:B:494:LEU:HG	2.02	0.41
1:A:529:VAL:HG12	1:A:530:TYR:CD1	2.55	0.41
1:A:205:LEU:CD1	1:A:242:LEU:HD22	2.51	0.41
1:A:276:LEU:O	3:B:431:ARG:HB2	2.21	0.41
1:A:466:VAL:HG23	3:B:345:PHE:CD2	2.56	0.41
1:A:279:LYS:HG2	3:B:357:MET:HE1	2.01	0.41
1:A:282:LYS:O	1:A:282:LYS:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:155:LEU:HD12	2:E:155:LEU:HA	1.79	0.41
3:B:190:PRO:O	3:B:191:SER:OG	2.26	0.41
3:B:490:LEU:HD12	3:B:490:LEU:O	2.21	0.41
5:P:24:DA:H8	5:P:24:DA:O5'	2.03	0.41
1:A:261:LEU:HD13	1:A:345:LEU:CB	2.50	0.41
1:A:273:ILE:HG21	1:A:366:LEU:HD13	2.03	0.41
1:A:316:THR:CG2	1:A:318:ARG:HH22	2.33	0.41
1:A:533:ASP:OD1	1:A:533:ASP:N	2.54	0.41
3:B:24:ILE:HG23	3:B:27:ILE:CD1	2.42	0.41
3:B:400:ARG:NH1	5:P:24:DA:N3	2.68	0.41
1:A:193:LEU:HD12	1:A:198:ILE:HD12	2.03	0.41
1:A:509:PRO:HG3	3:B:343:LEU:HD23	2.02	0.41
1:A:217:TYR:HA	1:A:220:ILE:HD12	2.02	0.41
1:A:319:SER:HB2	1:A:328:ILE:CD1	2.49	0.41
2:E:172:THR:O	2:E:172:THR:OG1	2.32	0.41
3:B:405:VAL:O	3:B:424:LEU:HB2	2.21	0.41
4:O:17:DG:N2	5:P:18:DT:H6	2.19	0.41
1:A:288:LEU:HD12	1:A:293:ASN:C	2.46	0.41
1:A:461:LYS:HZ2	1:A:524:GLU:HB3	1.85	0.41
3:B:46:VAL:HG22	3:B:86:PRO:HB2	2.02	0.41
3:B:384:LEU:HD23	3:B:384:LEU:HA	1.93	0.41
1:A:303:PHE:HD1	1:A:304:ASN:O	2.03	0.40
1:A:201:ASP:CG	1:A:249:LYS:HD3	2.47	0.40
1:A:317:LYS:NZ	1:A:330:GLU:OE2	2.41	0.40
1:A:580:MET:SD	1:A:581:LEU:CD2	3.09	0.40
1:A:121:GLN:HE22	1:A:130:ARG:CD	2.27	0.40
1:A:575:LYS:HA	2:E:149:ARG:CG	2.51	0.40
2:E:218:TYR:CD1	2:E:218:TYR:C	2.99	0.40
3:B:253:ILE:O	3:B:253:ILE:CG2	2.70	0.40
3:B:413:LYS:C	3:B:415:ASN:H	2.29	0.40
1:A:104:VAL:C	1:A:106:GLN:H	2.28	0.40
1:A:457:GLU:H	1:A:457:GLU:CD	2.19	0.40
1:A:462:MET:HA	1:A:462:MET:CE	2.48	0.40
2:E:49:PHE:HD1	2:E:218:TYR:CD2	2.39	0.40
2:E:73:LEU:HD12	2:E:74:SER:H	1.86	0.40
3:B:489:ARG:CD	3:B:508:ILE:HG12	2.52	0.40
4:O:17:DG:N1	5:P:18:DT:H72	2.25	0.40
5:P:25:DA:H2'	5:P:25:DA:N3	2.36	0.40
1:A:41:LEU:O	1:A:168:LEU:HA	2.22	0.40
1:A:277:VAL:O	1:A:277:VAL:HG23	2.22	0.40
1:A:376:ILE:HD13	1:A:376:ILE:HA	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:LEU:HD11	1:A:437:LEU:HD12	2.03	0.40
1:A:466:VAL:CG1	3:B:387:LEU:HD12	2.51	0.40
1:A:572:THR:O	1:A:574:GLY:N	2.50	0.40
1:A:580:MET:SD	1:A:580:MET:C	3.05	0.40
3:B:203:GLU:OE1	3:B:203:GLU:CA	2.67	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	550/609 (90%)	508 (92%)	40 (7%)	2 (0%)	30	59
2	E	214/1432 (15%)	204 (95%)	8 (4%)	2 (1%)	14	43
3	B	526/732 (72%)	505 (96%)	21 (4%)	0	100	100
All	All	1290/2773 (46%)	1217 (94%)	69 (5%)	4 (0%)	37	65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	ILE
1	A	231	VAL
2	E	206	THR
2	E	207	GLU

### 5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	408/548 (74%)	408 (100%)	0	100	100
2	E	150/1293 (12%)	149 (99%)	1 (1%)	76	79
3	B	431/649 (66%)	429 (100%)	2 (0%)	81	82
All	All	989/2490 (40%)	986 (100%)	3 (0%)	84	85

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	100	ILE
3	B	95	GLU
3	B	279	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	68	GLN
1	A	121	GLN
1	A	174	ASN
1	A	405	ASN
1	A	433	GLN
2	E	113	HIS
3	B	73	GLN
3	B	80	HIS
3	B	359	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	IHP	A	701	-	36,36,36	1.44	6 (16%)	54,60,60	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	IHP	A	701	-	-	8/30/54/54	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	701	IHP	P6-O16	3.11	1.65	1.59
6	A	701	IHP	P2-O12	3.11	1.65	1.59
6	A	701	IHP	P3-O13	3.10	1.65	1.59
6	A	701	IHP	P4-O14	3.06	1.65	1.59
6	A	701	IHP	P1-O11	3.04	1.65	1.59
6	A	701	IHP	P5-O15	2.99	1.65	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	701	IHP	C1-O11-P1-O31
6	A	701	IHP	C3-O13-P3-O33
6	A	701	IHP	C5-O15-P5-O25
6	A	701	IHP	C1-O11-P1-O21

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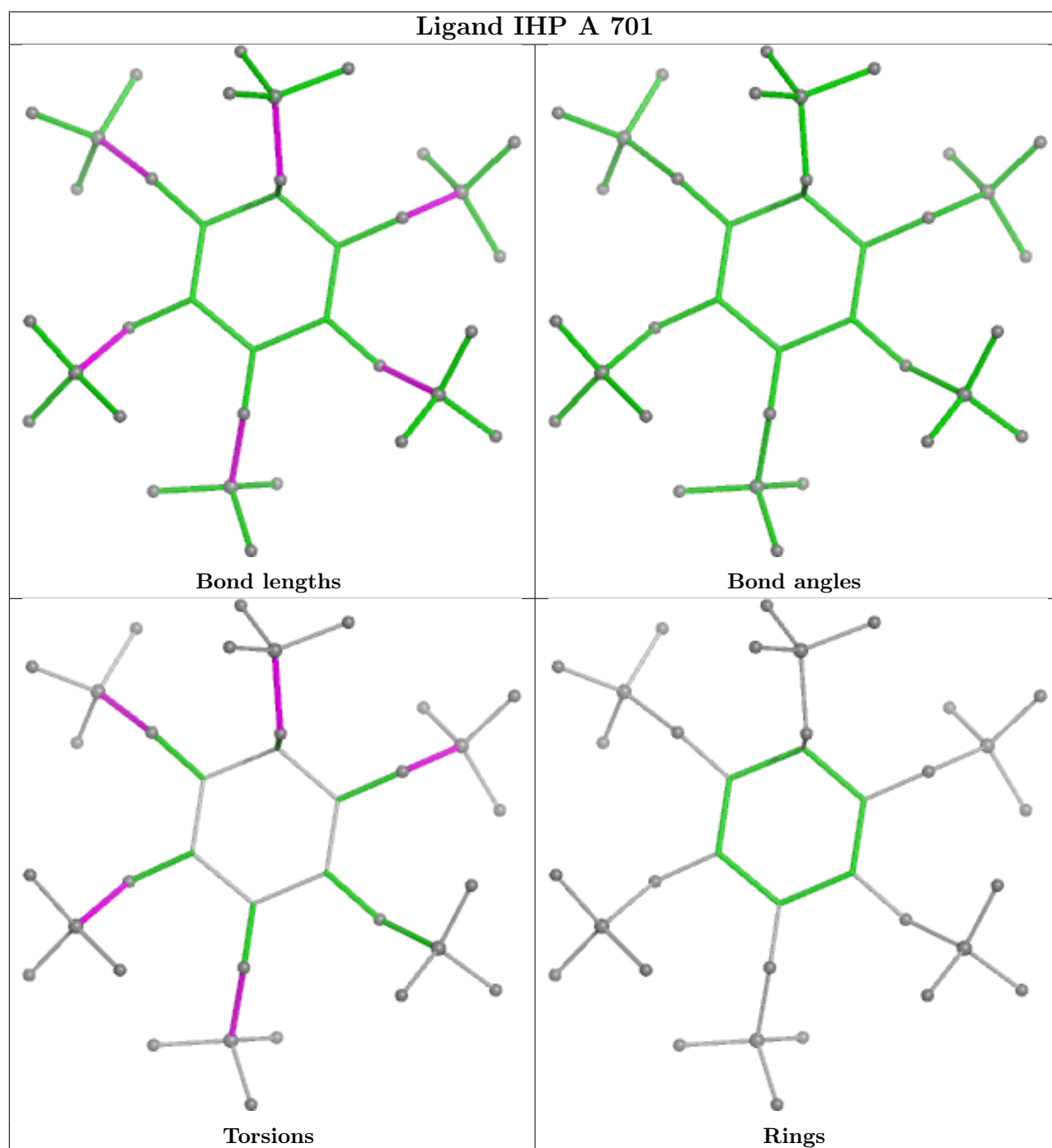
Mol	Chain	Res	Type	Atoms
6	A	701	IHP	C4-O14-P4-O44
6	A	701	IHP	C5-O15-P5-O45
6	A	701	IHP	C2-O12-P2-O22
6	A	701	IHP	C4-O14-P4-O34

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	701	IHP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

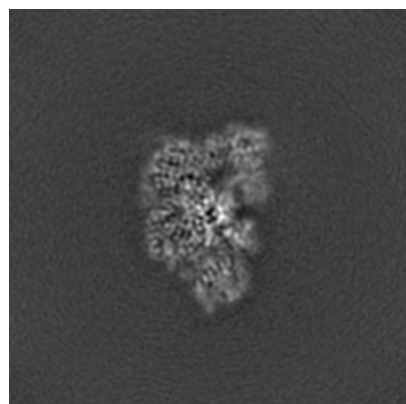
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52524. These allow visual inspection of the internal detail of the map and identification of artifacts.

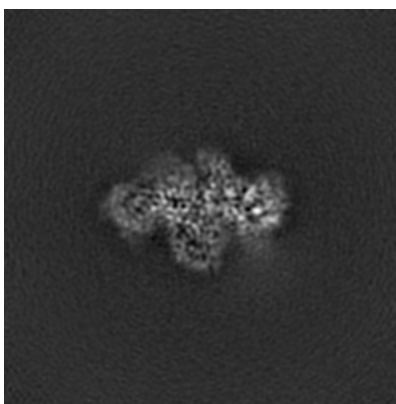
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

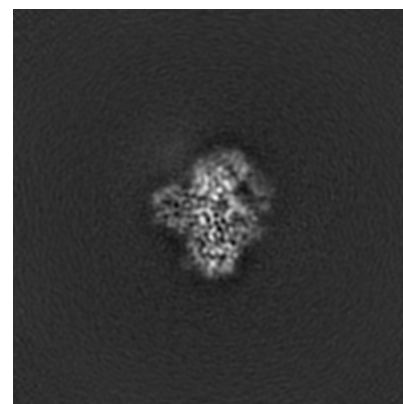
#### 6.1.1 Primary map



X

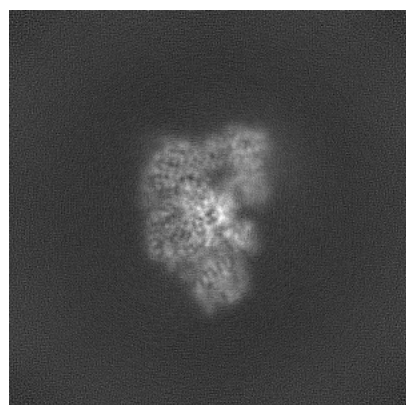


Y

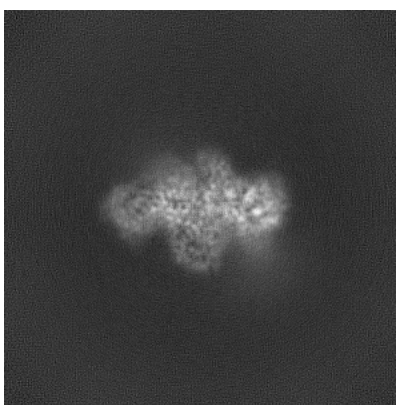


Z

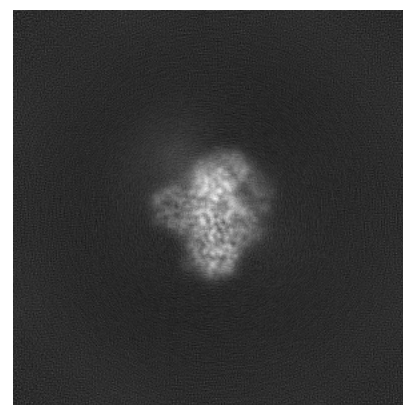
#### 6.1.2 Raw map



X



Y

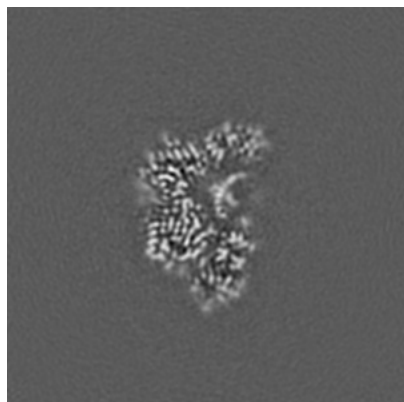


Z

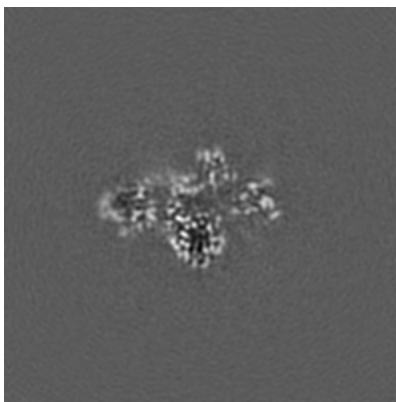
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

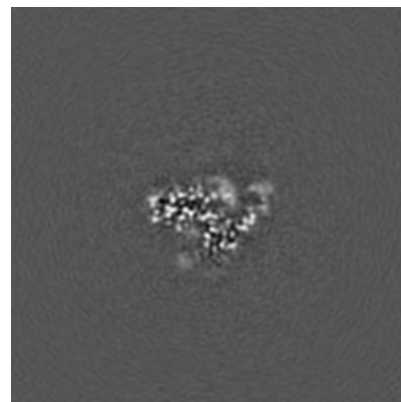
### 6.2.1 Primary map



X Index: 200

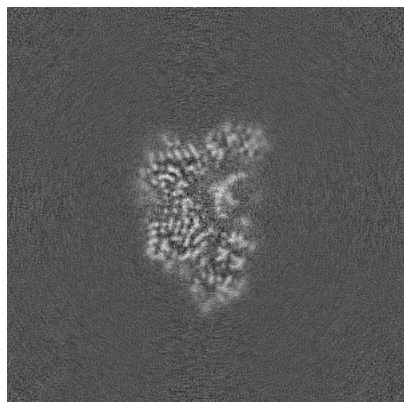


Y Index: 200

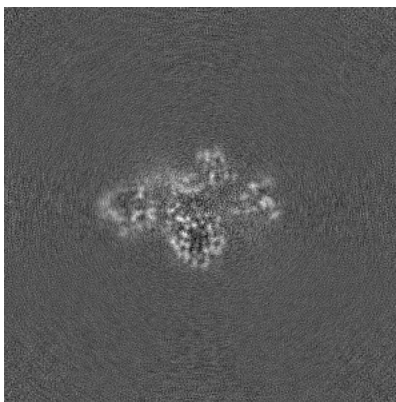


Z Index: 200

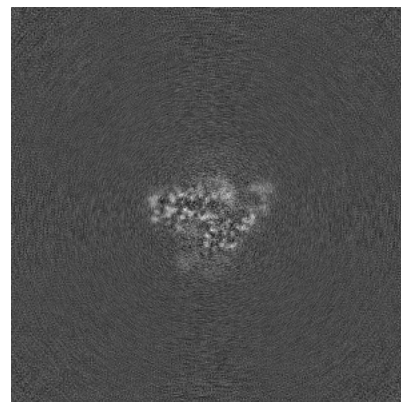
### 6.2.2 Raw map



X Index: 200



Y Index: 200

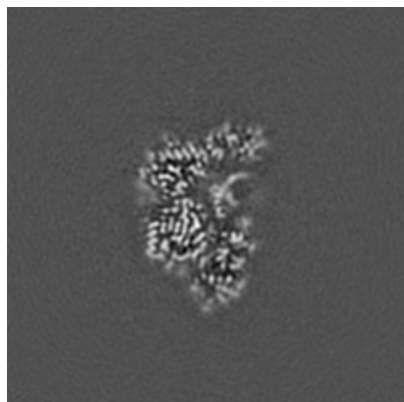


Z Index: 200

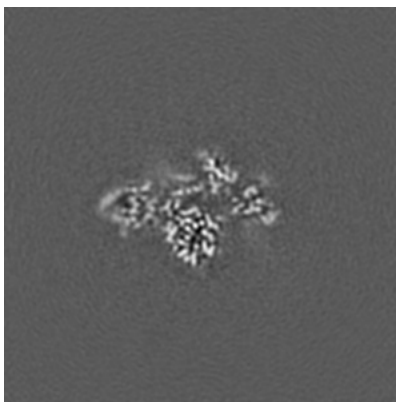
The images above show central slices of the map in three orthogonal directions.

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

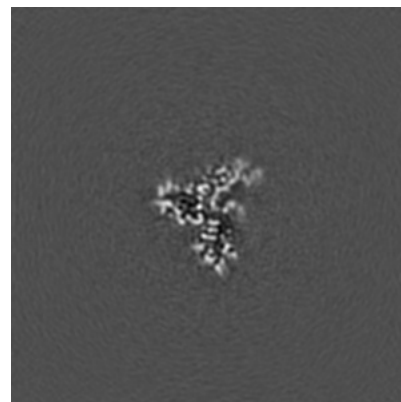
### 6.3.1 Primary map



X Index: 199

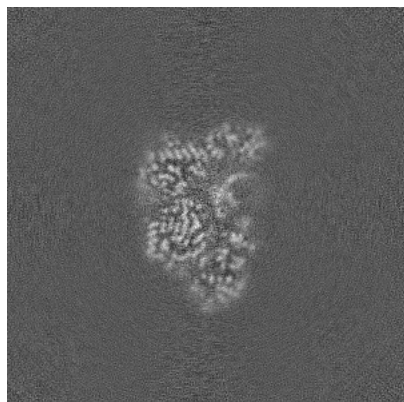


Y Index: 197

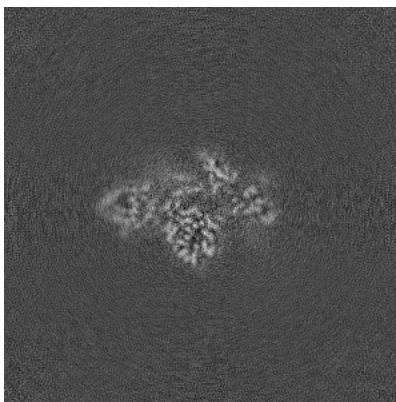


Z Index: 175

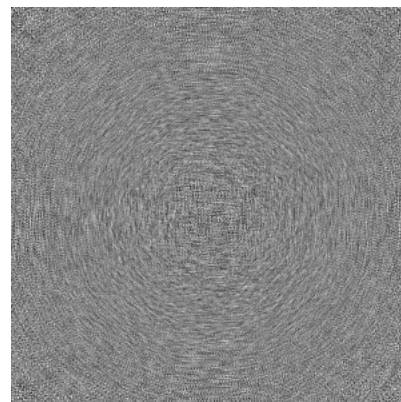
### 6.3.2 Raw map



X Index: 199



Y Index: 197

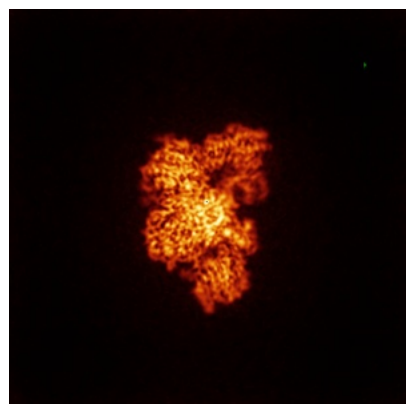


Z Index: 0

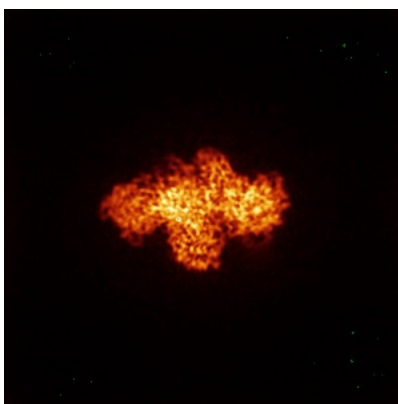
The images above show the largest variance slices of the map in three orthogonal directions.

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

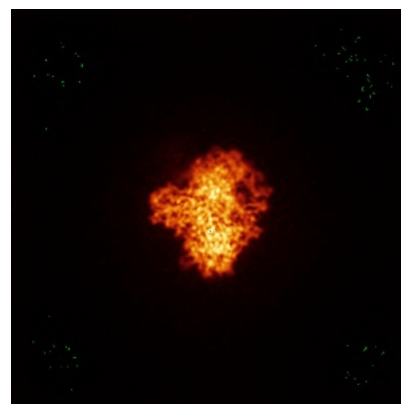
### 6.4.1 Primary map



X

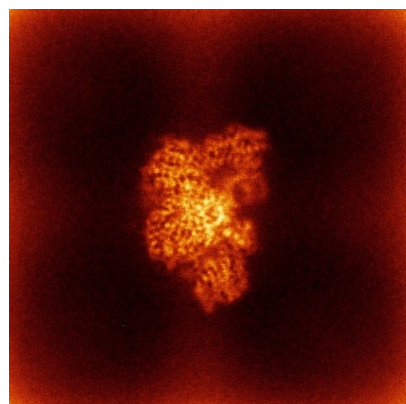


Y

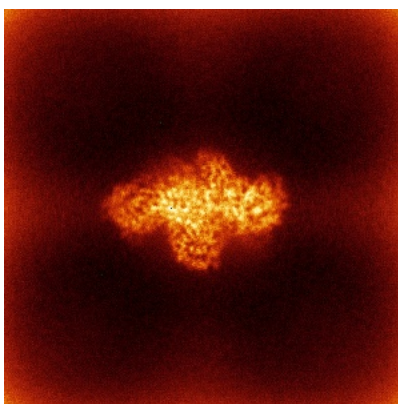


Z

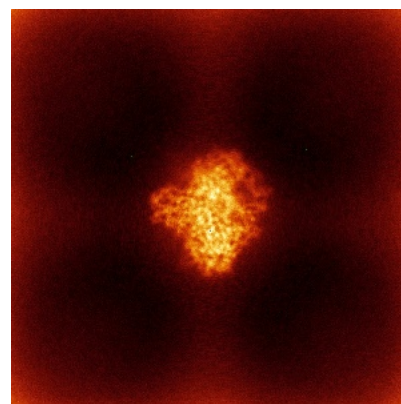
### 6.4.2 Raw map



X



Y

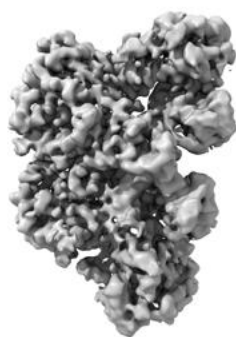


Z

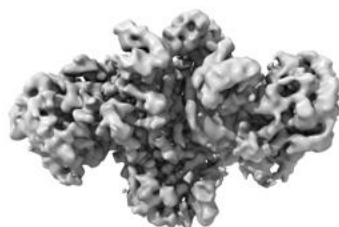
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

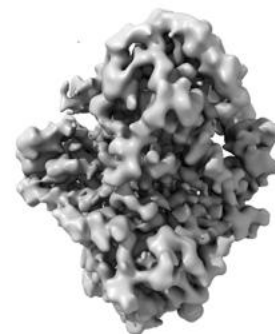
### 6.5.1 Primary map



X



Y



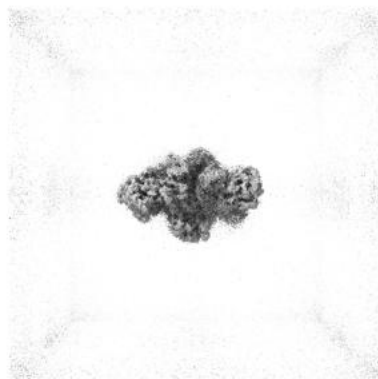
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0397. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

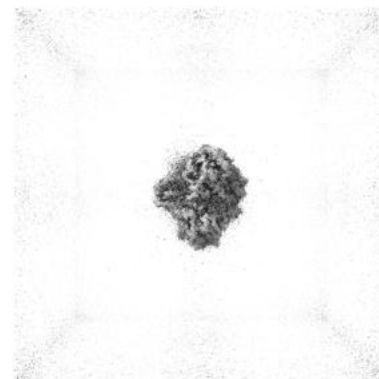
### 6.5.2 Raw map



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.

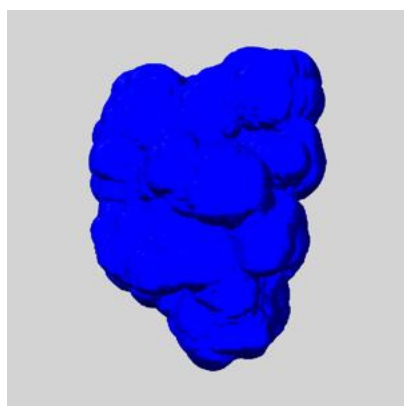
## 6.6 Mask visualisation [i](#)

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

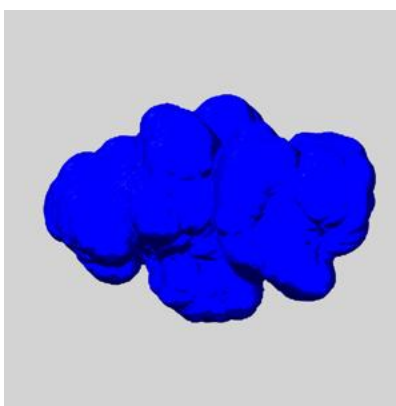
A mask typically either:

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

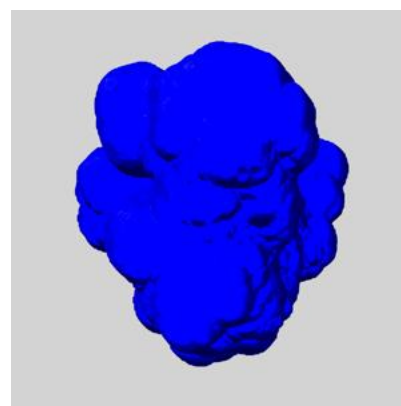
### 6.6.1 emd\_52524\_msk\_1.map [i](#)



X



Y

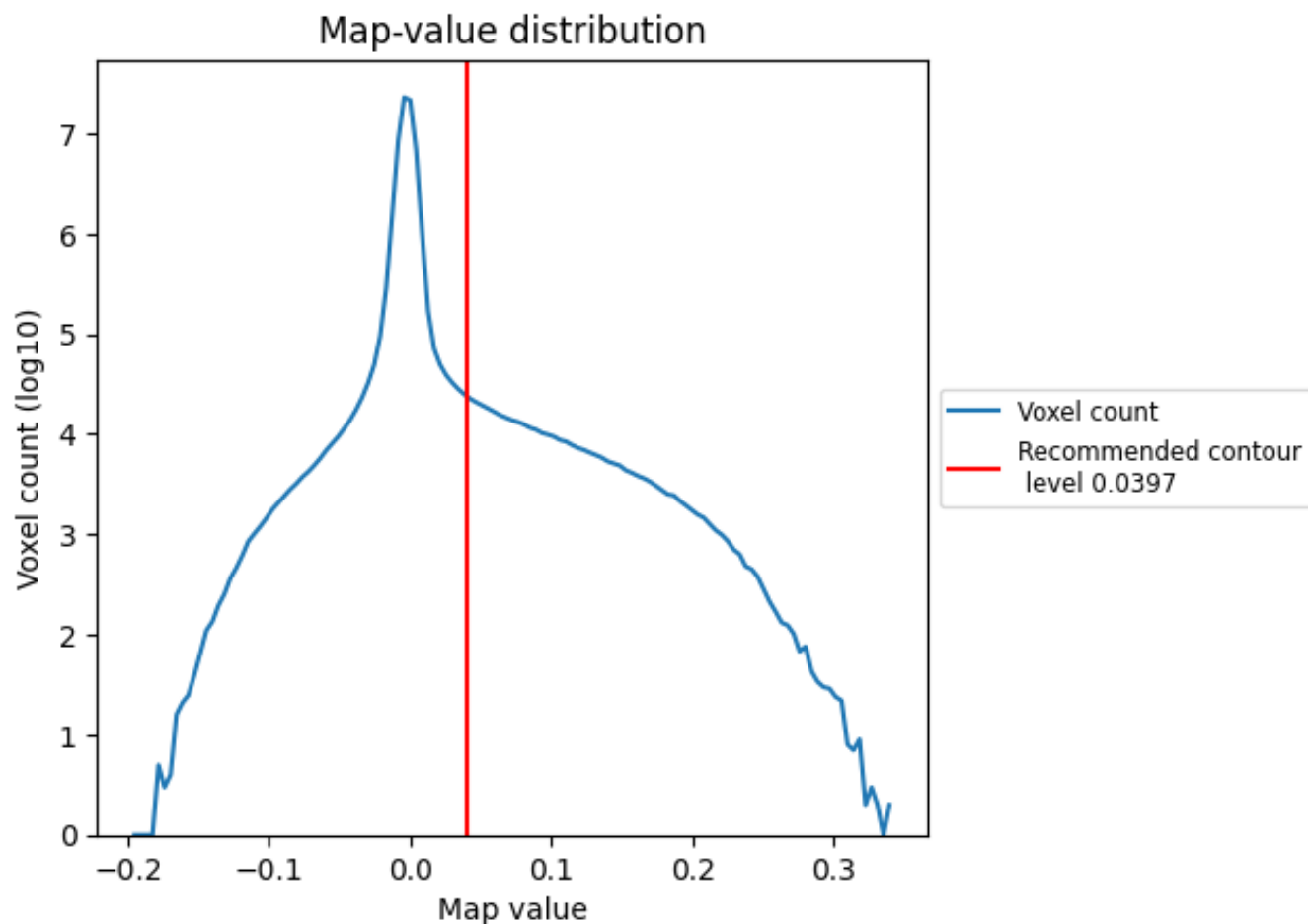


Z

## 7 Map analysis [i](#)

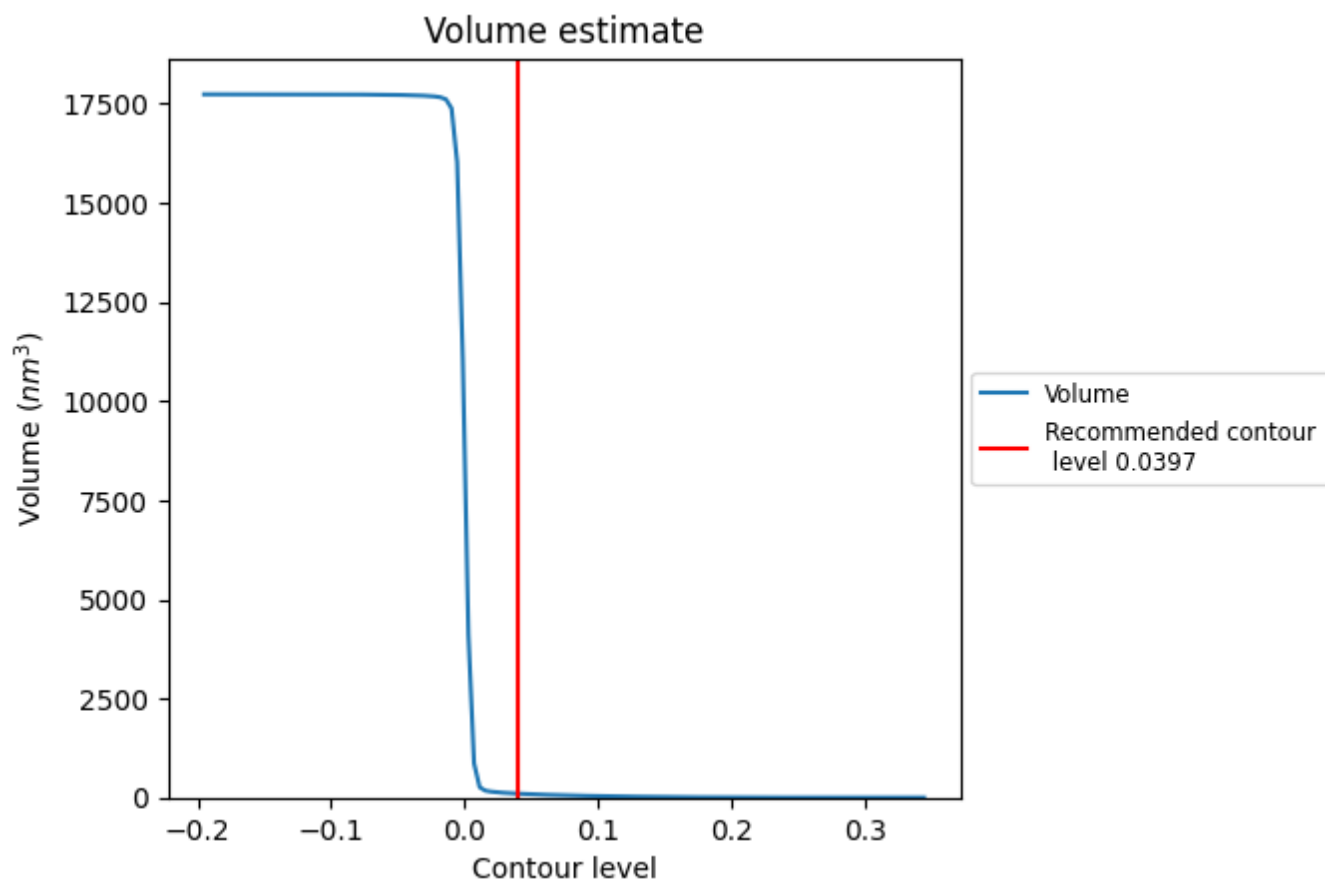
This section contains the results of statistical analysis of the map.

### 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.

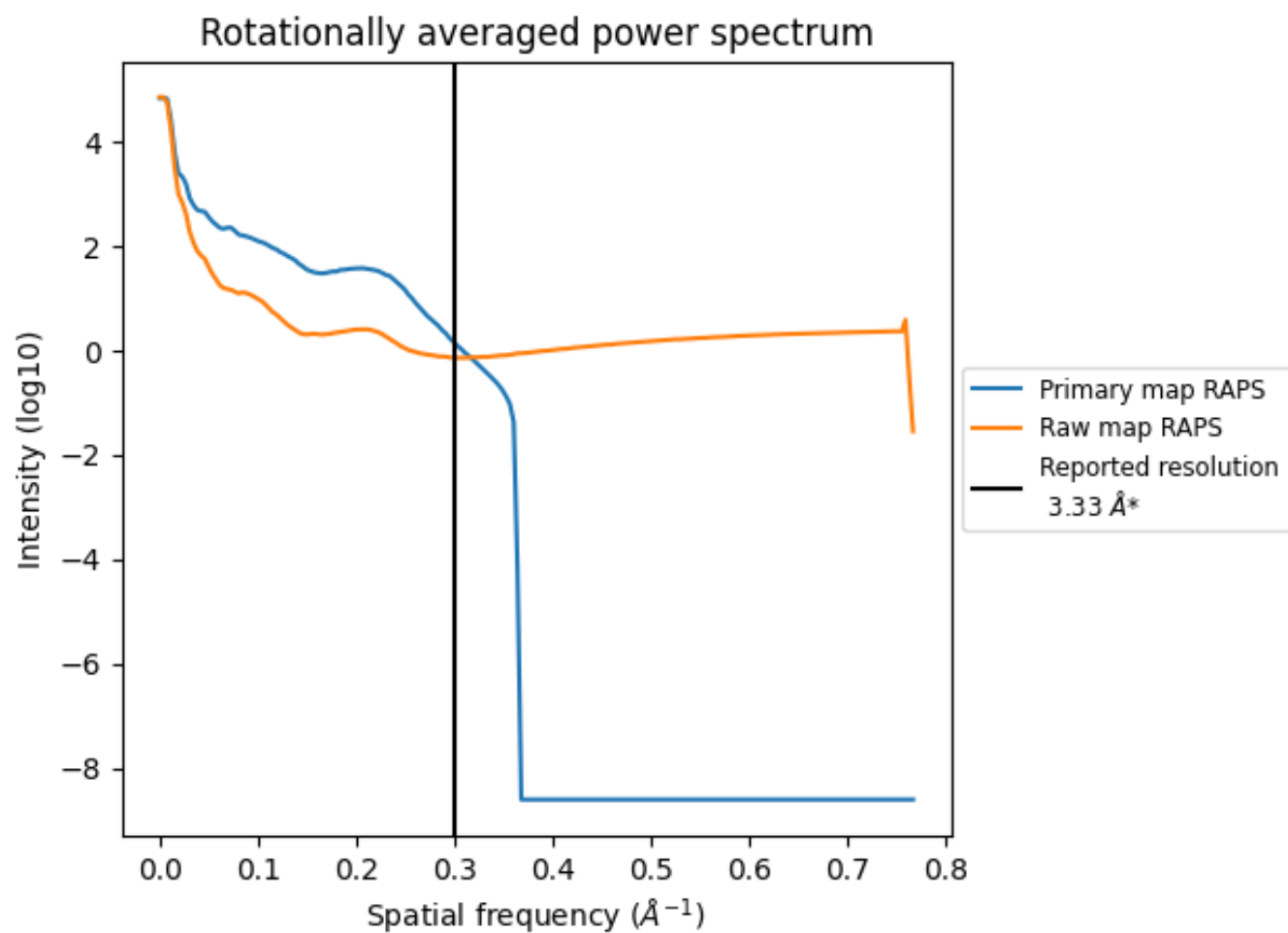
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 99  $\text{nm}^3$ ; this corresponds to an approximate mass of 89 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 ⓘ

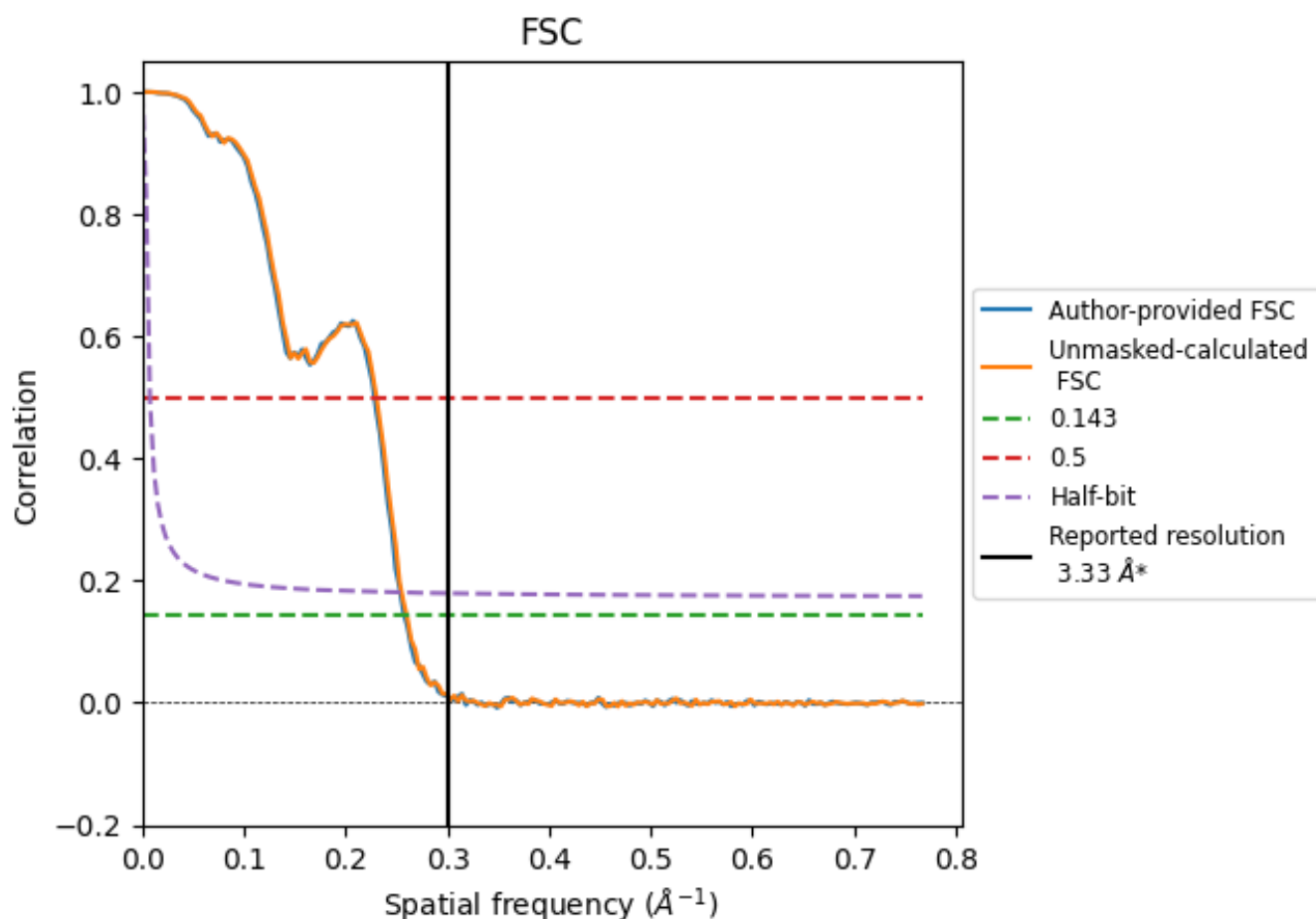


\*Reported resolution corresponds to spatial frequency of 0.300 Å<sup>-1</sup>

## 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 0.300  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.33	-	-
Author-provided FSC curve	3.88	4.38	3.94
Unmasked-calculated*	3.84	4.34	3.92

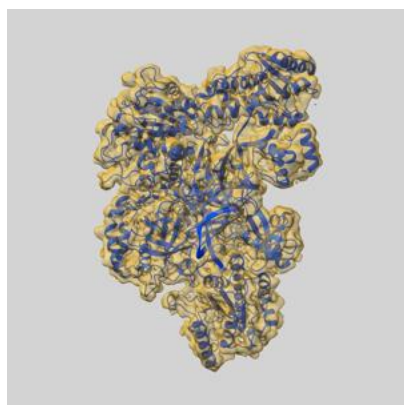
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.88 differs from the reported value 3.33 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.84 differs from the reported value 3.33 by more than 10 %

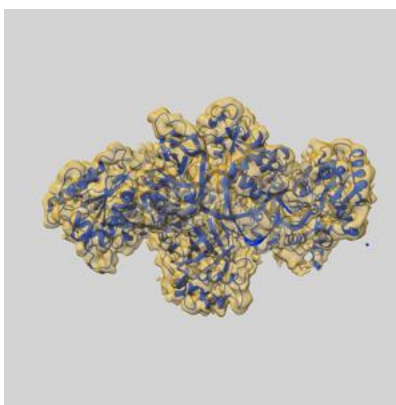
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52524 and PDB model 9HZG. Per-residue inclusion information can be found in section [3](#) on page [6](#).

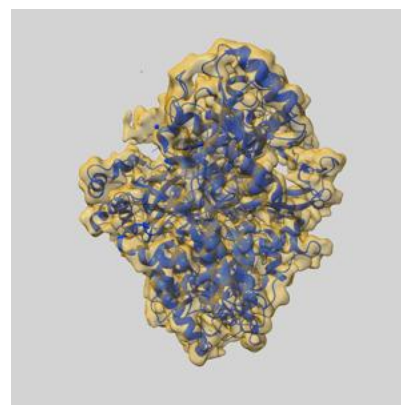
### 9.1 Map-model overlay [i](#)



X



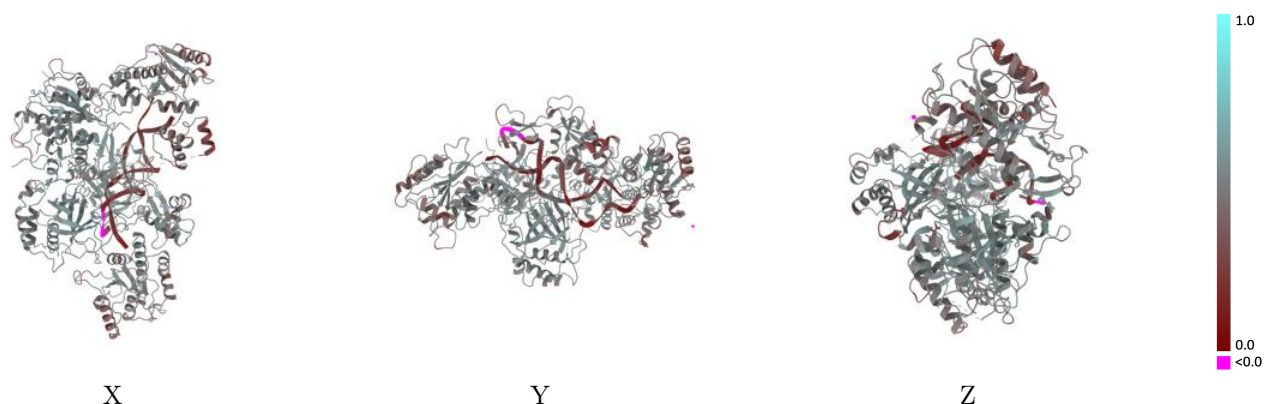
Y



Z

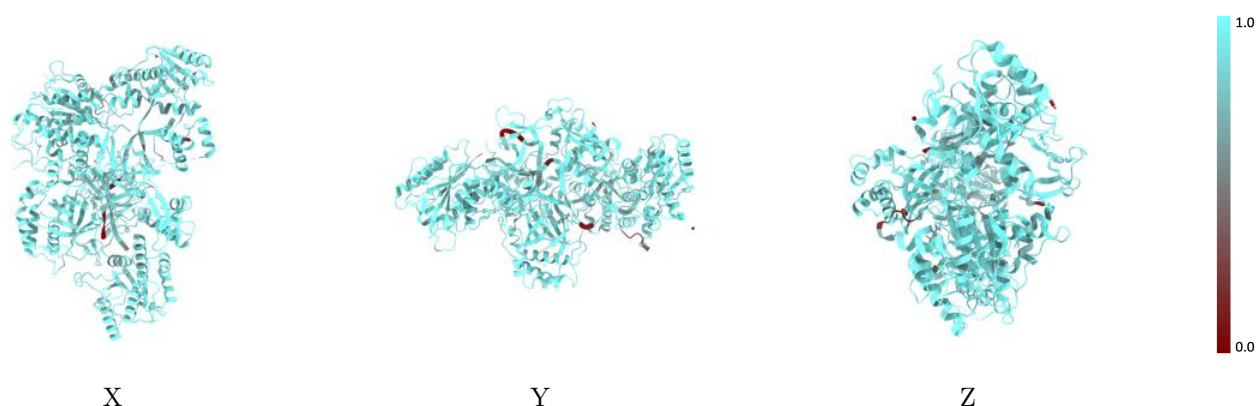
The images above show the 3D surface view of the map at the recommended contour level 0.0397 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



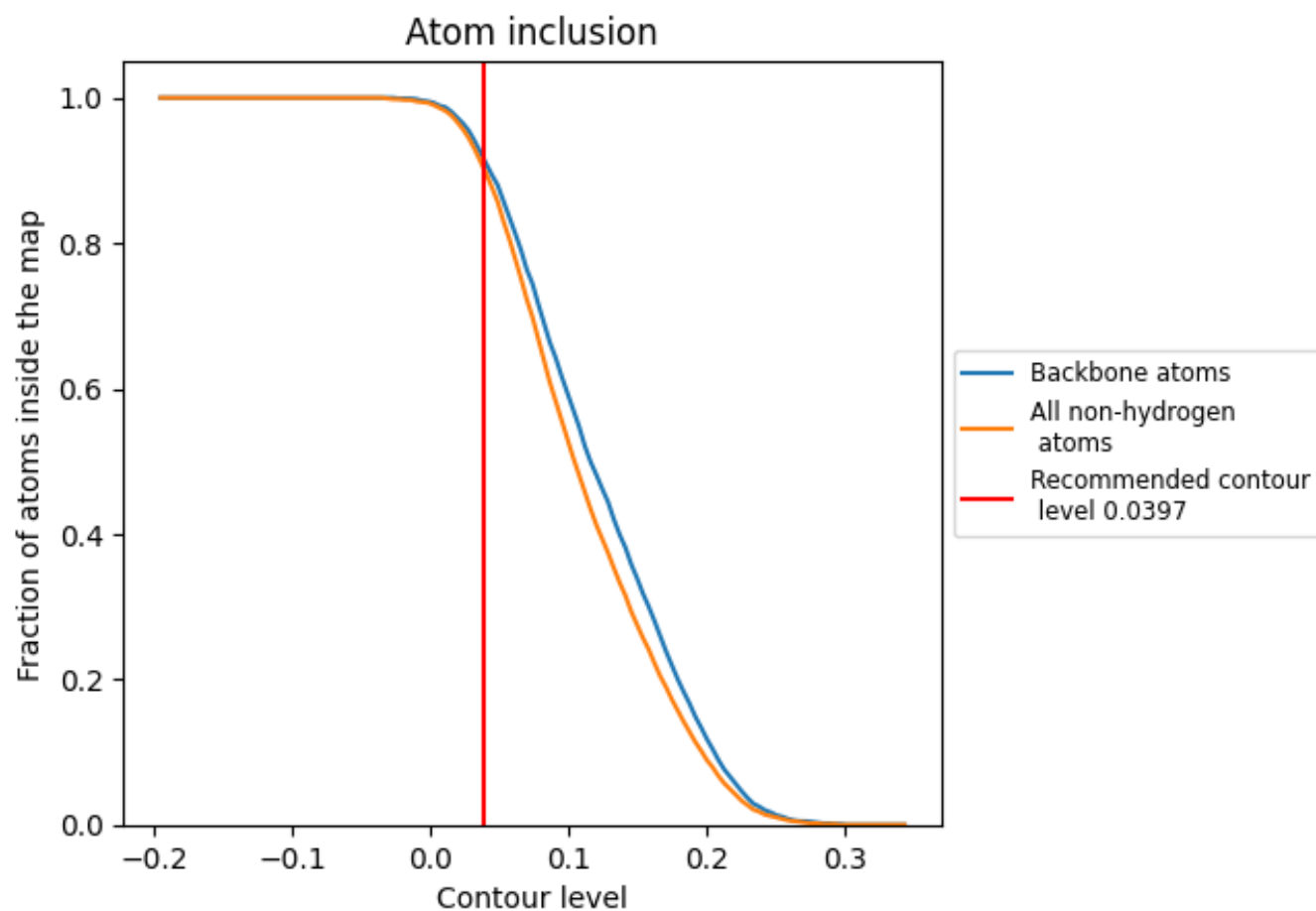
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0397).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 90% 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 (0.0397) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9000	<div></div> 0.4730
A	<div></div> 0.9170	<div></div> 0.4820
B	<div></div> 0.9210	<div></div> 0.5130
E	<div></div> 0.8930	<div></div> 0.4570
O	<div></div> 0.7180	<div></div> 0.2200
P	<div></div> 0.7110	<div></div> 0.2130

