



Full wwPDB EM Validation Report ⓘ

Jul 9, 2026 – 12:24 PM EDT

PDB ID : 9YC9 / pdb_00009yc9
EMDB ID : EMD-72764
Title : HSV replication fork complex bound to pritelivir
Authors : Yu, Z.; Abraham, J.
Deposited on : 2025-09-18
Resolution : 3.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

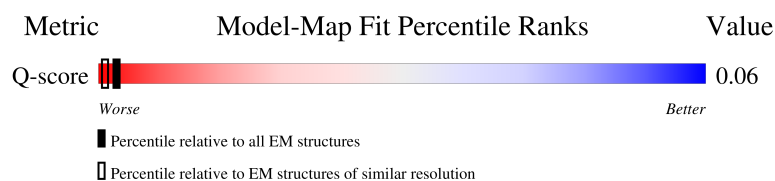
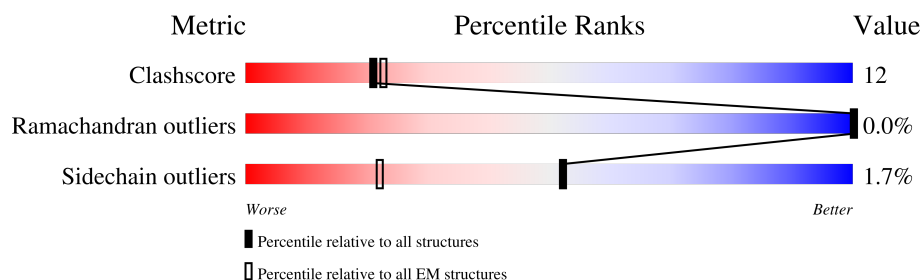
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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 3.80 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	10198 (3.30 - 4.30)

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

Mol	Chain	Length	Quality of chain
1	D	25	
2	P	25	
3	T	33	
4	C	1058	

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Mol	Chain	Length	Quality of chain
5	A	882	6% 55% 30% 13%
6	E	1235	16% 71% 15% 13%
7	B	750	92% 80% 19%
8	F	488	42% 11% 46%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 30757 atoms, of which 3 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	25	Total	C	N	O	P	0	0
			503	250	56	172	25		

- Molecule 2 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	25	Total	C	N	O	P	0	0
			517	244	98	150	25		

- Molecule 3 is a DNA chain called DNA (33-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	33	Total	C	N	O	P	0	0
			669	320	112	204	33		

- Molecule 4 is a protein called UL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	881	Total	C	N	O	S	0	0
			6803	4314	1232	1225	32		

- Molecule 5 is a protein called UL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	766	Total	C	N	O	S	0	0
			6107	3901	1065	1114	27		

- Molecule 6 is a protein called UL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	1071	Total	C	N	O	S	4	0
			8484	5431	1493	1519	41		

- Molecule 7 is a protein called UL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	746	Total	C	N	O	S	0	0
			5620	3609	996	996	19		

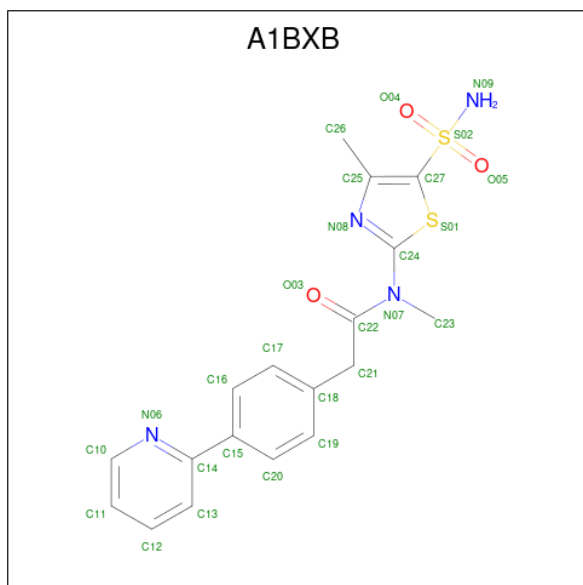
- Molecule 8 is a protein called UL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	262	Total	C	N	O	S	1	0
			2023	1286	356	373	8		

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
9	C	1	Total	Zn	0
			1	1	

- Molecule 10 is Pritelivir (CCD ID: A1BXB) (formula: C₁₈H₁₈N₄O₃S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
10	A	1	Total	C	H	N	O	S	0
			30	18	3	4	3	2	

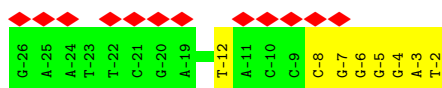
3 Residue-property plots [i](#)

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: DNA (25-MER)



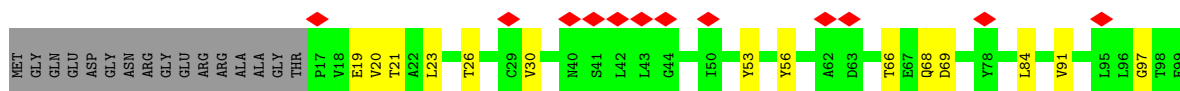
- Molecule 2: DNA (25-MER)

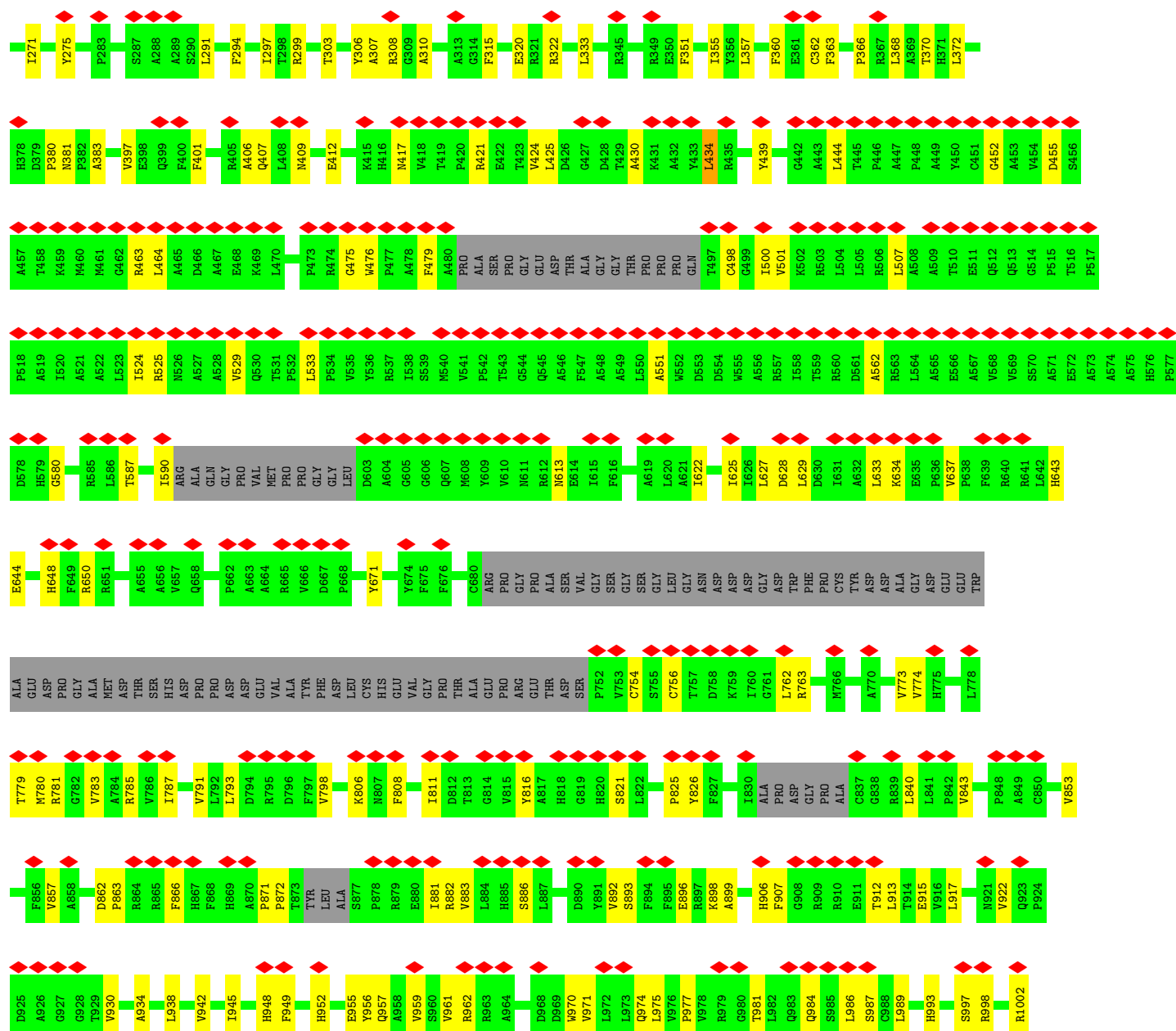


- Molecule 3: DNA (33-MER)

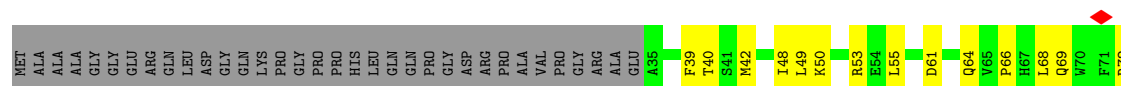


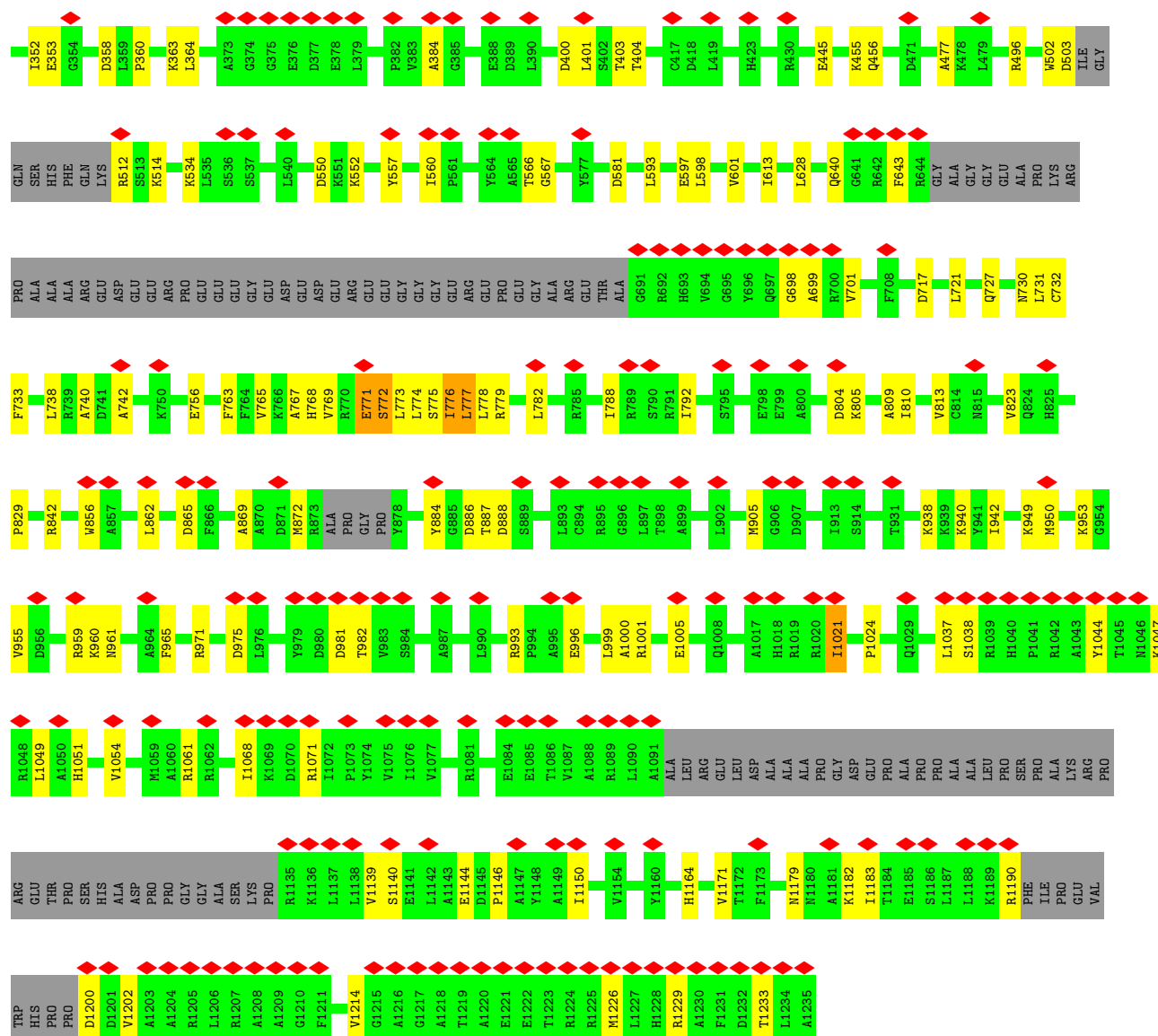
- Molecule 4: UL52



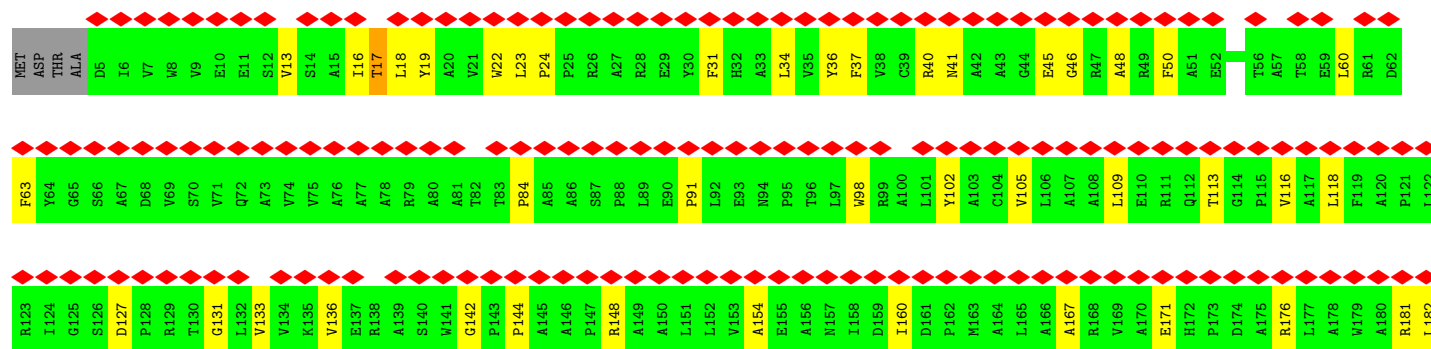
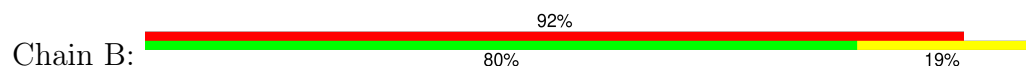


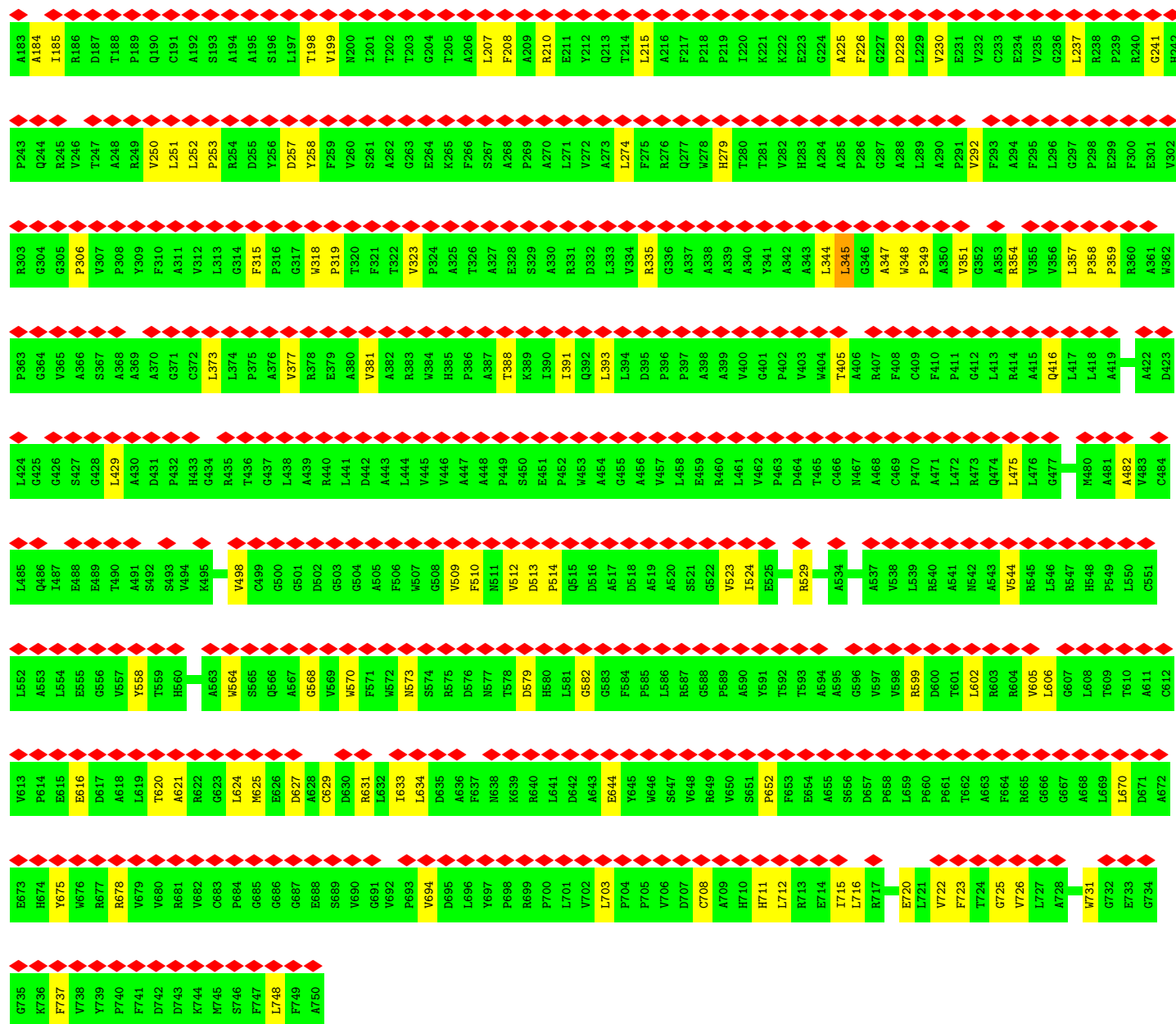
• Molecule 5: UL5



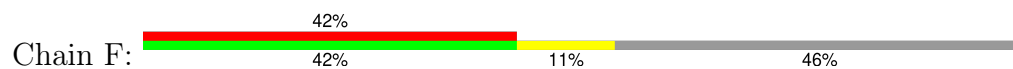


• Molecule 7: UL8





● Molecule 8: UL42



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.273	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.04	Depositor
Map size ($\text{\AA}$)	332.0, 332.0, 332.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, A1BXB

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	D	0.56	2/554 (0.4%)	0.75	0/854
2	P	0.83	0/580	0.79	0/894
3	T	1.31	1/746 (0.1%)	1.05	6/1148 (0.5%)
4	C	0.47	0/6961	0.66	0/9467
5	A	0.55	0/6241	0.79	5/8471 (0.1%)
6	E	0.87	0/8674	0.86	3/11745 (0.0%)
7	B	0.39	0/5778	0.57	0/7924
8	F	0.50	0/2058	0.79	1/2796 (0.0%)
All	All	0.65	3/31592 (0.0%)	0.76	15/43299 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	E	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	9	DG	O3'-P	27.63	2.02	1.61
1	D	10	DT	O3'-P	-6.15	1.51	1.61
1	D	11	DT	O3'-P	-5.77	1.52	1.61

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	9	DG	P-O3'-C3'	-17.86	93.42	120.20
3	T	9	DG	OP2-P-O3'	8.95	134.86	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	2	DA	P-O3'-C3'	7.31	131.17	120.20
3	T	17	DG	P-O3'-C3'	6.91	130.57	120.20
6	E	360	PRO	CA-C-N	6.28	134.87	122.31
6	E	360	PRO	C-N-CA	6.28	134.87	122.31
3	T	9	DG	OP1-P-O3'	-6.25	89.26	108.00
5	A	582	ALA	CA-C-N	-6.19	113.30	122.83
5	A	582	ALA	C-N-CA	-6.19	113.30	122.83
3	T	9	DG	O3'-P-O5'	-5.83	95.25	104.00
5	A	341	ILE	N-CA-CB	-5.60	105.03	112.26
8	F	319	LYS	CA-C-O	5.37	126.61	120.54
5	A	569	GLN	N-CA-C	-5.33	105.38	111.14
6	E	886	ASP	N-CA-C	-5.27	101.81	108.45
5	A	567	ALA	O-C-N	5.17	127.39	122.07

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	E	1024	PRO	Peptide
6	E	1190	ARG	Sidechain
6	E	323	ASN	Peptide
6	E	771	GLU	Mainchain

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	D	503	0	299	51	0
2	P	517	0	280	17	0
3	T	669	0	376	51	0
4	C	6803	0	6753	146	0
5	A	6107	0	6061	256	0
6	E	8484	0	8483	199	0
7	B	5620	0	5593	94	0
8	F	2023	0	2069	61	0
9	C	1	0	0	0	0
10	A	27	3	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	30754	3	29914	720	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (720) 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)
6:E:996:GLU:HB3	8:F:104:GLN:CG	1.10	1.49
1:D:6:DT:H2''	5:A:811:THR:CG2	1.51	1.40
1:D:6:DT:H2''	5:A:811:THR:CB	1.49	1.38
6:E:996:GLU:CB	8:F:104:GLN:CG	2.06	1.27
2:P:-12:DT:OP2	6:E:1182[B]:LYS:NZ	1.72	1.23
1:D:10:DT:C2	5:A:156:VAL:HG21	1.75	1.22
1:D:10:DT:P	5:A:123:ARG:HH21	1.63	1.21
6:E:1000:ALA:CB	8:F:99:LEU:HD12	1.70	1.20
3:T:9:DG:O3'	3:T:10:DG:P	2.02	1.18
6:E:996:GLU:CB	8:F:104:GLN:HG3	1.72	1.17
6:E:1000:ALA:HB2	8:F:99:LEU:HD12	1.22	1.16
3:T:-3:DT:H2'	6:E:502:TRP:CD1	1.83	1.13
4:C:226:GLN:HA	5:A:535:GLU:OE2	1.46	1.12
6:E:597:GLU:HB3	6:E:805:LYS:HG2	1.12	1.11
1:D:6:DT:H2''	5:A:811:THR:HG21	1.17	1.11
1:D:6:DT:H1'	5:A:811:THR:OG1	1.50	1.11
1:D:6:DT:C2'	5:A:811:THR:CB	2.31	1.08
1:D:6:DT:H71	5:A:311:VAL:HB	1.10	1.08
1:D:6:DT:C2'	5:A:811:THR:HG21	1.84	1.07
1:D:7:DT:H5'	5:A:811:THR:HG22	1.32	1.04
6:E:1000:ALA:CB	8:F:99:LEU:CD1	2.36	1.04
5:A:481:SER:HA	5:A:485:LEU:H	1.25	1.02
1:D:6:DT:C1'	5:A:811:THR:OG1	2.08	1.01
6:E:771:GLU:HG2	6:E:776:ILE:HG12	1.39	1.00
4:C:226:GLN:HB3	5:A:535:GLU:OE1	1.61	0.99
1:D:11:DT:H71	5:A:147:HIS:CE1	1.97	0.99
3:T:9:DG:C3'	3:T:10:DG:P	2.51	0.98
1:D:6:DT:C7	5:A:311:VAL:HB	1.92	0.98
6:E:597:GLU:CB	6:E:805:LYS:HG2	1.93	0.98
2:P:-12:DT:OP1	6:E:1182[A]:LYS:HD3	1.62	0.96
3:T:8:DG:OP1	6:E:1164:HIS:NE2	1.99	0.94
2:P:-12:DT:OP1	6:E:1182[A]:LYS:CD	2.05	0.94
6:E:996:GLU:HG3	8:F:104:GLN:NE2	1.82	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:DT:C2'	5:A:811:THR:CG2	2.44	0.94
3:T:-3:DT:H6	6:E:502:TRP:HE1	1.11	0.92
6:E:597:GLU:HB3	6:E:805:LYS:CG	2.00	0.92
1:D:10:DT:P	5:A:123:ARG:NH2	2.42	0.92
6:E:593:LEU:O	6:E:805:LYS:CE	2.18	0.92
6:E:593:LEU:C	6:E:805:LYS:NZ	2.28	0.91
3:T:9:DG:OP2	6:E:1139:VAL:HG12	1.71	0.91
1:D:6:DT:H2''	5:A:811:THR:HB	1.49	0.90
3:T:-3:DT:H6	6:E:502:TRP:NE1	1.69	0.89
5:A:343:ASN:HB2	10:A:901:A1BXB:C13	2.03	0.88
6:E:996:GLU:HB3	8:F:104:GLN:HG3	0.89	0.88
1:D:7:DT:H5'	5:A:811:THR:CG2	2.03	0.87
1:D:11:DT:C7	5:A:147:HIS:CE1	2.57	0.87
1:D:10:DT:N1	5:A:156:VAL:HG21	1.90	0.87
4:C:409:ASN:HA	4:C:793:LEU:HD13	1.54	0.86
6:E:1000:ALA:HB2	8:F:99:LEU:CD1	1.98	0.86
3:T:-3:DT:C2'	6:E:502:TRP:CD1	2.60	0.84
1:D:5:DT:H4'	5:A:396:SER:O	1.76	0.84
1:D:6:DT:O3'	5:A:811:THR:HB	1.75	0.84
3:T:8:DG:P	6:E:1164:HIS:HE2	2.01	0.84
6:E:593:LEU:HB2	6:E:805:LYS:NZ	1.93	0.84
6:E:1000:ALA:HB1	8:F:99:LEU:HD12	1.57	0.83
3:T:9:DG:P	6:E:1139:VAL:CG1	2.67	0.83
6:E:1000:ALA:HB1	8:F:99:LEU:CD1	2.08	0.83
6:E:593:LEU:O	6:E:805:LYS:HE2	1.77	0.82
1:D:10:DT:OP2	5:A:123:ARG:NH2	2.12	0.82
6:E:996:GLU:HG2	8:F:104:GLN:HB2	1.61	0.81
3:T:9:DG:P	6:E:1139:VAL:HG12	2.20	0.81
4:C:625:ILE:HA	4:C:780:MET:HE1	1.60	0.81
4:C:226:GLN:CA	5:A:535:GLU:OE2	2.28	0.80
1:D:6:DT:C2'	5:A:811:THR:OG1	2.29	0.79
3:T:-3:DT:H2'	6:E:502:TRP:NE1	1.97	0.78
5:A:765:VAL:HG22	5:A:775:VAL:HG22	1.66	0.78
7:B:716:LEU:O	7:B:720:GLU:HG3	1.83	0.77
6:E:996:GLU:CG	8:F:104:GLN:CD	2.33	0.77
2:P:-12:DT:P	6:E:1182[B]:LYS:NZ	2.57	0.77
1:D:6:DT:C2'	5:A:811:THR:HB	2.09	0.76
3:T:9:DG:H2''	3:T:10:DG:P	2.26	0.76
6:E:1037:LEU:O	6:E:1044:TYR:OH	2.02	0.76
6:E:996:GLU:CG	8:F:104:GLN:NE2	2.47	0.76
6:E:337:THR:OG1	6:E:342:GLU:OE2	2.03	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:-3:DT:C6	6:E:502:TRP:NE1	2.49	0.75
1:D:6:DT:OP1	5:A:398:HIS:N	2.20	0.75
5:A:557:TYR:HA	5:A:560:LEU:HG	1.69	0.74
4:C:333:LEU:HD13	4:C:362:CYS:HB3	1.69	0.74
8:F:32:GLN:OE1	8:F:90:ARG:NH2	2.20	0.74
4:C:226:GLN:HE21	5:A:138:LEU:HD11	1.53	0.74
1:D:7:DT:OP1	5:A:812:ARG:HB2	1.88	0.74
4:C:430:ALA:HB1	4:C:881:ILE:HD12	1.70	0.74
5:A:568:THR:HA	5:A:571:THR:HB	1.70	0.74
1:D:10:DT:C2	5:A:156:VAL:CG2	2.66	0.74
6:E:993:ARG:HH21	8:F:160:ARG:CZ	2.01	0.74
3:T:-3:DT:H2'	6:E:502:TRP:HD1	1.49	0.73
3:T:9:DG:C2'	3:T:10:DG:P	2.76	0.73
4:C:406:ALA:HA	4:C:412:GLU:HB3	1.71	0.73
5:A:421:VAL:H	5:A:496:LEU:HB3	1.54	0.72
5:A:432:SER:HB3	5:A:435:GLU:HG2	1.71	0.72
5:A:712:PRO:HG3	5:A:736:VAL:HG22	1.70	0.72
6:E:1183:ILE:HD12	8:F:104:GLN:HE22	1.53	0.72
1:D:6:DT:C3'	5:A:811:THR:HB	2.19	0.72
6:E:767:ALA:O	6:E:768:HIS:ND1	2.22	0.72
3:T:7:DC:OP1	6:E:1171:VAL:HG21	1.90	0.71
1:D:6:DT:H2''	5:A:811:THR:OG1	1.89	0.71
5:A:808:MET:HG2	5:A:812:ARG:HH12	1.54	0.71
5:A:92:VAL:HG22	5:A:331:ALA:HB1	1.73	0.71
6:E:999:LEU:HD12	8:F:104:GLN:NE2	2.06	0.71
5:A:463:ASN:HB3	5:A:466:GLN:HE21	1.56	0.71
4:C:628:ASP:HB2	4:C:763:ARG:HH12	1.56	0.70
7:B:226:PHE:HZ	7:B:251:LEU:HD21	1.55	0.70
4:C:981:THR:HB	4:C:984:GLN:HB2	1.74	0.69
5:A:48:ILE:HG23	5:A:93:TYR:HE2	1.57	0.69
5:A:521:GLU:HG3	5:A:677:PHE:CD2	2.27	0.69
5:A:106:CYS:HB2	5:A:340:PHE:CZ	2.27	0.69
3:T:-3:DT:C2'	6:E:502:TRP:NE1	2.54	0.69
4:C:248:TYR:HA	4:C:252:GLN:HB2	1.73	0.69
4:C:226:GLN:HA	5:A:535:GLU:CD	2.18	0.69
5:A:340:PHE:CD1	5:A:881:VAL:HB	2.28	0.68
6:E:1044:TYR:O	6:E:1047:LYS:NZ	2.26	0.68
1:D:10:DT:H1'	5:A:153:GLY:HA2	1.75	0.68
1:D:20:DT:H2'	6:E:496:ARG:HH22	1.58	0.68
2:P:-3:DA:P	6:E:534:LYS:HZ2	2.16	0.68
3:T:9:DG:P	6:E:1139:VAL:HG13	2.34	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:357:LEU:HD11	4:C:898:LYS:HB3	1.74	0.68
6:E:721:LEU:HD22	6:E:888:ASP:HB3	1.75	0.68
1:D:1:DT:H2''	1:D:2:DT:H2'	1.74	0.68
1:D:10:DT:OP1	5:A:123:ARG:NH2	2.26	0.68
4:C:397:VAL:HA	4:C:401:PHE:HB2	1.75	0.68
5:A:752:VAL:HG21	5:A:796:ILE:HD11	1.76	0.67
4:C:219:ARG:NH1	5:A:232:ALA:O	2.28	0.67
5:A:88:PHE:HB2	5:A:178:GLN:HE22	1.59	0.67
6:E:1229:ARG:O	6:E:1233:THR:OG1	2.07	0.67
7:B:181:ARG:O	7:B:185:ILE:HD12	1.95	0.67
1:D:7:DT:O4	5:A:300:SER:HB2	1.95	0.67
5:A:782:GLU:HG3	5:A:796:ILE:HG22	1.75	0.67
6:E:167:PHE:HB2	6:E:172:MET:HG2	1.75	0.66
7:B:405:THR:HG22	7:B:509:VAL:HG12	1.78	0.66
2:P:-12:DT:P	6:E:1182[B]:LYS:HZ3	2.19	0.66
3:T:9:DG:C6	3:T:10:DG:C5	2.83	0.66
4:C:291:LEU:HD23	4:C:297:ILE:HG12	1.78	0.66
6:E:993:ARG:HH21	8:F:160:ARG:NH2	1.94	0.66
4:C:351:PHE:O	4:C:355:ILE:HG23	1.97	0.65
5:A:68:LEU:CD2	5:A:72:ARG:HD2	2.27	0.65
6:E:311:VAL:HG22	6:E:352:ILE:HD11	1.79	0.65
6:E:1005:GLU:N	6:E:1005:GLU:OE1	2.28	0.65
8:F:267:VAL:HB	8:F:315:LEU:HD13	1.77	0.65
6:E:993:ARG:NH2	8:F:160:ARG:CZ	2.59	0.65
7:B:17:THR:HG22	7:B:36:TYR:HB3	1.78	0.65
6:E:1000:ALA:CB	8:F:99:LEU:HD11	2.26	0.64
7:B:602:LEU:HA	7:B:605:VAL:HG12	1.79	0.64
6:E:1183:ILE:CD1	8:F:104:GLN:HE22	2.11	0.64
5:A:733:TYR:CE2	6:E:242:GLY:O	2.51	0.64
3:T:8:DG:OP1	6:E:1164:HIS:CD2	2.50	0.64
4:C:245:THR:HG23	4:C:268:ILE:HG22	1.80	0.64
7:B:181:ARG:HD2	7:B:670:LEU:HB2	1.80	0.64
5:A:61:ASP:HB2	5:A:64:GLN:HG3	1.79	0.64
4:C:158:MET:HG2	5:A:229:LEU:HD13	1.81	0.63
5:A:412:LEU:HD21	5:A:420:PHE:HB2	1.80	0.63
5:A:48:ILE:HG23	5:A:93:TYR:CE2	2.34	0.63
6:E:732:CYS:SG	6:E:773:LEU:HB2	2.39	0.63
5:A:95:ILE:HB	5:A:289:VAL:HG22	1.81	0.63
6:E:503:ASP:N	6:E:503:ASP:OD1	2.30	0.63
6:E:593:LEU:O	6:E:805:LYS:NZ	2.32	0.62
6:E:228:MET:SD	6:E:282:LEU:HD21	2.39	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:9:DG:C6	3:T:10:DG:C6	2.88	0.62
3:T:9:DG:OP1	6:E:1139:VAL:HG13	1.99	0.62
3:T:9:DG:C2	3:T:10:DG:C4	2.88	0.62
4:C:68:GLN:NE2	4:C:381:ASN:OD1	2.33	0.62
5:A:99:ALA:HB3	5:A:294:GLN:NE2	2.13	0.62
5:A:416:ARG:HH22	5:A:422:VAL:HG23	1.65	0.62
7:B:354:ARG:HG2	7:B:359:PRO:HD3	1.81	0.62
6:E:228:MET:HB3	6:E:282:LEU:HD11	1.81	0.62
4:C:907:PHE:CD2	5:A:349:HIS:HB2	2.35	0.62
5:A:357:VAL:HG23	5:A:362:LEU:HB2	1.82	0.62
5:A:707:MET:HE1	5:A:729:MET:HG3	1.82	0.62
5:A:739:PHE:HB3	5:A:777:ASN:CG	2.24	0.62
5:A:559:PHE:HA	5:A:562:ARG:HH21	1.63	0.62
4:C:421:ARG:HD2	4:C:886:SER:HB3	1.82	0.61
5:A:387:ASN:O	5:A:393:ARG:NH2	2.33	0.61
8:F:292:LEU:O	8:F:319:LYS:NZ	2.31	0.61
5:A:480:HIS:HB2	5:A:487:VAL:HG23	1.81	0.61
4:C:938:LEU:HD21	4:C:959:VAL:HG23	1.82	0.61
4:C:226:GLN:CA	5:A:535:GLU:CD	2.73	0.61
7:B:13:VAL:HG12	7:B:118:LEU:HD23	1.83	0.61
7:B:22:TRP:HE1	7:B:241:GLY:HA3	1.66	0.61
5:A:53:ARG:HG3	5:A:114:LEU:HD21	1.82	0.60
5:A:102:GLY:HA3	5:A:344:LYS:NZ	2.15	0.60
5:A:544:PHE:CB	5:A:716:LEU:HD12	2.31	0.60
6:E:193:ARG:O	6:E:339:SER:HB2	2.01	0.60
6:E:1038:SER:N	6:E:1068:ILE:O	2.34	0.60
7:B:160:ILE:HD13	7:B:184:ALA:HB3	1.83	0.60
7:B:226:PHE:HZ	7:B:251:LEU:CD2	2.13	0.60
4:C:934:ALA:HB1	4:C:961:VAL:HG11	1.82	0.60
5:A:707:MET:HB3	5:A:732:THR:HB	1.83	0.60
6:E:996:GLU:HG3	8:F:104:GLN:CD	2.14	0.60
5:A:544:PHE:HB3	5:A:716:LEU:HD12	1.84	0.60
6:E:884:TYR:OH	6:E:938:LYS:O	2.11	0.60
4:C:66:THR:H	4:C:69:ASP:HB2	1.65	0.60
6:E:566:THR:HG22	6:E:567:GLY:H	1.67	0.60
8:F:61:MET:HE1	8:F:127:ILE:HD11	1.83	0.59
7:B:48:ALA:HB2	7:B:252:LEU:HD13	1.84	0.59
5:A:655:GLU:HB2	5:A:661:ALA:HB1	1.84	0.59
6:E:275:SER:O	6:E:278:VAL:HG12	2.02	0.59
7:B:627:ASP:HB3	7:B:631:ARG:HH12	1.67	0.59
4:C:893:SER:HB3	4:C:896:GLU:HG2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:157:GLN:HB3	5:A:785:GLU:HG2	1.85	0.59
7:B:34:LEU:HD21	7:B:237:LEU:HD13	1.84	0.58
6:E:593:LEU:CB	6:E:805:LYS:NZ	2.49	0.58
5:A:824:CYS:SG	5:A:851:ASN:ND2	2.77	0.58
6:E:996:GLU:CG	8:F:104:GLN:CG	2.78	0.58
5:A:830:LEU:HD21	5:A:854:PRO:HA	1.86	0.58
7:B:210:ARG:HH22	7:B:225:ALA:HA	1.68	0.58
8:F:302:THR:O	8:F:302:THR:OG1	2.21	0.58
5:A:393:ARG:HG3	5:A:393:ARG:HH11	1.69	0.58
6:E:699:ALA:CB	6:E:887:THR:HG23	2.33	0.57
5:A:103:LYS:HD3	5:A:289:VAL:HG12	1.86	0.57
3:T:-2:DT:OP2	6:E:514:LYS:HE3	2.05	0.57
1:D:6:DT:H5''	5:A:809:THR:HG21	1.86	0.57
3:T:6:DC:H5'	6:E:940:LYS:NZ	2.20	0.57
5:A:737:PHE:HA	5:A:740:ALA:HB3	1.87	0.57
7:B:510:PHE:CE2	7:B:524:ILE:HG12	2.39	0.57
2:P:-8:DC:H2'	2:P:-7:DG:C8	2.40	0.56
5:A:479:VAL:HA	5:A:486:VAL:HA	1.87	0.56
5:A:209:PHE:HB2	5:A:273:TYR:O	2.05	0.56
5:A:348:GLU:HB2	5:A:351:PHE:HB3	1.87	0.56
6:E:727:GLN:HE21	6:E:779:ARG:N	2.03	0.56
6:E:727:GLN:NE2	6:E:779:ARG:HA	2.20	0.56
7:B:644:GLU:OE1	7:B:678:ARG:NH2	2.38	0.56
6:E:971:ARG:NH1	6:E:975:ASP:OD1	2.38	0.56
4:C:355:ILE:HD11	5:A:341:ILE:HD11	1.86	0.56
7:B:629:CYS:O	7:B:633:ILE:HG13	2.05	0.56
8:F:298:SER:OG	8:F:314:LEU:HD23	2.05	0.56
3:T:4:DC:H5'	6:E:701:VAL:HG21	1.87	0.56
4:C:853:VAL:O	4:C:857:VAL:HG23	2.06	0.56
6:E:727:GLN:HE22	6:E:779:ARG:HA	1.70	0.56
7:B:570:TRP:HZ3	7:B:606:LEU:HD12	1.71	0.56
1:D:10:DT:N3	5:A:156:VAL:HG11	2.21	0.56
3:T:7:DC:OP1	6:E:1171:VAL:CG2	2.53	0.56
4:C:613:ASN:HB3	4:C:821:SER:HB2	1.88	0.56
8:F:214:THR:HG22	8:F:215:THR:H	1.71	0.56
2:P:-3:DA:OP1	6:E:960:LYS:HG3	2.06	0.55
3:T:7:DC:P	6:E:1171:VAL:HG21	2.47	0.55
7:B:84:PRO:HG3	7:B:279:HIS:CG	2.42	0.55
6:E:628:LEU:CD1	6:E:777:LEU:HB2	2.36	0.55
8:F:294:THR:OG1	8:F:296:VAL:O	2.23	0.55
8:F:56:ASP:HA	8:F:101:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:391:ILE:HD11	7:B:498:VAL:HG11	1.86	0.55
1:D:7:DT:C5'	5:A:811:THR:HG22	2.23	0.55
6:E:727:GLN:NE2	6:E:778:LEU:C	2.65	0.55
5:A:159:GLN:NE2	5:A:786:SER:O	2.40	0.55
5:A:438:GLU:HG3	5:A:441:ARG:HH21	1.70	0.55
6:E:1000:ALA:HA	8:F:99:LEU:HD11	1.88	0.55
7:B:558:TYR:HA	7:B:573:ASN:HB2	1.89	0.55
8:F:204:LEU:HD12	8:F:210:PHE:HA	1.89	0.55
5:A:256:ARG:HD3	5:A:315:GLU:HB3	1.89	0.55
4:C:110:THR:HG21	4:C:251:LEU:HD23	1.89	0.55
6:E:593:LEU:C	6:E:805:LYS:CE	2.76	0.55
7:B:127:ASP:O	7:B:131:GLY:N	2.34	0.55
4:C:425:LEU:HD22	7:B:634:LEU:HD21	1.89	0.54
4:C:780:MET:HG2	4:C:816:TYR:CD1	2.42	0.54
5:A:69:GLN:OE1	5:A:72:ARG:HD3	2.07	0.54
7:B:306:PRO:HA	7:B:675:TYR:CD2	2.43	0.54
5:A:117:VAL:HG23	5:A:243:SER:HB3	1.88	0.54
5:A:761:LEU:HD11	5:A:778:THR:HB	1.88	0.54
8:F:278:LEU:HD21	8:F:301:VAL:HG11	1.89	0.54
4:C:23:LEU:HD13	4:C:251:LEU:HD21	1.89	0.54
5:A:366:GLU:O	5:A:370:GLN:HG3	2.06	0.54
6:E:601:VAL:CG2	6:E:809:ALA:HB1	2.37	0.54
1:D:6:DT:H1'	5:A:811:THR:HG1	1.67	0.54
5:A:242:ARG:HG3	5:A:242:ARG:HH11	1.73	0.54
1:D:10:DT:OP1	5:A:123:ARG:CZ	2.55	0.54
4:C:368:LEU:O	4:C:372:LEU:HG	2.08	0.54
6:E:216:LEU:HB2	6:E:218:CYS:SG	2.48	0.54
7:B:113:THR:HG22	7:B:136:VAL:HG22	1.88	0.54
6:E:262:GLU:HB3	6:E:742:ALA:HB2	1.90	0.54
7:B:633:ILE:HD11	7:B:716:LEU:HD11	1.90	0.54
4:C:20:VAL:HB	4:C:91:VAL:HG22	1.89	0.54
5:A:539:GLU:HG3	5:A:662:VAL:HG21	1.89	0.54
7:B:225:ALA:N	7:B:228:ASP:OD2	2.41	0.54
5:A:508:LYS:HB3	5:A:720:ALA:HB2	1.89	0.54
6:E:732:CYS:SG	6:E:733:PHE:N	2.81	0.54
4:C:629:LEU:HB2	4:C:762:LEU:HB2	1.90	0.53
4:C:226:GLN:HB3	5:A:535:GLU:CD	2.31	0.53
5:A:197:LEU:HD22	5:A:272:LEU:HD11	1.90	0.53
5:A:684:PHE:HB2	5:A:688:PHE:HB2	1.91	0.53
5:A:736:VAL:HG12	5:A:738:ALA:H	1.72	0.53
6:E:601:VAL:HG23	6:E:809:ALA:HB1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:981:ASP:OD1	6:E:982:THR:N	2.40	0.53
5:A:781:SER:O	5:A:796:ILE:HA	2.08	0.53
5:A:808:MET:HG2	5:A:812:ARG:NH1	2.24	0.53
4:C:226:GLN:CB	5:A:535:GLU:OE1	2.46	0.53
7:B:381:VAL:HG21	7:B:475:LEU:HD12	1.91	0.53
7:B:568:GLY:HA2	7:B:582:GLY:O	2.09	0.53
4:C:156:ALA:HA	4:C:159:ILE:HD12	1.91	0.53
5:A:483:GLN:HB3	5:A:751:ASN:HB3	1.90	0.53
4:C:942:VAL:HA	4:C:945:ILE:HG22	1.91	0.53
5:A:853:ASN:HB3	5:A:856:ARG:HB2	1.90	0.53
7:B:258:TYR:HB3	7:B:319:PRO:HG2	1.90	0.53
1:D:8:DT:H4'	5:A:122:THR:HG22	1.90	0.53
4:C:299:ARG:O	4:C:303:THR:HG22	2.08	0.53
5:A:565:LEU:HB2	5:A:570:ARG:HE	1.72	0.53
6:E:727:GLN:NE2	6:E:779:ARG:N	2.57	0.53
7:B:723:PHE:HA	7:B:726:VAL:HG12	1.91	0.53
7:B:621:ALA:O	7:B:625:MET:HG3	2.09	0.52
5:A:779:ASN:O	5:A:798:ALA:HA	2.09	0.52
5:A:546:SER:HB3	5:A:665:GLN:HE22	1.74	0.52
5:A:673:PHE:O	5:A:674:LEU:C	2.50	0.52
6:E:740:ALA:HB2	6:E:763:PHE:CZ	2.44	0.52
6:E:942:ILE:HD11	6:E:955:VAL:HG21	1.91	0.52
6:E:765:VAL:HG21	6:E:769:VAL:HG11	1.90	0.52
1:D:6:DT:O4	5:A:311:VAL:O	2.27	0.52
2:P:-5:DG:N3	6:E:959:ARG:NH2	2.56	0.52
6:E:244:SER:OG	6:E:245:ALA:N	2.42	0.52
6:E:1061:ARG:NH1	6:E:1144:GLU:OE2	2.39	0.52
2:P:-4:DG:C5'	6:E:961:ASN:OD1	2.58	0.52
4:C:562:ALA:HB3	4:C:826:TYR:HE2	1.75	0.52
5:A:368:HIS:O	5:A:372:VAL:HG23	2.09	0.52
7:B:207:LEU:HD23	7:B:208:PHE:N	2.25	0.52
5:A:463:ASN:HB3	5:A:466:GLN:NE2	2.24	0.52
5:A:694:SER:HB2	5:A:696:TYR:HE1	1.75	0.52
5:A:66:PRO:O	5:A:278:TYR:OH	2.27	0.52
5:A:451:GLU:CD	5:A:451:GLU:H	2.18	0.52
6:E:228:MET:HG2	6:E:286:PHE:CZ	2.45	0.52
7:B:357:LEU:HD21	7:B:429:LEU:HD21	1.92	0.52
2:P:-4:DG:H5''	6:E:961:ASN:OD1	2.10	0.52
8:F:57:SER:OG	8:F:58:LEU:N	2.42	0.52
4:C:226:GLN:CB	5:A:535:GLU:CD	2.84	0.51
3:T:-3:DT:C2'	6:E:502:TRP:HE1	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:425:LEU:HB3	5:A:800:TYR:HE2	1.74	0.51
4:C:19:GLU:HB2	4:C:56:TYR:CE1	2.46	0.51
4:C:825:PRO:HA	4:C:840:LEU:HB3	1.92	0.51
4:C:320:GLU:HA	4:C:320:GLU:OE2	2.10	0.51
5:A:99:ALA:CB	5:A:294:GLN:HE21	2.24	0.51
5:A:106:CYS:HB2	5:A:340:PHE:HZ	1.73	0.51
7:B:176:ARG:HD3	7:B:652:PRO:HB3	1.91	0.51
7:B:226:PHE:CZ	7:B:230:VAL:HG21	2.46	0.51
5:A:385:PRO:HB3	5:A:408:LEU:HD12	1.93	0.51
5:A:507:ARG:HH12	5:A:741:ASP:HB2	1.76	0.51
6:E:232:LEU:HD13	6:E:243:ILE:HD13	1.93	0.51
7:B:176:ARG:N	7:B:176:ARG:HD2	2.25	0.51
3:T:-2:DT:P	6:E:514:LYS:HE3	2.51	0.51
4:C:115:VAL:H	4:C:151:THR:HG23	1.76	0.51
4:C:53:TYR:CG	4:C:131:LEU:HD11	2.46	0.51
4:C:899:ALA:HB1	10:A:901:A1BXB:O04	2.10	0.51
3:T:9:DG:N1	3:T:10:DG:C5	2.79	0.51
1:D:6:DT:OP1	5:A:398:HIS:HB2	2.11	0.50
3:T:9:DG:OP1	6:E:1139:VAL:CG1	2.58	0.50
5:A:250:GLU:N	5:A:289:VAL:O	2.43	0.50
6:E:176:THR:HB	6:E:177:PRO:HD3	1.93	0.50
8:F:289:LYS:O	8:F:299:LEU:HD12	2.12	0.50
6:E:965:PHE:CE2	6:E:1021:ILE:HD12	2.46	0.50
3:T:6:DC:H5''	6:E:1171:VAL:CG1	2.42	0.50
3:T:9:DG:O3'	3:T:10:DG:H5'	2.12	0.50
4:C:424:VAL:HG22	4:C:882:ARG:HG2	1.93	0.50
4:C:945:ILE:HG13	4:C:949:PHE:HB2	1.92	0.50
4:C:959:VAL:HG12	4:C:977:PRO:HB3	1.93	0.50
5:A:345:ARG:HB3	5:A:843:THR:HG22	1.92	0.50
5:A:80:PRO:HB3	5:A:186:TRP:CD2	2.47	0.50
5:A:479:VAL:HG13	5:A:486:VAL:HG22	1.92	0.50
5:A:726:TYR:HB3	5:A:766:LEU:HB3	1.92	0.50
6:E:775:SER:O	6:E:776:ILE:C	2.54	0.50
3:T:8:DG:H3'	6:E:1139:VAL:CG1	2.42	0.50
5:A:98:ASN:HB2	5:A:101:SER:HB3	1.94	0.50
8:F:121:ARG:HE	8:F:149:ALA:HB2	1.77	0.50
6:E:403:THR:O	6:E:404:THR:OG1	2.26	0.50
7:B:226:PHE:CZ	7:B:251:LEU:HD21	2.43	0.50
7:B:347:ALA:HB1	7:B:351:VAL:HB	1.93	0.50
4:C:533:LEU:HD22	4:C:551:ALA:HA	1.94	0.50
5:A:393:ARG:HD2	5:A:404:TYR:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:873:LEU:HD23	5:A:880:ILE:HD12	1.93	0.49
7:B:391:ILE:CD1	7:B:498:VAL:HG11	2.42	0.49
7:B:605:VAL:HG22	7:B:731:TRP:HH2	1.76	0.49
8:F:278:LEU:HD11	8:F:283:VAL:HG21	1.93	0.49
5:A:566:ASP:HB3	5:A:569:GLN:HB2	1.94	0.49
6:E:315:TRP:NE1	6:E:358:ASP:O	2.42	0.49
2:P:-2:DT:OP1	6:E:953:LYS:HD3	2.12	0.49
5:A:808:MET:SD	5:A:812:ARG:CZ	3.01	0.49
6:E:593:LEU:O	6:E:805:LYS:CD	2.59	0.49
8:F:35:LEU:HD21	8:F:43:ILE:HD12	1.94	0.49
4:C:243:VAL:HG11	4:C:307:ALA:HB2	1.93	0.49
6:E:730:ASN:OD1	6:E:772:SER:HB3	2.13	0.49
7:B:711:HIS:O	7:B:715:ILE:HG13	2.13	0.49
2:P:-6:DG:H5''	6:E:1049:LEU:HD11	1.93	0.49
5:A:146:PHE:HA	5:A:149:PHE:CE2	2.48	0.49
6:E:222:ARG:O	6:E:226:GLU:HG2	2.13	0.49
7:B:335:ARG:HH11	7:B:335:ARG:HG2	1.78	0.49
4:C:229:PHE:O	4:C:233:SER:OG	2.27	0.49
7:B:393:LEU:HD23	7:B:498:VAL:HG12	1.94	0.49
4:C:912:THR:N	4:C:915:GLU:OE1	2.46	0.49
6:E:1000:ALA:CA	8:F:99:LEU:HD11	2.42	0.49
5:A:343:ASN:CB	10:A:901:A1BXB:C13	2.85	0.49
5:A:822:ALA:HA	5:A:849:ARG:O	2.13	0.49
6:E:1200:ASP:C	6:E:1202:VAL:H	2.21	0.49
7:B:116:VAL:HG23	7:B:345:LEU:HD11	1.95	0.49
7:B:199:VAL:HG21	7:B:274:LEU:HD13	1.93	0.48
4:C:989:LEU:H	4:C:1021:GLN:HE22	1.60	0.48
5:A:108:GLN:O	5:A:112:GLU:HG3	2.13	0.48
6:E:384:ALA:HB1	6:E:477:ALA:HB3	1.94	0.48
7:B:40:ARG:HA	7:B:46:GLY:HA2	1.94	0.48
4:C:209:HIS:CD2	4:C:212:ARG:HH21	2.31	0.48
6:E:154:GLU:OE1	6:E:299:ALA:HB3	2.13	0.48
7:B:644:GLU:HG2	7:B:694:VAL:HG11	1.95	0.48
6:E:225:CYS:HA	6:E:228:MET:HE2	1.95	0.48
1:D:12:DT:H4'	1:D:13:DT:H5'	1.95	0.48
3:T:9:DG:H3'	3:T:10:DG:P	2.48	0.48
3:T:24:DT:H2''	3:T:25:DT:H71	1.96	0.48
6:E:597:GLU:CG	6:E:805:LYS:HG2	2.43	0.48
6:E:730:ASN:HA	6:E:775:SER:OG	2.14	0.48
7:B:37:PHE:CE1	7:B:109:LEU:HD21	2.49	0.48
4:C:97:GLY:HA3	4:C:221:TYR:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:49:LEU:HD21	5:A:113:VAL:HG11	1.95	0.48
5:A:783:PHE:CE1	5:A:785:GLU:HB2	2.49	0.48
6:E:593:LEU:O	6:E:805:LYS:HD3	2.14	0.48
6:E:1233:THR:HG22	8:F:172:GLY:H	1.79	0.48
3:T:8:DG:P	6:E:1164:HIS:NE2	2.78	0.48
5:A:379:GLU:OE1	5:A:851:ASN:ND2	2.46	0.48
5:A:420:PHE:HB3	5:A:496:LEU:O	2.14	0.48
6:E:203:GLN:HG2	6:E:299:ALA:HB2	1.96	0.48
7:B:148:ARG:O	7:B:257:ASP:HB3	2.13	0.48
8:F:283:VAL:HG13	8:F:303:ALA:HB2	1.96	0.48
4:C:930:VAL:HG11	4:C:971:VAL:HG11	1.94	0.47
5:A:832:LEU:HD13	5:A:859:HIS:CG	2.49	0.47
6:E:999:LEU:CD1	8:F:104:GLN:NE2	2.75	0.47
7:B:18:LEU:HD11	7:B:105:VAL:HG21	1.97	0.47
7:B:512:VAL:HG11	7:B:523:VAL:HG21	1.97	0.47
4:C:993:HIS:HB3	4:C:997:SER:HB2	1.96	0.47
5:A:320:TYR:O	5:A:324:ASN:HB2	2.14	0.47
5:A:698:ASP:O	5:A:700:VAL:HG23	2.13	0.47
6:E:856:TRP:NE1	6:E:865:ASP:OD2	2.39	0.47
6:E:872:MET:HE1	6:E:905:MET:SD	2.54	0.47
4:C:162:LEU:HD13	4:C:213:VAL:HG22	1.96	0.47
6:E:1146:PRO:O	6:E:1150:ILE:HG13	2.15	0.47
4:C:226:GLN:CB	5:A:535:GLU:OE2	2.63	0.47
4:C:773:VAL:O	4:C:883:VAL:HA	2.14	0.47
4:C:863:PRO:HA	4:C:866:PHE:CZ	2.50	0.47
6:E:598:LEU:HD13	6:E:613:ILE:HG12	1.95	0.47
6:E:981:ASP:O	6:E:982:THR:HG22	2.15	0.47
7:B:31:PHE:HE2	7:B:60:LEU:HD13	1.80	0.47
4:C:115:VAL:HG13	4:C:154:LEU:HD11	1.97	0.47
4:C:650:ARG:NH2	4:C:671:TYR:O	2.46	0.47
6:E:273:VAL:HG11	6:E:279:LEU:HB2	1.97	0.47
4:C:244:LEU:HD13	4:C:315:PHE:HB2	1.95	0.47
5:A:416:ARG:HE	5:A:416:ARG:HA	1.79	0.47
6:E:317:ARG:NH2	6:E:353:GLU:OE2	2.47	0.47
6:E:731:LEU:O	6:E:774:LEU:HB2	2.14	0.47
6:E:996:GLU:HG2	8:F:104:GLN:CB	2.39	0.47
7:B:344:LEU:HD12	7:B:348:TRP:HB2	1.96	0.47
5:A:55:LEU:HD22	5:A:91:ALA:HB1	1.96	0.47
3:T:19:DT:H5"	8:F:279:ARG:HG2	1.96	0.47
4:C:587:THR:HG21	4:C:843:VAL:HG22	1.95	0.47
7:B:116:VAL:HG12	7:B:136:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:754:CYS:HB3	4:C:756:CYS:SG	2.56	0.46
6:E:727:GLN:NE2	6:E:779:ARG:CA	2.78	0.46
7:B:564:TRP:HB3	7:B:725:GLY:HA3	1.96	0.46
4:C:993:HIS:H	4:C:998:ARG:HG3	1.80	0.46
4:C:141:HIS:O	4:C:145:THR:OG1	2.30	0.46
4:C:258:GLY:HA3	4:C:320:GLU:OE1	2.15	0.46
5:A:250:GLU:HB3	5:A:253:LEU:HD12	1.98	0.46
5:A:513:PHE:HB2	5:A:772:PHE:CE2	2.50	0.46
5:A:830:LEU:HD12	5:A:830:LEU:HA	1.79	0.46
7:B:616:GLU:O	7:B:620:THR:HG22	2.15	0.46
5:A:61:ASP:OD2	5:A:64:GLN:NE2	2.48	0.46
5:A:472:ALA:HA	5:A:491:ASP:O	2.15	0.46
1:D:7:DT:OP1	5:A:809:THR:OG1	2.33	0.46
4:C:362:CYS:C	4:C:363:PHE:HD1	2.23	0.46
4:C:952:HIS:NE2	4:C:998:ARG:HD2	2.30	0.46
5:A:88:PHE:HB2	5:A:178:GLN:NE2	2.29	0.46
7:B:230:VAL:HG21	7:B:251:LEU:HD23	1.97	0.46
1:D:6:DT:H2'	5:A:811:THR:HG21	1.85	0.46
5:A:169:SER:HB2	5:A:172:ALA:HA	1.98	0.46
7:B:50:PHE:CZ	7:B:250:VAL:HG11	2.51	0.46
7:B:91:PRO:HA	7:B:98:TRP:CD1	2.49	0.46
7:B:579:ASP:OD1	7:B:599:ARG:NH2	2.48	0.46
4:C:452:GLY:HA2	4:C:524:ILE:HG23	1.97	0.46
4:C:644:GLU:HG2	4:C:648:HIS:NE2	2.30	0.46
5:A:209:PHE:HD1	5:A:273:TYR:HB3	1.80	0.46
5:A:304:HIS:CD2	5:A:787:ILE:HG23	2.50	0.46
5:A:541:ALA:HA	5:A:716:LEU:HD11	1.98	0.46
7:B:16:ILE:O	7:B:102:TYR:OH	2.33	0.46
7:B:102:TYR:HA	7:B:105:VAL:HG22	1.98	0.46
4:C:23:LEU:HD22	4:C:250:LEU:HD13	1.97	0.46
5:A:50:LYS:HG2	5:A:53:ARG:NH2	2.30	0.46
6:E:364:LEU:HB2	6:E:401:LEU:HD13	1.96	0.46
2:P:-4:DG:P	6:E:1071:ARG:HH12	2.39	0.46
6:E:194:VAL:HA	6:E:341:VAL:O	2.16	0.46
5:A:102:GLY:HA3	5:A:344:LYS:CE	2.45	0.46
6:E:593:LEU:C	6:E:805:LYS:HE2	2.40	0.46
7:B:215:LEU:HD12	7:B:215:LEU:HA	1.72	0.46
4:C:962:ARG:O	4:C:974:GLN:N	2.46	0.45
5:A:68:LEU:HD23	5:A:72:ARG:CD	2.46	0.45
5:A:90:PHE:HB3	5:A:263:VAL:HG11	1.98	0.45
6:E:66:THR:HG22	6:E:66:THR:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:216:LEU:HD11	6:E:287:CYS:SG	2.55	0.45
3:T:8:DG:H3'	6:E:1139:VAL:HG11	1.98	0.45
4:C:240:LYS:HG3	4:C:306:TYR:CD2	2.51	0.45
5:A:340:PHE:HD1	5:A:881:VAL:HB	1.79	0.45
6:E:216:LEU:O	6:E:217:GLN:C	2.60	0.45
8:F:185:LEU:HA	8:F:188:VAL:HG22	1.99	0.45
3:T:-1:DT:OP1	6:E:512:ARG:N	2.50	0.45
4:C:580:GLY:HA2	4:C:643:HIS:CE1	2.51	0.45
4:C:956:TYR:CE1	4:C:986:LEU:HD22	2.51	0.45
5:A:39:PHE:HA	5:A:42:MET:HE2	1.98	0.45
5:A:388:LEU:HB3	5:A:391:TRP:CG	2.52	0.45
3:T:-3:DT:H2''	6:E:502:TRP:NE1	2.31	0.45
5:A:443:THR:C	5:A:445:GLN:H	2.25	0.45
7:B:251:LEU:HD13	7:B:315:PHE:CE1	2.51	0.45
2:P:-3:DA:OP2	6:E:534:LYS:NZ	2.49	0.45
4:C:21:THR:O	4:C:53:TYR:HA	2.17	0.45
4:C:476:TRP:HE1	4:C:479:PHE:HE1	1.65	0.45
4:C:622:ILE:HD12	4:C:780:MET:HE2	1.97	0.45
4:C:899:ALA:HA	10:A:901:A1BXB:N09	2.31	0.45
5:A:160:LEU:HD12	5:A:185:TYR:HE1	1.82	0.45
5:A:340:PHE:HE1	5:A:881:VAL:HG11	1.81	0.45
5:A:423:PHE:HE1	5:A:425:LEU:HD12	1.81	0.45
6:E:552:LYS:NZ	6:E:581:ASP:OD1	2.42	0.45
1:D:11:DT:C7	5:A:147:HIS:NE2	2.79	0.45
4:C:271:ILE:HG12	4:C:322:ARG:NH1	2.32	0.45
5:A:388:LEU:HD23	5:A:391:TRP:CE3	2.52	0.45
5:A:480:HIS:HB2	5:A:487:VAL:CG2	2.46	0.45
8:F:35:LEU:HD21	8:F:43:ILE:CD1	2.47	0.45
1:D:11:DT:C5	1:D:12:DT:O4	2.70	0.45
6:E:823:VAL:O	6:E:829:PRO:HB3	2.17	0.45
6:E:1001:ARG:HD2	8:F:160:ARG:HH12	1.81	0.45
7:B:50:PHE:O	7:B:133:VAL:HG23	2.17	0.45
4:C:955:GLU:OE2	4:C:987:SER:OG	2.30	0.44
4:C:989:LEU:HD12	4:C:1036:LEU:HD13	1.98	0.44
5:A:345:ARG:HB3	5:A:843:THR:CG2	2.46	0.44
5:A:713:ARG:HD2	5:A:713:ARG:HA	1.80	0.44
7:B:41:ASN:HD21	7:B:45:GLU:HB2	1.81	0.44
7:B:708:CYS:O	7:B:712:LEU:HB2	2.17	0.44
8:F:301:VAL:O	8:F:310:SER:HA	2.16	0.44
4:C:107:ARG:O	4:C:254:GLN:NE2	2.51	0.44
4:C:781:ARG:O	4:C:785:ARG:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:185:TYR:CE1	5:A:257:HIS:ND1	2.86	0.44
2:P:-3:DA:OP1	6:E:959:ARG:HA	2.17	0.44
4:C:974:GLN:NE2	4:C:1002:ARG:HD3	2.33	0.44
7:B:22:TRP:HH2	7:B:34:LEU:HD13	1.83	0.44
7:B:167:ALA:O	7:B:171:GLU:HG3	2.18	0.44
7:B:357:LEU:HD22	7:B:358:PRO:HD2	1.98	0.44
4:C:1021:GLN:NE2	4:C:1036:LEU:HD11	2.32	0.44
5:A:472:ALA:HB1	5:A:490:ASN:HD22	1.82	0.44
5:A:507:ARG:HA	5:A:719:VAL:HA	1.99	0.44
5:A:683:LEU:HD22	5:A:683:LEU:HA	1.85	0.44
6:E:788:ILE:O	6:E:792:ILE:HG13	2.18	0.44
6:E:862:LEU:HD21	6:E:905:MET:HE1	1.98	0.44
7:B:529:ARG:HG3	7:B:529:ARG:HH11	1.81	0.44
1:D:5:DT:O3'	5:A:397:SER:HA	2.18	0.44
6:E:640:GLN:HA	6:E:643:PHE:HB2	1.99	0.44
1:D:7:DT:H5''	5:A:812:ARG:CA	2.48	0.44
4:C:913:LEU:HD21	4:C:971:VAL:HG23	2.00	0.44
4:C:917:LEU:HD22	4:C:922:VAL:HG11	2.00	0.44
6:E:221:PRO:O	6:E:224:LEU:HB3	2.17	0.44
6:E:244:SER:OG	6:E:246:ASP:OD1	2.35	0.44
6:E:756:GLU:OE1	6:E:756:GLU:N	2.50	0.44
8:F:189:LEU:HD21	8:F:278:LEU:HB3	2.00	0.44
3:T:-3:DT:H6	6:E:502:TRP:CD1	2.34	0.44
3:T:9:DG:C4	3:T:10:DG:C8	3.06	0.44
5:A:816:LEU:HD23	5:A:816:LEU:HA	1.81	0.44
6:E:699:ALA:HB1	6:E:887:THR:HG23	1.99	0.44
8:F:201:THR:HG22	8:F:268:VAL:HG22	1.98	0.44
5:A:752:VAL:CG2	5:A:796:ILE:HD11	2.46	0.44
6:E:1214:VAL:HG23	6:E:1214:VAL:O	2.18	0.44
7:B:253:PRO:HD3	7:B:318:TRP:HE1	1.83	0.44
5:A:246:ILE:HD11	5:A:266:TRP:CD1	2.53	0.43
6:E:101:ARG:NH2	6:E:445:GLU:OE2	2.51	0.43
4:C:219:ARG:HD2	5:A:232:ALA:HA	1.99	0.43
4:C:948:HIS:O	5:A:380:ASN:ND2	2.51	0.43
5:A:69:GLN:NE2	5:A:73:ASP:OD1	2.51	0.43
6:E:229:ALA:HA	6:E:232:LEU:HD12	1.99	0.43
4:C:246:THR:HG23	4:C:250:LEU:HD12	2.00	0.43
5:A:40:THR:HG21	5:A:882:TYR:HB3	2.00	0.43
5:A:266:TRP:CZ3	5:A:284:PRO:HD3	2.54	0.43
5:A:581:THR:HA	5:A:584:ILE:HB	2.01	0.43
4:C:107:ARG:HB3	5:A:113:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:226:GLN:NE2	5:A:138:LEU:HD11	2.27	0.43
4:C:363:PHE:CD2	5:A:40:THR:HG23	2.53	0.43
4:C:407:GLN:O	4:C:407:GLN:HG3	2.19	0.43
4:C:633:LEU:HD23	4:C:633:LEU:HA	1.79	0.43
4:C:634:LYS:HG2	4:C:806:LYS:HE3	2.00	0.43
4:C:779:THR:O	4:C:783:VAL:HG23	2.19	0.43
5:A:111:ASN:HA	5:A:116:CYS:SG	2.59	0.43
1:D:10:DT:OP1	5:A:123:ARG:NE	2.51	0.43
4:C:475:GLY:HA3	7:B:703:LEU:HD23	2.00	0.43
5:A:167:LEU:HD11	5:A:180:ARG:HB2	1.99	0.43
4:C:439:TYR:HD2	4:C:444:LEU:HD11	1.84	0.43
4:C:109:ARG:HD3	4:C:249:TYR:O	2.19	0.43
5:A:134:SER:HA	5:A:137:PHE:O	2.18	0.43
8:F:135:THR:OG1	8:F:159:LYS:O	2.27	0.43
5:A:733:TYR:CZ	6:E:242:GLY:HA2	2.53	0.43
6:E:338:SER:HB3	6:E:455:LYS:HE3	2.00	0.43
3:T:23:DA:H2'	3:T:24:DT:H72	2.01	0.43
4:C:434:LEU:HD12	4:C:434:LEU:HA	1.83	0.43
5:A:104:SER:CB	5:A:132:LYS:HD3	2.49	0.43
5:A:854:PRO:O	5:A:859:HIS:ND1	2.43	0.43
6:E:1226:MET:HE3	6:E:1229:ARG:HB2	1.99	0.43
3:T:9:DG:C5	3:T:10:DG:N7	2.87	0.42
4:C:529:VAL:HG13	4:C:551:ALA:HB2	2.01	0.42
5:A:242:ARG:HG3	5:A:242:ARG:NH1	2.34	0.42
8:F:267:VAL:CB	8:F:315:LEU:HD13	2.48	0.42
4:C:507:LEU:HD23	4:C:507:LEU:HA	1.85	0.42
5:A:254:LEU:HB3	5:A:258:LEU:HD13	2.02	0.42
5:A:669:LEU:HD23	5:A:669:LEU:HA	1.90	0.42
7:B:63:PHE:HA	7:B:359:PRO:HD2	2.00	0.42
7:B:351:VAL:CG1	7:B:354:ARG:HB2	2.48	0.42
1:D:6:DT:OP1	5:A:398:HIS:CB	2.67	0.42
4:C:633:LEU:HD12	4:C:756:CYS:HB2	2.00	0.42
5:A:245:VAL:HA	5:A:285:VAL:HG13	2.00	0.42
5:A:727:THR:N	5:A:767:ARG:O	2.52	0.42
5:A:448:LEU:HD12	5:A:452:LYS:HE3	2.00	0.42
4:C:975:LEU:HD23	4:C:975:LEU:HA	1.83	0.42
5:A:68:LEU:HD23	5:A:72:ARG:HG3	2.00	0.42
7:B:142:GLY:O	7:B:144:PRO:HD3	2.19	0.42
7:B:357:LEU:CD2	7:B:358:PRO:HD2	2.49	0.42
2:P:-4:DG:O4'	6:E:959:ARG:NH2	2.52	0.42
5:A:511:PHE:HZ	5:A:712:PRO:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:708:LEU:HD13	5:A:710:GLY:H	1.85	0.42
6:E:248:PHE:HZ	6:E:278:VAL:HG21	1.85	0.42
4:C:498:CYS:O	4:C:501:VAL:HG12	2.20	0.42
4:C:798:VAL:HG12	4:C:808:PHE:HE2	1.85	0.42
4:C:970:TRP:HB2	5:A:370:GLN:NE2	2.35	0.42
5:A:443:THR:HA	5:A:787:ILE:HD11	2.01	0.42
5:A:693:PHE:CZ	5:A:695:THR:HB	2.54	0.42
4:C:533:LEU:HD23	4:C:533:LEU:HA	1.88	0.42
4:C:871:PRO:HA	4:C:872:PRO:HD3	1.93	0.42
5:A:206:ARG:O	5:A:208:GLU:HG2	2.20	0.42
5:A:209:PHE:CD1	5:A:273:TYR:HB3	2.55	0.42
6:E:130:TRP:CZ3	6:E:456:GLN:HG3	2.55	0.42
6:E:224:LEU:O	6:E:228:MET:HG3	2.20	0.42
7:B:18:LEU:HD13	7:B:102:TYR:CE1	2.54	0.42
5:A:837:VAL:O	5:A:841:ARG:HG2	2.20	0.42
8:F:121:ARG:HB3	8:F:143:THR:HG23	2.01	0.42
8:F:204:LEU:HD12	8:F:210:PHE:CA	2.49	0.42
4:C:228:PRO:HD3	4:C:294:PHE:HE1	1.85	0.42
4:C:464:LEU:HD12	4:C:500:ILE:HG13	2.01	0.42
5:A:409:HIS:HE1	5:A:493:THR:O	2.02	0.42
7:B:720:GLU:HB3	7:B:737:PHE:O	2.19	0.42
8:F:142:THR:HG23	8:F:152:LEU:HD11	2.02	0.42
4:C:26:THR:HG23	4:C:30:VAL:HG23	2.01	0.41
4:C:152:PHE:HA	4:C:155:HIS:NE2	2.35	0.41
4:C:160:LEU:O	4:C:164:VAL:HG23	2.20	0.41
5:A:328:ARG:HG3	5:A:333:LEU:HB2	2.02	0.41
7:B:377:VAL:HG12	7:B:482:ALA:HB2	2.02	0.41
3:T:6:DC:H5"	6:E:1171:VAL:HG13	2.02	0.41
4:C:627:LEU:HD22	4:C:811:ILE:HG21	2.02	0.41
4:C:989:LEU:H	4:C:1021:GLN:NE2	2.17	0.41
5:A:258:LEU:O	5:A:262:VAL:HG23	2.20	0.41
7:B:19:TYR:O	7:B:292:VAL:HG23	2.20	0.41
3:T:9:DG:OP1	6:E:1140:SER:N	2.52	0.41
4:C:562:ALA:HA	4:C:590:ILE:HD12	2.02	0.41
5:A:388:LEU:HD22	5:A:822:ALA:HB2	2.02	0.41
5:A:453:TRP:HE3	5:A:454:LEU:HG	1.85	0.41
6:E:194:VAL:HG13	6:E:341:VAL:HG13	2.02	0.41
6:E:698:GLY:O	6:E:842:ARG:NH1	2.47	0.41
7:B:348:TRP:CD2	7:B:349:PRO:HA	2.55	0.41
5:A:68:LEU:HD23	5:A:72:ARG:HD2	2.02	0.41
5:A:702:PHE:HB3	5:A:707:MET:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:778:THR:OG1	5:A:779:ASN:N	2.53	0.41
5:A:808:MET:SD	5:A:812:ARG:NH2	2.93	0.41
5:A:354:LEU:HA	5:A:357:VAL:HG12	2.03	0.41
5:A:544:PHE:HB2	5:A:716:LEU:HD12	2.01	0.41
5:A:777:ASN:OD1	5:A:778:THR:N	2.49	0.41
5:A:808:MET:CG	5:A:812:ARG:NH1	2.84	0.41
6:E:207:MET:HE1	6:E:224:LEU:HD11	2.03	0.41
6:E:772:SER:O	6:E:773:LEU:C	2.64	0.41
8:F:94:PRO:O	8:F:134:ARG:NH1	2.53	0.41
5:A:112:GLU:OE1	5:A:137:PHE:HB2	2.21	0.41
5:A:351:PHE:CD1	5:A:845:SER:HB3	2.54	0.41
6:E:62:THR:HG23	6:E:63:GLN:H	1.85	0.41
6:E:557:TYR:HA	6:E:560:ILE:HD12	2.03	0.41
6:E:950:MET:SD	6:E:971:ARG:NH1	2.94	0.41
7:B:182:LEU:HD23	7:B:182:LEU:HA	1.91	0.41
4:C:355:ILE:CD1	5:A:341:ILE:HD11	2.51	0.41
4:C:622:ILE:HG12	4:C:774:VAL:O	2.20	0.41
4:C:787:ILE:O	4:C:791:VAL:HG22	2.21	0.41
5:A:187:GLU:OE2	5:A:187:GLU:N	2.54	0.41
5:A:489:ARG:NH1	6:E:234:GLU:HG2	2.36	0.41
6:E:127:SER:HB3	6:E:456:GLN:HA	2.02	0.41
6:E:363:LYS:NZ	6:E:400:ASP:OD2	2.51	0.41
7:B:620:THR:O	7:B:624:LEU:HD13	2.21	0.41
8:F:139:ARG:HB2	8:F:141:TRP:CZ3	2.55	0.41
4:C:333:LEU:HD23	4:C:333:LEU:HA	1.86	0.41
6:E:260:TYR:HE1	6:E:738:LEU:HG	1.86	0.41
6:E:872:MET:HE1	6:E:905:MET:HE2	2.02	0.41
7:B:373:LEU:HB3	7:B:377:VAL:HG23	2.01	0.41
3:T:6:DC:H5"	6:E:1171:VAL:HG11	2.03	0.41
3:T:9:DG:N1	3:T:10:DG:C6	2.89	0.41
5:A:230:ALA:HB3	5:A:231:PRO:HD3	2.02	0.41
5:A:517:PHE:HB3	5:A:677:PHE:CD1	2.56	0.41
5:A:557:TYR:O	5:A:560:LEU:HB2	2.21	0.41
5:A:707:MET:HB2	5:A:707:MET:HE3	1.78	0.41
6:E:148:HIS:O	6:E:186:GLY:HA3	2.21	0.41
6:E:219:ARG:HA	6:E:219:ARG:HD3	1.86	0.41
7:B:154:ALA:HA	7:B:198:THR:O	2.20	0.41
7:B:748:LEU:HD23	7:B:748:LEU:HA	1.94	0.41
8:F:210:PHE:O	8:F:220:THR:HG23	2.21	0.41
4:C:68:GLN:HE21	4:C:383:ALA:H	1.69	0.41
4:C:155:HIS:O	4:C:159:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:166:ILE:HD12	4:C:205:LEU:HD22	2.03	0.41
4:C:275:TYR:OH	4:C:380:PRO:HB3	2.20	0.41
5:A:354:LEU:HD11	5:A:855:LEU:HD11	2.03	0.41
5:A:824:CYS:HA	5:A:851:ASN:CG	2.45	0.41
4:C:244:LEU:HD23	4:C:244:LEU:HA	1.82	0.40
4:C:248:TYR:HD2	4:C:268:ILE:HD12	1.86	0.40
4:C:455:ASP:HB2	4:C:463:ARG:HH21	1.85	0.40
4:C:862:ASP:OD1	4:C:862:ASP:C	2.63	0.40
5:A:102:GLY:HA3	5:A:344:LYS:HZ2	1.85	0.40
5:A:172:ALA:O	5:A:326:THR:OG1	2.30	0.40
5:A:353:ASN:O	5:A:357:VAL:HG12	2.21	0.40
5:A:435:GLU:HB3	5:A:794:MET:CG	2.51	0.40
6:E:1051:HIS:HA	6:E:1054:VAL:HG12	2.03	0.40
7:B:226:PHE:CZ	7:B:251:LEU:CD2	3.00	0.40
7:B:513:ASP:HA	7:B:514:PRO:HD3	1.80	0.40
4:C:209:HIS:CG	4:C:212:ARG:HE	2.39	0.40
5:A:353:ASN:HA	5:A:356:LYS:HD2	2.03	0.40
6:E:869:ALA:HA	6:E:872:MET:HE3	2.02	0.40
7:B:564:TRP:CZ2	7:B:722:VAL:HG22	2.56	0.40
4:C:360:PHE:CE1	4:C:906:HIS:HD2	2.38	0.40
5:A:55:LEU:HD23	5:A:55:LEU:HA	1.97	0.40
5:A:870:LEU:HD12	5:A:870:LEU:HA	1.80	0.40
4:C:159:ILE:HG23	4:C:205:LEU:HD12	2.03	0.40
4:C:310:ALA:HB1	4:C:380:PRO:HG2	2.03	0.40
4:C:366:PRO:O	4:C:370:THR:HG23	2.21	0.40
4:C:525:ARG:HH11	4:C:525:ARG:HG2	1.86	0.40
5:A:97:GLY:HA2	5:A:340:PHE:O	2.21	0.40
7:B:23:LEU:HD23	7:B:24:PRO:O	2.21	0.40
6:E:156:VAL:HA	6:E:179:GLY:O	2.22	0.40
6:E:730:ASN:CG	6:E:772:SER:HB3	2.46	0.40
8:F:58:LEU:CD2	8:F:167:VAL:HG11	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	C	865/1058 (82%)	817 (94%)	48 (6%)	0	100	100
5	A	754/882 (86%)	709 (94%)	45 (6%)	0	100	100
6	E	1061/1235 (86%)	1046 (99%)	14 (1%)	1 (0%)	48	79
7	B	744/750 (99%)	701 (94%)	43 (6%)	0	100	100
8	F	257/488 (53%)	256 (100%)	1 (0%)	0	100	100
All	All	3681/4413 (83%)	3529 (96%)	151 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	E	177	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	C	702/832 (84%)	695 (99%)	7 (1%)	68	74
5	A	657/742 (88%)	638 (97%)	19 (3%)	37	58
6	E	885/995 (89%)	869 (98%)	16 (2%)	51	67
7	B	557/560 (100%)	551 (99%)	6 (1%)	65	73
8	F	225/388 (58%)	221 (98%)	4 (2%)	51	67
All	All	3026/3517 (86%)	2974 (98%)	52 (2%)	52	67

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	C	84	LEU
4	C	308	ARG
4	C	417	ASN
4	C	434	LEU

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Mol	Chain	Res	Type
4	C	637	VAL
4	C	892	VAL
4	C	957	GLN
5	A	416	ARG
5	A	481	SER
5	A	511	PHE
5	A	572	LEU
5	A	580	LEU
5	A	583	GLU
5	A	584	ILE
5	A	648	TYR
5	A	652	THR
5	A	671	ARG
5	A	683	LEU
5	A	697	VAL
5	A	702	PHE
5	A	707	MET
5	A	708	LEU
5	A	716	LEU
5	A	818	LEU
5	A	829	ASN
5	A	860	GLU
6	E	156	VAL
6	E	203	GLN
6	E	233	ARG
6	E	550	ASP
6	E	717	ASP
6	E	772	SER
6	E	776	ILE
6	E	777	LEU
6	E	782	LEU
6	E	804	ASP
6	E	810	ILE
6	E	813	VAL
6	E	949[A]	LYS
6	E	949[B]	LYS
6	E	1021	ILE
6	E	1179	ASN
7	B	17	THR
7	B	323	VAL
7	B	345	LEU
7	B	388	THR

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Mol	Chain	Res	Type
7	B	416	GLN
7	B	544	VAL
8	F	77	VAL
8	F	105[A]	LYS
8	F	105[B]	LYS
8	F	128	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
4	C	68	GLN
4	C	613	ASN
5	A	127	GLN
5	A	147	HIS
5	A	155	HIS
5	A	159	GLN
5	A	234	HIS
5	A	294	GLN
5	A	409	HIS
5	A	466	GLN
5	A	499	GLN
5	A	533	GLN
5	A	699	ASN
5	A	797	ASN
5	A	851	ASN
6	E	155	ASN
6	E	203	GLN
6	E	215	HIS
6	E	587	GLN
6	E	727	GLN
6	E	729	HIS
6	E	832	HIS
6	E	1018	HIS
6	E	1228	HIS
7	B	283	HIS
8	F	104	GLN
8	F	282	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
10	A1BXB	A	901	-	28,29,29	6.23	12 (42%)	34,42,42	3.75	9 (26%)

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
10	A1BXB	A	901	-	-	7/21/22/22	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	901	A1BXB	C24-N08	15.86	1.66	1.31
10	A	901	A1BXB	C27-S01	-14.72	1.42	1.72
10	A	901	A1BXB	O05-S02	14.10	1.65	1.43
10	A	901	A1BXB	O04-S02	13.73	1.64	1.43
10	A	901	A1BXB	C27-S02	10.55	1.90	1.74
10	A	901	A1BXB	S02-N09	5.24	1.70	1.58
10	A	901	A1BXB	C26-C25	-4.75	1.40	1.49
10	A	901	A1BXB	C22-N07	4.61	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	901	A1BXB	C25-N08	4.39	1.46	1.38
10	A	901	A1BXB	C15-C14	2.74	1.53	1.49
10	A	901	A1BXB	C24-S01	-2.73	1.69	1.75
10	A	901	A1BXB	O03-C22	-2.47	1.17	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	901	A1BXB	C26-C25-C27	-11.85	109.02	127.41
10	A	901	A1BXB	S01-C27-S02	-9.51	105.71	120.10
10	A	901	A1BXB	S01-C24-N08	-8.35	104.16	116.44
10	A	901	A1BXB	C24-S01-C27	7.70	103.07	89.75
10	A	901	A1BXB	O05-S02-O04	-7.36	109.75	120.27
10	A	901	A1BXB	C27-C25-N08	-3.88	108.02	114.78
10	A	901	A1BXB	C10-N06-C14	2.98	121.41	117.24
10	A	901	A1BXB	O04-S02-N09	2.75	112.22	108.39
10	A	901	A1BXB	C11-C12-C13	-2.08	117.67	120.24

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	901	A1BXB	C21-C22-N07-C23
10	A	901	A1BXB	N08-C24-N07-C22
10	A	901	A1BXB	N08-C24-N07-C23
10	A	901	A1BXB	S01-C27-S02-O05
10	A	901	A1BXB	O03-C22-N07-C23
10	A	901	A1BXB	C25-C27-S02-O04
10	A	901	A1BXB	S01-C27-S02-N09

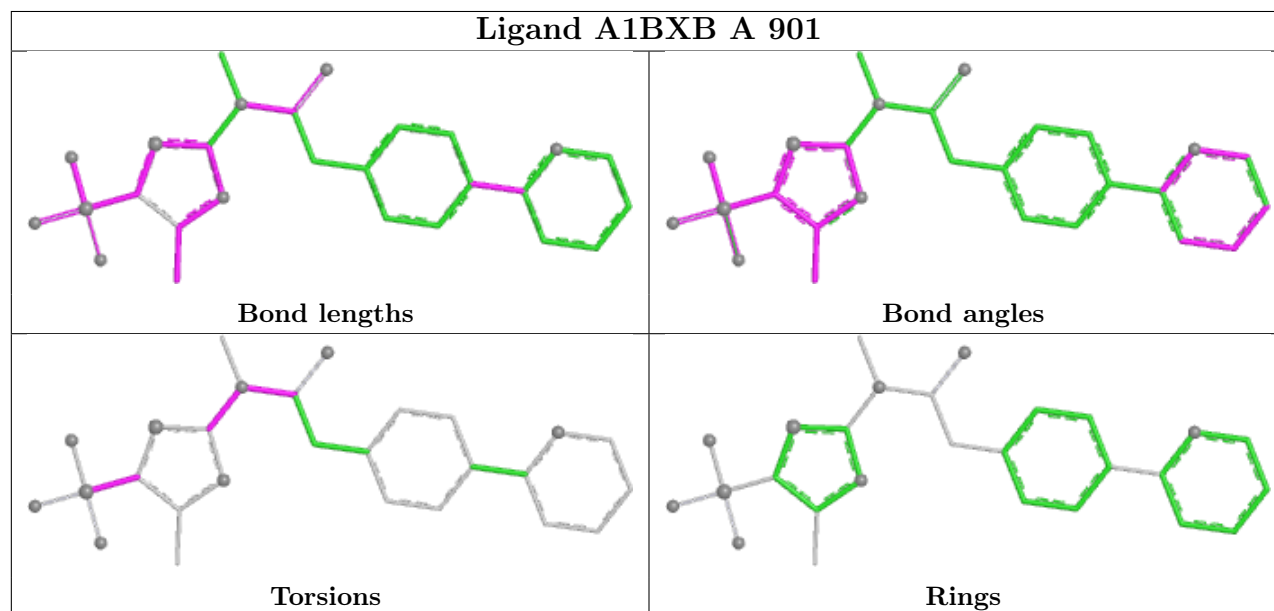
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	901	A1BXB	4	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	T	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	T	9:DG	O3'	10:DG	P	2.02

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72764. These allow visual inspection of the internal detail of the map and identification of artifacts.

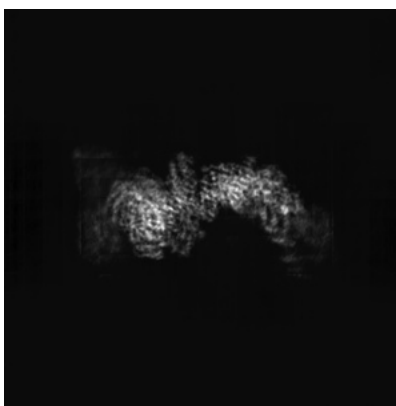
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

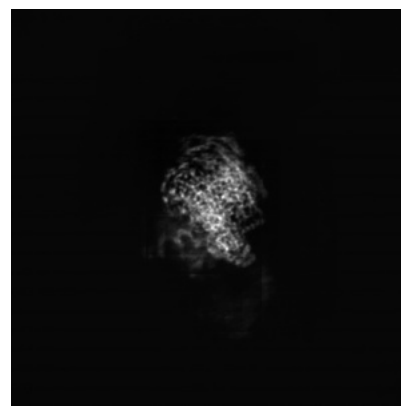
6.1.1 Primary map



X

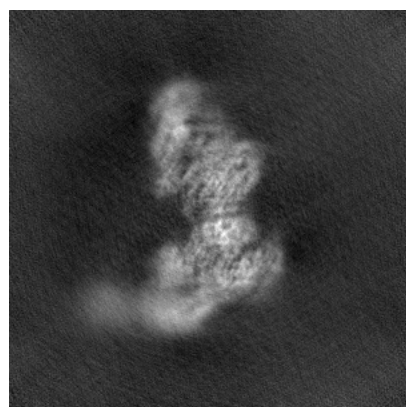


Y

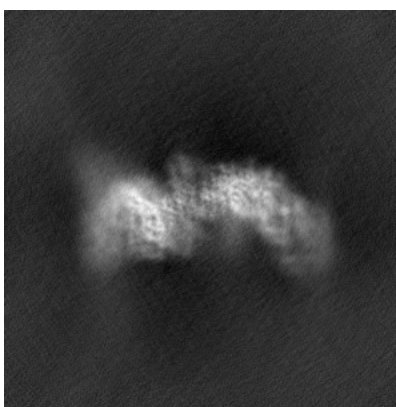


Z

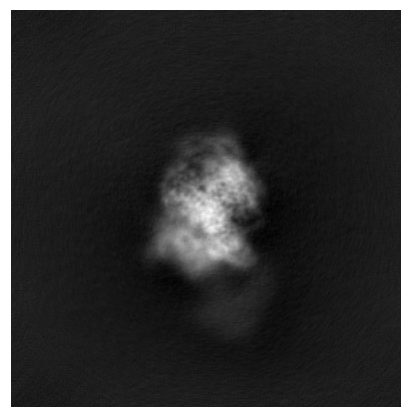
6.1.2 Raw map



X



Y

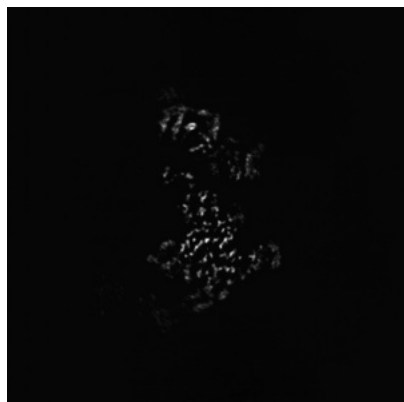


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 200

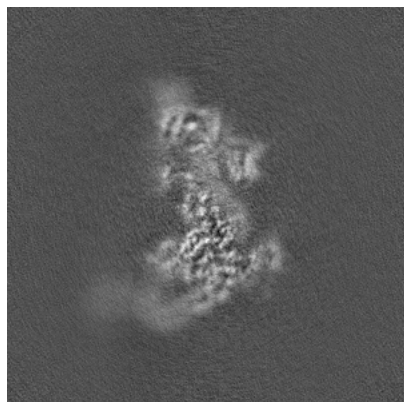


Y Index: 200



Z Index: 200

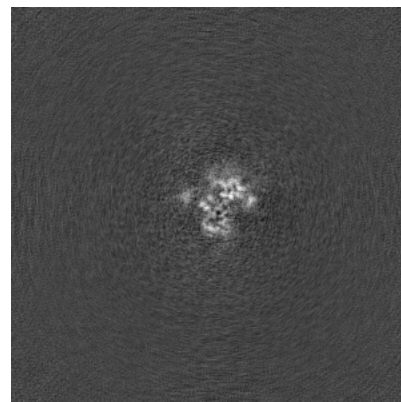
6.2.2 Raw map



X Index: 200



Y Index: 200

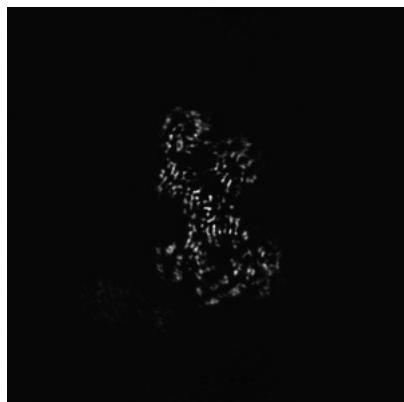


Z Index: 200

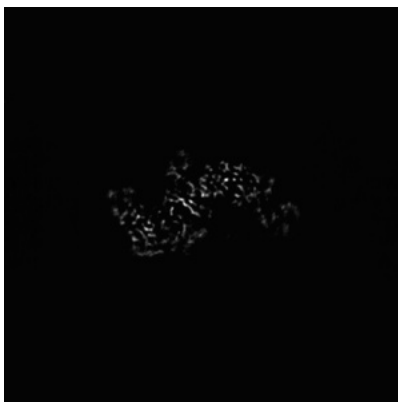
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 209

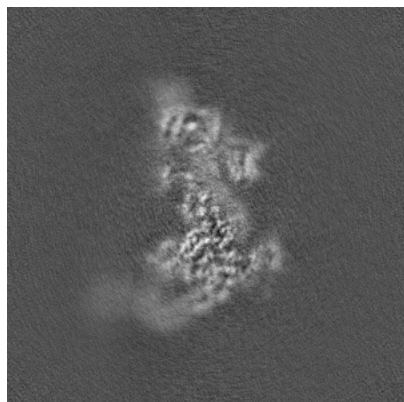


Y Index: 211

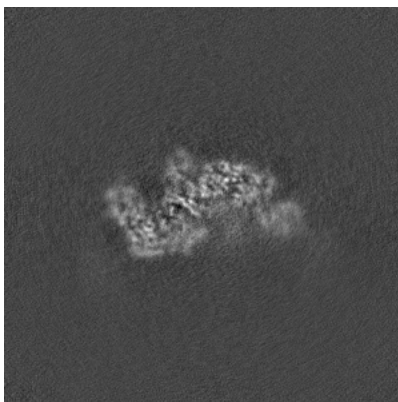


Z Index: 146

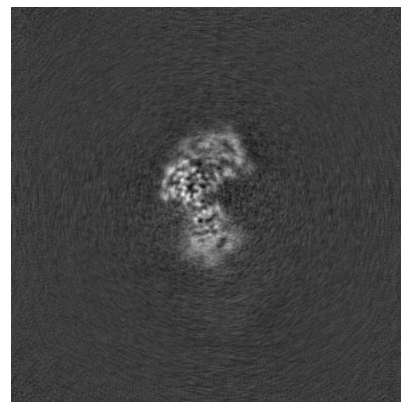
6.3.2 Raw map



X Index: 200



Y Index: 211

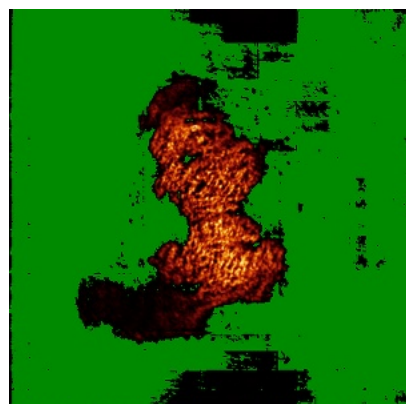


Z Index: 145

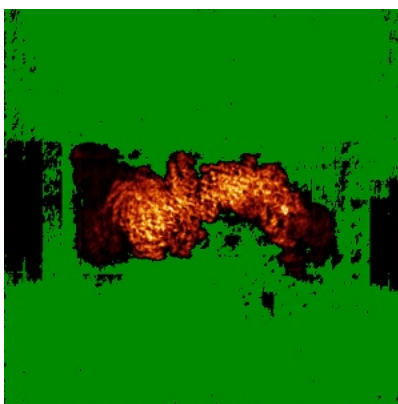
The images above show the largest variance slices of the map in three orthogonal directions.

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

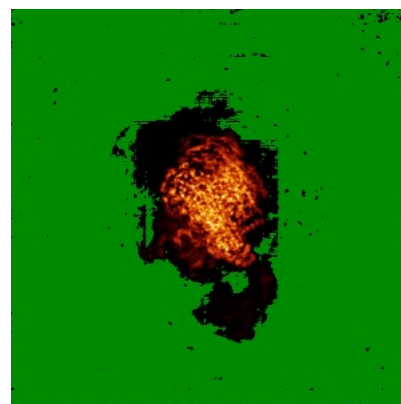
6.4.1 Primary map



X

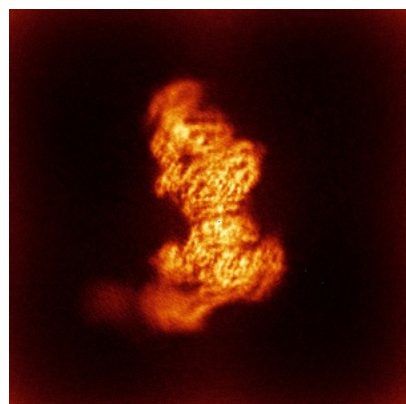


Y

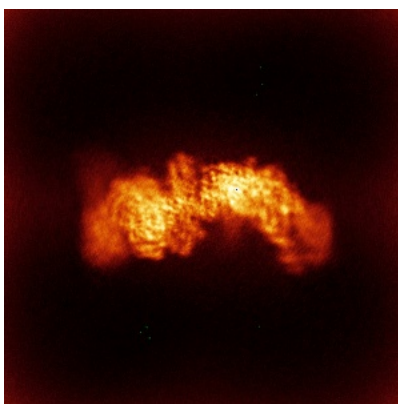


Z

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.

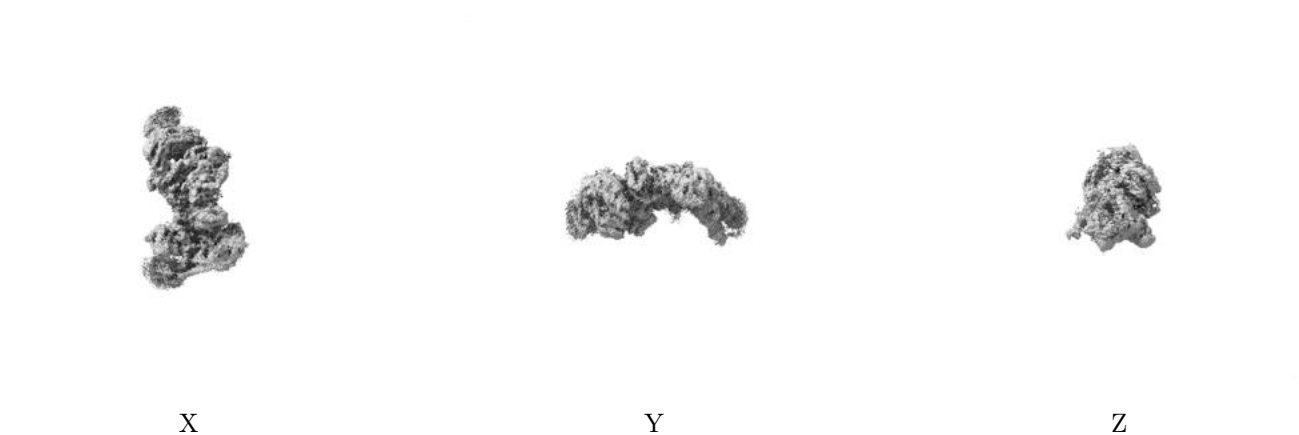
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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



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

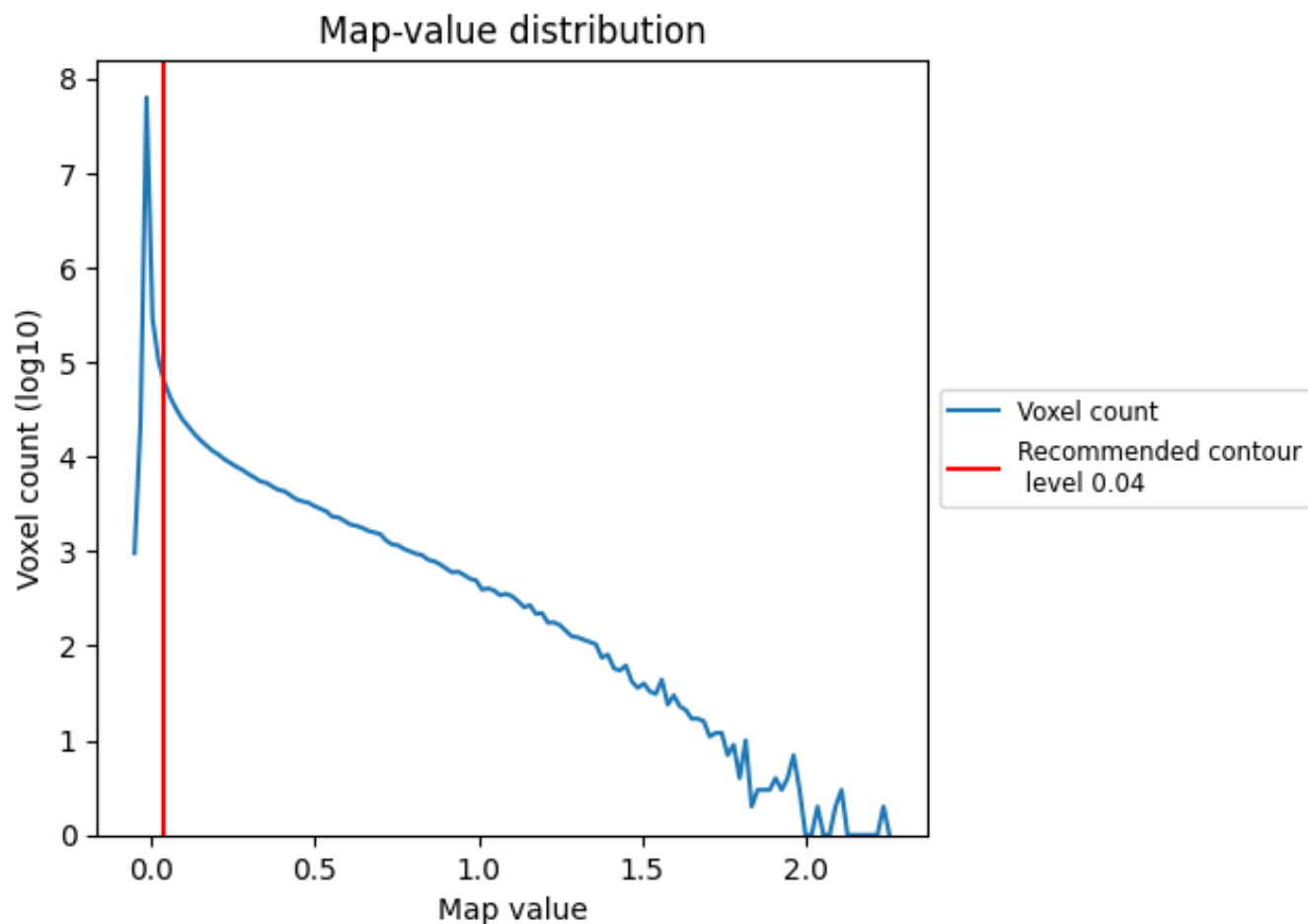
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

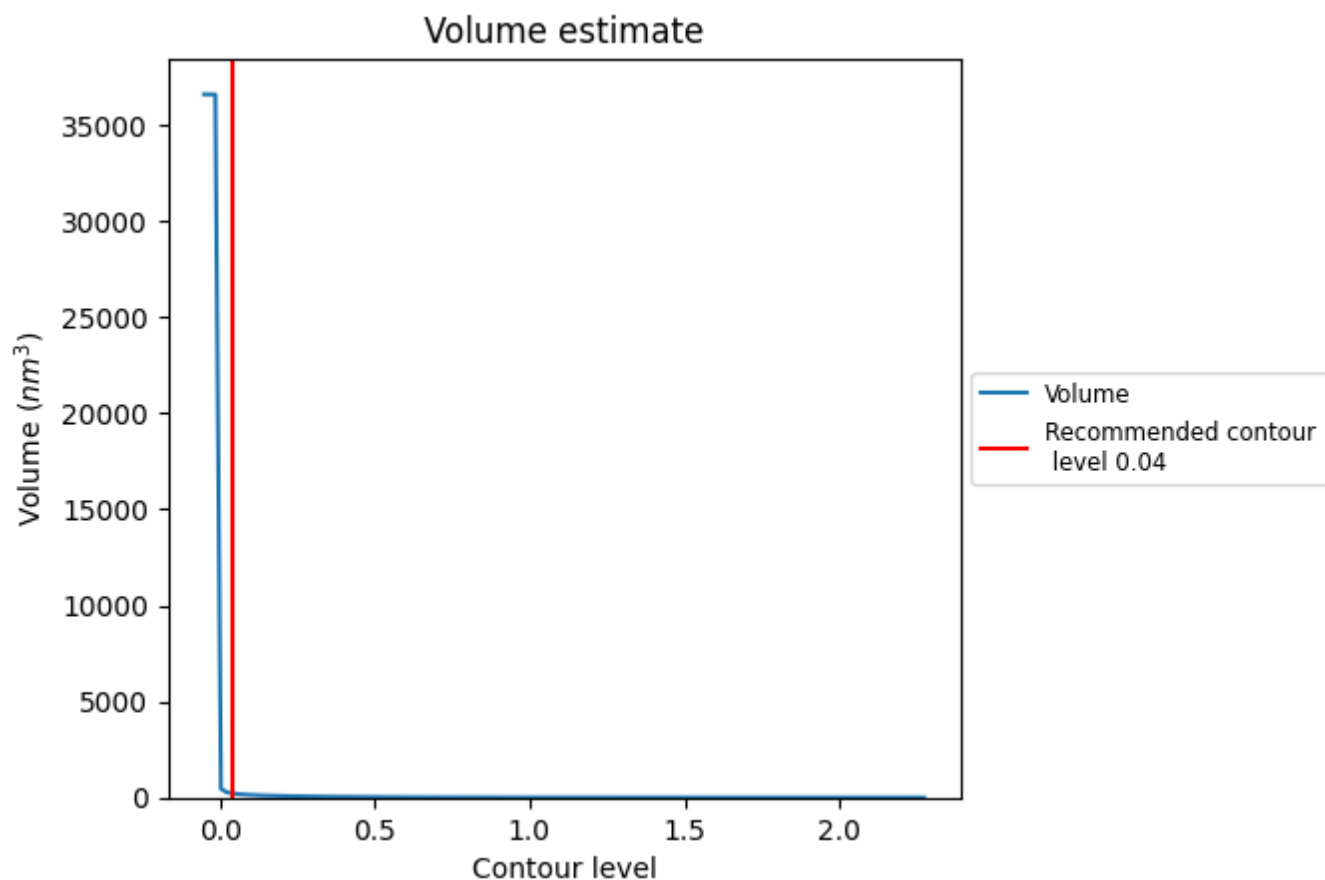
This section contains the results of statistical analysis of the map.

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.

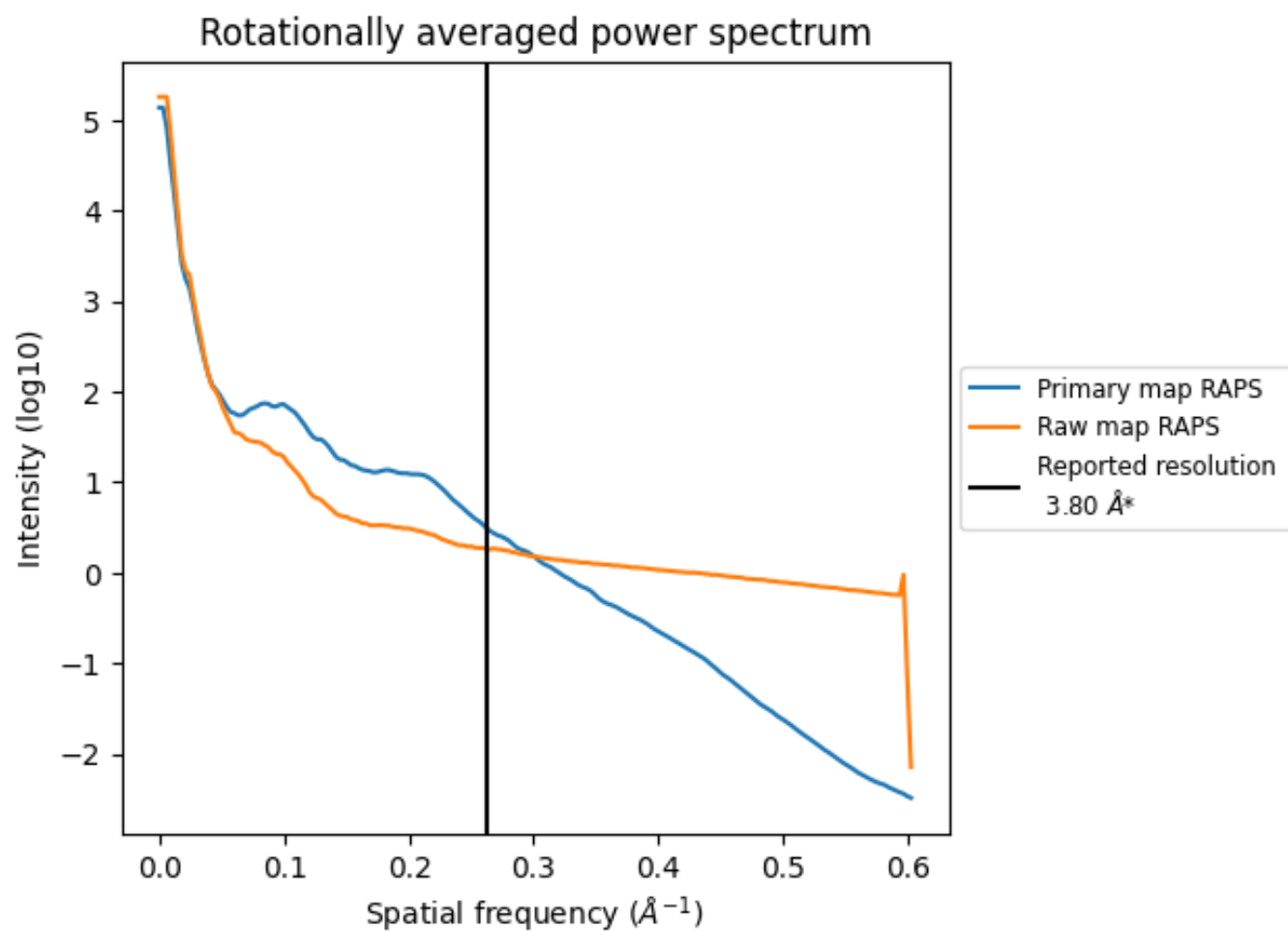
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 219 nm³; this corresponds to an approximate mass of 198 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 ⓘ

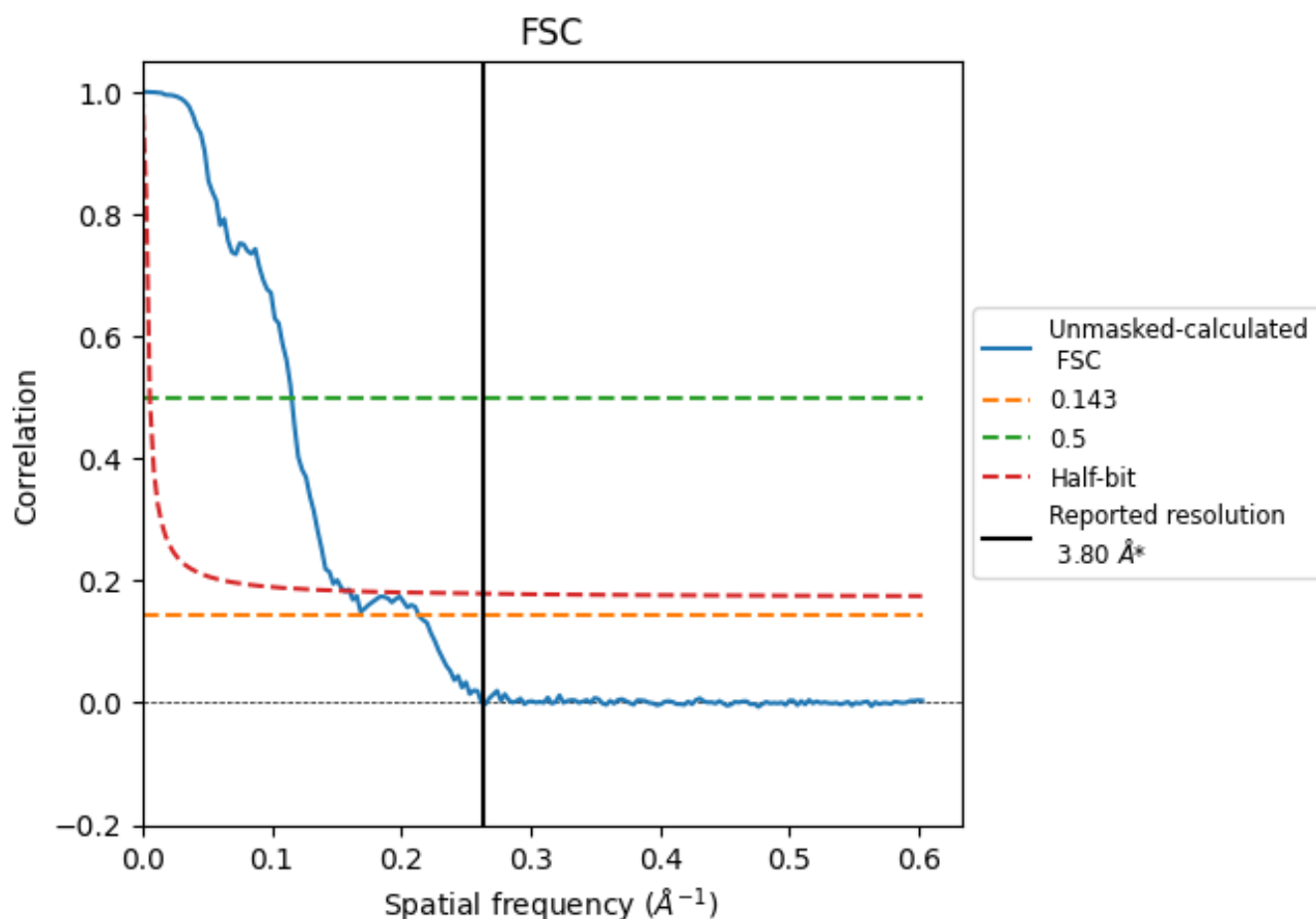


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 $0.263 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

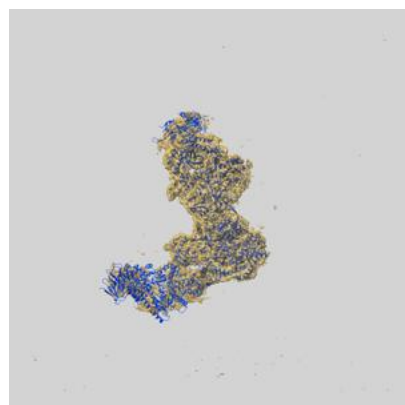
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.68	8.67	6.40

*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 4.68 differs from the reported value 3.8 by more than 10 %

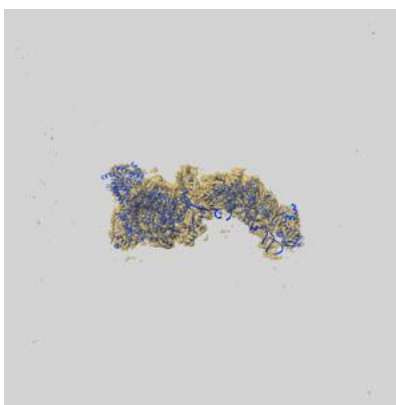
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72764 and PDB model 9YC9. Per-residue inclusion information can be found in section [3](#) on page [6](#).

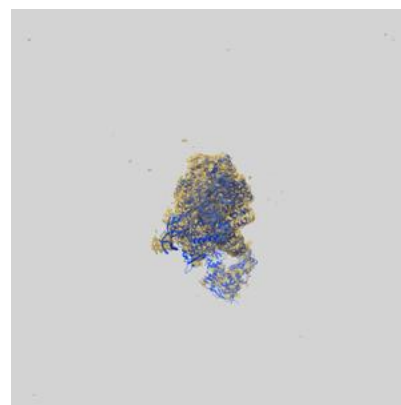
9.1 Map-model overlay [i](#)



X



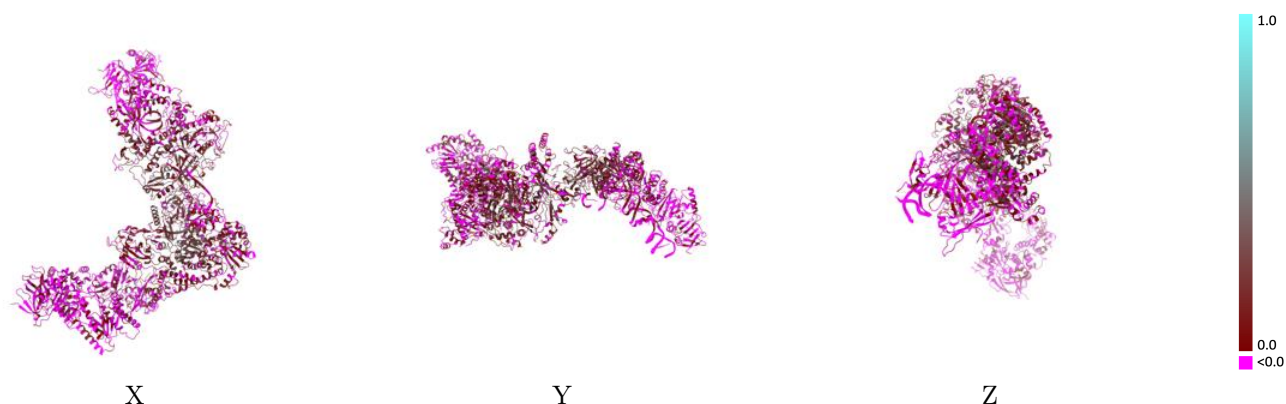
Y



Z

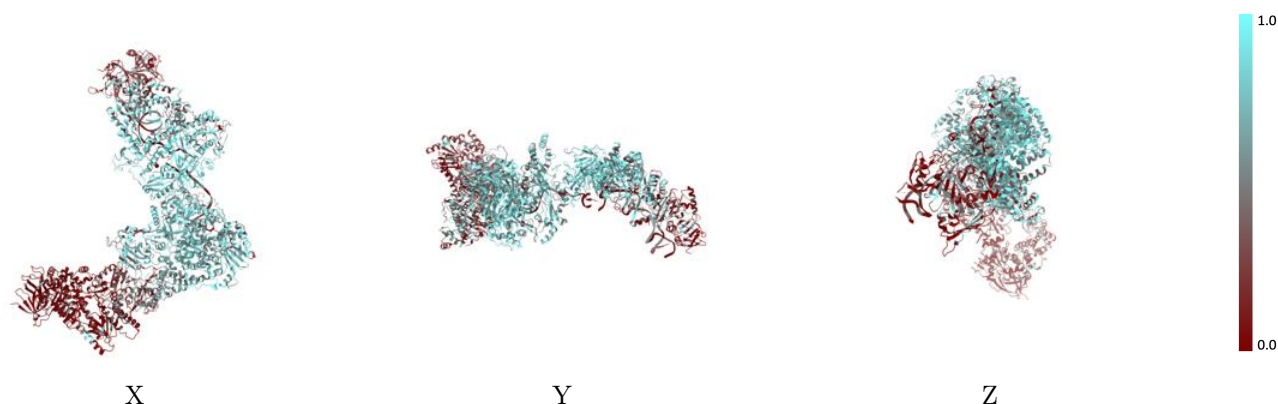
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



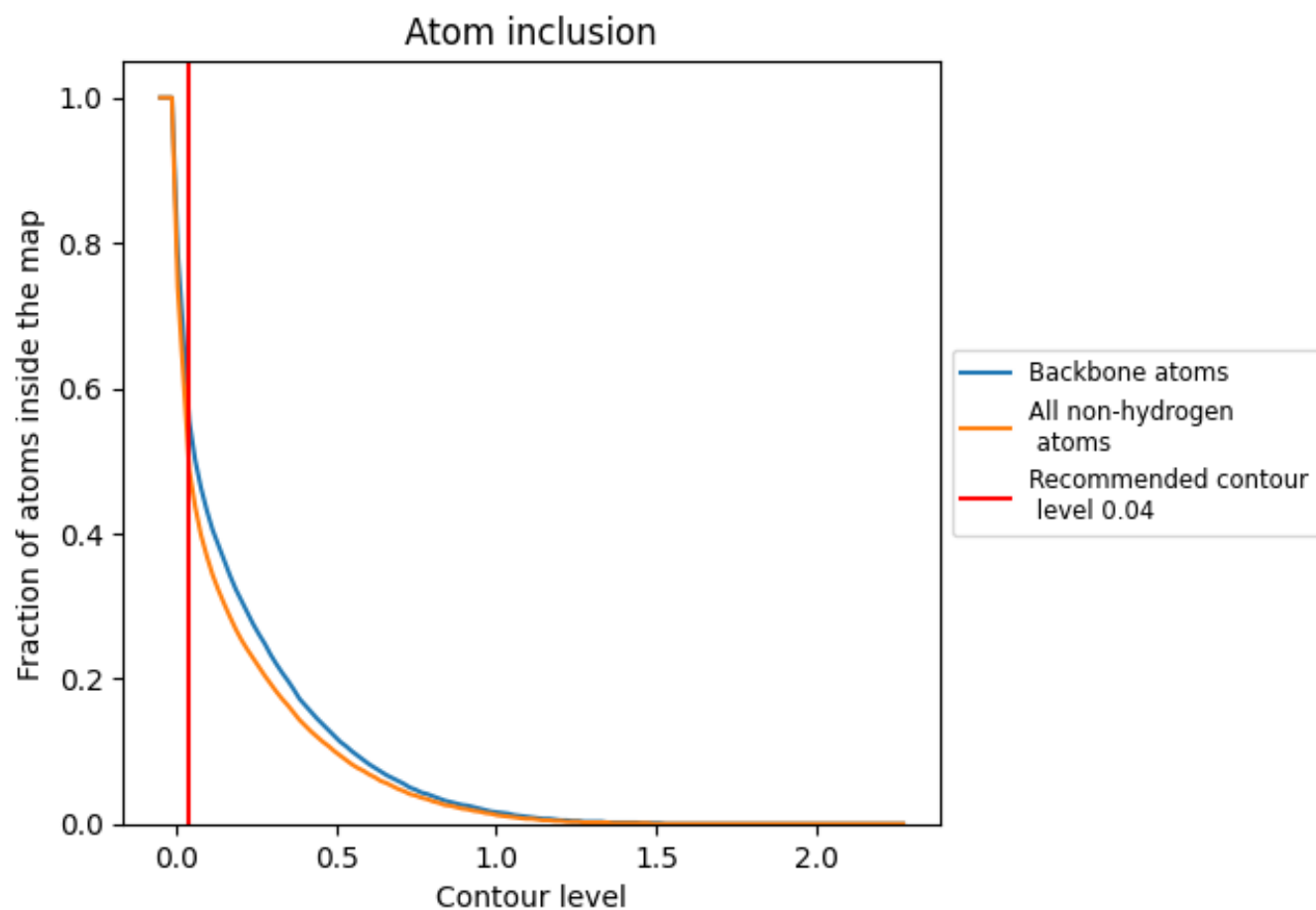
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion ⓘ



At the recommended contour level, 56% of all backbone atoms, 49% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4890	0.0600
A	0.7430	0.1670
B	0.0930	-0.0400
C	0.5130	0.0410
D	0.3060	0.0700
E	0.6660	0.1090
F	0.1940	-0.0750
P	0.3890	-0.0250
T	0.3030	-0.0360

1.0

0.0

<0.0