



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:53 AM UTC

PDB ID : 6GH6 / pdb_00006gh6
EMDB ID : EMD-0002
Title : Cryo-EM structure of bacterial RNA polymerase-sigma54 holoenzyme intermediate partially loaded complex
Authors : Glyde, R.; Ye, F.Z.; Zhang, X.D.
Deposited on : 2018-05-04
Resolution : 4.10 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:

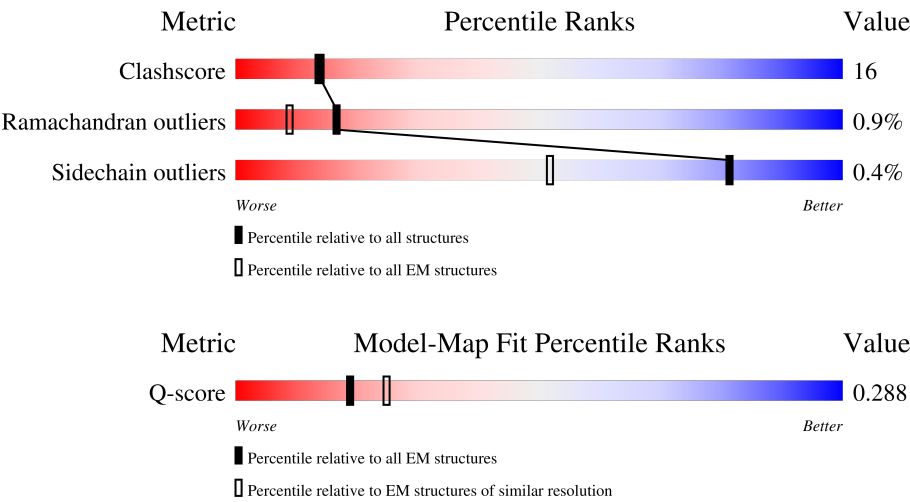
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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	6458 (3.60 - 4.60)

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	A	329	
1	B	329	
2	C	1342	
3	D	1407	

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Mol	Chain	Length	Quality of chain
4	E	91	67%15%18%
5	M	497	51%12%37%
6	N	63	44%27%5%24%
7	T	63	5%49%24%24%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 28051 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	233	Total	C	N	O	S	0	0
			1776	1107	312	351	6		
1	B	235	Total	C	N	O	S	0	0
			1729	1085	301	337	6		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1341	Total	C	N	O	S	0	0
			10068	6315	1744	1972	37		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1334	Total	C	N	O	S	0	0
			10063	6297	1791	1933	42		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	75	Total	C	N	O	S	0	0
			568	349	110	107	2		

- Molecule 5 is a protein called RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	315	Total	C	N	O	S	0	0
			1875	1168	331	373	3		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-19	MET	-	initiating methionine	UNP A0A0J4U551
M	-18	GLY	-	expression tag	UNP A0A0J4U551
M	-17	SER	-	expression tag	UNP A0A0J4U551
M	-16	SER	-	expression tag	UNP A0A0J4U551
M	-15	HIS	-	expression tag	UNP A0A0J4U551
M	-14	HIS	-	expression tag	UNP A0A0J4U551
M	-13	HIS	-	expression tag	UNP A0A0J4U551
M	-12	HIS	-	expression tag	UNP A0A0J4U551
M	-11	HIS	-	expression tag	UNP A0A0J4U551
M	-10	HIS	-	expression tag	UNP A0A0J4U551
M	-9	SER	-	expression tag	UNP A0A0J4U551
M	-8	SER	-	expression tag	UNP A0A0J4U551
M	-7	GLY	-	expression tag	UNP A0A0J4U551
M	-6	LEU	-	expression tag	UNP A0A0J4U551
M	-5	VAL	-	expression tag	UNP A0A0J4U551
M	-4	PRO	-	expression tag	UNP A0A0J4U551
M	-3	ARG	-	expression tag	UNP A0A0J4U551
M	-2	GLY	-	expression tag	UNP A0A0J4U551
M	-1	SER	-	expression tag	UNP A0A0J4U551
M	0	HIS	-	expression tag	UNP A0A0J4U551
M	336	ALA	ARG	engineered mutation	UNP A0A0J4U551

- Molecule 6 is a DNA chain called nifH promoter non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	48	Total	C	N	O	P	0	0
			988	467	184	289	48		

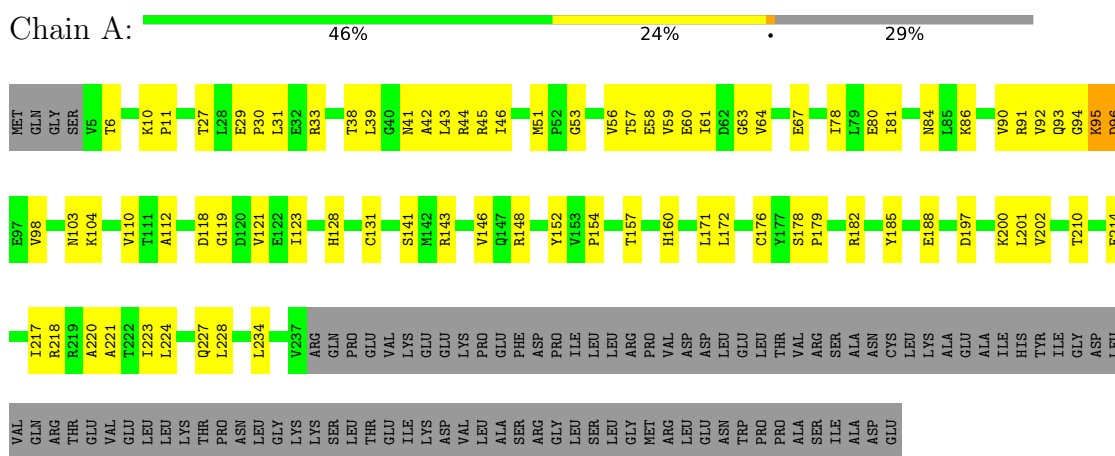
- Molecule 7 is a DNA chain called nifH promoter template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	48	Total	C	N	O	P	0	0
			984	464	187	285	48		

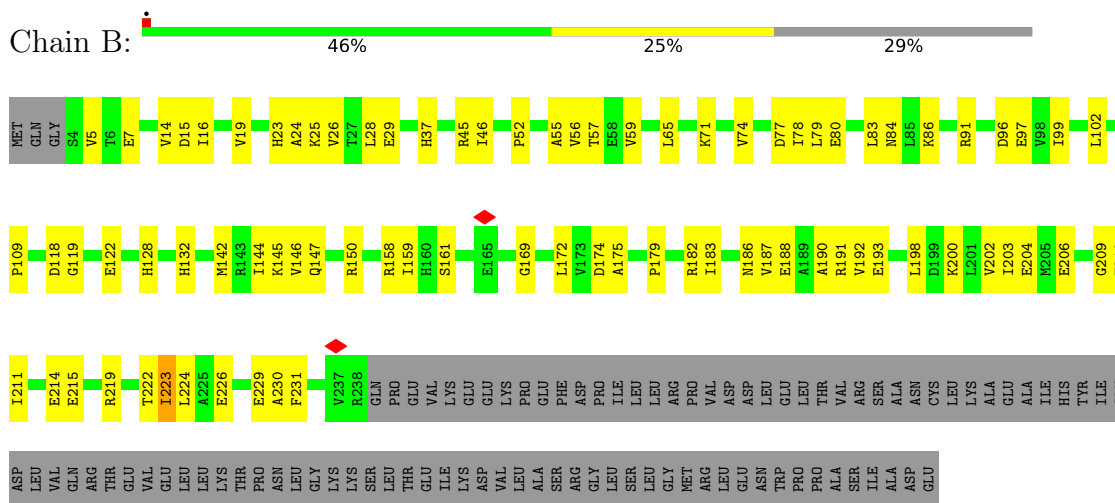
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA-directed RNA polymerase subunit alpha

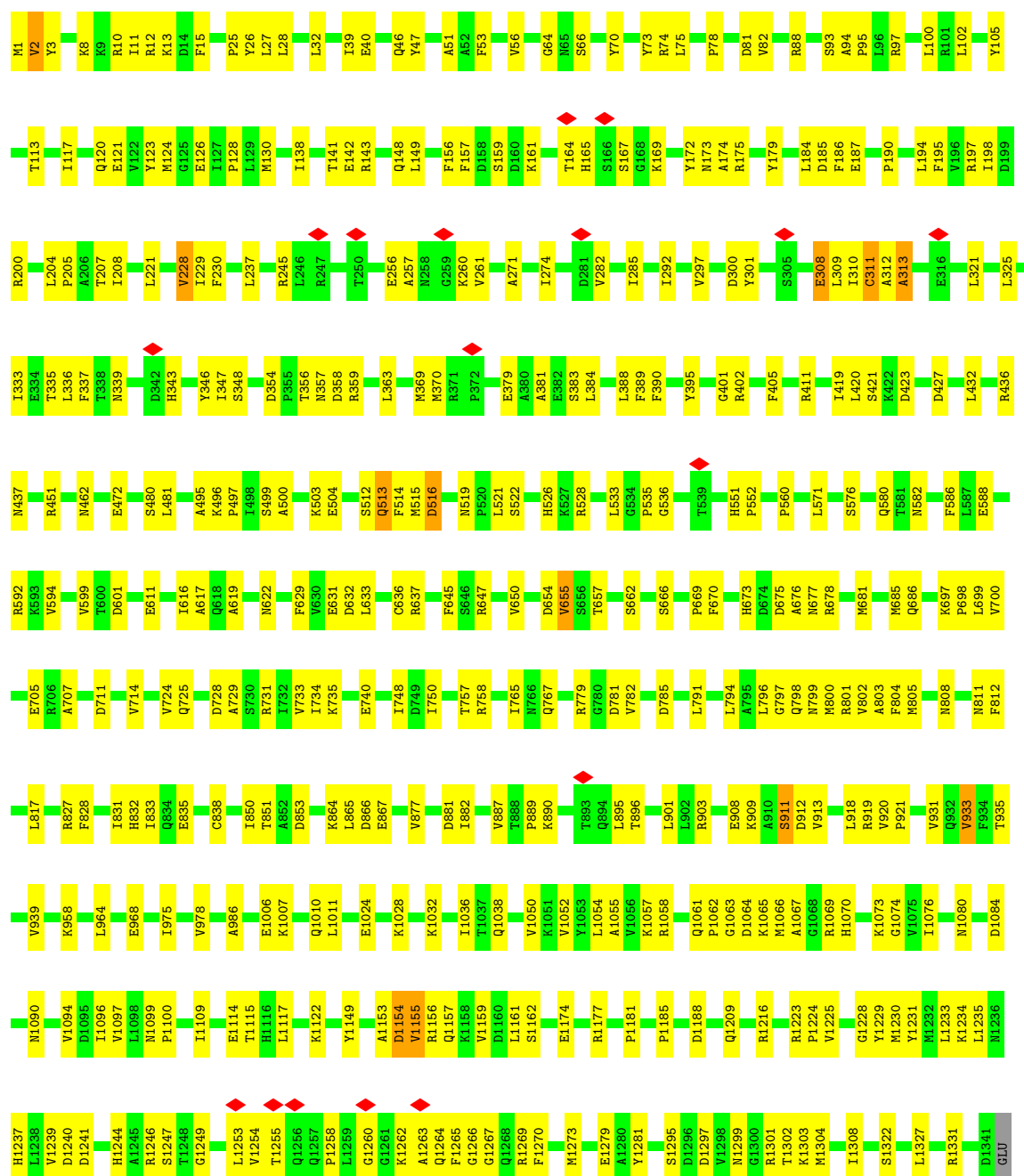


• Molecule 1: DNA-directed RNA polymerase subunit alpha

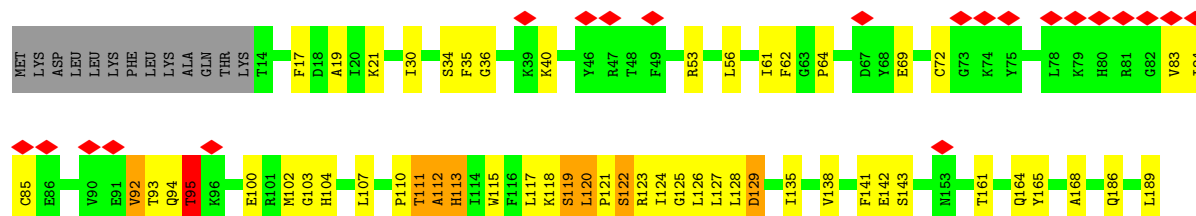


• Molecule 2: DNA-directed RNA polymerase subunit beta

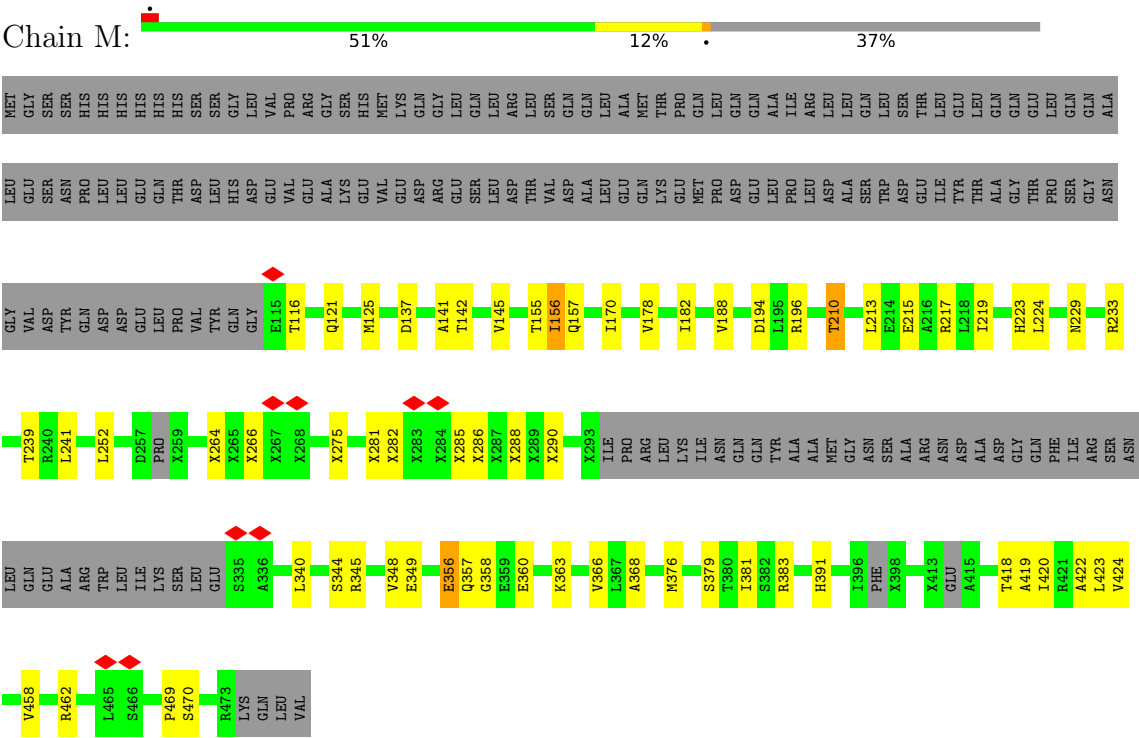




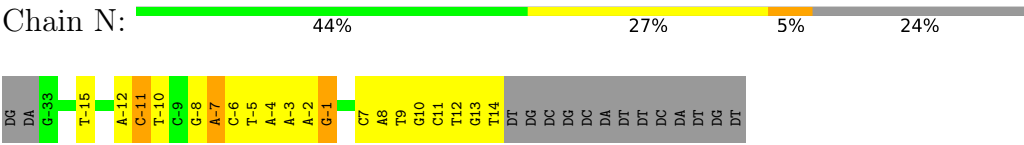
• Molecule 3: DNA-directed RNA polymerase subunit beta'



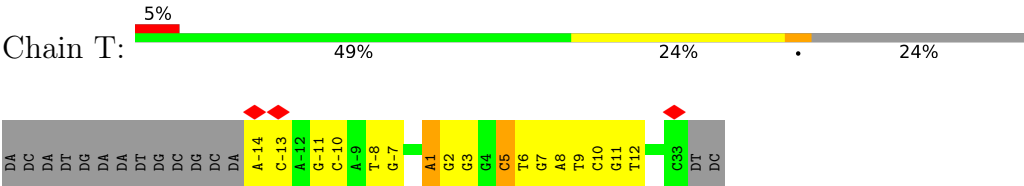
- Molecule 5: RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor,RNA polymerase sigma-54 factor



- Molecule 6: nifH promoter non-tmeplate DNA



- Molecule 7: nifH promoter template DNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53709	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.191	Depositor
Minimum map value	-0.081	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.16	0/1798	0.51	2/2442 (0.1%)
1	B	0.14	0/1748	0.45	0/2380
2	C	0.17	0/10223	0.48	5/13870 (0.0%)
3	D	0.33	1/10200 (0.0%)	0.56	13/13816 (0.1%)
4	E	0.12	0/570	0.43	0/770
5	M	0.42	2/1631 (0.1%)	0.80	6/2260 (0.3%)
6	N	0.33	0/1108	0.87	13/1709 (0.8%)
7	T	0.34	1/1104 (0.1%)	0.76	4/1701 (0.2%)
All	All	0.27	4/28382 (0.0%)	0.57	43/38948 (0.1%)

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
2	C	0	1
3	D	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	514	THR	C-N	-26.87	0.96	1.33
5	M	356	GLU	C-N	12.50	1.51	1.33
5	M	210	THR	C-N	7.58	1.51	1.33
7	T	1	DA	O3'-P	5.27	1.69	1.61

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	356	GLU	O-C-N	17.95	146.82	123.12
5	M	356	GLU	CA-C-N	-16.63	89.78	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	356	GLU	C-N-CA	-16.63	89.78	121.54
7	T	5	DC	O3'-P-O5'	14.60	125.91	104.00
7	T	5	DC	C5'-C4'-O4'	13.03	128.94	109.40
6	N	-1	DG	O3'-P-O5'	12.17	122.26	104.00
6	N	-6	DC	C2'-C3'-O3'	-10.39	95.92	111.50
2	C	356	THR	N-CA-C	9.43	124.59	107.99
6	N	-7	DA	C4'-C3'-O3'	9.27	123.91	110.00
7	T	6	DT	O3'-P-O5'	9.10	117.65	104.00
7	T	6	DT	C5'-C4'-O4'	8.65	122.38	109.40
6	N	-11	DC	C4'-C3'-O3'	8.47	122.70	110.00
6	N	-11	DC	C2'-C3'-O3'	-8.26	99.11	111.50
2	C	357	ASN	N-CA-C	-7.87	102.79	111.36
3	D	111	THR	N-CA-C	7.44	120.17	108.79
3	D	120	LEU	C-N-CD	7.41	136.91	120.60
1	A	95	LYS	N-CA-C	-7.39	103.30	111.36
3	D	529	GLY	C-N-CD	7.05	136.10	120.60
6	N	-1	DG	OP1-P-O3'	-6.84	87.48	108.00
3	D	125	GLY	N-CA-C	-6.48	106.74	115.36
6	N	-7	DA	C2'-C3'-O3'	-6.45	101.83	111.50
6	N	-7	DA	C4-N9-C1'	-6.27	117.65	127.05
3	D	888	CYS	N-CA-C	-6.22	103.59	111.92
6	N	-7	DA	C8-N9-C1'	5.93	135.95	127.05
2	C	911	SER	CB-CA-C	-5.90	109.76	116.54
5	M	363	LYS	CA-C-N	-5.80	113.78	119.76
5	M	363	LYS	C-N-CA	-5.80	113.78	119.76
6	N	-6	DC	O5'-C5'-C4'	5.74	119.41	110.80
3	D	141	PHE	CB-CA-C	-5.74	109.98	116.63
6	N	-6	DC	C4'-C3'-O3'	5.72	118.59	110.00
3	D	545	HIS	N-CA-C	5.70	117.94	108.20
3	D	92	VAL	N-CA-C	-5.58	97.74	109.34
3	D	1324	SER	N-CA-C	-5.43	106.32	113.17
1	A	93	GLN	N-CA-C	-5.40	105.50	111.71
3	D	547	ARG	N-CA-C	-5.39	99.66	108.76
6	N	-15	DT	C5'-C4'-O4'	5.34	117.41	109.40
3	D	548	VAL	N-CA-C	5.18	115.58	108.12
5	M	233	ARG	CB-CA-C	-5.14	110.23	117.23
2	C	986	ALA	CB-CA-C	-5.13	110.25	117.23
2	C	1154	ASP	CB-CA-C	-5.11	110.29	117.23
3	D	586	GLY	CA-C-N	-5.09	112.95	120.68
3	D	586	GLY	C-N-CA	-5.09	112.95	120.68
6	N	-7	DA	C3'-C2'-C1'	-5.01	94.08	101.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1263	ALA	Peptide
3	D	343	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1776	0	1774	54	0
1	B	1729	0	1723	60	0
2	C	10068	0	9713	293	0
3	D	10063	0	10044	332	0
4	E	568	0	570	10	0
5	M	1875	0	1337	41	0
6	N	988	0	539	50	0
7	T	984	0	536	38	0
All	All	28051	0	26236	810	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (810) 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:N:-11:DC:H1'	6:N:-10:DT:OP1	1.21	1.27
2:C:141:THR:HG21	2:C:514:PHE:CE1	1.73	1.21
5:M:288:UNK:CB	5:M:349:GLU:HA	1.71	1.20
1:B:79:LEU:HD21	3:D:526:VAL:CG2	1.72	1.18
2:C:142:GLU:HG3	2:C:515:MET:CE	1.75	1.16
1:B:83:LEU:HD12	3:D:526:VAL:CG1	1.77	1.14
3:D:118:LYS:HA	3:D:122:SER:HA	1.30	1.11
6:N:-11:DC:H2''	6:N:-10:DT:O5'	1.41	1.11
6:N:-12:DA:H4'	6:N:-11:DC:OP1	1.29	1.10
1:B:79:LEU:CD2	3:D:526:VAL:HG21	1.82	1.10
2:C:142:GLU:CB	2:C:515:MET:HE2	1.82	1.08
6:N:-2:DA:H2	7:T:2:DG:N2	1.53	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1168:GLU:CB	3:D:1179:PRO:HD3	1.85	1.05
1:B:83:LEU:HD12	3:D:526:VAL:HG12	1.36	1.03
3:D:527:LEU:HD11	3:D:535:ARG:NH2	1.73	1.03
1:A:95:LYS:O	1:A:96:ASP:HB2	1.55	1.02
3:D:523:GLU:OE2	3:D:524:GLY:N	1.93	1.01
3:D:1168:GLU:CB	3:D:1178:THR:HB	1.90	1.01
3:D:121:PRO:HA	3:D:122:SER:HB3	1.42	0.97
6:N:-11:DC:C1'	6:N:-10:DT:OP1	2.12	0.96
2:C:141:THR:HG21	2:C:514:PHE:CD1	2.01	0.95
6:N:-1:DG:N1	7:T:1:DA:C2	2.36	0.93
2:C:142:GLU:CG	2:C:515:MET:HE2	2.00	0.92
6:N:-1:DG:H1	7:T:1:DA:H2	0.98	0.91
3:D:542:ALA:HB3	3:D:545:HIS:CB	2.01	0.90
2:C:142:GLU:CG	2:C:515:MET:CE	2.48	0.90
3:D:118:LYS:CB	3:D:122:SER:HB2	2.02	0.89
6:N:-2:DA:H2	7:T:2:DG:H22	0.89	0.89
2:C:300:ASP:HA	2:C:311:CYS:O	1.73	0.88
6:N:-1:DG:N1	7:T:1:DA:H2	1.69	0.88
3:D:118:LYS:CA	3:D:122:SER:HA	2.02	0.88
3:D:527:LEU:HD11	3:D:535:ARG:HH21	1.39	0.88
1:B:79:LEU:HD21	3:D:526:VAL:HG21	0.91	0.87
1:B:83:LEU:HD12	3:D:526:VAL:HG11	1.53	0.87
3:D:529:GLY:N	3:D:530:PRO:HA	1.89	0.87
2:C:142:GLU:HG3	2:C:515:MET:HE2	1.54	0.86
2:C:310:ILE:O	2:C:311:CYS:HB2	1.75	0.86
1:A:94:GLY:HA3	1:A:148:ARG:HE	1.40	0.86
3:D:527:LEU:CD1	3:D:535:ARG:NH2	2.39	0.86
6:N:13:DG:H2''	6:N:14:DT:H71	1.57	0.85
2:C:141:THR:CG2	2:C:514:PHE:CE1	2.58	0.84
6:N:-11:DC:H1'	6:N:-10:DT:P	2.17	0.84
2:C:1007:LYS:O	2:C:1011:LEU:HB2	1.78	0.83
5:M:288:UNK:CB	5:M:349:GLU:CA	2.54	0.83
1:A:92:VAL:HG22	1:A:94:GLY:H	1.42	0.83
1:B:83:LEU:CD1	3:D:526:VAL:CG1	2.56	0.82
3:D:119:SER:H	3:D:122:SER:HA	1.42	0.82
1:A:11:PRO:HA	1:A:30:PRO:HG2	1.60	0.82
3:D:517:CYS:CB	3:D:544:LEU:O	2.26	0.82
6:N:-7:DA:H2	7:T:7:DG:H22	1.27	0.82
3:D:528:THR:C	3:D:530:PRO:HA	2.05	0.81
2:C:310:ILE:O	2:C:310:ILE:HD12	1.79	0.81
7:T:10:DC:H4'	7:T:11:DG:OP1	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:110:PRO:O	3:D:111:THR:HG23	1.82	0.80
2:C:384:LEU:O	2:C:388:LEU:HB3	1.80	0.80
3:D:519:ASN:HD22	3:D:709:ARG:HD3	1.46	0.80
3:D:517:CYS:HB3	3:D:545:HIS:HA	1.62	0.80
3:D:110:PRO:O	3:D:111:THR:CG2	2.30	0.79
3:D:1168:GLU:CB	3:D:1178:THR:H	1.94	0.79
2:C:142:GLU:HB3	2:C:515:MET:HE2	1.65	0.79
6:N:10:DG:H2''	6:N:11:DC:C5	2.18	0.79
3:D:1175:LEU:HD22	3:D:1196:LEU:HD13	1.63	0.79
6:N:-11:DC:C2'	6:N:-10:DT:O5'	2.29	0.79
2:C:141:THR:HG21	2:C:514:PHE:HE1	1.46	0.79
3:D:309:ASN:HB3	3:D:324:LEU:CB	2.13	0.79
2:C:88:ARG:HH22	2:C:1038:GLN:HE21	1.29	0.79
2:C:141:THR:CG2	2:C:514:PHE:CD1	2.67	0.78
3:D:323:PRO:O	3:D:324:LEU:CB	2.29	0.78
2:C:301:TYR:H	2:C:311:CYS:HB3	1.49	0.77
3:D:480:ALA:HA	3:D:484:MET:HE3	1.67	0.77
1:B:83:LEU:CD1	3:D:526:VAL:HG12	2.12	0.77
6:N:-12:DA:C4'	6:N:-11:DC:OP1	2.22	0.77
3:D:527:LEU:CD1	3:D:535:ARG:HH21	1.96	0.77
3:D:544:LEU:N	3:D:544:LEU:HD12	2.00	0.77
3:D:535:ARG:HE	3:D:541:LEU:HD22	1.48	0.77
2:C:513:GLN:HE21	2:C:513:GLN:N	1.83	0.77
3:D:517:CYS:HB3	3:D:544:LEU:O	1.84	0.77
3:D:92:VAL:HG13	3:D:100:GLU:OE1	1.85	0.76
3:D:119:SER:H	3:D:122:SER:CA	1.99	0.76
3:D:326:SER:O	3:D:330:MET:CB	2.34	0.76
3:D:724:MET:O	3:D:728:SER:HB3	1.85	0.76
7:T:10:DC:OP2	7:T:10:DC:H3'	1.86	0.75
3:D:119:SER:N	3:D:122:SER:HA	2.02	0.74
3:D:1168:GLU:CB	3:D:1178:THR:CB	2.65	0.74
3:D:61:ILE:HG22	3:D:62:PHE:H	1.52	0.74
3:D:535:ARG:HB2	3:D:535:ARG:NH1	2.03	0.73
1:A:95:LYS:O	1:A:96:ASP:CB	2.35	0.73
3:D:958:ILE:HA	3:D:983:LYS:O	1.88	0.73
6:N:-2:DA:C2	7:T:2:DG:N1	2.57	0.73
2:C:187:GLU:O	2:C:194:LEU:HA	1.89	0.72
6:N:13:DG:C2'	6:N:14:DT:H71	2.19	0.72
3:D:118:LYS:HA	3:D:122:SER:CA	2.15	0.72
2:C:142:GLU:CB	2:C:515:MET:CE	2.66	0.71
1:A:10:LYS:HD2	1:A:11:PRO:HD2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:527:LEU:HB3	3:D:530:PRO:HB2	1.70	0.71
6:N:8:DA:C2'	6:N:9:DT:H72	2.20	0.71
1:A:59:VAL:O	1:A:171:LEU:HB2	1.89	0.71
2:C:1322:SER:OG	3:D:332:LYS:NZ	2.22	0.71
2:C:673:HIS:HB3	2:C:1109:ILE:HB	1.74	0.70
2:C:803:ALA:HB3	2:C:1097:VAL:HG22	1.73	0.70
3:D:723:TYR:O	3:D:727:ASP:HB3	1.91	0.70
3:D:1288:ALA:O	3:D:1292:LEU:HB2	1.92	0.70
2:C:522:SER:O	2:C:526:HIS:HB2	1.91	0.70
3:D:544:LEU:HD12	3:D:544:LEU:H	1.56	0.70
6:N:-2:DA:H2	7:T:2:DG:C2	2.09	0.69
5:M:340:LEU:CB	7:T:10:DC:OP1	2.40	0.69
6:N:-7:DA:C2	7:T:7:DG:N2	2.51	0.69
2:C:310:ILE:HD12	2:C:310:ILE:C	2.17	0.69
3:D:1060:VAL:HG23	3:D:1107:VAL:H	1.58	0.69
3:D:352:ARG:HA	3:D:466:MET:O	1.94	0.68
3:D:519:ASN:HD22	3:D:709:ARG:CD	2.07	0.68
2:C:1270:PHE:HB2	3:D:347:VAL:HG12	1.74	0.68
3:D:121:PRO:CA	3:D:122:SER:HB3	2.20	0.68
1:B:83:LEU:CD1	3:D:526:VAL:HG11	2.22	0.67
2:C:312:ALA:O	2:C:313:ALA:HB2	1.92	0.67
2:C:1209:GLN:HB3	2:C:1224:PRO:HB2	1.77	0.67
6:N:8:DA:H8	6:N:8:DA:OP2	1.78	0.67
3:D:127:LEU:HD22	3:D:223:LEU:HB3	1.77	0.67
3:D:523:GLU:CD	3:D:524:GLY:H	1.99	0.67
2:C:798:GLN:HB3	2:C:827:ARG:HH21	1.59	0.67
1:A:46:ILE:HG13	1:A:224:LEU:HD12	1.76	0.66
2:C:363:LEU:HB3	2:C:381:ALA:HB1	1.76	0.66
6:N:-8:DG:H21	7:T:8:DA:H62	1.42	0.66
2:C:516:ASP:OD1	2:C:516:ASP:N	2.24	0.66
3:D:120:LEU:N	3:D:121:PRO:HA	2.09	0.66
2:C:358:ASP:OD1	2:C:359:ARG:N	2.29	0.65
2:C:256:GLU:HA	2:C:261:VAL:HA	1.78	0.65
2:C:533:LEU:HD11	2:C:571:LEU:HD13	1.77	0.65
2:C:533:LEU:N	2:C:533:LEU:HD12	2.11	0.65
1:A:234:LEU:HD22	1:B:214:GLU:HB2	1.77	0.65
2:C:142:GLU:HG3	2:C:515:MET:HE1	1.73	0.65
5:M:356:GLU:C	5:M:358:GLY:N	2.50	0.65
1:A:10:LYS:HZ1	1:B:230:ALA:H	1.44	0.65
2:C:105:TYR:HA	2:C:113:THR:HA	1.79	0.65
2:C:512:SER:C	2:C:513:GLN:HE21	2.05	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:164:GLN:O	3:D:168:ALA:HB2	1.96	0.64
1:B:19:VAL:HB	1:B:23:HIS:HB3	1.79	0.64
5:M:366:VAL:HG12	5:M:368:ALA:H	1.62	0.64
3:D:384:LYS:HD2	3:D:415:VAL:HG22	1.79	0.64
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.80	0.64
2:C:636:CYS:SG	2:C:637:ARG:N	2.69	0.64
2:C:724:VAL:HG22	2:C:734:ILE:HG12	1.80	0.64
2:C:812:PHE:HB3	3:D:357:VAL:HG11	1.79	0.64
3:D:110:PRO:C	3:D:111:THR:HG23	2.22	0.64
3:D:934:THR:HG23	3:D:936:HIS:H	1.62	0.64
3:D:94:GLN:O	3:D:95:THR:HG23	1.98	0.64
7:T:-14:DA:H2''	7:T:-13:DC:C5	2.33	0.64
3:D:709:ARG:NH2	3:D:710:ASP:OD1	2.32	0.63
3:D:547:ARG:HA	3:D:572:THR:O	1.97	0.63
1:A:214:GLU:O	1:A:218:ARG:HB2	1.98	0.63
3:D:1228:ALA:O	3:D:1232:TYR:HB2	1.98	0.63
3:D:56:LEU:HD12	3:D:273:ILE:HD11	1.81	0.63
3:D:1265:THR:HG22	3:D:1277:GLY:HA2	1.79	0.63
1:B:191:ARG:NH1	3:D:413:ASP:OD2	2.32	0.63
3:D:976:THR:HG22	3:D:1026:PRO:HB2	1.81	0.63
1:B:102:LEU:HD11	1:B:142:MET:HE3	1.80	0.63
6:N:-7:DA:N1	7:T:7:DG:N2	2.45	0.63
3:D:119:SER:H	3:D:122:SER:N	1.97	0.63
3:D:128:LEU:CD2	3:D:189:LEU:HD13	2.29	0.63
2:C:142:GLU:HB2	2:C:515:MET:HE2	1.77	0.63
2:C:560:PRO:O	3:D:780:ARG:NH1	2.32	0.63
3:D:1317:GLU:OE2	3:D:1345:ARG:NH2	2.32	0.63
3:D:121:PRO:HA	3:D:122:SER:CB	2.25	0.62
2:C:13:LYS:NZ	2:C:1149:TYR:O	2.32	0.62
3:D:161:THR:O	3:D:165:TYR:N	2.31	0.62
3:D:1153:PRO:O	3:D:1194:ARG:NH2	2.32	0.62
6:N:8:DA:H2''	6:N:9:DT:OP2	1.99	0.62
6:N:10:DG:H2''	6:N:11:DC:H5	1.64	0.62
3:D:473:THR:HG22	3:D:474:LEU:H	1.64	0.62
7:T:10:DC:H1'	7:T:11:DG:H5'	1.81	0.62
1:B:190:ALA:HB2	1:B:200:LYS:HG3	1.82	0.62
2:C:70:TYR:HA	2:C:100:LEU:HA	1.82	0.62
2:C:1295:SER:O	2:C:1301:ARG:NH1	2.33	0.62
3:D:527:LEU:CB	3:D:530:PRO:HB2	2.29	0.62
7:T:9:DT:H2''	7:T:10:DC:H5'	1.82	0.62
7:T:10:DC:H1'	7:T:11:DG:C5'	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1061:GLN:HB2	2:C:1062:PRO:HD2	1.80	0.61
3:D:120:LEU:O	3:D:120:LEU:HD23	1.99	0.61
2:C:56:VAL:HG11	2:C:472:GLU:HG3	1.82	0.61
3:D:128:LEU:HD21	3:D:189:LEU:HD13	1.83	0.61
3:D:806:ASP:OD1	3:D:1259:GLN:NE2	2.33	0.61
1:A:94:GLY:HA3	1:A:148:ARG:NE	2.14	0.61
3:D:1100:PHE:HA	3:D:1196:LEU:HD23	1.83	0.61
3:D:535:ARG:NE	3:D:541:LEU:HD22	2.15	0.61
2:C:805:MET:HE2	2:C:1225:VAL:HG11	1.82	0.61
3:D:93:THR:O	3:D:93:THR:HG22	2.00	0.61
6:N:-11:DC:C1'	6:N:-10:DT:P	2.74	0.61
3:D:709:ARG:NH2	3:D:710:ASP:O	2.34	0.61
2:C:901:LEU:HD11	5:M:229:ASN:HD22	1.66	0.60
3:D:1354:GLY:O	3:D:1355:ARG:HG3	2.01	0.60
5:M:155:THR:O	5:M:156:ILE:HG13	2.00	0.60
3:D:364:HIS:HD2	3:D:487:THR:HG21	1.66	0.60
7:T:-8:DT:H2''	7:T:-7:DG:C8	2.37	0.60
3:D:1268:ASN:OD1	3:D:1269:ALA:N	2.33	0.60
1:B:80:GLU:O	1:B:84:ASN:ND2	2.34	0.60
2:C:46:GLN:HA	2:C:51:ALA:HB2	1.83	0.60
2:C:617:ALA:HB2	2:C:650:VAL:HG21	1.84	0.60
2:C:699:LEU:HD13	2:C:799:ASN:HD21	1.66	0.60
2:C:499:SER:O	2:C:503:LYS:HB3	2.02	0.59
3:D:364:HIS:O	3:D:365:GLN:HG3	2.01	0.59
3:D:1355:ARG:HH12	3:D:1366:HIS:CD2	2.20	0.59
6:N:-2:DA:C2	7:T:2:DG:N2	2.44	0.59
2:C:312:ALA:O	2:C:313:ALA:CB	2.50	0.59
3:D:535:ARG:HD2	3:D:541:LEU:HB2	1.84	0.59
3:D:551:ARG:HA	3:D:568:SER:O	2.02	0.59
6:N:12:DT:O2	7:T:-11:DG:N2	2.35	0.59
2:C:13:LYS:HE3	2:C:15:PHE:HE1	1.67	0.59
2:C:197:ARG:HD3	2:C:200:ARG:HA	1.84	0.59
3:D:889:ASP:N	3:D:889:ASP:OD1	2.35	0.59
1:A:57:THR:HG22	1:A:58:GLU:HG3	1.84	0.59
3:D:809:VAL:HG13	3:D:896:ALA:HB2	1.85	0.59
1:B:158:ARG:HD3	1:B:172:LEU:HD22	1.84	0.59
2:C:801:ARG:HD2	2:C:1094:VAL:HA	1.84	0.59
3:D:30:ILE:HD13	3:D:243:PRO:HD3	1.83	0.59
3:D:1270:GLY:HA2	3:D:1299:GLY:HA2	1.84	0.59
7:T:-11:DG:H2''	7:T:-10:DC:C6	2.37	0.59
2:C:142:GLU:HB3	2:C:515:MET:CE	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:205:PRO:HG2	2:C:208:ILE:HG12	1.84	0.59
2:C:519:ASN:ND2	2:C:686:GLN:O	2.36	0.59
4:E:27:ALA:O	4:E:31:GLN:HB2	2.02	0.59
3:D:631:TYR:HA	3:D:634:ARG:HG2	1.83	0.58
1:A:80:GLU:O	1:A:84:ASN:ND2	2.36	0.58
1:B:91:ARG:HB2	1:B:122:GLU:HB3	1.85	0.58
2:C:804:PHE:HB3	2:C:1100:PRO:HG3	1.84	0.58
3:D:422:LEU:HD23	3:D:436:ALA:HB2	1.85	0.58
1:B:186:ASN:OD1	1:B:187:VAL:N	2.36	0.58
3:D:517:CYS:HB2	3:D:544:LEU:O	2.02	0.58
3:D:1368:ASP:OD1	3:D:1371:ARG:NH2	2.36	0.58
2:C:156:PHE:O	2:C:174:ALA:HA	2.04	0.58
1:A:157:THR:O	1:A:160:HIS:ND1	2.29	0.58
3:D:288:PRO:HD2	3:D:291:ILE:HD12	1.85	0.58
3:D:344:GLY:O	3:D:346:ARG:NH1	2.37	0.58
3:D:749:LYS:HD2	3:D:750:PRO:HD2	1.86	0.58
6:N:8:DA:H2'	6:N:9:DT:H72	1.85	0.58
2:C:1240:ASP:OD1	2:C:1241:ASP:N	2.37	0.58
3:D:886:VAL:H	3:D:1258:ARG:HD2	1.69	0.57
6:N:8:DA:H2''	6:N:9:DT:C7	2.33	0.57
2:C:169:LYS:HE3	2:C:190:PRO:HA	1.85	0.57
2:C:411:ARG:NH2	2:C:427:ASP:OD2	2.37	0.57
3:D:724:MET:O	3:D:728:SER:CB	2.52	0.57
1:B:15:ASP:O	1:B:26:VAL:HA	2.03	0.57
2:C:309:LEU:N	2:C:309:LEU:HD12	2.19	0.57
2:C:1174:GLU:HA	2:C:1177:ARG:HE	1.69	0.57
2:C:1267:GLY:O	3:D:347:VAL:HG22	2.04	0.57
3:D:403:ARG:NH1	3:D:405:GLU:OE2	2.37	0.57
3:D:961:SER:HB3	3:D:981:GLU:HB2	1.87	0.57
2:C:74:ARG:HG2	2:C:75:LEU:H	1.69	0.57
2:C:797:GLY:N	2:C:1231:TYR:OH	2.37	0.57
3:D:40:LYS:HG3	3:D:53:ARG:HH12	1.70	0.57
3:D:121:PRO:CA	3:D:122:SER:CB	2.82	0.57
3:D:576:ARG:NH1	3:D:593:ASN:O	2.37	0.57
3:D:368:LEU:HD12	3:D:369:PRO:HD2	1.86	0.57
2:C:379:GLU:O	2:C:383:SER:HB3	2.05	0.57
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.86	0.56
1:B:52:PRO:HG2	1:B:219:ARG:HH22	1.69	0.56
3:D:568:SER:OG	3:D:570:LYS:NZ	2.34	0.56
2:C:1007:LYS:HA	2:C:1011:LEU:HD13	1.88	0.56
5:M:419:ALA:O	5:M:423:LEU:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:VAL:HG12	1:B:193:GLU:OE1	2.05	0.56
2:C:935:THR:HB	2:C:939:VAL:HG11	1.87	0.56
5:M:288:UNK:CB	5:M:349:GLU:CB	2.83	0.56
5:M:376:MET:HB2	5:M:381:ILE:HD11	1.88	0.56
2:C:500:ALA:O	2:C:504:GLU:HB2	2.05	0.56
3:D:161:THR:H	3:D:164:GLN:HB2	1.70	0.56
2:C:337:PHE:HD2	2:C:339:ASN:HB2	1.70	0.56
3:D:1342:ASP:O	3:D:1343:GLU:HG2	2.05	0.56
3:D:751:ASP:OD1	3:D:752:GLY:N	2.38	0.56
6:N:-7:DA:H2	7:T:7:DG:N2	1.97	0.56
2:C:237:LEU:HD21	2:C:292:ILE:HD11	1.86	0.56
2:C:308:GLU:O	2:C:309:LEU:HB2	2.05	0.56
2:C:1297:ASP:O	2:C:1301:ARG:NH2	2.39	0.56
2:C:632:ASP:HA	2:C:647:ARG:HH11	1.71	0.55
2:C:707:ALA:O	2:C:711:ASP:HB2	2.06	0.55
7:T:10:DC:H1'	7:T:11:DG:O5'	2.06	0.55
2:C:95:PRO:HB3	2:C:123:TYR:HE1	1.71	0.55
3:D:303:VAL:HG13	3:D:306:LEU:HD12	1.89	0.55
6:N:-1:DG:C2	7:T:1:DA:H2	2.25	0.55
2:C:838:CYS:HB2	2:C:918:LEU:HD22	1.89	0.55
2:C:890:LYS:HE3	2:C:912:ASP:HB2	1.87	0.55
2:C:297:VAL:HA	2:C:335:THR:HG22	1.89	0.55
3:D:552:ILE:O	3:D:567:THR:HA	2.06	0.55
2:C:499:SER:O	2:C:503:LYS:CB	2.54	0.55
3:D:1168:GLU:O	3:D:1176:VAL:O	2.25	0.55
1:A:118:ASP:HB3	1:A:121:VAL:HB	1.87	0.55
3:D:17:PHE:HB3	3:D:1355:ARG:HD2	1.89	0.55
1:A:188:GLU:OE2	1:A:200:LYS:NZ	2.33	0.54
1:B:222:THR:O	1:B:226:GLU:HB2	2.06	0.54
3:D:117:LEU:CB	3:D:124:ILE:CB	2.86	0.54
3:D:265:LEU:HD21	3:D:326:SER:HB2	1.88	0.54
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.41	0.54
1:B:84:ASN:O	1:B:128:HIS:NE2	2.33	0.54
2:C:629:PHE:O	2:C:647:ARG:NH2	2.40	0.54
2:C:866:ASP:OD1	2:C:867:GLU:N	2.39	0.54
3:D:535:ARG:O	3:D:538:ARG:N	2.40	0.54
6:N:8:DA:C2'	6:N:9:DT:C7	2.85	0.54
2:C:669:PRO:HD2	2:C:1069:ARG:HH12	1.71	0.54
2:C:802:VAL:HG21	2:C:1230:MET:HB3	1.90	0.54
2:C:811:ASN:HB2	2:C:1099:ASN:HB2	1.89	0.54
2:C:1299:ASN:OD1	2:C:1302:THR:OG1	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:32:LEU:HD23	2:C:130:MET:HE2	1.90	0.54
2:C:78:PRO:HG3	2:C:94:ALA:HB2	1.88	0.54
2:C:120:GLN:HG2	2:C:121:GLU:H	1.72	0.54
2:C:175:ARG:HA	2:C:184:LEU:O	2.07	0.54
3:D:482:ALA:O	3:D:488:ASN:ND2	2.41	0.54
2:C:1267:GLY:HA3	3:D:346:ARG:HB3	1.90	0.54
6:N:-8:DG:H21	7:T:8:DA:N6	2.06	0.54
2:C:669:PRO:HG2	2:C:700:VAL:HG12	1.89	0.54
2:C:141:THR:CG2	2:C:514:PHE:HE1	2.12	0.54
3:D:21:LYS:HB3	3:D:1341:ARG:HD2	1.89	0.54
3:D:535:ARG:HB2	3:D:535:ARG:HH11	1.68	0.54
2:C:142:GLU:CG	2:C:515:MET:HE1	2.34	0.54
3:D:111:THR:O	3:D:112:ALA:HB3	2.07	0.54
3:D:737:ILE:HD13	3:D:740:LEU:HD12	1.89	0.54
5:M:275:UNK:HA	5:M:391:HIS:HB2	1.89	0.54
1:A:56:VAL:HG22	1:A:146:VAL:HG22	1.89	0.54
2:C:148:GLN:HE22	2:C:535:PRO:HD2	1.72	0.54
2:C:1223:ARG:NH2	3:D:719:PHE:HB3	2.23	0.54
3:D:360:TYR:CD2	3:D:361:LEU:HG	2.43	0.54
3:D:824:PRO:HD3	3:D:835:LEU:HD13	1.89	0.54
1:A:31:LEU:HD11	1:A:201:LEU:HB2	1.90	0.53
1:B:179:PRO:HG3	1:B:211:ILE:HD13	1.89	0.53
3:D:117:LEU:CA	3:D:124:ILE:CB	2.85	0.53
3:D:535:ARG:CB	3:D:535:ARG:CZ	2.86	0.53
2:C:1185:PRO:HB2	2:C:1188:ASP:OD1	2.07	0.53
2:C:142:GLU:HG3	2:C:515:MET:HE3	1.81	0.53
2:C:731:ARG:HH11	2:C:958:LYS:HE3	1.73	0.53
2:C:1154:ASP:O	2:C:1155:VAL:HG22	2.09	0.53
2:C:13:LYS:HA	2:C:1157:GLN:HE22	1.72	0.53
3:D:532:GLU:HA	3:D:535:ARG:NH2	2.22	0.53
3:D:885:VAL:HB	3:D:1258:ARG:HD2	1.89	0.53
4:E:15:ASN:ND2	4:E:17:PHE:HB2	2.24	0.53
5:M:420:ILE:O	5:M:424:VAL:CB	2.56	0.53
1:A:61:ILE:HG12	1:A:63:GLY:H	1.72	0.53
2:C:785:ASP:OD2	2:C:791:LEU:N	2.39	0.53
3:D:324:LEU:O	3:D:326:SER:N	2.42	0.53
2:C:611:GLU:HB2	2:C:616:ILE:HD11	1.89	0.53
2:C:740:GLU:OE1	2:C:779:ARG:NH1	2.41	0.53
2:C:877:VAL:HG13	2:C:881:ASP:HB2	1.91	0.53
1:A:60:GLU:OE2	1:A:143:ARG:NH2	2.41	0.53
2:C:257:ALA:HB1	2:C:282:VAL:HG11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:747:MET:HE2	3:D:775:SER:HA	1.90	0.53
2:C:53:PHE:HE2	2:C:73:TYR:HB3	1.74	0.53
2:C:102:LEU:HB3	2:C:117:ILE:O	2.08	0.53
3:D:83:VAL:HG22	3:D:84:ILE:H	1.74	0.53
4:E:27:ALA:O	4:E:31:GLN:CB	2.57	0.53
2:C:714:VAL:O	2:C:767:GLN:NE2	2.42	0.53
2:C:801:ARG:NH2	2:C:1229:TYR:OH	2.43	0.52
2:C:257:ALA:N	2:C:260:LYS:O	2.41	0.52
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.91	0.52
2:C:1260:GLY:HA2	3:D:346:ARG:HE	1.73	0.52
3:D:117:LEU:HA	3:D:124:ILE:CB	2.40	0.52
3:D:967:VAL:HB	3:D:1030:GLU:HB3	1.90	0.52
6:N:-8:DG:N2	7:T:8:DA:H62	2.07	0.52
2:C:421:SER:OG	2:C:423:ASP:OD1	2.27	0.52
2:C:1157:GLN:HG2	2:C:1159:VAL:HG12	1.90	0.52
3:D:123:ARG:O	3:D:126:LEU:HB2	2.09	0.52
3:D:529:GLY:N	3:D:530:PRO:CA	2.70	0.52
3:D:1266:ILE:HA	3:D:1302:TYR:HA	1.90	0.52
2:C:1032:LYS:O	2:C:1036:ILE:HG12	2.09	0.52
2:C:1066:MET:HG2	2:C:1234:LYS:HG2	1.92	0.52
2:C:1115:THR:HB	2:C:1228:GLY:HA3	1.92	0.52
7:T:-14:DA:H2"	7:T:-13:DC:C6	2.45	0.52
1:A:64:VAL:HG21	1:A:78:ILE:HG13	1.91	0.52
6:N:-5:DT:H3	7:T:5:DC:H42	1.56	0.52
2:C:903:ARG:HA	2:C:908:GLU:HA	1.92	0.52
3:D:338:PHE:HA	3:D:342:LEU:HD22	1.90	0.52
3:D:826:ILE:HG21	3:D:831:VAL:HG23	1.92	0.52
3:D:921:GLN:O	3:D:925:GLU:HB3	2.09	0.52
3:D:836:ARG:NH2	3:D:866:GLU:OE1	2.43	0.52
3:D:1060:VAL:HA	3:D:1107:VAL:HB	1.92	0.52
1:A:92:VAL:HG22	1:A:94:GLY:N	2.21	0.51
2:C:582:ASN:HD22	2:C:586:PHE:HB2	1.75	0.51
3:D:918:ILE:O	3:D:922:SER:HB3	2.10	0.51
1:B:71:LYS:O	1:B:74:VAL:HG23	2.11	0.51
3:D:530:PRO:O	3:D:531:LYS:CB	2.57	0.51
2:C:138:ILE:HB	2:C:143:ARG:HD2	1.92	0.51
2:C:533:LEU:N	2:C:533:LEU:CD1	2.73	0.51
2:C:728:ASP:OD1	2:C:729:ALA:N	2.43	0.51
3:D:848:VAL:HG23	3:D:857:LEU:HB2	1.91	0.51
2:C:10:ARG:NH2	2:C:697:LYS:HD3	2.25	0.51
2:C:12:ARG:HG2	2:C:1181:PRO:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:555:TYR:O	3:D:556:GLU:HG3	2.10	0.51
5:M:213:LEU:HD13	5:M:252:LEU:HD22	1.91	0.51
1:A:81:ILE:HG12	1:A:131:CYS:HB3	1.92	0.51
1:A:228:LEU:HD11	1:B:224:LEU:HD22	1.92	0.51
2:C:221:LEU:HD21	2:C:336:LEU:HD23	1.92	0.51
3:D:94:GLN:HA	3:D:94:GLN:NE2	2.25	0.51
3:D:364:HIS:O	3:D:364:HIS:ND1	2.44	0.51
5:M:275:UNK:CB	5:M:391:HIS:HB3	2.41	0.51
2:C:179:TYR:OH	2:C:462:ASN:OD1	2.28	0.51
2:C:887:VAL:HB	2:C:913:VAL:HG12	1.91	0.51
3:D:973:LEU:H	3:D:1006:GLY:HA2	1.76	0.51
5:M:264:UNK:O	5:M:266:UNK:N	2.44	0.51
5:M:137:ASP:O	5:M:141:ALA:HB2	2.10	0.51
6:N:-2:DA:C2	7:T:2:DG:C2	2.93	0.51
1:B:182:ARG:HG2	1:B:206:GLU:HB3	1.92	0.51
1:A:33:ARG:NH2	1:A:197:ASP:OD1	2.44	0.51
2:C:533:LEU:CD1	2:C:533:LEU:H	2.23	0.51
2:C:933:VAL:HG22	2:C:1050:VAL:HG13	1.92	0.51
2:C:1246:ARG:NH2	2:C:1249:GLY:H	2.08	0.51
3:D:34:SER:HB3	3:D:103:GLY:H	1.75	0.50
3:D:226:ALA:O	3:D:230:SER:CB	2.59	0.50
3:D:535:ARG:NH1	3:D:535:ARG:CB	2.73	0.50
3:D:987:GLU:HG3	3:D:988:PHE:H	1.76	0.50
5:M:458:VAL:O	5:M:462:ARG:CB	2.60	0.50
2:C:528:ARG:NH1	2:C:576:SER:O	2.45	0.50
2:C:592:ARG:NH2	2:C:601:ASP:OD1	2.43	0.50
3:D:113:HIS:O	3:D:115:TRP:N	2.42	0.50
2:C:1:MET:C	2:C:3:TYR:H	2.19	0.50
2:C:1223:ARG:HH21	3:D:719:PHE:HB3	1.77	0.50
2:C:1254:VAL:HG12	2:C:1255:THR:HG23	1.94	0.50
3:D:61:ILE:HG22	3:D:62:PHE:N	2.25	0.50
3:D:916:GLY:HA2	3:D:919:ALA:HB3	1.91	0.50
6:N:13:DG:H2"	6:N:14:DT:C7	2.34	0.50
2:C:346:TYR:C	2:C:348:SER:H	2.20	0.50
2:C:402:ARG:NH2	2:C:419:ILE:O	2.44	0.50
2:C:622:ASN:HD21	2:C:631:GLU:HB2	1.77	0.50
2:C:828:PHE:HB2	2:C:1234:LYS:HD2	1.93	0.50
2:C:1244:HIS:CE1	2:C:1265:PHE:HA	2.47	0.50
6:N:12:DT:H2"	6:N:13:DG:N7	2.27	0.50
1:A:58:GLU:HG2	1:A:172:LEU:HG	1.93	0.50
1:A:91:ARG:HG2	1:A:210:THR:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:175:ARG:NH2	2:C:185:ASP:OD2	2.45	0.50
3:D:816:THR:HG21	3:D:888:CYS:CB	2.41	0.50
3:D:1168:GLU:CB	3:D:1178:THR:N	2.70	0.50
4:E:20:VAL:O	4:E:24:ALA:HB2	2.12	0.50
2:C:887:VAL:HB	2:C:913:VAL:CG1	2.42	0.50
3:D:120:LEU:N	3:D:121:PRO:CA	2.75	0.50
3:D:522:GLY:O	3:D:523:GLU:HB2	2.11	0.50
3:D:1101:LEU:H	3:D:1196:LEU:HB3	1.76	0.50
2:C:310:ILE:O	2:C:311:CYS:CB	2.50	0.50
2:C:675:ASP:OD1	2:C:676:ALA:N	2.44	0.50
2:C:817:LEU:HD21	2:C:1080:ASN:HD22	1.77	0.50
3:D:272:VAL:HG21	3:D:306:LEU:HD11	1.93	0.49
2:C:186:PHE:HD2	2:C:432:LEU:HD13	1.76	0.49
3:D:164:GLN:O	3:D:168:ALA:CB	2.60	0.49
3:D:455:ALA:O	3:D:458:ASN:ND2	2.44	0.49
3:D:1080:ILE:HB	3:D:1097:ALA:HA	1.93	0.49
3:D:918:ILE:O	3:D:922:SER:CB	2.60	0.49
1:A:53:GLY:O	1:A:148:ARG:HA	2.12	0.49
1:B:16:ILE:HD11	1:B:24:ALA:HB1	1.94	0.49
2:C:337:PHE:CD2	2:C:339:ASN:HB2	2.47	0.49
3:D:1174:ARG:H	3:D:1192:LYS:HB3	1.77	0.49
5:M:290:UNK:CB	5:M:345:ARG:CB	2.90	0.49
1:B:118:ASP:OD1	1:B:119:GLY:N	2.46	0.49
2:C:39:ILE:O	2:C:40:GLU:HG2	2.12	0.49
3:D:186:GLN:O	3:D:190:LYS:HB2	2.13	0.49
4:E:5:THR:HG22	4:E:7:GLN:H	1.77	0.49
1:A:104:LYS:HD3	1:A:110:VAL:HG22	1.94	0.49
2:C:343:HIS:HA	2:C:437:ASN:ND2	2.27	0.49
2:C:1064:ASP:OD2	2:C:1076:ILE:HG13	2.13	0.49
3:D:110:PRO:O	3:D:111:THR:HG22	2.12	0.49
1:A:217:ILE:O	1:A:221:ALA:CB	2.61	0.49
2:C:516:ASP:OD2	2:C:522:SER:OG	2.31	0.49
3:D:142:GLU:HG2	3:D:143:SER:N	2.28	0.49
1:A:6:THR:HB	1:B:150:ARG:HH12	1.78	0.48
2:C:95:PRO:HA	2:C:126:GLU:HG2	1.95	0.48
3:D:226:ALA:O	3:D:230:SER:OG	2.30	0.48
5:M:210:THR:HB	5:M:213:LEU:HB2	1.95	0.48
1:B:55:ALA:HB3	1:B:175:ALA:HB1	1.95	0.48
1:B:188:GLU:HB2	1:B:200:LYS:HB2	1.95	0.48
2:C:384:LEU:O	2:C:388:LEU:CB	2.55	0.48
3:D:118:LYS:C	3:D:122:SER:HA	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:723:TYR:O	3:D:727:ASP:CB	2.61	0.48
1:B:159:ILE:C	1:B:161:SER:H	2.20	0.48
1:B:219:ARG:O	1:B:222:THR:OG1	2.23	0.48
2:C:308:GLU:C	2:C:309:LEU:CD1	2.85	0.48
2:C:533:LEU:HD12	2:C:533:LEU:H	1.77	0.48
3:D:528:THR:OG1	3:D:551:ARG:NH1	2.46	0.48
1:B:14:VAL:HG12	1:B:28:LEU:HG	1.96	0.48
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.49	0.48
3:D:309:ASN:CB	3:D:324:LEU:CB	2.89	0.48
1:B:29:GLU:HB2	1:B:200:LYS:HG2	1.96	0.48
2:C:522:SER:O	2:C:526:HIS:CB	2.60	0.48
3:D:1159:ILE:HA	3:D:1205:GLU:HA	1.96	0.48
6:N:-3:DA:H2	7:T:3:DG:H22	1.54	0.48
1:A:118:ASP:OD1	1:A:119:GLY:N	2.47	0.48
1:A:218:ARG:NH2	1:B:231:PHE:O	2.46	0.48
2:C:1006:GLU:O	2:C:1010:GLN:CB	2.61	0.48
3:D:351:GLY:HA3	3:D:372:MET:HE3	1.96	0.48
2:C:1247:SER:HB3	3:D:375:GLU:HG2	1.96	0.47
3:D:1342:ASP:C	3:D:1344:LEU:H	2.21	0.47
3:D:1362:GLY:O	3:D:1366:HIS:ND1	2.44	0.47
3:D:591:ILE:HD11	3:D:604:MET:HA	1.95	0.47
3:D:1184:ASP:O	3:D:1186:TYR:N	2.47	0.47
2:C:120:GLN:HG2	2:C:121:GLU:N	2.30	0.47
3:D:523:GLU:HG2	3:D:546:ALA:HB1	1.95	0.47
3:D:641:ILE:O	3:D:764:ARG:NH1	2.40	0.47
6:N:-1:DG:N2	7:T:1:DA:H2	2.13	0.47
2:C:159:SER:C	2:C:161:LYS:H	2.21	0.47
2:C:802:VAL:HA	2:C:1096:ILE:O	2.14	0.47
2:C:1067:ALA:O	2:C:1233:LEU:HB2	2.13	0.47
3:D:478:LEU:HB2	4:E:20:VAL:HG13	1.96	0.47
3:D:902:ASP:OD1	3:D:906:GLY:HA2	2.15	0.47
1:B:219:ARG:O	1:B:223:ILE:HD12	2.14	0.47
2:C:817:LEU:O	2:C:1096:ILE:HG13	2.14	0.47
2:C:1065:LYS:HG2	2:C:1235:LEU:HD12	1.96	0.47
2:C:1281:TYR:OH	3:D:434:ILE:O	2.29	0.47
5:M:213:LEU:O	5:M:217:ARG:CB	2.63	0.47
1:A:39:LEU:O	1:A:43:LEU:HB2	2.14	0.47
2:C:93:SER:HA	2:C:128:PRO:HA	1.96	0.47
2:C:500:ALA:O	2:C:504:GLU:CB	2.62	0.47
3:D:361:LEU:O	3:D:450:HIS:ND1	2.48	0.47
3:D:527:LEU:HD13	3:D:532:GLU:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:10:VAL:HG21	4:E:16:ARG:HE	1.79	0.47
6:N:12:DT:H2"	6:N:13:DG:C8	2.49	0.47
2:C:148:GLN:HE22	2:C:536:GLY:H	1.63	0.47
3:D:381:ILE:HD13	3:D:415:VAL:HG21	1.96	0.47
3:D:805:GLN:HB2	3:D:1347:LEU:HD23	1.96	0.47
5:M:155:THR:C	5:M:156:ILE:HG13	2.40	0.47
1:A:46:ILE:HG22	1:A:220:ALA:HB1	1.97	0.47
2:C:594:VAL:HG22	2:C:599:VAL:HG13	1.97	0.47
3:D:369:PRO:HG2	3:D:372:MET:HB3	1.97	0.47
4:E:19:LEU:O	4:E:23:ALA:HB3	2.15	0.47
6:N:-1:DG:H22	7:T:1:DA:H2	1.61	0.47
2:C:309:LEU:N	2:C:309:LEU:CD1	2.78	0.47
2:C:758:ARG:HD2	2:C:835:GLU:HB2	1.97	0.47
2:C:64:GLY:C	2:C:66:SER:H	2.22	0.46
2:C:228:VAL:HG22	2:C:229:ILE:H	1.79	0.46
3:D:107:LEU:HD22	3:D:299:LEU:HD21	1.97	0.46
3:D:417:ARG:HG3	3:D:418:GLU:HG3	1.96	0.46
3:D:850:LYS:HB3	3:D:851:PRO:HD2	1.97	0.46
2:C:781:ASP:OD1	2:C:782:VAL:N	2.49	0.46
2:C:796:LEU:N	2:C:1231:TYR:OH	2.48	0.46
3:D:1154:ALA:HB3	3:D:1215:GLU:HA	1.95	0.46
2:C:733:VAL:HG12	2:C:750:ILE:HA	1.97	0.46
2:C:832:HIS:O	2:C:1055:ALA:HA	2.15	0.46
2:C:1070:HIS:NE2	2:C:1114:GLU:OE1	2.48	0.46
3:D:399:LYS:HA	3:D:402:GLU:OE2	2.15	0.46
3:D:420:PRO:HA	3:D:439:PRO:HD3	1.98	0.46
1:A:41:ASN:ND2	2:C:1216:ARG:O	2.49	0.46
2:C:174:ALA:O	2:C:185:ASP:HA	2.14	0.46
2:C:174:ALA:HB3	2:C:432:LEU:HD12	1.98	0.46
2:C:395:TYR:CE2	2:C:420:LEU:HG	2.50	0.46
3:D:528:THR:O	3:D:528:THR:HG23	2.14	0.46
5:M:344:SER:O	5:M:348:VAL:CB	2.63	0.46
3:D:1206:ARG:NE	3:D:1223:LEU:O	2.46	0.46
1:A:182:ARG:HH22	2:C:1090:ASN:HB3	1.81	0.46
1:B:190:ALA:HB3	1:B:198:LEU:HB2	1.97	0.46
2:C:310:ILE:C	2:C:310:ILE:CD1	2.86	0.46
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.50	0.46
2:C:1299:ASN:ND2	2:C:1303:LYS:HE2	2.31	0.46
3:D:36:GLY:H	3:D:104:HIS:CE1	2.34	0.46
2:C:964:LEU:O	2:C:968:GLU:HB2	2.16	0.46
2:C:799:ASN:HA	2:C:1230:MET:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1161:LEU:O	2:C:1162:SER:OG	2.25	0.46
3:D:110:PRO:C	3:D:111:THR:CG2	2.85	0.46
3:D:121:PRO:HB2	3:D:122:SER:OG	2.16	0.46
3:D:127:LEU:HD11	3:D:224:LEU:HG	1.98	0.46
3:D:702:GLN:HE22	3:D:717:VAL:HA	1.81	0.46
3:D:450:HIS:HE1	3:D:625:MET:HE1	1.80	0.46
5:M:239:THR:HG23	5:M:241:LEU:H	1.80	0.46
2:C:379:GLU:O	2:C:383:SER:CB	2.63	0.45
3:D:112:ALA:O	3:D:113:HIS:CB	2.63	0.45
5:M:418:THR:O	5:M:422:ALA:CB	2.63	0.45
2:C:245:ARG:O	2:C:339:ASN:ND2	2.49	0.45
3:D:664:ILE:HG22	3:D:678:ARG:HG3	1.99	0.45
3:D:1308:GLY:C	3:D:1310:THR:H	2.25	0.45
3:D:1362:GLY:O	3:D:1365:TYR:HB3	2.16	0.45
1:B:215:GLU:O	1:B:219:ARG:HG3	2.16	0.45
2:C:705:GLU:HB3	2:C:794:LEU:H	1.82	0.45
3:D:411:ILE:O	3:D:415:VAL:HG23	2.16	0.45
6:N:-7:DA:N1	7:T:7:DG:C2	2.84	0.45
2:C:580:GLN:NE2	2:C:588:GLU:OE1	2.34	0.45
2:C:1064:ASP:OD1	2:C:1066:MET:HG3	2.17	0.45
3:D:62:PHE:CE1	3:D:102:MET:HA	2.51	0.45
3:D:883:ARG:HB3	3:D:898:CYS:SG	2.55	0.45
3:D:1308:GLY:O	3:D:1310:THR:N	2.49	0.45
1:B:59:VAL:HG22	1:B:144:ILE:HD12	1.98	0.45
2:C:1:MET:O	2:C:2:VAL:HG22	2.17	0.45
2:C:148:GLN:NE2	2:C:535:PRO:HD2	2.32	0.45
3:D:19:ALA:HB1	3:D:1343:GLU:H	1.80	0.45
3:D:370:LYS:HB2	3:D:409:TRP:CZ3	2.51	0.45
3:D:966:VAL:HG21	3:D:976:THR:HG23	1.99	0.45
3:D:1136:GLY:HA2	3:D:1240:VAL:HG22	1.98	0.45
3:D:1236:GLU:O	3:D:1240:VAL:HG23	2.16	0.45
2:C:97:ARG:HB3	2:C:121:GLU:HB3	1.99	0.45
2:C:321:LEU:HG	2:C:325:LEU:HD23	1.99	0.45
2:C:975:ILE:HA	2:C:978:VAL:HG12	1.98	0.45
3:D:226:ALA:O	3:D:230:SER:HB3	2.16	0.45
3:D:845:ALA:HB2	3:D:883:ARG:HG3	1.98	0.45
5:M:223:HIS:O	5:M:224:LEU:HG	2.16	0.45
3:D:517:CYS:N	3:D:544:LEU:O	2.50	0.45
3:D:845:ALA:HB3	3:D:881:LYS:HG3	1.98	0.45
2:C:582:ASN:N	2:C:586:PHE:O	2.36	0.45
2:C:670:PHE:HB3	2:C:673:HIS:HD2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:700:VAL:HG22	2:C:1117:LEU:HD22	1.98	0.45
3:D:639:VAL:HG12	3:D:640:GLY:N	2.32	0.45
2:C:25:PRO:HG2	2:C:27:LEU:HD12	1.98	0.45
2:C:207:THR:OG1	2:C:354:ASP:OD2	2.33	0.45
2:C:257:ALA:HA	2:C:285:ILE:HG21	1.99	0.45
2:C:1327:LEU:O	2:C:1331:ARG:HB2	2.16	0.45
3:D:128:LEU:HD22	3:D:189:LEU:HD13	1.99	0.45
2:C:662:SER:O	2:C:666:SER:OG	2.27	0.45
2:C:757:THR:HB	2:C:765:ILE:HD11	1.99	0.45
3:D:35:PHE:HA	3:D:104:HIS:CE1	2.52	0.45
3:D:308:ASP:OD1	3:D:328:ALA:HB2	2.17	0.45
3:D:1208:ASP:O	3:D:1224:ARG:NH2	2.50	0.45
2:C:8:LYS:HA	2:C:11:ILE:HD11	2.00	0.44
2:C:186:PHE:HA	2:C:195:PHE:O	2.17	0.44
2:C:889:PRO:HA	2:C:913:VAL:HG22	1.99	0.44
2:C:1262:LYS:HA	2:C:1266:GLY:H	1.83	0.44
1:B:57:THR:HB	1:B:147:GLN:HG2	1.99	0.44
1:A:10:LYS:HE3	1:B:229:GLU:HG2	1.99	0.44
2:C:931:VAL:HG22	2:C:1052:VAL:HG22	1.99	0.44
2:C:1024:GLU:HG3	2:C:1028:LYS:NZ	2.32	0.44
3:D:1040:MET:HG2	3:D:1061:VAL:HG13	1.99	0.44
2:C:204:LEU:HD23	2:C:208:ILE:HD11	1.98	0.44
2:C:1154:ASP:C	2:C:1156:ARG:H	2.25	0.44
2:C:1279:GLU:OE1	3:D:1347:LEU:HD21	2.18	0.44
3:D:545:HIS:O	3:D:546:ALA:HB3	2.17	0.44
2:C:480:SER:O	2:C:481:LEU:HG	2.18	0.44
2:C:864:LYS:HG3	2:C:865:LEU:HD12	1.99	0.44
3:D:72:CYS:CB	3:D:85:CYS:SG	3.06	0.44
3:D:1081:VAL:HA	3:D:1088:VAL:HB	2.00	0.44
2:C:157:PHE:HA	2:C:173:ASN:O	2.18	0.44
3:D:1268:ASN:HB3	3:D:1300:ALA:HB3	2.00	0.44
1:B:29:GLU:OE1	1:B:200:LYS:NZ	2.35	0.44
3:D:907:HIS:HD1	3:D:908:ILE:C	2.26	0.44
3:D:1135:THR:HA	3:D:1140:ARG:HG2	2.00	0.44
6:N:8:DA:C8	6:N:9:DT:H72	2.53	0.44
2:C:401:GLY:O	2:C:405:PHE:HB2	2.18	0.44
2:C:496:LYS:HB2	2:C:497:PRO:HD3	2.00	0.44
2:C:592:ARG:HD2	2:C:655:VAL:HG22	2.00	0.44
2:C:1153:ALA:O	2:C:1155:VAL:HG13	2.18	0.44
3:D:535:ARG:CZ	3:D:535:ARG:HB3	2.48	0.44
3:D:822:MET:HB3	3:D:880:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1221:LEU:HB2	3:D:1229:VAL:HG21	2.00	0.44
5:M:282:UNK:N	5:M:285:UNK:O	2.50	0.44
2:C:619:ALA:HB1	2:C:657:THR:HG22	1.99	0.44
2:C:895:LEU:O	2:C:896:THR:OG1	2.27	0.44
2:C:1065:LYS:HA	2:C:1074:GLY:O	2.17	0.44
2:C:1269:ARG:HH12	3:D:343:LEU:HD21	1.82	0.44
3:D:118:LYS:CB	3:D:122:SER:CB	2.86	0.44
3:D:639:VAL:HG12	3:D:640:GLY:H	1.83	0.44
5:M:356:GLU:O	5:M:357:GLN:C	2.44	0.44
2:C:677:ASN:OD1	2:C:678:ARG:N	2.51	0.43
3:D:1332:LEU:O	3:D:1336:ALA:HB2	2.17	0.43
1:B:96:ASP:OD1	1:B:97:GLU:N	2.50	0.43
1:B:99:ILE:HG13	1:B:145:LYS:HG3	2.00	0.43
2:C:230:PHE:N	2:C:333:ILE:O	2.51	0.43
2:C:619:ALA:HA	2:C:654:ASP:HB2	1.99	0.43
2:C:882:ILE:HG12	2:C:919:ARG:HB3	2.00	0.43
3:D:127:LEU:HD13	3:D:223:LEU:HD12	2.00	0.43
5:M:194:ASP:C	5:M:196:ARG:H	2.27	0.43
7:T:10:DC:H3'	7:T:10:DC:P	2.58	0.43
2:C:149:LEU:HD21	2:C:451:ARG:HH12	1.83	0.43
3:D:117:LEU:O	3:D:124:ILE:N	2.49	0.43
3:D:841:GLY:HA3	3:D:901:ARG:HB2	1.99	0.43
3:D:1164:SER:O	3:D:1199:PHE:HA	2.18	0.43
6:N:-1:DG:O6	7:T:1:DA:N1	2.51	0.43
2:C:370:MET:HE2	2:C:388:LEU:HD11	1.99	0.43
2:C:1253:LEU:HG	5:M:116:THR:HB	1.99	0.43
3:D:810:THR:HG23	3:D:811:GLU:N	2.34	0.43
2:C:632:ASP:OD1	2:C:633:LEU:N	2.51	0.43
5:M:121:GLN:O	5:M:125:MET:CB	2.67	0.43
1:A:217:ILE:O	1:A:221:ALA:HB2	2.18	0.43
1:B:37:HIS:CG	2:C:1216:ARG:HD2	2.53	0.43
1:B:186:ASN:HB3	1:B:202:VAL:HB	2.00	0.43
2:C:725:GLN:HB3	2:C:733:VAL:HG23	2.01	0.43
2:C:802:VAL:HG22	2:C:1096:ILE:HG23	2.00	0.43
2:C:833:ILE:HA	2:C:1054:LEU:O	2.19	0.43
3:D:421:VAL:HG23	3:D:470:VAL:HG22	2.00	0.43
3:D:811:GLU:HG2	3:D:812:ASP:H	1.84	0.43
1:B:46:ILE:HD11	1:B:224:LEU:HD12	2.01	0.43
1:B:109:PRO:HA	1:B:132:HIS:HA	1.99	0.43
2:C:800:MET:HE1	2:C:828:PHE:HE2	1.84	0.43
2:C:1063:GLY:HA3	2:C:1239:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:343:LEU:HD23	3:D:344:GLY:N	2.34	0.43
2:C:53:PHE:CE2	2:C:73:TYR:HB3	2.52	0.43
2:C:909:LYS:C	2:C:911:SER:H	2.26	0.43
3:D:127:LEU:HD13	3:D:223:LEU:HB2	2.00	0.43
3:D:480:ALA:O	3:D:485:MET:HG2	2.18	0.43
3:D:1183:SER:OG	3:D:1184:ASP:N	2.51	0.43
5:M:215:GLU:O	5:M:219:ILE:HD12	2.19	0.43
2:C:10:ARG:NE	2:C:791:LEU:HD12	2.34	0.43
2:C:685:MET:HE1	2:C:1073:LYS:NZ	2.34	0.43
2:C:735:LYS:HA	2:C:748:ILE:HG22	2.00	0.43
3:D:224:LEU:O	3:D:228:VAL:HG23	2.19	0.43
3:D:348:ASP:O	3:D:349:TYR:HB2	2.19	0.43
3:D:557:LYS:HE2	3:D:611:ILE:HG23	2.01	0.43
3:D:625:MET:HG3	3:D:629:PHE:HE2	1.83	0.43
3:D:628:GLY:O	3:D:632:ALA:CB	2.67	0.43
2:C:681:MET:O	2:C:685:MET:HG2	2.19	0.43
2:C:1244:HIS:NE2	2:C:1246:ARG:HB2	2.34	0.43
3:D:544:LEU:N	3:D:544:LEU:CD1	2.73	0.43
3:D:827:GLU:HB2	3:D:832:LYS:HG3	2.01	0.43
2:C:81:ASP:OD1	2:C:82:VAL:N	2.44	0.42
2:C:204:LEU:HD11	2:C:369:MET:HG2	2.01	0.42
3:D:135:ILE:HA	3:D:138:VAL:HG22	2.00	0.42
2:C:164:THR:HG23	2:C:165:HIS:H	1.84	0.42
2:C:165:HIS:HD2	2:C:167:SER:HB2	1.84	0.42
2:C:187:GLU:OE2	2:C:197:ARG:NH1	2.38	0.42
2:C:1304:MET:O	2:C:1308:ILE:HG12	2.19	0.42
1:A:45:ARG:HH12	2:C:1084:ASP:HB3	1.83	0.42
1:B:65:LEU:HB3	1:B:169:GLY:HA3	2.01	0.42
2:C:46:GLN:HG2	2:C:47:TYR:CD2	2.53	0.42
3:D:64:PRO:HB3	3:D:69:GLU:H	1.84	0.42
3:D:548:VAL:O	3:D:549:LYS:C	2.59	0.42
3:D:746:LEU:HD13	3:D:754:ILE:HG21	2.02	0.42
3:D:937:ILE:HD12	3:D:939:GLY:N	2.33	0.42
1:A:67:GLU:HB3	1:A:171:LEU:HD22	2.01	0.42
2:C:184:LEU:HG	2:C:198:ILE:HG12	2.01	0.42
3:D:128:LEU:O	3:D:129:ASP:HB3	2.19	0.42
3:D:984:LEU:HD22	3:D:993:GLU:HB3	2.01	0.42
3:D:1355:ARG:HH12	3:D:1366:HIS:HD2	1.63	0.42
5:M:156:ILE:HD12	5:M:157:GLN:H	1.83	0.42
1:A:112:ALA:HB2	1:A:128:HIS:HB3	2.00	0.42
2:C:831:ILE:HD12	2:C:1057:LYS:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:246:PRO:HB2	3:D:249:LEU:HD13	2.01	0.42
3:D:1137:GLY:O	3:D:1141:VAL:HG23	2.20	0.42
7:T:9:DT:C2'	7:T:10:DC:H5'	2.48	0.42
7:T:11:DG:H2''	7:T:12:DT:C6	2.54	0.42
1:A:51:MET:HB2	1:A:178:SER:HB2	2.01	0.42
1:B:77:ASP:OD1	1:B:78:ILE:N	2.52	0.42
2:C:389:PHE:CG	2:C:390:PHE:N	2.87	0.42
3:D:102:MET:HB3	3:D:244:VAL:O	2.20	0.42
3:D:115:TRP:CG	3:D:115:TRP:O	2.70	0.42
3:D:481:ARG:NH2	4:E:3:ARG:HB2	2.34	0.42
3:D:528:THR:C	3:D:530:PRO:CA	2.85	0.42
3:D:1231:ARG:O	3:D:1235:ASN:HB2	2.20	0.42
5:M:142:THR:HA	5:M:145:VAL:HG22	2.00	0.42
1:A:44:ARG:HD2	1:A:185:TYR:HE1	1.85	0.42
1:A:86:LYS:NZ	1:A:176:CYS:SG	2.73	0.42
2:C:1254:VAL:O	2:C:1255:THR:OG1	2.32	0.42
3:D:347:VAL:HG21	3:D:350:SER:OG	2.19	0.42
3:D:1238:GLN:O	3:D:1242:ARG:HG3	2.20	0.42
1:B:56:VAL:HA	1:B:146:VAL:HG12	2.02	0.42
5:M:178:VAL:O	5:M:182:ILE:HG12	2.20	0.42
6:N:-5:DT:C5	6:N:-4:DA:C6	3.08	0.42
2:C:164:THR:HG23	2:C:165:HIS:N	2.35	0.42
2:C:172:TYR:HD2	2:C:436:ARG:HA	1.85	0.42
3:D:119:SER:N	3:D:122:SER:CA	2.73	0.42
3:D:689:ALA:HA	3:D:692:ARG:HE	1.85	0.42
5:M:275:UNK:CB	5:M:391:HIS:CB	2.98	0.42
2:C:124:MET:HA	2:C:495:ALA:HB2	2.02	0.41
3:D:272:VAL:HG22	3:D:302:ALA:HB1	2.01	0.41
3:D:505:ASP:HB2	3:D:629:PHE:CE1	2.55	0.41
6:N:13:DG:C2'	6:N:14:DT:C7	2.92	0.41
2:C:308:GLU:C	2:C:309:LEU:HD13	2.44	0.41
2:C:1122:LYS:HB3	2:C:1229:TYR:CE2	2.55	0.41
3:D:94:GLN:HA	3:D:94:GLN:HE21	1.83	0.41
3:D:112:ALA:HB1	3:D:303:VAL:HB	2.01	0.41
1:A:29:GLU:HB2	1:A:30:PRO:HD3	2.03	0.41
2:C:74:ARG:HG2	2:C:75:LEU:N	2.34	0.41
3:D:552:ILE:HB	3:D:570:LYS:NZ	2.35	0.41
1:B:5:VAL:C	1:B:7:GLU:H	2.28	0.41
1:B:25:LYS:HA	1:B:203:ILE:O	2.20	0.41
1:B:209:GLY:C	1:B:210:THR:HG1	2.23	0.41
3:D:35:PHE:HA	3:D:104:HIS:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:397:ALA:O	3:D:401:VAL:HG23	2.20	0.41
3:D:828:GLY:HA2	3:D:994:SER:O	2.21	0.41
3:D:959:LYS:HB2	3:D:983:LYS:HB2	2.02	0.41
2:C:519:ASN:ND2	2:C:521:LEU:HB2	2.35	0.41
3:D:950:ILE:HB	3:D:1018:ALA:HB3	2.02	0.41
3:D:1156:LEU:HD22	3:D:1224:ARG:NH2	2.35	0.41
1:A:152:TYR:CE2	1:A:154:PRO:HG3	2.55	0.41
2:C:698:PRO:HG3	2:C:1231:TYR:CE1	2.55	0.41
3:D:94:GLN:C	3:D:95:THR:HG1	2.28	0.41
3:D:481:ARG:HH12	4:E:51:LEU:HD22	1.86	0.41
3:D:1278:GLU:HG2	3:D:1279:GLN:H	1.85	0.41
5:M:469:PRO:HA	5:M:470:SER:HA	1.81	0.41
1:A:42:ALA:HB1	1:A:224:LEU:HD11	2.03	0.41
2:C:1062:PRO:HA	2:C:1076:ILE:HB	2.02	0.41
3:D:704:GLU:H	3:D:718:SER:HG	1.63	0.41
3:D:786:THR:O	3:D:790:THR:OG1	2.25	0.41
3:D:810:THR:HG23	3:D:811:GLU:H	1.85	0.41
3:D:900:GLY:O	3:D:901:ARG:HB3	2.20	0.41
2:C:141:THR:CG2	2:C:514:PHE:HD1	2.29	0.41
2:C:808:ASN:H	3:D:633:ALA:CB	2.34	0.41
2:C:808:ASN:H	3:D:633:ALA:HB2	1.86	0.41
2:C:851:THR:C	2:C:853:ASP:H	2.29	0.41
3:D:980:THR:HB	3:D:997:VAL:HB	2.03	0.41
1:A:27:THR:HG22	1:A:202:VAL:HG23	2.02	0.41
1:A:103:ASN:HD22	1:A:141:SER:HA	1.86	0.41
3:D:250:ARG:HH22	3:D:266:ASN:HB2	1.86	0.41
3:D:275:ARG:HH11	3:D:298:MET:HB2	1.86	0.41
5:M:281:UNK:HA	5:M:286:UNK:HA	2.02	0.41
5:M:379:SER:O	5:M:383:ARG:CB	2.68	0.41
1:A:223:ILE:O	1:A:227:GLN:HG2	2.21	0.41
2:C:73:TYR:HD2	2:C:74:ARG:O	2.03	0.41
2:C:920:VAL:HG12	2:C:921:PRO:O	2.20	0.41
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.95	0.41
3:D:365:GLN:HA	3:D:438:GLU:O	2.21	0.41
3:D:34:SER:CB	3:D:103:GLY:H	2.34	0.40
3:D:929:GLN:OE1	3:D:929:GLN:N	2.54	0.40
1:B:86:LYS:HE2	1:B:174:ASP:HB2	2.03	0.40
2:C:271:ALA:HA	2:C:274:ILE:HD12	2.04	0.40
2:C:1273:MET:HG2	3:D:428:THR:OG1	2.20	0.40
6:N:-4:DA:C2	6:N:-3:DA:C6	3.08	0.40
6:N:7:DC:H2"	6:N:8:DA:C8	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1065:LYS:HD3	2:C:1237:HIS:HB2	2.03	0.40
2:C:1258:PRO:HG2	3:D:346:ARG:HB2	2.03	0.40
3:D:350:SER:HA	3:D:468:VAL:O	2.21	0.40
3:D:629:PHE:O	3:D:633:ALA:HB2	2.21	0.40
3:D:769:VAL:O	3:D:773:PHE:HB2	2.21	0.40
5:M:418:THR:O	5:M:422:ALA:HB3	2.22	0.40
1:B:183:ILE:HD12	1:B:204:GLU:O	2.21	0.40
2:C:698:PRO:HG3	2:C:1231:TYR:CZ	2.57	0.40
2:C:908:GLU:O	2:C:911:SER:N	2.54	0.40
3:D:112:ALA:CB	3:D:303:VAL:HB	2.52	0.40
3:D:263:SER:HB2	3:D:266:ASN:HB2	2.03	0.40
3:D:792:ASN:HA	3:D:795:TYR:HB3	2.03	0.40
3:D:1027:VAL:O	3:D:1121:LEU:HB3	2.21	0.40
1:A:90:VAL:HG23	1:A:123:ILE:HD13	2.04	0.40
2:C:228:VAL:HG13	2:C:229:ILE:N	2.37	0.40
2:C:636:CYS:HB3	2:C:645:PHE:HD2	1.87	0.40
2:C:832:HIS:CD2	2:C:1058:ARG:HD2	2.57	0.40
5:M:137:ASP:O	5:M:141:ALA:CB	2.69	0.40
5:M:156:ILE:HD12	5:M:157:GLN:N	2.35	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	231/329 (70%)	212 (92%)	16 (7%)	3 (1%)	9	41
1	B	233/329 (71%)	214 (92%)	19 (8%)	0	100	100
2	C	1339/1342 (100%)	1224 (91%)	105 (8%)	10 (1%)	18	55
3	D	1324/1407 (94%)	1151 (87%)	158 (12%)	15 (1%)	11	44
4	E	73/91 (80%)	68 (93%)	5 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	M	258/497 (52%)	220 (85%)	34 (13%)	4 (2%)	7	37
All	All	3458/3995 (87%)	3089 (89%)	337 (10%)	32 (1%)	16	49

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	ASP
2	C	2	VAL
2	C	313	ALA
2	C	347	ILE
3	D	122	SER
3	D	129	ASP
3	D	1309	ILE
2	C	308	GLU
2	C	311	CYS
2	C	1155	VAL
3	D	113	HIS
3	D	324	LEU
3	D	523	GLU
3	D	886	VAL
2	C	228	VAL
2	C	1264	GLN
3	D	95	THR
3	D	349	TYR
5	M	156	ILE
5	M	360	GLU
2	C	655	VAL
3	D	112	ALA
3	D	907	HIS
5	M	188	VAL
3	D	416	ILE
1	A	98	VAL
3	D	885	VAL
1	A	179	PRO
3	D	499	ILE
3	D	1134	ILE
2	C	933	VAL
5	M	170	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/286 (68%)	193 (100%)	0	100	100
1	B	182/286 (64%)	181 (100%)	1 (0%)	81	82
2	C	1038/1157 (90%)	1035 (100%)	3 (0%)	86	85
3	D	1048/1168 (90%)	1042 (99%)	6 (1%)	78	80
4	E	57/75 (76%)	57 (100%)	0	100	100
5	M	107/394 (27%)	107 (100%)	0	100	100
All	All	2625/3366 (78%)	2615 (100%)	10 (0%)	81	83

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

Mol	Chain	Res	Type
1	B	223	ILE
2	C	513	GLN
2	C	516	ASP
2	C	850	ILE
3	D	95	THR
3	D	119	SER
3	D	523	GLU
3	D	544	LEU
3	D	889	ASP
3	D	1049	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	132	HIS
1	B	194	GLN
1	B	227	GLN
2	C	133	ASN
2	C	148	GLN
2	C	165	HIS

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Mol	Chain	Res	Type
2	C	513	GLN
2	C	518	ASN
2	C	526	HIS
2	C	582	ASN
2	C	618	GLN
2	C	686	GLN
2	C	688	GLN
2	C	760	ASN
2	C	761	GLN
2	C	799	ASN
2	C	832	HIS
2	C	1017	GLN
2	C	1038	GLN
2	C	1072	ASN
2	C	1136	GLN
2	C	1256	GLN
2	C	1288	GLN
3	D	94	GLN
3	D	104	HIS
3	D	157	GLN
3	D	341	ASN
3	D	424	ASN
3	D	458	ASN
3	D	465	GLN
3	D	469	HIS
3	D	519	ASN
3	D	560	ASN
3	D	702	GLN
3	D	716	GLN
3	D	777	HIS
3	D	897	HIS
3	D	910	ASN
3	D	1023	HIS
3	D	1238	GLN
4	E	15	ASN
5	M	202	GLN
5	M	229	ASN
5	M	357	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](#)

There are no ligands in this entry.

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	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	514:THR	C	515:ARG	N	0.96

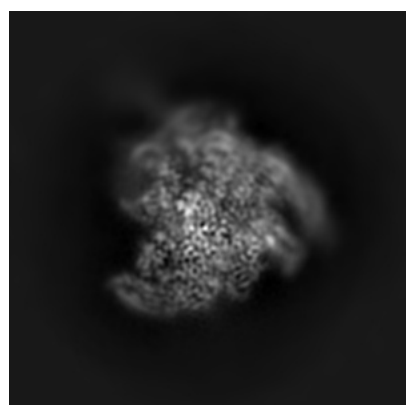
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0002. These allow visual inspection of the internal detail of the map and identification of artifacts.

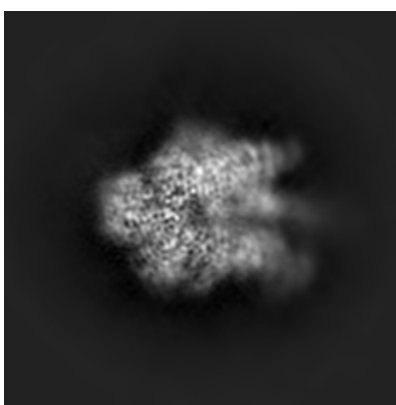
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

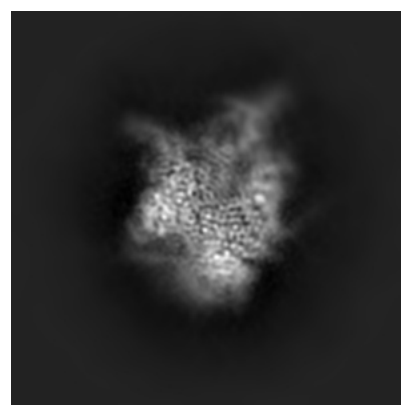
6.1.1 Primary map



X



Y

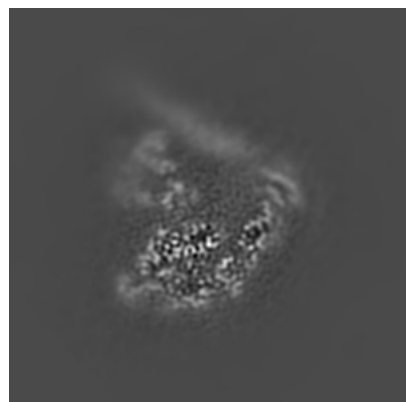


Z

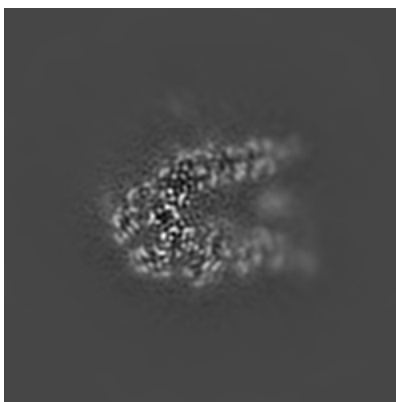
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

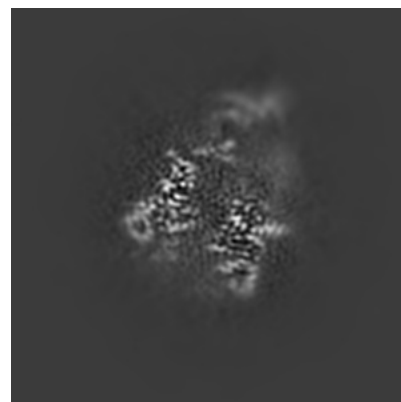
6.2.1 Primary map



X Index: 128



Y Index: 128

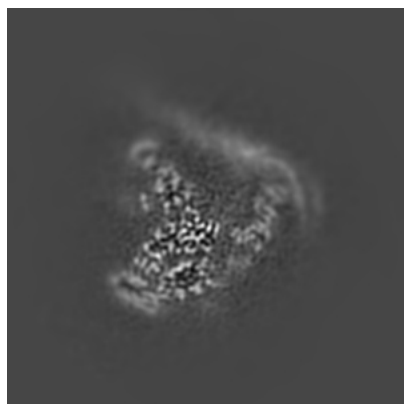


Z Index: 128

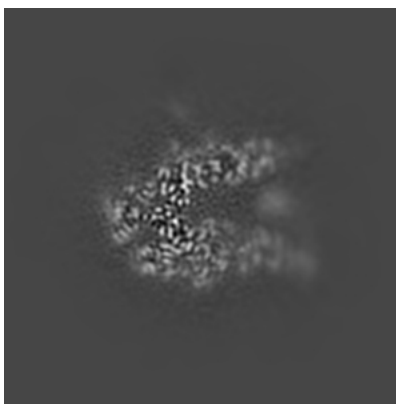
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

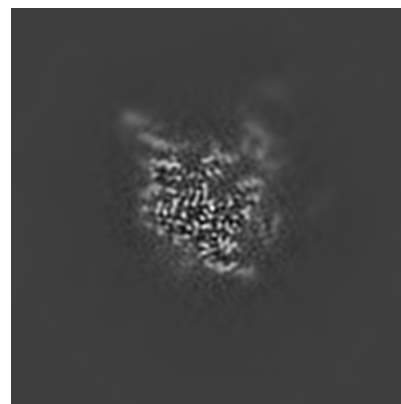
6.3.1 Primary map



X Index: 136



Y Index: 126

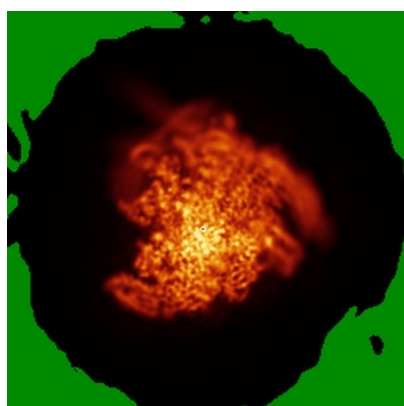


Z Index: 104

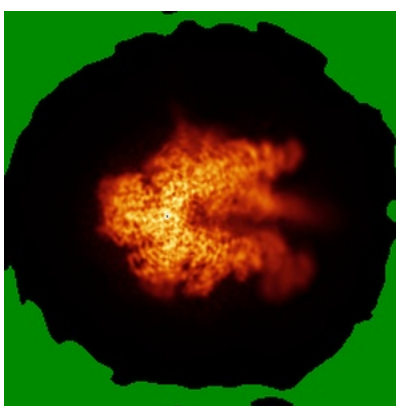
The images above show the largest variance slices of the map in three orthogonal directions.

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

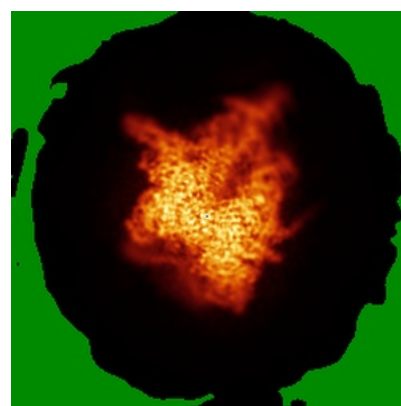
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

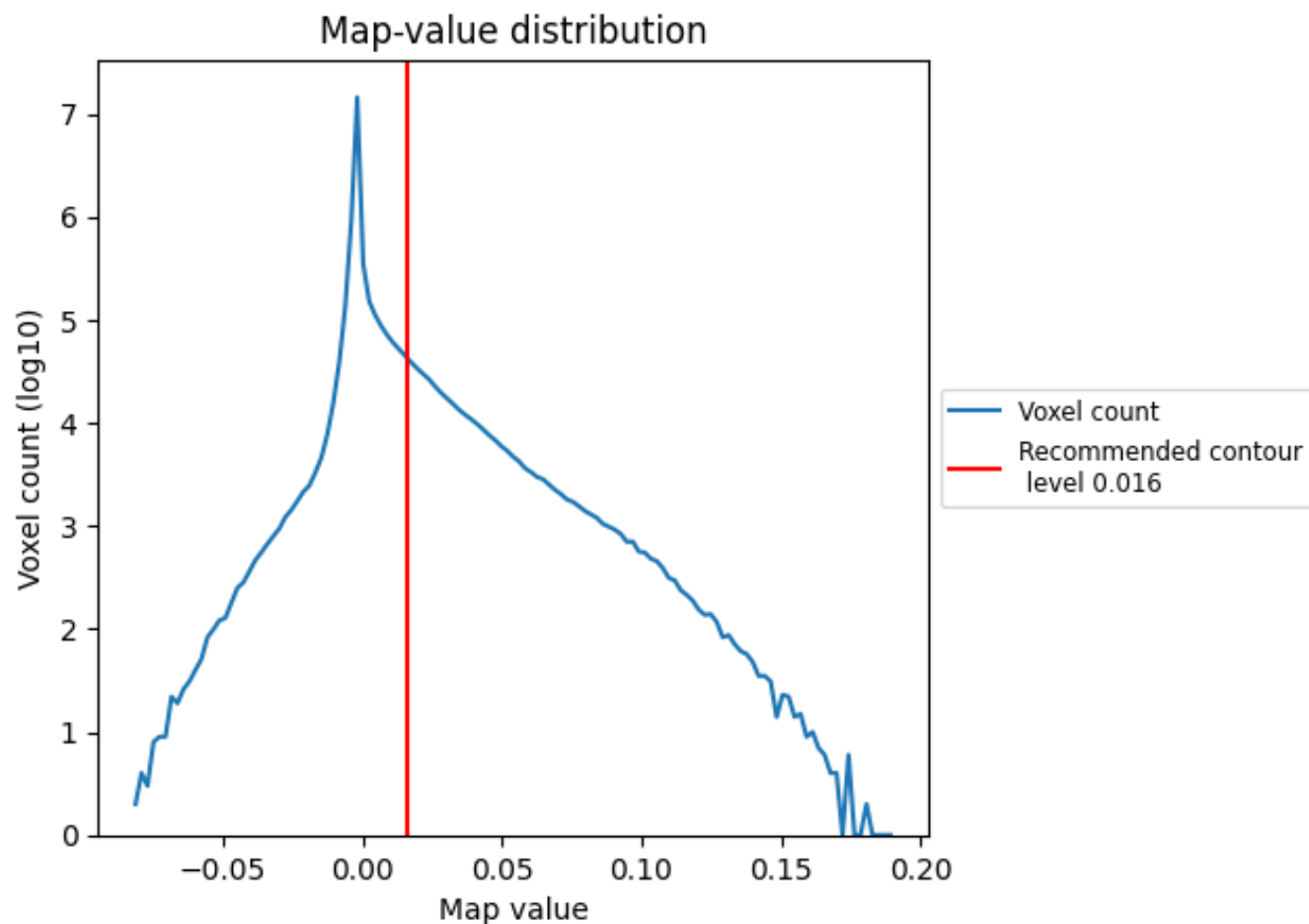
6.6 Mask visualisation

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

7 Map analysis [i](#)

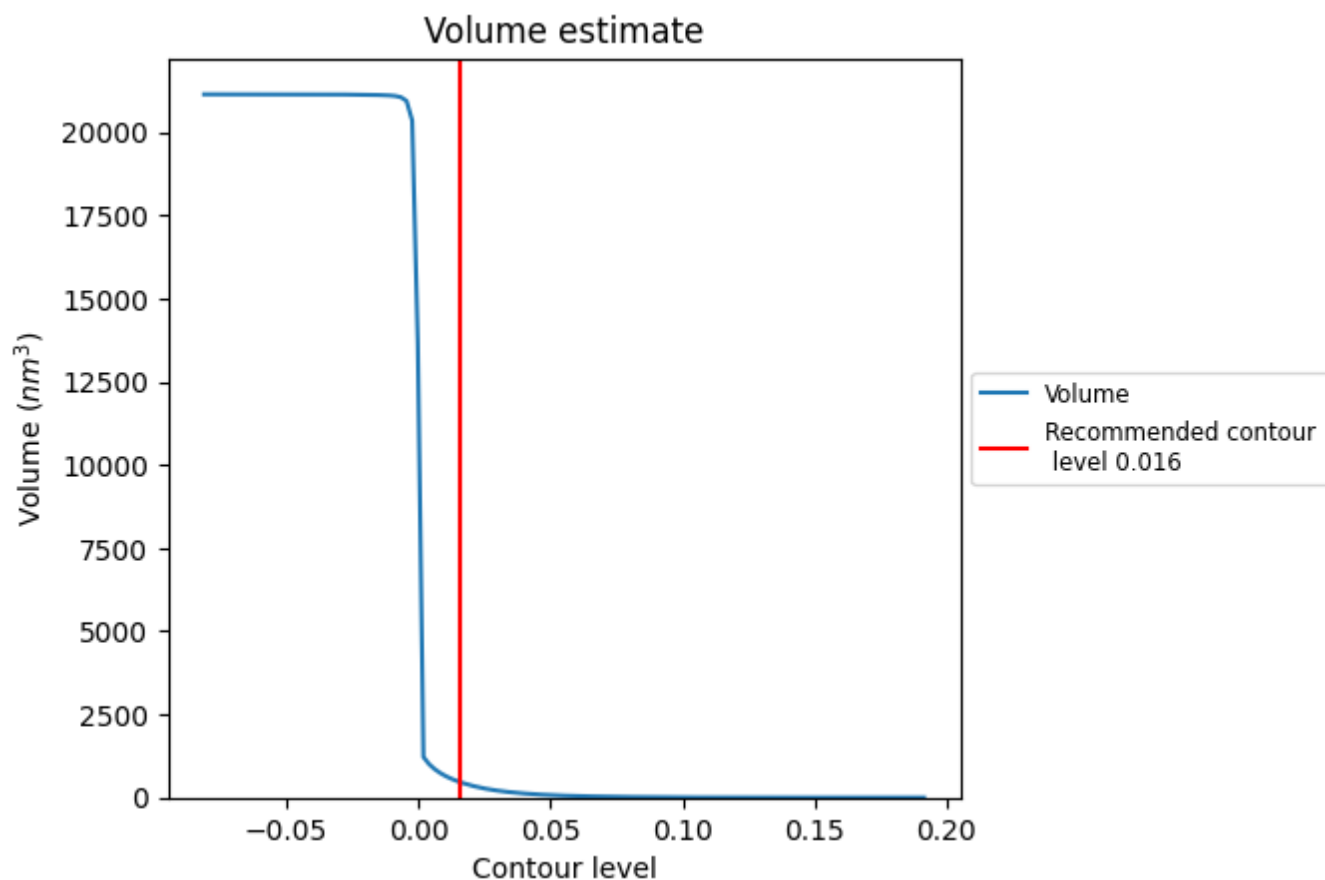
This section contains the results of statistical analysis of the map.

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.

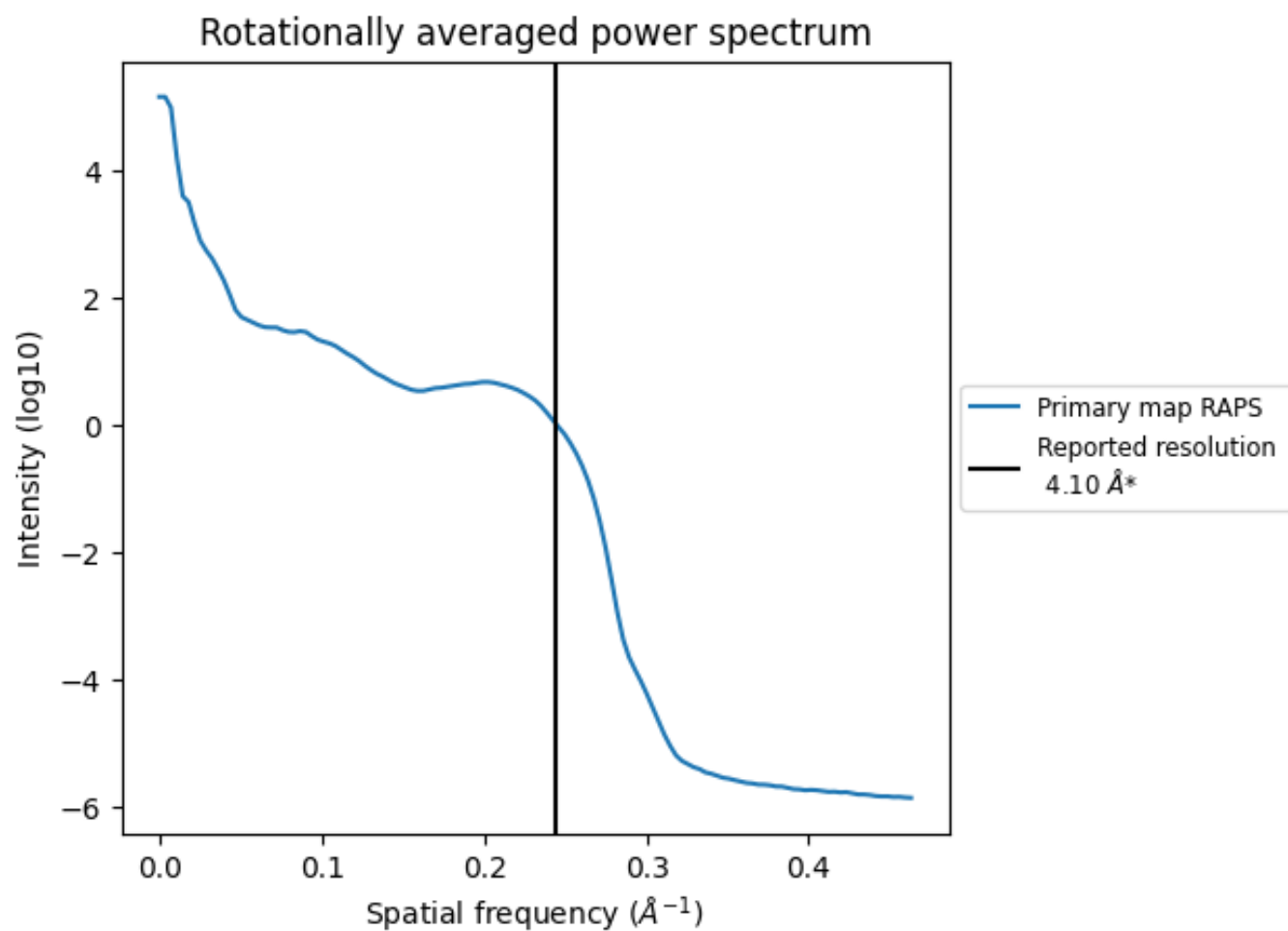
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 457 nm^3 ; this corresponds to an approximate mass of 413 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 0.244 Å⁻¹

8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0002 and PDB model 6GH6. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

This section was not generated.

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

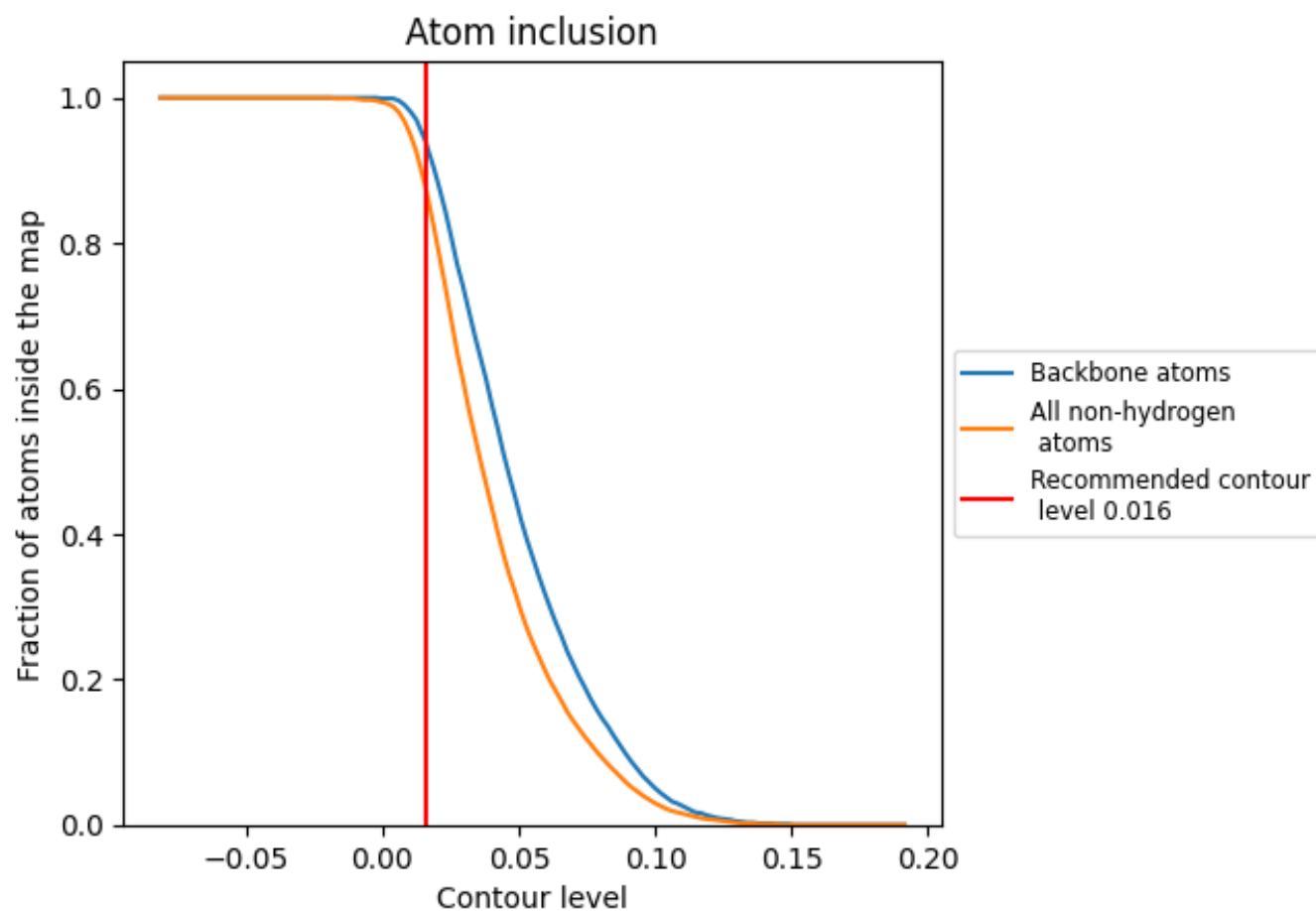


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 88% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8750	0.2880
A	0.9480	0.3880
B	0.9330	0.3330
C	0.9110	0.3370
D	0.8180	0.2560
E	0.8370	0.3230
M	0.9160	0.2220
N	0.8180	0.1160
T	0.8570	0.1200

