



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 11:58 AM UTC

PDB ID : 6HV9 / pdb_00006hv9
EMDB ID : EMD-0288
Title : S. cerevisiae CMG-Pol epsilon-DNA
Authors : Abid Ali, F.; Purkiss, A.G.; Cheung, A.; Costa, A.
Deposited on : 2018-10-10
Resolution : 4.98 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:

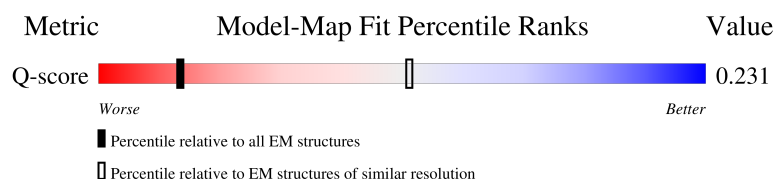
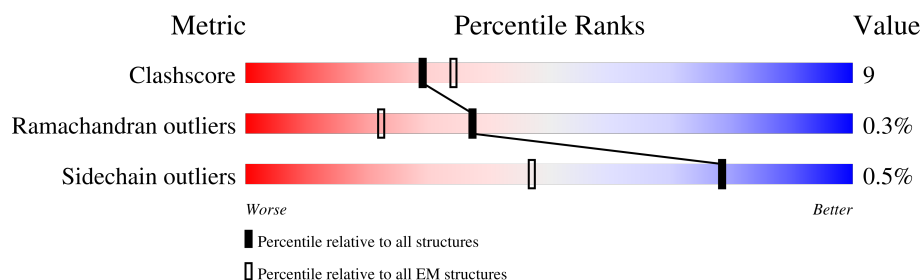
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 4.98 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	1031 (4.48 - 5.48)

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	3	971	5% 45% 12% 43%
2	4	933	16% 50% 13% 37%
3	5	775	13% 60% 20% 19%
4	6	1017	10% 43% 13% 44%

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Mol	Chain	Length	Quality of chain
5	2	868	
6	7	845	
7	C	208	
8	D	213	
9	E	194	
10	F	294	
11	G	650	
12	X	21	
13	Y	21	
14	J	7	
15	B	689	
16	A	914	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 47617 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 replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	558	Total	C	N	O	S	0	0
			4270	2689	753	818	10		

- Molecule 2 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	589	Total	C	N	O	S	0	0
			4543	2848	796	873	26		

- Molecule 3 is a protein called DNA replication licensing factor MCM5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	628	Total	C	N	O	S	0	0
			4690	2942	820	907	21		

- Molecule 4 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	571	Total	C	N	O	S	0	0
			4307	2704	766	821	16		

- Molecule 5 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	2	549	Total	C	N	O	S	0	0
			4184	2639	745	785	15		

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	616	Total	C	N	O	S	0	0
			4785	3024	820	916	25		

- Molecule 7 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	194	Total	C	N	O	S	0	0
			1492	934	265	287	6		

- Molecule 8 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	181	Total	C	N	O	S	0	0
			1461	935	257	265	4		

- Molecule 9 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	159	Total	C	N	O	S	0	0
			1262	824	207	226	5		

- Molecule 10 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	218	Total	C	N	O	S	0	0
			1743	1099	292	339	13		

- Molecule 11 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	541	Total	C	N	O	S	0	0
			4239	2684	737	808	10		

- Molecule 12 is a DNA chain called DNA (5'-D(*GP*CP*AP*GP*CP*CP*AP*CP*GP*CP*TP*GP*GP*CP*CP*GP*TP*TP*TP*TP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	21	Total	C	N	O	P	0	0
			425	203	76	126	20		

- Molecule 13 is a DNA chain called DNA (5'-D(P*TP*AP*AP*AP*AP*CP*GP*GP*CP*C*P*AP*GP*CP*GP*TP*GP*GP*CP*TP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Y	21	Total	C	N	O	P	0	0
			433	204	84	124	21		

- Molecule 14 is a DNA chain called DNA (5'-D(P*TP*TP*TP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	7	Total	C	N	O	P	0	0
			140	70	14	49	7		

- Molecule 15 is a protein called DNA polymerase epsilon subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	B	465	Total	C	N	O	S	0	0
			3661	2346	620	681	14		

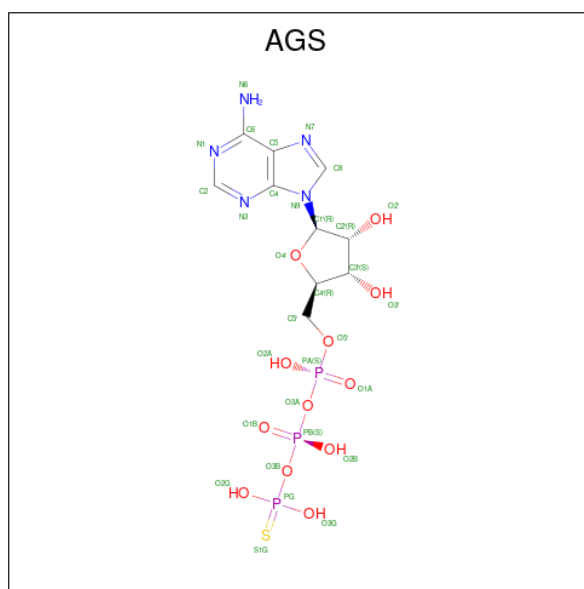
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	266	ASN	MET	conflict	UNP P24482

- Molecule 16 is a protein called DNA polymerase epsilon catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A	771	Total	C	N	O	S	0	0
			5918	3797	988	1101	32		

- Molecule 17 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						AltConf
17	5	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
17	5	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

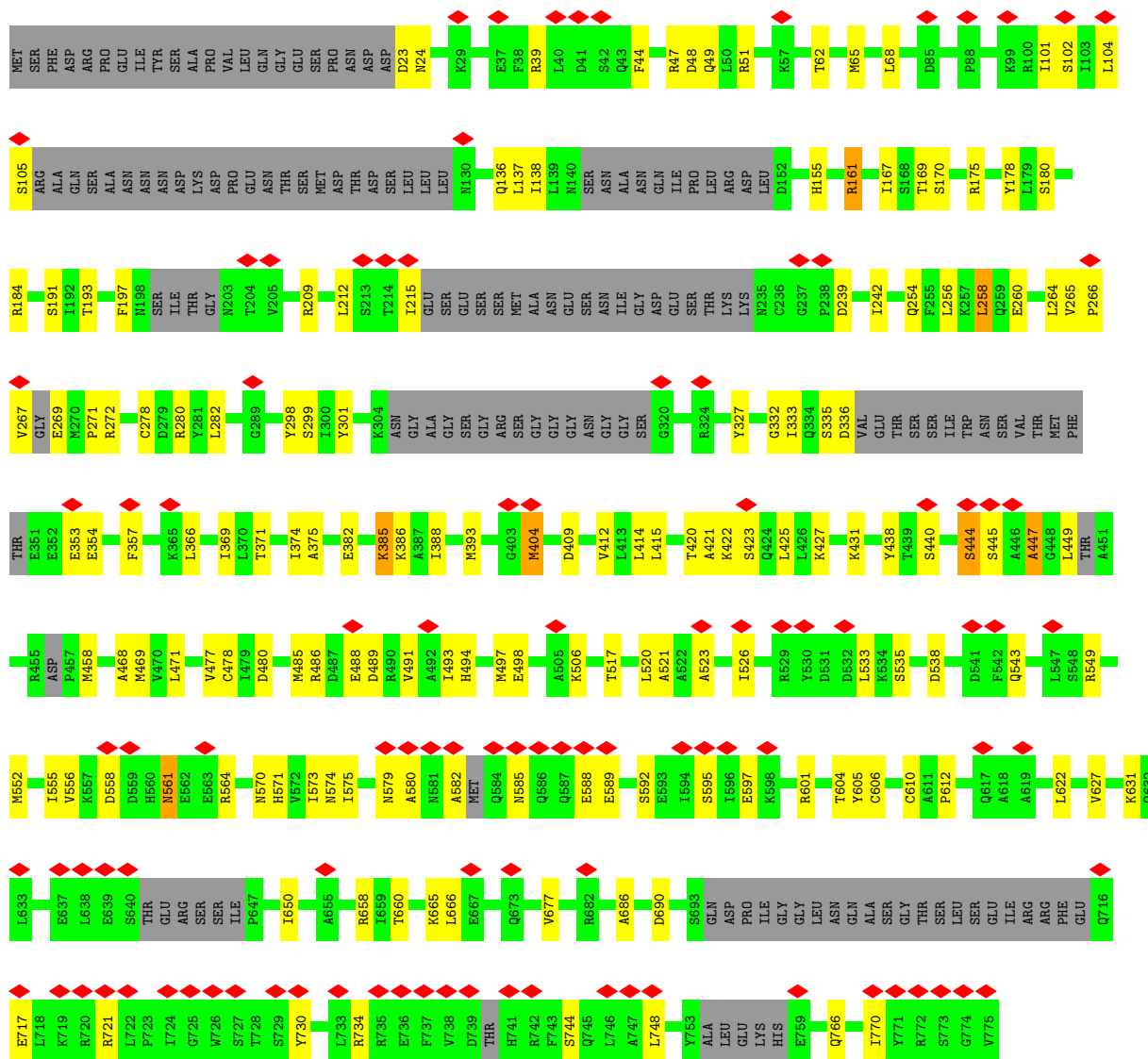
- Molecule 18 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
18	A	2	Total	Zn	0
			2	2	

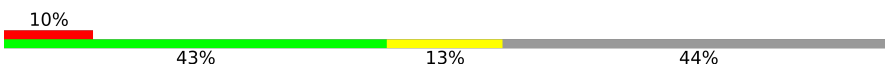
LEU
GLY
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SER
VAL
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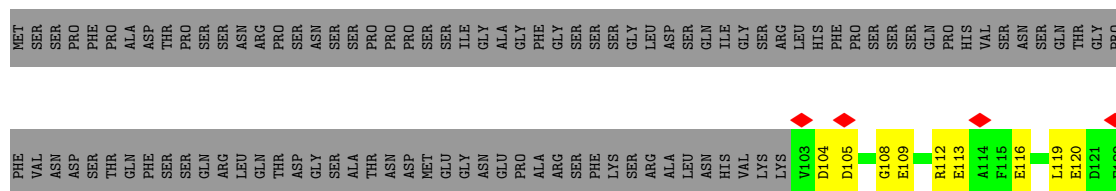
• Molecule 3: DNA replication licensing factor MCM5

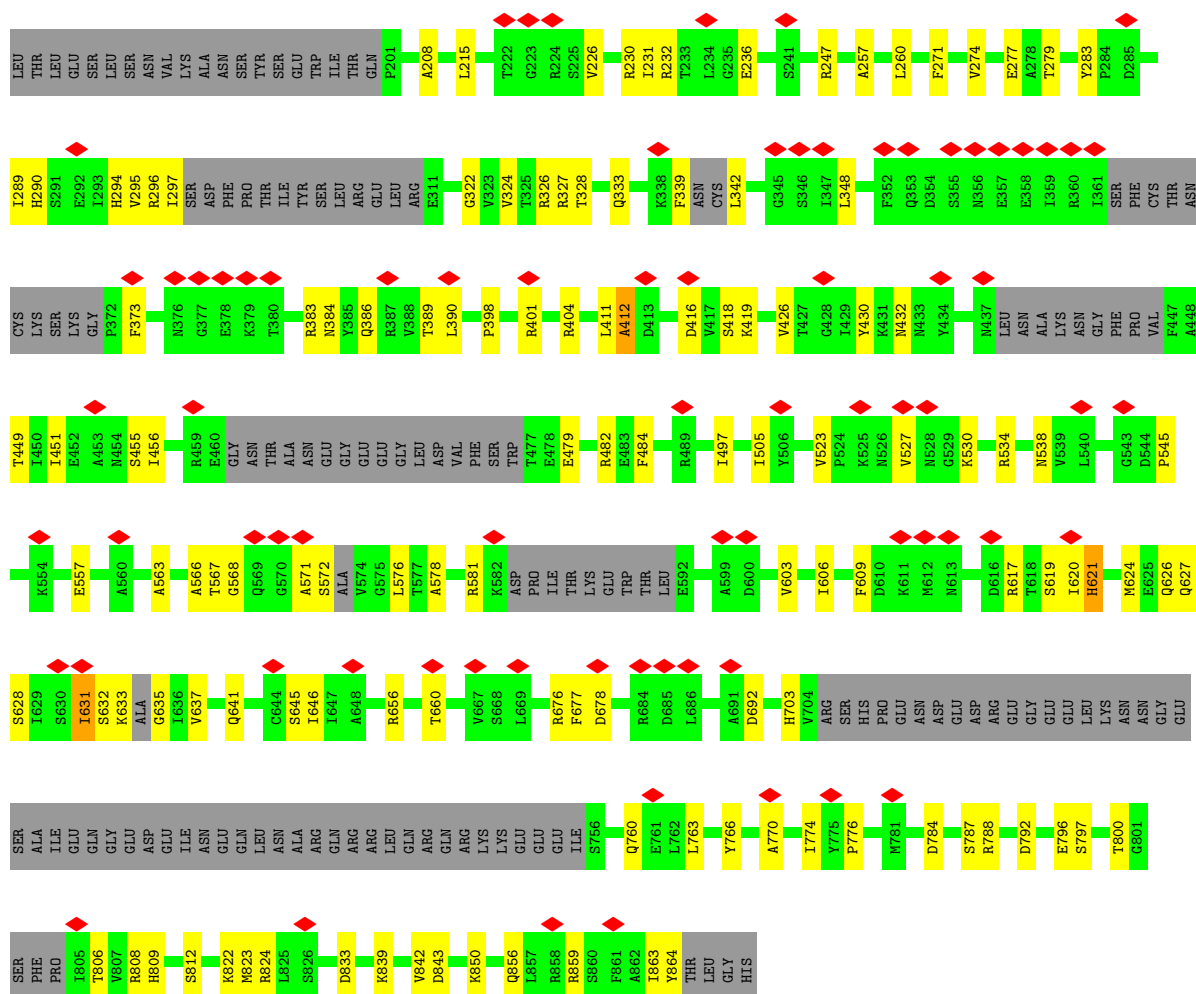
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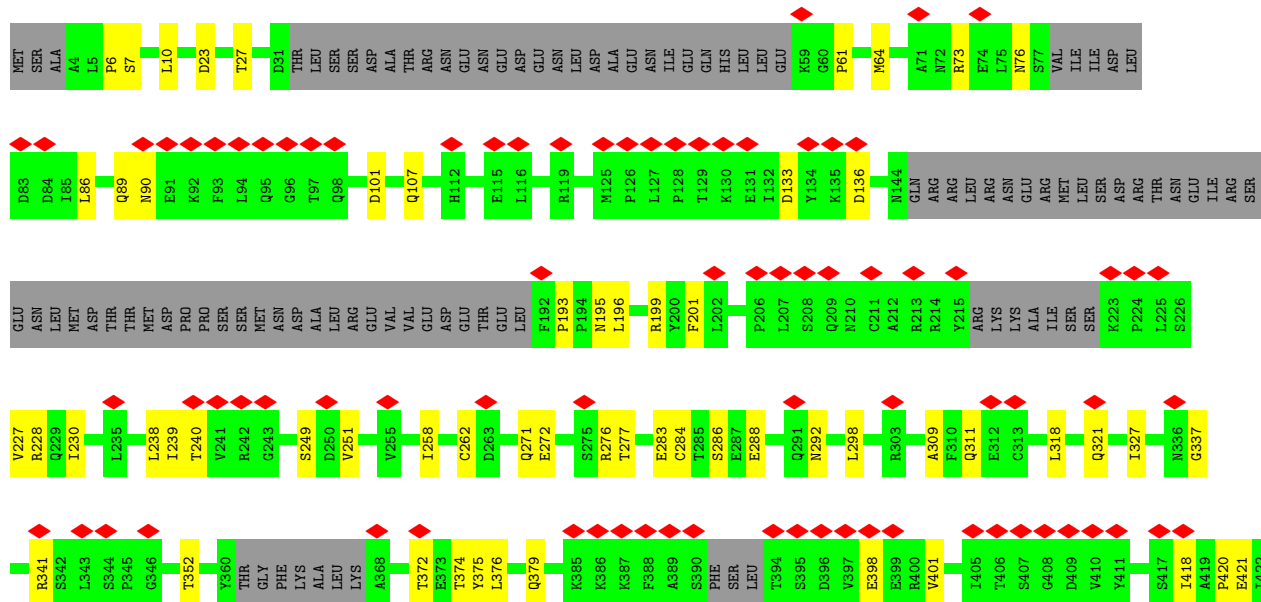
• Molecule 4: DNA replication licensing factor MCM6

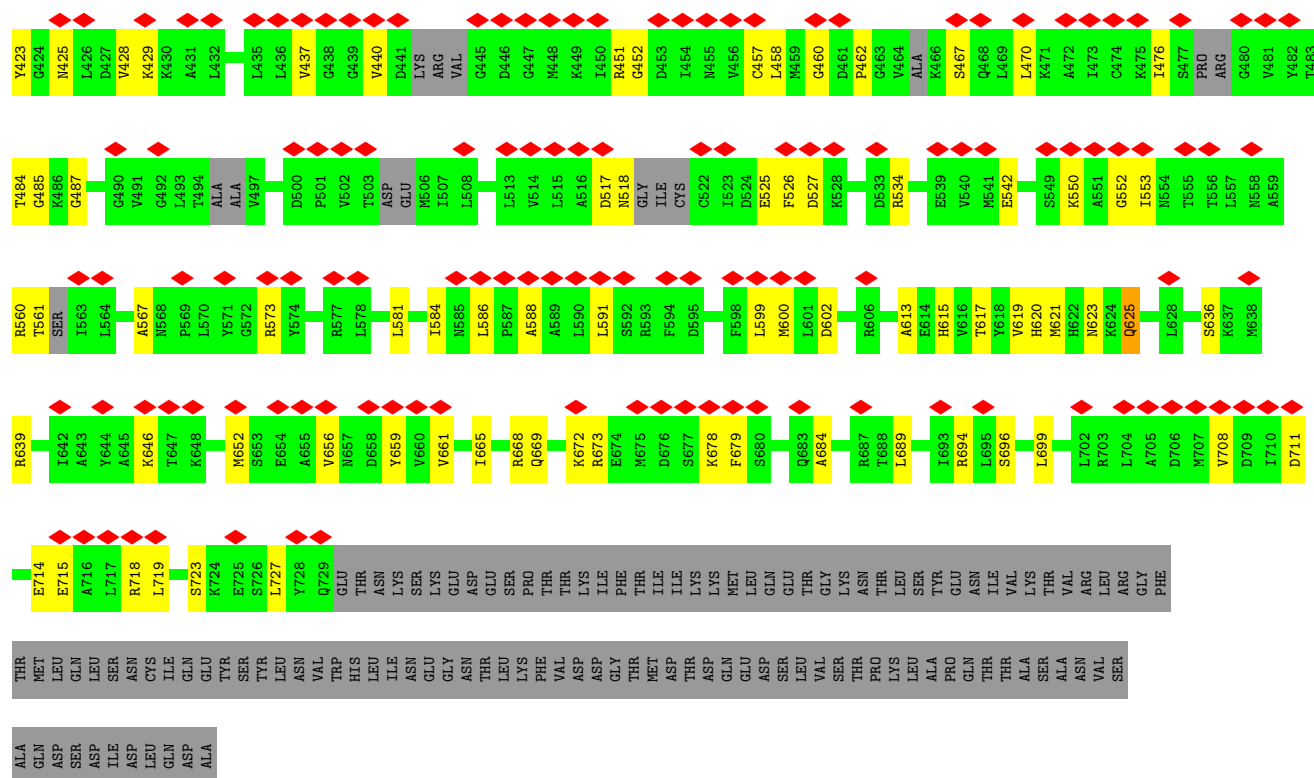
Chain 6: 



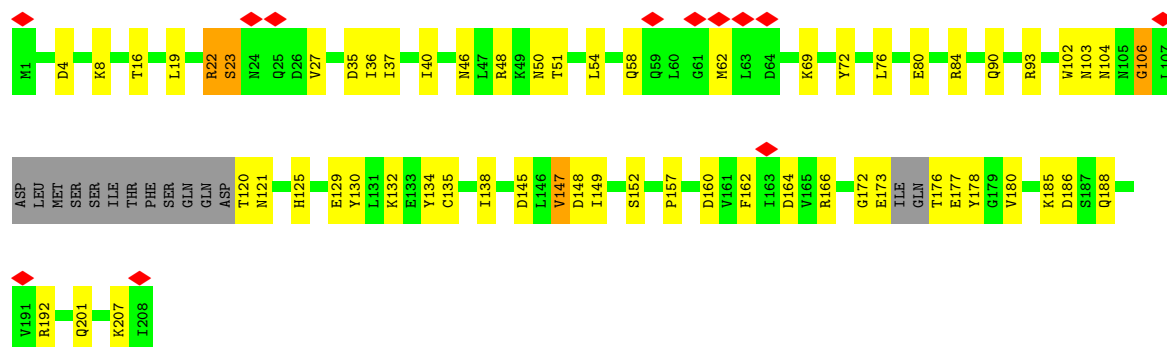


• Molecule 6: DNA replication licensing factor MCM7

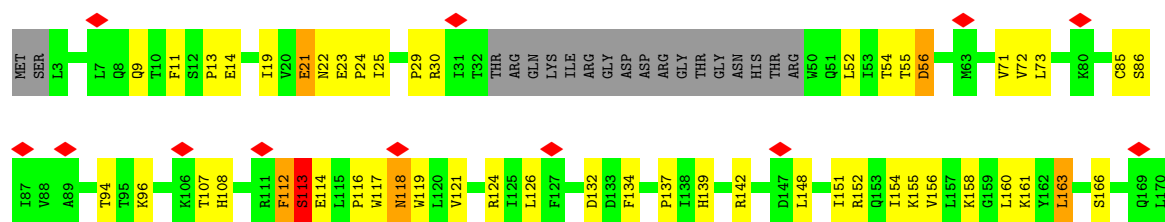


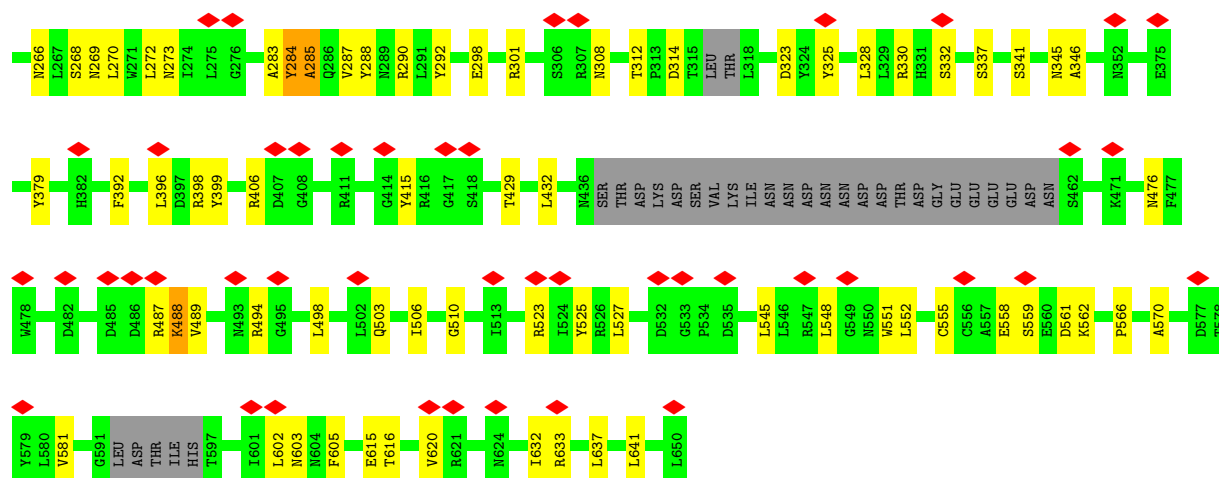


• Molecule 7: DNA replication complex GINS protein PSF1

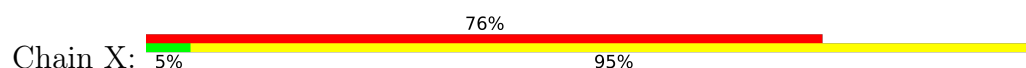


• Molecule 8: DNA replication complex GINS protein PSF2

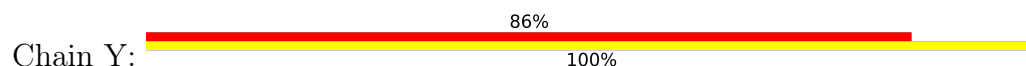




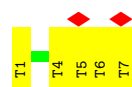
- Molecule 12: DNA (5'-D(*GP*CP*AP*GP*CP*CP*AP*CP*GP*CP*TP*GP*GP*CP*CP*GP*TP*TP*TP*TP*A)-3')



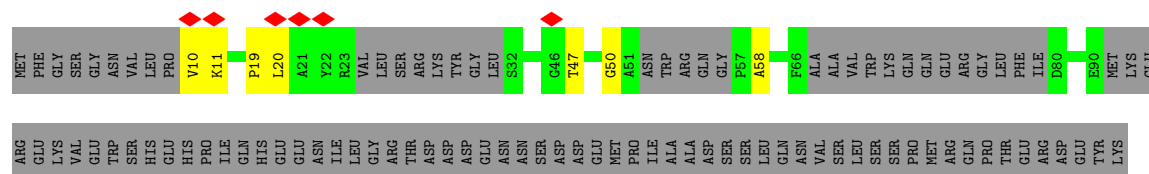
- Molecule 13: DNA (5'-D(P*TP*AP*AP*AP*AP*CP*GP*GP*CP*CP*AP*GP*CP*GP*TP*GP*GP*CP*TP*GP*C)-3')

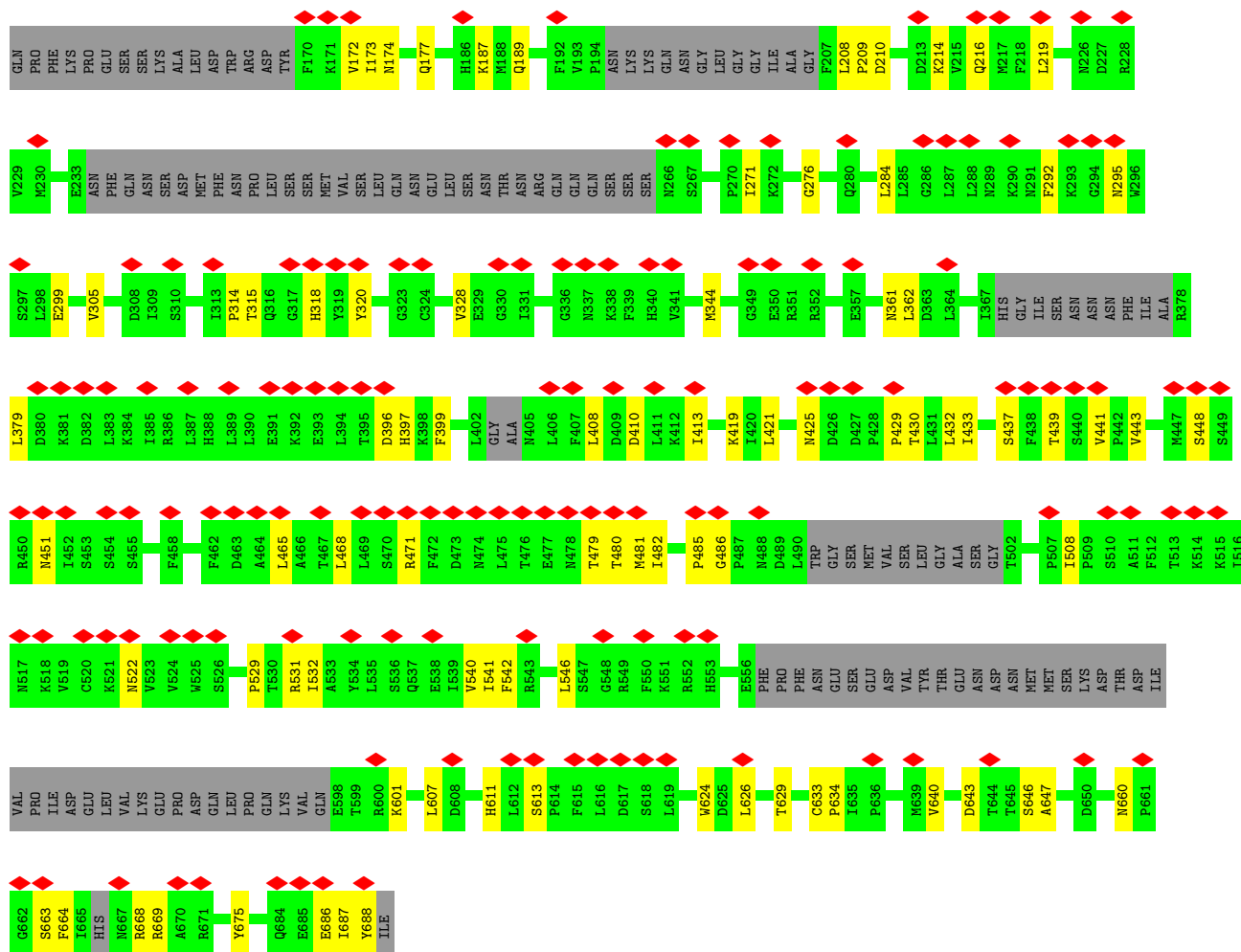


- Molecule 14: DNA (5'-D(P*TP*TP*TP*TP*TP*TP*T)-3')

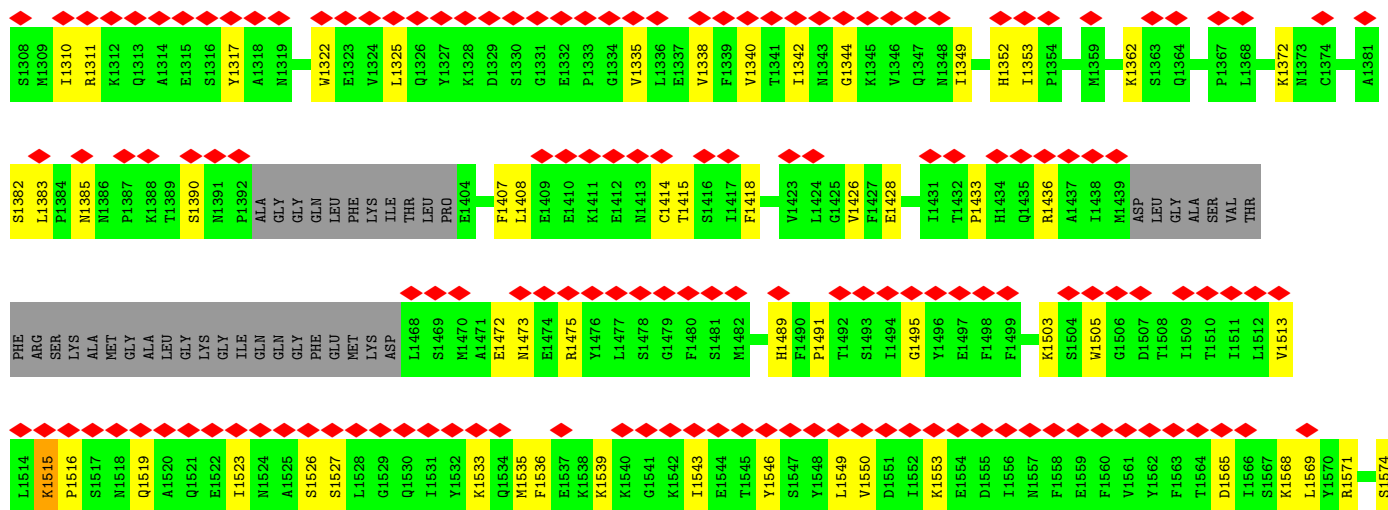
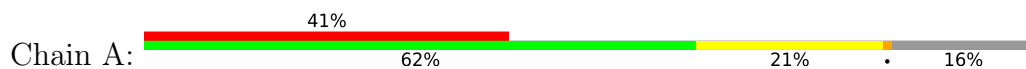


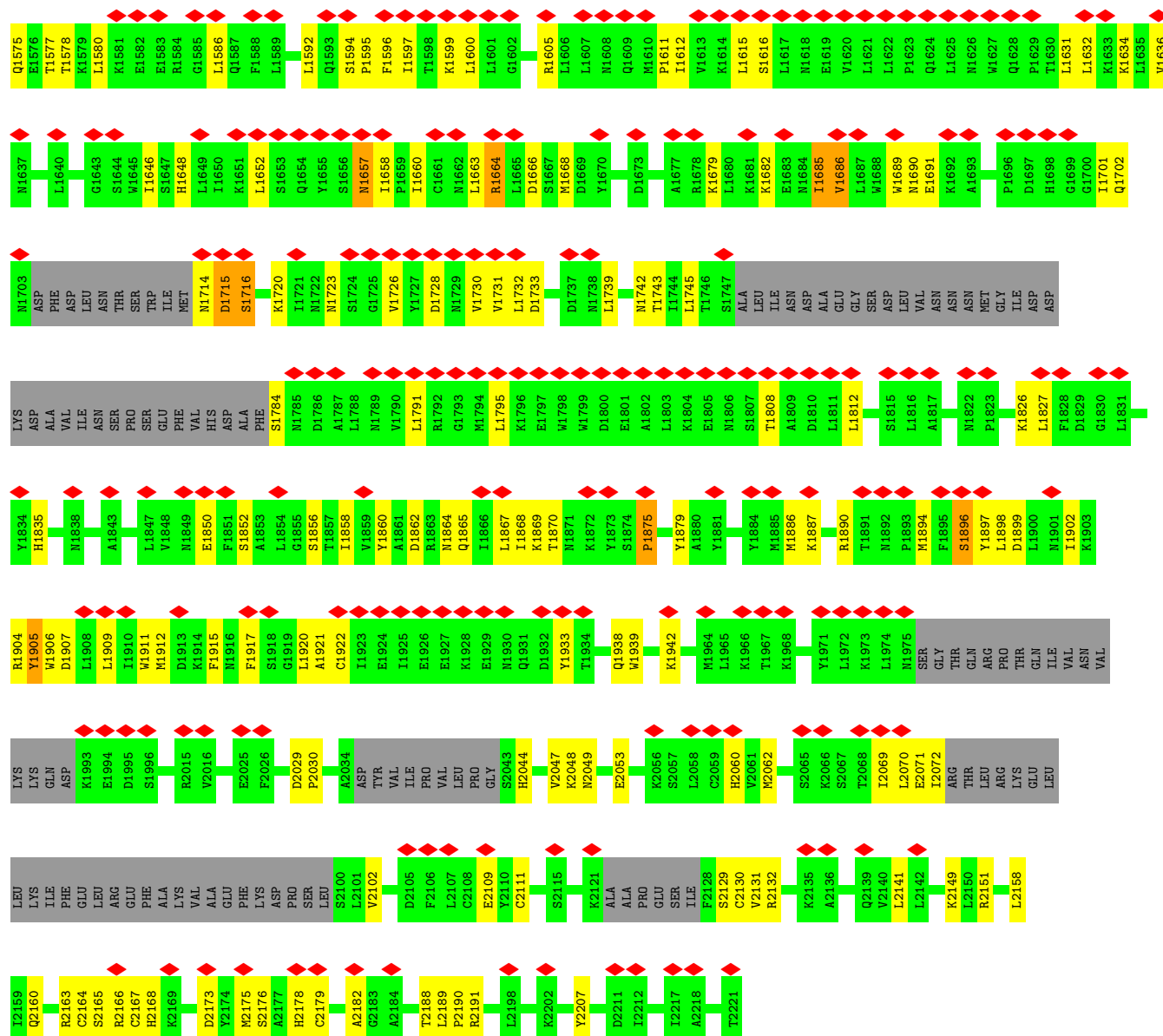
- Molecule 15: DNA polymerase epsilon subunit B





• Molecule 16: DNA polymerase epsilon catalytic subunit





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	78556	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 ($e^-/\text{\AA}^2$)	4.2	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	5.270	Depositor
Minimum map value	-2.822	Depositor
Average map value	0.035	Depositor
Map value standard deviation	0.184	Depositor
Recommended contour level	1.01	Depositor
Map size (Å)	353.28, 353.28, 353.28	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

5 Model quality

5.1 Standard geometry

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

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	3	0.60	0/4330	1.12	19/5872 (0.3%)
2	4	0.40	0/4594	0.89	6/6203 (0.1%)
3	5	0.75	0/4741	1.31	24/6405 (0.4%)
4	6	0.49	0/4359	0.97	3/5882 (0.1%)
5	2	0.65	0/4241	1.16	12/5720 (0.2%)
6	7	0.40	0/4853	0.84	2/6553 (0.0%)
7	C	0.61	0/1511	1.30	15/2039 (0.7%)
8	D	0.63	0/1489	1.29	8/2016 (0.4%)
9	E	0.63	0/1294	1.14	2/1750 (0.1%)
10	F	0.55	0/1771	1.22	15/2386 (0.6%)
11	G	0.52	0/4311	1.18	28/5832 (0.5%)
12	X	0.41	0/475	0.76	0/731
13	Y	0.40	0/486	0.71	0/748
14	J	0.79	0/153	1.16	0/234
15	B	0.47	0/3727	0.98	3/5041 (0.1%)
16	A	0.45	0/6029	1.09	23/8179 (0.3%)
All	All	0.54	0/48364	1.09	160/65591 (0.2%)

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
10	F	0	4
11	G	0	3
All	All	0	7

There are no bond length outliers.

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	F	216	VAL	CA-C-N	11.38	143.44	122.84
10	F	216	VAL	C-N-CA	11.38	143.44	122.84
11	G	98	ILE	CA-C-N	10.85	148.27	121.80
11	G	98	ILE	C-N-CA	10.85	148.27	121.80
10	F	200	LYS	CA-C-N	9.54	138.87	121.70
10	F	200	LYS	C-N-CA	9.54	138.87	121.70
3	5	444	SER	CB-CA-C	-8.68	95.44	110.45
7	C	149	ILE	CA-C-N	8.55	137.10	121.70
7	C	149	ILE	C-N-CA	8.55	137.10	121.70
16	A	1715	ASP	CA-C-N	8.41	137.61	121.54
16	A	1715	ASP	C-N-CA	8.41	137.61	121.54
10	F	212	THR	CA-C-N	8.37	135.50	122.94
10	F	212	THR	C-N-CA	8.37	135.50	122.94
11	G	415	TYR	N-CA-C	7.81	121.75	111.75
11	G	605	PHE	N-CA-C	7.77	127.34	110.80
11	G	558	GLU	CA-C-N	7.59	135.36	121.70
11	G	558	GLU	C-N-CA	7.59	135.36	121.70
16	A	1911	TRP	CA-C-N	7.57	136.01	122.08
16	A	1911	TRP	C-N-CA	7.57	136.01	122.08
7	C	145	ASP	CA-C-N	7.47	135.15	121.70
7	C	145	ASP	C-N-CA	7.47	135.15	121.70
11	G	308	ASN	CA-C-N	7.38	134.98	121.70
11	G	308	ASN	C-N-CA	7.38	134.98	121.70
11	G	559	SER	CA-C-N	7.34	134.91	121.70
11	G	559	SER	C-N-CA	7.34	134.91	121.70
1	3	175	HIS	N-CA-C	-7.23	95.40	110.80
16	A	1657	ASN	N-CA-C	7.19	126.11	110.80
5	2	631	ILE	CB-CA-C	-7.18	99.52	111.29
4	6	383	GLY	N-CA-C	7.03	129.83	113.18
3	5	280	ARG	N-CA-C	7.01	125.74	110.80
3	5	485	MET	CA-C-N	7.00	134.22	121.06
3	5	485	MET	C-N-CA	7.00	134.22	121.06
11	G	151	THR	CA-C-N	6.94	134.20	121.70
11	G	151	THR	C-N-CA	6.94	134.20	121.70
9	E	101	ASN	CA-C-N	6.92	134.16	121.70
9	E	101	ASN	C-N-CA	6.92	134.16	121.70
1	3	175	HIS	CA-CB-CG	6.90	120.70	113.80
16	A	1896	SER	CA-C-N	6.80	133.94	121.70
16	A	1896	SER	C-N-CA	6.80	133.94	121.70
2	4	373	ARG	CA-C-N	6.77	134.16	121.97
2	4	373	ARG	C-N-CA	6.77	134.16	121.97
1	3	175	HIS	CA-C-N	6.75	133.61	122.07
1	3	175	HIS	C-N-CA	6.75	133.61	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	174	GLN	N-CA-C	-6.71	98.03	109.24
1	3	172	THR	CA-C-N	6.66	134.25	121.54
1	3	172	THR	C-N-CA	6.66	134.25	121.54
11	G	283	ALA	N-CA-C	-6.59	95.50	107.75
10	F	135	ARG	CB-CG-CD	6.58	126.44	111.30
3	5	444	SER	CA-CB-OG	6.57	124.24	111.10
5	2	626	GLN	CA-C-N	6.42	133.29	123.47
5	2	626	GLN	C-N-CA	6.42	133.29	123.47
5	2	412	ALA	N-CA-C	6.33	124.28	110.80
3	5	385	LYS	CA-CB-CG	6.32	126.74	114.10
7	C	23	SER	CA-C-N	6.31	133.05	121.70
7	C	23	SER	C-N-CA	6.31	133.05	121.70
8	D	113	SER	N-CA-C	6.22	124.04	110.80
11	G	149	ASP	CA-C-N	6.13	132.73	121.70
11	G	149	ASP	C-N-CA	6.13	132.73	121.70
8	D	56	ASP	N-CA-C	6.11	121.67	113.72
3	5	136	GLN	CA-C-N	-6.11	111.63	122.07
3	5	136	GLN	C-N-CA	-6.11	111.63	122.07
3	5	374	ILE	N-CA-C	6.04	116.23	110.74
3	5	427	LYS	CA-CB-CG	6.03	126.17	114.10
11	G	62	PHE	CA-C-N	6.00	126.80	120.43
11	G	62	PHE	C-N-CA	6.00	126.80	120.43
3	5	404	MET	N-CA-CB	6.00	120.09	110.85
2	4	820	GLU	CA-C-N	5.99	136.74	126.32
2	4	820	GLU	C-N-CA	5.99	136.74	126.32
1	3	273	SER	N-CA-C	5.96	118.02	109.14
1	3	418	LEU	N-CA-C	-5.94	106.19	113.50
3	5	458	MET	N-CA-C	-5.90	100.88	110.20
4	6	323	GLN	N-CA-C	5.89	119.78	112.47
6	7	542	GLU	N-CA-C	-5.88	99.69	109.46
7	C	147	VAL	CA-C-N	5.84	132.22	121.70
7	C	147	VAL	C-N-CA	5.84	132.22	121.70
16	A	1912	MET	N-CA-C	-5.83	100.66	108.19
11	G	140	ILE	CA-C-N	5.83	132.19	121.70
11	G	140	ILE	C-N-CA	5.83	132.19	121.70
16	A	2030	PRO	N-CA-CB	5.80	109.43	103.23
10	F	267	VAL	CA-C-N	5.79	132.13	121.70
10	F	267	VAL	C-N-CA	5.79	132.13	121.70
16	A	1905	TYR	CA-C-N	-5.79	112.42	122.37
16	A	1905	TYR	C-N-CA	-5.79	112.42	122.37
3	5	161	ARG	CG-CD-NE	5.78	124.72	112.00
5	2	621	HIS	N-CA-CB	-5.78	101.63	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	160	ASP	CA-C-N	5.77	132.09	121.70
7	C	160	ASP	C-N-CA	5.77	132.09	121.70
1	3	174	GLN	CA-C-N	5.74	132.49	121.54
1	3	174	GLN	C-N-CA	5.74	132.49	121.54
5	2	627	GLN	N-CA-C	5.68	120.16	113.23
4	6	599	SER	N-CA-C	-5.67	101.72	109.71
15	B	669	ARG	CB-CA-C	5.66	119.92	111.89
3	5	137	LEU	CA-CB-CG	5.65	136.07	116.30
16	A	1716	SER	N-CA-C	5.65	122.83	110.80
16	A	1515	LYS	N-CA-C	5.63	122.26	109.81
5	2	631	ILE	CA-C-N	5.61	133.43	123.34
5	2	631	ILE	C-N-CA	5.61	133.43	123.34
1	3	324	ASN	N-CA-C	5.57	118.81	109.95
16	A	1664	ARG	CA-CB-CG	5.57	125.24	114.10
11	G	284	TYR	N-CA-C	5.50	122.52	110.80
15	B	451	ASN	CA-C-N	-5.48	115.21	123.27
15	B	451	ASN	C-N-CA	-5.48	115.21	123.27
3	5	264	LEU	CA-C-N	5.48	132.27	122.13
3	5	264	LEU	C-N-CA	5.48	132.27	122.13
7	C	22	ARG	CA-C-N	5.47	131.55	121.70
7	C	22	ARG	C-N-CA	5.47	131.55	121.70
16	A	1428	GLU	N-CA-CB	5.44	118.62	110.14
16	A	2047	VAL	N-CA-C	-5.43	107.53	112.96
16	A	2151	ARG	CG-CD-NE	5.43	123.95	112.00
16	A	1685	ILE	CA-C-N	5.43	131.74	121.97
16	A	1685	ILE	C-N-CA	5.43	131.74	121.97
16	A	1922	CYS	CA-C-N	5.42	131.73	121.97
16	A	1922	CYS	C-N-CA	5.42	131.73	121.97
3	5	517	THR	N-CA-C	5.42	117.08	110.41
5	2	627	GLN	CB-CA-C	-5.40	102.24	111.26
16	A	1875	PRO	N-CA-C	5.39	123.57	112.47
5	2	631	ILE	N-CA-C	5.38	120.53	109.34
3	5	447	ALA	CA-C-N	5.37	129.34	121.67
3	5	447	ALA	C-N-CA	5.37	129.34	121.67
10	F	256	TYR	CA-C-N	5.37	131.36	121.70
10	F	256	TYR	C-N-CA	5.37	131.36	121.70
5	2	505	ILE	CB-CA-C	5.34	118.09	111.15
3	5	258	LEU	CA-CB-CG	5.32	134.92	116.30
7	C	106	GLY	CA-C-N	5.29	131.21	121.70
7	C	106	GLY	C-N-CA	5.29	131.21	121.70
1	3	264	MET	CA-CB-CG	5.27	124.64	114.10
1	3	316	GLY	N-CA-C	5.27	120.14	112.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	F	255	CYS	CA-C-N	5.24	132.32	121.32
10	F	255	CYS	C-N-CA	5.24	132.32	121.32
11	G	330	ARG	CA-CB-CG	-5.23	103.63	114.10
3	5	506	LYS	N-CA-C	5.23	117.96	109.86
8	D	112	PHE	CA-C-N	5.22	131.52	121.54
8	D	112	PHE	C-N-CA	5.22	131.52	121.54
1	3	319	THR	N-CA-C	5.21	117.78	109.81
1	3	563	GLU	CB-CA-C	-5.21	99.43	110.31
10	F	268	GLU	N-CA-C	5.20	125.56	111.00
16	A	2207	TYR	CA-CB-CG	5.20	123.26	113.90
8	D	116	PRO	CA-C-N	5.18	131.44	121.54
8	D	116	PRO	C-N-CA	5.18	131.44	121.54
3	5	427	LYS	CB-CA-C	-5.17	102.06	110.85
11	G	285	ALA	CA-C-N	5.17	131.01	121.70
11	G	285	ALA	C-N-CA	5.17	131.01	121.70
11	G	285	ALA	CB-CA-C	5.17	120.71	110.42
11	G	488	LYS	CA-CB-CG	-5.17	103.76	114.10
10	F	155	SER	N-CA-C	5.16	117.30	111.11
8	D	21	GLU	CB-CA-C	-5.15	100.48	110.46
1	3	443	THR	CA-C-N	5.14	131.36	121.54
1	3	443	THR	C-N-CA	5.14	131.36	121.54
3	5	561	ASN	N-CA-C	-5.14	99.73	108.26
8	D	163	LEU	N-CA-C	5.13	117.61	109.96
2	4	641	THR	CA-C-N	5.13	131.34	121.54
2	4	641	THR	C-N-CA	5.13	131.34	121.54
11	G	150	ASP	CA-C-N	5.12	130.92	121.70
11	G	150	ASP	C-N-CA	5.12	130.92	121.70
7	C	106	GLY	N-CA-C	5.12	128.16	113.30
6	7	625	GLN	N-CA-C	5.11	121.10	109.81
11	G	345	ASN	N-CA-C	5.09	117.23	111.02
3	5	301	TYR	CA-CB-CG	5.06	123.01	113.90
5	2	247	ARG	CA-CB-CG	5.03	124.16	114.10
1	3	324	ASN	N-CA-CB	-5.01	102.83	110.85

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	F	212	THR	Mainchain,Peptide
10	F	216	VAL	Mainchain,Peptide
11	G	523	ARG	Sidechain
11	G	98	ILE	Mainchain,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	3	4270	0	4259	79	0
2	4	4543	0	4517	78	0
3	5	4690	0	4526	105	0
4	6	4307	0	4166	88	0
5	2	4184	0	4126	85	0
6	7	4785	0	4761	83	0
7	C	1492	0	1394	36	0
8	D	1461	0	1445	46	0
9	E	1262	0	1240	32	0
10	F	1743	0	1672	41	0
11	G	4239	0	4083	51	0
12	X	425	0	238	18	0
13	Y	433	0	235	20	0
14	J	140	0	85	7	0
15	B	3661	0	3656	56	0
16	A	5918	0	5682	121	0
17	5	62	0	24	8	0
18	A	2	0	0	0	0
All	All	47617	0	46109	871	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 9.

All (871) 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)
6:7:460:GLY:HA3	6:7:600:MET:HB2	1.62	0.81
5:2:617:ARG:O	5:2:621:HIS:HB2	1.84	0.77
9:E:48:LEU:O	9:E:52:ARG:HB2	1.85	0.76
11:G:244:GLY:HA3	11:G:603:ASN:HB2	1.67	0.76
3:5:447:ALA:HA	5:2:637:VAL:HA	1.69	0.73
7:C:58:GLN:HA	7:C:62:MET:HB2	1.71	0.73
16:A:1383:LEU:HB2	16:A:1686:VAL:HG21	1.70	0.73
4:6:551:MET:O	4:6:759:ARG:NH2	2.22	0.72
2:4:434:GLU:H	2:4:467:LYS:HB3	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:339:PHE:HB2	5:2:348:LEU:HB2	1.73	0.71
10:F:266:GLU:HB3	10:F:268:GLU:HG3	1.73	0.70
5:2:328:THR:O	5:2:386:GLN:NE2	2.25	0.70
11:G:85:GLY:N	11:G:123:LEU:O	2.25	0.69
7:C:164:ASP:O	7:C:207:LYS:NZ	2.26	0.69
5:2:676:ARG:HD3	5:2:808:ARG:HH22	1.58	0.68
4:6:794:ARG:HD3	5:2:656:ARG:HH22	1.59	0.68
6:7:719:LEU:O	6:7:723:SER:HB3	1.92	0.68
1:3:435:ARG:HH12	3:5:489:ASP:HA	1.59	0.68
4:6:828:TYR:OH	4:6:832:ARG:NH2	2.27	0.68
1:3:435:ARG:NH1	3:5:488:GLU:O	2.28	0.67
5:2:633:LYS:O	5:2:635:GLY:N	2.28	0.67
11:G:570:ALA:HB2	11:G:581:VAL:HG22	1.76	0.67
2:4:293:LEU:O	2:4:297:GLU:HB2	1.94	0.67
3:5:412:VAL:HB	3:5:520:LEU:HG	1.77	0.67
1:3:417:GLN:HE22	3:5:404:MET:HB2	1.60	0.66
8:D:124:ARG:NH2	9:E:190:TRP:O	2.29	0.66
10:F:229:PHE:HA	10:F:276:VAL:HG22	1.77	0.66
16:A:1733:ASP:HB2	16:A:1904:ARG:H	1.60	0.66
3:5:588:GLU:O	3:5:592:SER:N	2.25	0.66
7:C:106:GLY:HA2	7:C:201:GLN:HE21	1.60	0.66
5:2:842:VAL:HG11	5:2:863:ILE:HG21	1.77	0.66
1:3:277:ILE:O	1:3:324:ASN:ND2	2.30	0.65
3:5:266:PRO:O	3:5:269:GLU:N	2.29	0.65
16:A:2062:MET:SD	16:A:2062:MET:N	2.71	0.64
16:A:2164:CYS:HB3	16:A:2167:CYS:SG	2.38	0.64
2:4:367:GLU:H	4:6:422:ASP:H	1.46	0.64
1:3:314:LEU:O	3:5:175:ARG:NH2	2.30	0.64
2:4:662:ILE:HD12	4:6:390:LYS:HZ1	1.63	0.64
3:5:335:SER:OG	3:5:336:ASP:N	2.30	0.64
16:A:2164:CYS:SG	16:A:2165:SER:N	2.71	0.64
16:A:1906:TRP:HB3	16:A:1909:LEU:HD11	1.80	0.63
3:5:574:ASN:HB3	3:5:580:ALA:HB3	1.81	0.63
6:7:288:GLU:O	6:7:292:ASN:ND2	2.31	0.63
2:4:336:THR:O	2:4:395:GLN:NE2	2.30	0.63
2:4:655:SER:HA	2:4:664:THR:HG22	1.81	0.63
7:C:102:TRP:NE1	7:C:134:TYR:OH	2.30	0.63
11:G:432:LEU:O	11:G:476:ASN:ND2	2.31	0.63
7:C:46:ASN:O	7:C:50:ASN:ND2	2.31	0.63
16:A:1860:TYR:HB3	16:A:1867:LEU:HD13	1.81	0.63
1:3:39:ARG:HH22	1:3:132:LEU:HD11	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:346:ALA:HB2	11:G:555:CYS:HA	1.81	0.62
15:B:208:LEU:O	16:A:2191:ARG:NH2	2.30	0.62
5:2:660:THR:HB	5:2:850:LYS:HG3	1.82	0.62
1:3:686:LEU:HB3	1:3:697:ILE:HD12	1.82	0.61
15:B:647:ALA:O	15:B:660:ASN:ND2	2.33	0.61
3:5:375:ALA:HB3	3:5:385:LYS:HE3	1.82	0.61
5:2:226:VAL:O	5:2:230:ARG:HB2	2.00	0.61
6:7:588:ALA:HA	6:7:591:LEU:HD13	1.82	0.61
2:4:367:GLU:O	4:6:422:ASP:N	2.34	0.61
8:D:113:SER:OG	8:D:114:GLU:N	2.33	0.60
16:A:1414:CYS:SG	16:A:1415:THR:N	2.74	0.60
3:5:438:TYR:HA	3:5:478:CYS:HB2	1.83	0.60
8:D:25:ILE:N	8:D:71:VAL:O	2.30	0.60
4:6:704:PRO:HB3	5:2:545:PRO:HB3	1.83	0.60
10:F:248:GLU:N	10:F:250:GLU:OE1	2.34	0.60
16:A:2163:ARG:NH2	16:A:2168:HIS:O	2.34	0.60
3:5:444:SER:OG	5:2:631:ILE:N	2.33	0.60
1:3:29:GLN:HE22	1:3:132:LEU:HB2	1.67	0.60
6:7:518:ASN:H	6:7:561:THR:HA	1.67	0.60
4:6:308:SER:HA	4:6:319:ASP:HA	1.83	0.60
6:7:258:ILE:HB	6:7:271:GLN:HB3	1.82	0.60
4:6:109:GLU:HG2	4:6:112:ARG:HH21	1.66	0.60
8:D:9:GLN:O	8:D:182:ARG:NH1	2.35	0.60
16:A:1533:LYS:HA	16:A:1536:PHE:HB3	1.81	0.60
16:A:1612:ILE:O	16:A:1664:ARG:NH2	2.35	0.60
6:7:193:PRO:HG2	6:7:196:LEU:HB2	1.84	0.59
15:B:410:ASP:HB3	15:B:413:ILE:HG12	1.84	0.59
16:A:1720:LYS:HE2	16:A:1860:TYR:HB2	1.84	0.59
11:G:298:GLU:OE1	11:G:301:ARG:NH1	2.35	0.59
1:3:431:ALA:HA	1:3:471:CYS:HB2	1.83	0.59
7:C:147:VAL:H	7:C:148:ASP:HA	1.67	0.59
15:B:174:ASN:ND2	15:B:177:GLN:OE1	2.35	0.59
1:3:29:GLN:NE2	1:3:128:ALA:O	2.35	0.59
2:4:388:ARG:NH1	4:6:104:ASP:OD2	2.32	0.59
2:4:569:ASP:O	2:4:574:LYS:NZ	2.35	0.59
5:2:788:ARG:HB2	16:A:2070:LEU:HD22	1.83	0.59
16:A:1701:ILE:HG22	16:A:1702:GLN:HG3	1.84	0.59
2:4:329:LYS:HA	2:4:434:GLU:HA	1.85	0.59
5:2:774:ILE:HG12	5:2:822:LYS:HA	1.83	0.59
15:B:531:ARG:HG2	15:B:540:VAL:HG22	1.83	0.59
2:4:563:ASN:ND2	2:4:649:MET:SD	2.71	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:662:SER:O	5:2:572:SER:OG	2.21	0.59
16:A:1890:ARG:NH1	16:A:1894:MET:SD	2.76	0.59
2:4:574:LYS:HA	2:4:577:ILE:HD12	1.85	0.59
3:5:414:LEU:HD13	3:5:422:LYS:HB2	1.85	0.59
3:5:440:SER:HA	3:5:480:ASP:HB2	1.85	0.59
11:G:292:TYR:OH	11:G:406:ARG:NH1	2.36	0.59
2:4:315:ARG:HH12	6:7:251:VAL:H	1.51	0.59
4:6:104:ASP:HA	4:6:176:ARG:HH11	1.67	0.58
11:G:285:ALA:HB1	11:G:288:TYR:HB3	1.85	0.58
15:B:611:HIS:CD2	15:B:613:SER:H	2.22	0.58
3:5:412:VAL:O	3:5:521:ALA:N	2.33	0.58
4:6:112:ARG:HH12	4:6:187:ARG:HH12	1.51	0.58
6:7:669:GLN:O	6:7:673:ARG:HB3	2.03	0.58
1:3:298:PHE:HA	1:3:321:ILE:HG12	1.86	0.58
6:7:249:SER:O	6:7:311:GLN:NE2	2.36	0.58
16:A:1611:PRO:HB2	16:A:1664:ARG:HH12	1.69	0.58
15:B:210:ASP:OD1	16:A:2191:ARG:NH2	2.37	0.58
1:3:536:PRO:HD2	1:3:539:LEU:HD12	1.86	0.58
5:2:257:ALA:HA	5:2:260:LEU:HD12	1.86	0.58
15:B:437:SER:H	15:B:486:GLY:HA3	1.69	0.58
1:3:564:HIS:O	1:3:568:THR:OG1	2.14	0.58
5:2:326:ARG:O	5:2:389:THR:OG1	2.20	0.58
6:7:668:ARG:O	6:7:672:LYS:HB2	2.04	0.58
15:B:439:THR:HG22	15:B:441:VAL:H	1.68	0.58
8:D:195:ILE:HG22	9:E:109:ILE:HD13	1.86	0.58
10:F:70:GLU:O	10:F:150:LYS:NZ	2.37	0.58
15:B:448:SER:N	16:A:2109:GLU:OE2	2.36	0.58
3:5:254:GLN:HB3	3:5:278:CYS:HB2	1.85	0.57
8:D:194:GLU:O	8:D:198:ALA:CB	2.51	0.57
11:G:269:ASN:O	11:G:273:ASN:ND2	2.37	0.57
16:A:1495:GLY:HA3	16:A:1515:LYS:HB2	1.86	0.57
4:6:632:ASP:OD1	4:6:675:ARG:NH1	2.37	0.57
3:5:175:ARG:NH1	3:5:197:PHE:O	2.38	0.57
17:5:801:AGS:O3G	17:5:801:AGS:O2B	2.22	0.57
10:F:78:PRO:HA	10:F:174:LEU:HA	1.87	0.57
1:3:233:THR:HG22	1:3:234:GLU:HG2	1.86	0.57
2:4:334:ARG:NH2	6:7:552:GLY:O	2.35	0.57
6:7:617:THR:O	6:7:621:MET:HB2	2.03	0.57
4:6:696:ARG:HH21	4:6:793:TYR:HA	1.70	0.57
6:7:284:CYS:HA	6:7:298:LEU:HD23	1.85	0.57
11:G:503:GLN:HA	11:G:506:ILE:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:21:GLU:HA	8:D:73:LEU:HD23	1.85	0.57
1:3:233:THR:HA	1:3:241:LEU:HB2	1.87	0.57
3:5:260:GLU:OE1	3:5:272:ARG:NE	2.38	0.57
3:5:184:ARG:HE	3:5:242:ILE:HD11	1.70	0.57
4:6:127:THR:OG1	4:6:128:ASP:N	2.38	0.57
16:A:1543:ILE:HG12	16:A:1553:LYS:HD3	1.87	0.57
4:6:601:LYS:HD3	4:6:643:LYS:HB3	1.87	0.56
8:D:30:ARG:NH1	8:D:86:SER:OG	2.38	0.56
6:7:89:GLN:HE22	6:7:101:ASP:HA	1.70	0.56
1:3:176:LEU:HD23	1:3:177:ASN:HB2	1.86	0.56
3:5:267:VAL:O	3:5:269:GLU:N	2.37	0.56
3:5:409:ASP:O	3:5:658:ARG:NH1	2.38	0.56
4:6:303:GLU:OE1	4:6:356:TRP:NE1	2.38	0.56
7:C:102:TRP:O	7:C:152:SER:OG	2.23	0.56
8:D:121:VAL:HG13	9:E:190:TRP:HH2	1.70	0.56
8:D:139:HIS:H	8:D:142:ARG:HH11	1.52	0.56
1:3:394:GLU:HB2	6:7:623:ASN:HB3	1.86	0.56
3:5:101:ILE:O	3:5:105:SER:N	2.39	0.56
7:C:35:ASP:OD1	7:C:35:ASP:N	2.38	0.56
9:E:186:ASP:OD1	9:E:189:ARG:NH2	2.39	0.56
12:X:16:DG:H1'	12:X:17:DT:H5'	1.88	0.56
3:5:498:GLU:HG2	3:5:549:ARG:HD2	1.88	0.56
13:Y:2:DA:H1'	13:Y:3:DA:H5'	1.88	0.56
17:5:801:AGS:H4'	5:2:534:ARG:HH12	1.71	0.56
1:3:433:THR:HA	1:3:473:ASP:HB2	1.86	0.56
3:5:449:LEU:O	3:5:468:ALA:N	2.38	0.56
6:7:262:CYS:SG	6:7:286:SER:OG	2.63	0.56
10:F:97:LEU:O	10:F:99:GLU:N	2.39	0.56
15:B:209:PRO:HB2	15:B:624:TRP:HE3	1.71	0.56
16:A:1915:PHE:HB2	16:A:1938:GLN:HG3	1.88	0.56
15:B:314:PRO:HB3	15:B:344:MET:H	1.71	0.55
15:B:663:SER:HB3	15:B:668:ARG:HG2	1.87	0.55
2:4:293:LEU:O	2:4:297:GLU:CB	2.54	0.55
9:E:96:ASP:HA	9:E:168:LYS:HD3	1.89	0.55
6:7:240:THR:HG23	6:7:352:THR:HG22	1.89	0.55
2:4:433:ILE:HG12	2:4:468:LYS:HA	1.87	0.55
4:6:113:GLU:OE2	4:6:187:ARG:NH2	2.40	0.55
4:6:763:PRO:HD3	4:6:812:ARG:HD3	1.88	0.55
16:A:1549:LEU:HB3	16:A:1646:ILE:HD11	1.88	0.55
2:4:590:TYR:HA	2:4:630:CYS:HB2	1.89	0.55
6:7:76:ASN:O	6:7:201:PHE:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:146:CYS:O	10:F:149:SER:OG	2.21	0.55
16:A:2102:VAL:O	16:A:2149:LYS:NZ	2.39	0.55
1:3:33:ASP:HA	1:3:39:ARG:HH11	1.72	0.55
1:3:363:LEU:HD22	1:3:656:LEU:HD12	1.88	0.55
2:4:774:TYR:OH	2:4:778:ARG:NH2	2.40	0.55
4:6:124:VAL:HG12	4:6:126:SER:H	1.72	0.55
6:7:525:GLU:HA	6:7:567:ALA:HA	1.87	0.55
2:4:344:VAL:HA	2:4:359:GLU:HA	1.89	0.55
5:2:432:ASN:HA	5:2:449:THR:HA	1.89	0.55
4:6:105:ASP:O	4:6:109:GLU:HB2	2.06	0.55
4:6:303:GLU:HG3	4:6:304:LEU:H	1.72	0.55
7:C:129:GLU:HA	7:C:132:LYS:HE3	1.88	0.55
4:6:663:ILE:HG12	5:2:572:SER:HA	1.88	0.54
4:6:777:TYR:HE2	5:2:692:ASP:HB3	1.73	0.54
16:A:2173:ASP:OD2	16:A:2176:SER:OG	2.23	0.54
6:7:421:GLU:O	6:7:625:GLN:NE2	2.39	0.54
11:G:49:PHE:HB3	11:G:54:VAL:HB	1.88	0.54
3:5:744:SER:O	3:5:748:LEU:N	2.36	0.54
6:7:656:VAL:HG11	6:7:708:VAL:HG12	1.89	0.54
7:C:84:ARG:HH22	10:F:217:ASN:HB3	1.71	0.54
11:G:392:PHE:HA	11:G:396:LEU:HD23	1.90	0.54
7:C:120:THR:OG1	7:C:121:ASN:N	2.40	0.54
8:D:56:ASP:OD1	8:D:56:ASP:N	2.35	0.54
15:B:172:VAL:HG22	15:B:532:ILE:HG12	1.89	0.54
2:4:454:LYS:HA	6:7:277:THR:HG22	1.90	0.54
5:2:322:GLY:HA3	5:2:390:LEU:HD21	1.90	0.54
16:A:1732:LEU:HD13	16:A:1909:LEU:HD13	1.90	0.54
3:5:570:ASN:O	3:5:574:ASN:ND2	2.41	0.54
5:2:479:GLU:HA	5:2:482:ARG:HG2	1.89	0.54
5:2:624:MET:HG3	5:2:646:ILE:HD12	1.89	0.54
11:G:137:SER:OG	11:G:140:ILE:O	2.24	0.54
16:A:2111:CYS:HB2	16:A:2132:ARG:HB3	1.90	0.54
3:5:558:ASP:OD1	3:5:558:ASP:N	2.40	0.54
5:2:566:ALA:HB3	5:2:606:ILE:HA	1.90	0.54
2:4:601:LEU:HG	2:4:620:ALA:HB3	1.89	0.54
3:5:415:LEU:HB3	3:5:523:ALA:HB3	1.89	0.54
16:A:1383:LEU:HD12	16:A:1686:VAL:HG11	1.90	0.54
5:2:557:GLU:HG3	5:2:563:ALA:HB3	1.90	0.54
6:7:239:ILE:HD11	6:7:376:LEU:HD13	1.89	0.54
4:6:830:LEU:O	4:6:834:SER:OG	2.16	0.53
1:3:210:HIS:HA	6:7:7:SER:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:568:ASP:O	4:6:805:ARG:NH1	2.36	0.53
1:3:96:ILE:HD13	1:3:129:LEU:HD11	1.89	0.53
4:6:187:ARG:HA	4:6:190:ARG:HG2	1.90	0.53
5:2:839:LYS:HD3	5:2:864:TYR:HD1	1.71	0.53
8:D:161:LYS:HA	9:E:133:GLN:HE22	1.72	0.53
11:G:92:LEU:HA	11:G:95:PHE:HB3	1.91	0.53
16:A:1473:ASN:OD1	16:A:1475:ARG:NH2	2.42	0.53
16:A:1631:LEU:HD13	16:A:1634:LYS:HD2	1.89	0.53
1:3:487:HIS:HB3	1:3:542:ARG:HH21	1.73	0.53
2:4:616:LEU:HD22	2:4:661:ILE:HD12	1.91	0.53
8:D:24:PRO:HA	8:D:72:VAL:HA	1.90	0.53
8:D:11:PHE:HA	10:F:71:ARG:HH22	1.72	0.53
8:D:126:LEU:HB3	8:D:134:PHE:HZ	1.74	0.53
15:B:50:GLY:HA3	15:B:58:ALA:H	1.73	0.53
8:D:189:MET:HA	8:D:192:LEU:HD13	1.91	0.53
11:G:323:ASP:N	11:G:406:ARG:O	2.42	0.53
16:A:2129:SER:OG	16:A:2130:CYS:N	2.42	0.53
1:3:116:VAL:HA	1:3:178:LYS:HE3	1.90	0.52
15:B:292:PHE:H	15:B:295:ASN:HB3	1.75	0.52
1:3:659:TYR:OH	1:3:715:VAL:O	2.28	0.52
4:6:691:ARG:HH11	4:6:716:LEU:HD22	1.74	0.52
10:F:203:PRO:HG2	10:F:206:LEU:HD12	1.91	0.52
12:X:15:DC:H1'	12:X:16:DG:H5'	1.91	0.52
5:2:824:ARG:NH2	5:2:833:ASP:OD1	2.35	0.52
6:7:23:ASP:O	6:7:27:THR:N	2.35	0.52
9:E:55:ALA:HB2	9:E:72:VAL:HB	1.90	0.52
11:G:633:ARG:O	11:G:637:LEU:N	2.42	0.52
5:2:538:ASN:HB3	5:2:677:PHE:HD1	1.75	0.52
1:3:315:ILE:HA	3:5:175:ARG:HE	1.75	0.52
2:4:564:ILE:HG13	2:4:703:ASP:HB3	1.92	0.52
5:2:581:ARG:NH2	14:J:6:DT:OP1	2.42	0.52
9:E:81:SER:HB2	9:E:84:VAL:HG23	1.91	0.52
11:G:14:LYS:NZ	11:G:141:GLN:OE1	2.34	0.52
2:4:189:GLU:O	2:4:193:ASN:HB2	2.09	0.52
2:4:521:LEU:HD11	2:4:741:VAL:HB	1.91	0.52
11:G:227:LYS:O	11:G:231:HIS:ND1	2.29	0.52
16:A:1513:VAL:HG11	16:A:1569:LEU:HD22	1.92	0.52
16:A:2164:CYS:CB	16:A:2167:CYS:SG	2.95	0.52
2:4:543:GLN:HA	2:4:562:ILE:HD11	1.91	0.52
6:7:584:ILE:HG22	6:7:586:LEU:H	1.74	0.52
9:E:94:ALA:O	9:E:168:LYS:NZ	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:1594:SER:HA	16:A:1615:LEU:HD23	1.90	0.52
3:5:161:ARG:NH2	11:G:379:TYR:OH	2.40	0.52
6:7:228:ARG:NH2	6:7:327:ILE:O	2.42	0.52
6:7:73:ARG:NH1	6:7:136:ASP:OD2	2.43	0.52
2:4:256:ASP:OD2	2:4:260:GLN:NE2	2.43	0.51
2:4:367:GLU:H	4:6:422:ASP:N	2.09	0.51
3:5:209:ARG:HA	3:5:239:ASP:HA	1.91	0.51
5:2:274:VAL:HA	5:2:277:GLU:HG2	1.91	0.51
6:7:107:GLN:HG2	6:7:238:LEU:HB3	1.92	0.51
15:B:397:HIS:HA	15:B:430:THR:HG21	1.92	0.51
4:6:134:LYS:HB3	4:6:137:ARG:HB2	1.91	0.51
10:F:285:LEU:O	10:F:289:ASP:N	2.43	0.51
15:B:663:SER:OG	15:B:664:PHE:N	2.43	0.51
16:A:1690:ASN:HB3	16:A:1827:LEU:HD12	1.92	0.51
1:3:367:LEU:HD21	1:3:656:LEU:HD13	1.93	0.51
2:4:393:ASP:N	2:4:421:ASP:OD1	2.38	0.51
7:C:157:PRO:HG3	10:F:138:PHE:CE2	2.46	0.51
1:3:259:GLN:NE2	1:3:271:PRO:O	2.43	0.51
3:5:371:THR:HG21	3:5:386:LYS:HG2	1.93	0.51
3:5:606:CYS:HB3	3:5:665:LYS:HG2	1.92	0.51
16:A:2049:ASN:O	16:A:2053:GLU:HB2	2.10	0.51
6:7:440:VAL:H	6:7:452:GLY:HA3	1.76	0.51
13:Y:3:DA:H1'	13:Y:4:DA:H5'	1.92	0.51
1:3:186:VAL:O	1:3:289:GLY:N	2.33	0.51
5:2:784:ASP:O	5:2:787:SER:OG	2.24	0.51
1:3:211:TYR:HB3	6:7:6:PRO:HG2	1.92	0.51
3:5:555:ILE:HD12	3:5:690:ASP:HB3	1.93	0.51
3:5:717:GLU:O	3:5:721:ARG:CB	2.59	0.51
6:7:425:ASN:HB3	6:7:428:VAL:HB	1.93	0.51
15:B:432:LEU:HD12	15:B:481:MET:HG2	1.93	0.51
16:A:1864:ASN:OD1	16:A:1865:GLN:NE2	2.43	0.51
11:G:551:TRP:HE3	11:G:552:LEU:HD12	1.76	0.51
2:4:551:THR:HG22	2:4:557:ARG:HA	1.93	0.50
5:2:497:ILE:HD12	5:2:823:MET:HE3	1.92	0.50
1:3:368:ALA:HB2	1:3:378:LYS:HE2	1.92	0.50
3:5:660:THR:HB	3:5:677:VAL:HG22	1.92	0.50
11:G:325:TYR:OH	11:G:406:ARG:NH2	2.40	0.50
16:A:1550:VAL:HB	16:A:1553:LYS:HE3	1.93	0.50
17:5:801:AGS:O2B	17:5:801:AGS:O2A	2.29	0.50
5:2:333:GLN:N	5:2:383:ARG:O	2.39	0.50
5:2:567:THR:HG21	5:2:571:ALA:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:1568:LYS:HA	16:A:1571:ARG:HB3	1.94	0.50
12:X:10:DC:H1'	12:X:11:DT:H5'	1.94	0.50
4:6:582:SER:HA	4:6:585:LEU:HD12	1.93	0.50
3:5:491:VAL:HA	3:5:494:HIS:HD2	1.75	0.50
17:5:802:AGS:S1G	17:5:802:AGS:O2B	2.70	0.50
11:G:615:GLU:HG2	11:G:616:THR:H	1.76	0.50
16:A:1353:ILE:HB	16:A:1436:ARG:HD3	1.93	0.50
1:3:680:VAL:HG22	6:7:613:ALA:HB1	1.94	0.50
4:6:116:GLU:OE1	4:6:187:ARG:NH2	2.45	0.50
2:4:392:ALA:O	4:6:281:SER:OG	2.26	0.50
3:5:477:VAL:O	3:5:520:LEU:N	2.35	0.50
2:4:360:ILE:HA	2:4:365:ILE:HG12	1.94	0.49
2:4:455:SER:OG	2:4:456:LEU:N	2.45	0.49
3:5:260:GLU:OE2	3:5:271:PRO:HA	2.12	0.49
16:A:1726:VAL:HG12	16:A:1728:ASP:H	1.77	0.49
4:6:581:LYS:HA	4:6:584:PHE:CD2	2.47	0.49
4:6:757:TYR:O	4:6:760:THR:OG1	2.29	0.49
11:G:398:ARG:HH21	11:G:399:TYR:HE1	1.60	0.49
16:A:1317:TYR:CE2	16:A:1472:GLU:HG2	2.48	0.49
2:4:616:LEU:O	4:6:362:GLN:NE2	2.43	0.49
6:7:420:PRO:HA	6:7:429:LYS:HZ1	1.77	0.49
1:3:228:PRO:O	1:3:230:ILE:N	2.45	0.49
9:E:87:ALA:O	9:E:90:THR:OG1	2.26	0.49
15:B:408:LEU:HD21	15:B:465:LEU:HD22	1.95	0.49
7:C:135:CYS:HA	7:C:138:ILE:HG22	1.94	0.49
12:X:17:DT:H1'	12:X:18:DT:H5'	1.93	0.49
15:B:531:ARG:NH2	15:B:629:THR:O	2.45	0.49
16:A:1385:ASN:ND2	16:A:1390:SER:OG	2.36	0.49
16:A:1595:PRO:HB2	16:A:1600:LEU:HD12	1.94	0.49
1:3:202:TYR:N	1:3:242:THR:O	2.36	0.49
3:5:491:VAL:HA	3:5:494:HIS:CD2	2.48	0.49
3:5:730:TYR:O	3:5:734:ARG:CB	2.60	0.49
5:2:797:SER:O	5:2:800:THR:OG1	2.25	0.49
7:C:176:THR:HA	7:C:180:VAL:HA	1.94	0.49
8:D:155:LYS:HA	8:D:158:LYS:HG2	1.94	0.49
9:E:180:SER:O	9:E:183:SER:OG	2.21	0.49
13:Y:9:DC:H1'	13:Y:10:DC:H5'	1.94	0.49
16:A:1850:GLU:OE1	16:A:1890:ARG:NH2	2.46	0.49
1:3:209:PHE:HE2	6:7:10:LEU:HB2	1.78	0.49
3:5:49:GLN:NE2	3:5:62:THR:O	2.39	0.49
11:G:287:VAL:HG13	11:G:290:ARG:HH11	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:297:THR:HA	4:6:359:VAL:HG12	1.94	0.49
5:2:788:ARG:HD3	16:A:2070:LEU:HB2	1.95	0.49
12:X:7:DA:H1'	12:X:8:DC:H5'	1.95	0.49
13:Y:7:DG:H1'	13:Y:8:DG:H5'	1.95	0.49
1:3:259:GLN:HE21	1:3:271:PRO:C	2.19	0.49
4:6:565:LEU:HD22	5:2:703:HIS:CD2	2.48	0.49
5:2:620:ILE:HG22	5:2:624:MET:HE2	1.95	0.49
1:3:344:ASP:HA	1:3:347:ILE:HG22	1.94	0.48
5:2:215:LEU:HD21	5:2:231:ILE:HD11	1.94	0.48
8:D:55:THR:OG1	8:D:56:ASP:OD1	2.30	0.48
9:E:26:GLY:H	9:E:36:ARG:HG3	1.78	0.48
10:F:231:HIS:HB3	10:F:292:ALA:HB3	1.94	0.48
16:A:1546:TYR:O	16:A:1553:LYS:NZ	2.35	0.48
16:A:1690:ASN:HB2	16:A:1826:LYS:HD3	1.94	0.48
2:4:261:LEU:HD12	2:4:265:PRO:HA	1.95	0.48
2:4:341:ASP:O	2:4:392:ALA:N	2.46	0.48
3:5:686:ALA:HB2	16:A:2182:ALA:HB2	1.95	0.48
6:7:437:VAL:O	6:7:646:LYS:NZ	2.46	0.48
7:C:37:ILE:HA	7:C:40:ILE:HD12	1.94	0.48
8:D:29:PRO:HA	8:D:85:CYS:HA	1.95	0.48
16:A:1730:VAL:HG23	16:A:1732:LEU:HD11	1.95	0.48
1:3:195:LYS:NZ	1:3:216:ASP:OD2	2.44	0.48
1:3:374:HIS:HB3	1:3:377:ILE:HD12	1.95	0.48
5:2:809:HIS:O	5:2:812:SER:OG	2.21	0.48
6:7:659:TYR:OH	6:7:714:GLU:OE1	2.27	0.48
11:G:545:LEU:HA	11:G:548:LEU:HB3	1.94	0.48
1:3:521:GLY:N	3:5:543:GLN:OE1	2.44	0.48
6:7:283:GLU:O	6:7:298:LEU:N	2.46	0.48
15:B:529:PRO:HB3	15:B:542:PHE:HB2	1.95	0.48
1:3:390:GLU:OE1	1:3:509:ARG:NH2	2.46	0.48
9:E:12:ASP:HA	9:E:48:LEU:HB3	1.95	0.48
15:B:626:LEU:O	15:B:629:THR:OG1	2.26	0.48
16:A:1733:ASP:HB3	16:A:1906:TRP:HD1	1.77	0.48
16:A:1742:ASN:HD21	16:A:1899:ASP:HB3	1.78	0.48
5:2:271:PHE:HD2	5:2:295:VAL:HG21	1.78	0.48
16:A:1691:GLU:N	16:A:1691:GLU:OE1	2.47	0.48
7:C:90:GLN:HA	7:C:93:ARG:HB3	1.96	0.48
13:Y:8:DG:H1'	13:Y:9:DC:H5'	1.96	0.48
15:B:315:THR:OG1	15:B:320:TYR:OH	2.29	0.48
16:A:1860:TYR:OH	16:A:1862:ASP:OD2	2.24	0.48
16:A:1870:THR:HG21	16:A:1879:TYR:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:426:VAL:HG12	5:2:456:ILE:HG13	1.95	0.48
7:C:162:PHE:HA	7:C:192:ARG:HA	1.95	0.48
9:E:20:PHE:HD2	9:E:24:ILE:HD13	1.78	0.48
15:B:429:PRO:HG2	15:B:479:THR:HG21	1.95	0.48
3:5:445:SER:HA	5:2:578:ALA:HB3	1.96	0.48
7:C:76:LEU:O	7:C:80:GLU:HG3	2.14	0.48
16:A:1433:PRO:HD3	16:A:1689:TRP:NE1	2.29	0.48
3:5:650:ILE:HD11	17:5:802:AGS:C8	2.44	0.48
13:Y:17:DG:H1'	13:Y:18:DC:H5'	1.96	0.48
15:B:299:GLU:OE2	16:A:2175:MET:N	2.47	0.48
16:A:1733:ASP:OD1	16:A:1733:ASP:N	2.46	0.48
4:6:402:ILE:HD13	4:6:455:LEU:HD22	1.96	0.47
13:Y:10:DC:H1'	13:Y:11:DA:H5'	1.96	0.47
16:A:1879:TYR:OH	16:A:1886:MET:SD	2.67	0.47
1:3:499:LYS:HG2	1:3:500:ALA:H	1.80	0.47
3:5:354:GLU:HG2	3:5:605:TYR:CE1	2.49	0.47
4:6:533:ILE:HB	4:6:544:LYS:HD2	1.97	0.47
6:7:318:LEU:HD23	6:7:321:GLN:HG3	1.96	0.47
13:Y:13:DC:H1'	13:Y:14:DG:H5'	1.96	0.47
1:3:100:LEU:HB3	1:3:111:TRP:HH2	1.79	0.47
1:3:446:VAL:HG22	14:J:1:DT:H4'	1.96	0.47
6:7:672:LYS:HE3	6:7:684:ALA:H	1.79	0.47
8:D:132:ASP:OD1	8:D:132:ASP:N	2.46	0.47
9:E:43:LYS:HD3	9:E:75:LEU:HD13	1.95	0.47
11:G:270:LEU:HA	11:G:273:ASN:HD22	1.79	0.47
13:Y:19:DT:H1'	13:Y:20:DG:H5'	1.96	0.47
16:A:1516:PRO:HB2	16:A:1519:GLN:HB2	1.95	0.47
2:4:605:ILE:HD12	2:4:616:LEU:HG	1.97	0.47
4:6:751:LEU:O	4:6:755:ILE:HG12	2.15	0.47
7:C:69:LYS:HA	7:C:72:TYR:HD2	1.79	0.47
13:Y:18:DC:H1'	13:Y:19:DT:H5'	1.95	0.47
16:A:1523:ILE:HG23	16:A:1527:SER:HB3	1.95	0.47
16:A:1852:SER:HB2	16:A:1858:ILE:HD11	1.95	0.47
16:A:1856:SER:HB2	16:A:1868:ILE:HB	1.96	0.47
16:A:2160:GLN:OE1	16:A:2188:THR:OG1	2.32	0.47
3:5:239:ASP:OD1	3:5:239:ASP:N	2.45	0.47
3:5:766:GLN:O	3:5:770:ILE:N	2.48	0.47
12:X:9:DG:H1'	12:X:10:DC:H5'	1.95	0.47
12:X:11:DT:H1'	12:X:12:DG:H5'	1.97	0.47
16:A:1574:SER:HB2	16:A:1605:ARG:HG2	1.96	0.47
5:2:232:ARG:O	5:2:236:GLU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:289:ILE:HG22	5:2:290:HIS:CD2	2.50	0.47
1:3:259:GLN:HG3	1:3:273:SER:HB3	1.95	0.47
1:3:565:VAL:O	1:3:569:HIS:ND1	2.48	0.47
2:4:234:ARG:NH1	2:4:290:ASP:OD2	2.45	0.47
2:4:393:ASP:OD1	4:6:281:SER:OG	2.33	0.47
2:4:549:ASN:OD1	2:4:560:GLY:N	2.48	0.47
4:6:120:GLU:O	4:6:137:ARG:NH1	2.47	0.47
5:2:527:VAL:HB	5:2:530:LYS:HB2	1.96	0.47
6:7:86:LEU:HD23	6:7:90:ASN:HD21	1.79	0.47
6:7:195:ASN:ND2	6:7:272:GLU:OE2	2.47	0.47
10:F:131:THR:O	10:F:135:ARG:HB2	2.14	0.47
10:F:138:PHE:HA	10:F:141:ARG:HH11	1.80	0.47
10:F:170:SER:HB3	10:F:175:LEU:HD22	1.97	0.47
4:6:307:ALA:O	4:6:320:ASN:N	2.47	0.47
6:7:467:SER:HA	6:7:470:LEU:HD12	1.96	0.47
12:X:1:DG:H1'	12:X:2:DC:H5'	1.97	0.47
2:4:446:ALA:HB3	2:4:452:VAL:HG23	1.96	0.47
2:4:743:PRO:HB2	2:4:746:PHE:HB2	1.97	0.47
6:7:719:LEU:O	6:7:723:SER:CB	2.61	0.47
15:B:216:GLN:HA	15:B:219:LEU:HD12	1.96	0.47
16:A:1730:VAL:HG21	16:A:1869:LYS:HG2	1.96	0.47
1:3:315:ILE:HG13	3:5:175:ARG:HH21	1.80	0.47
12:X:6:DC:H1'	12:X:7:DA:H5'	1.97	0.47
5:2:342:LEU:HG	5:2:373:PHE:HA	1.97	0.46
5:2:856:GLN:HA	5:2:859:ARG:HG2	1.97	0.46
7:C:16:THR:HA	7:C:19:LEU:HD12	1.97	0.46
11:G:312:THR:OG1	11:G:314:ASP:O	2.34	0.46
14:J:5:DT:H2''	14:J:6:DT:H5'	1.96	0.46
16:A:1382:SER:N	16:A:1685:ILE:O	2.42	0.46
16:A:1580:LEU:HD13	16:A:1580:LEU:HA	1.76	0.46
1:3:722:ASN:OD1	1:3:723:LYS:N	2.49	0.46
3:5:382:GLU:HA	3:5:385:LYS:HB3	1.97	0.46
16:A:1372:LYS:HB3	16:A:1407:PHE:HB2	1.97	0.46
16:A:1907:ASP:HB3	16:A:1921:ALA:H	1.80	0.46
1:3:360:PHE:O	1:3:364:SER:OG	2.28	0.46
7:C:185:LYS:NZ	7:C:186:ASP:OD2	2.48	0.46
9:E:74:LEU:HD13	9:E:114:LEU:HD21	1.96	0.46
15:B:187:LYS:HD3	15:B:189:GLN:HE21	1.81	0.46
16:A:1310:ILE:HG22	16:A:1311:ARG:HG2	1.97	0.46
16:A:1648:HIS:O	16:A:1652:LEU:HB2	2.14	0.46
6:7:352:THR:O	6:7:379:GLN:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:711:ASP:HA	6:7:714:GLU:HB3	1.98	0.46
7:C:177:GLU:HA	15:B:20:LEU:HD11	1.97	0.46
1:3:304:GLY:HA3	1:3:317:PHE:CE2	2.50	0.46
13:Y:12:DG:H1'	13:Y:13:DC:H5'	1.98	0.46
2:4:349:CYS:SG	2:4:371:CYS:HB3	2.55	0.46
3:5:23:ASP:HB3	3:5:24:ASN:H	1.53	0.46
3:5:180:SER:HA	3:5:191:SER:HA	1.97	0.46
8:D:156:VAL:O	8:D:160:LEU:HB2	2.15	0.46
8:D:194:GLU:O	8:D:198:ALA:HB3	2.15	0.46
3:5:48:ASP:HA	3:5:51:ARG:HG2	1.96	0.46
4:6:776:LYS:HD3	4:6:828:TYR:HB2	1.96	0.46
6:7:193:PRO:HD2	6:7:196:LEU:HD13	1.97	0.46
6:7:484:THR:HG23	6:7:487:GLY:H	1.80	0.46
16:A:2130:CYS:SG	16:A:2131:VAL:N	2.89	0.46
3:5:212:LEU:HD22	3:5:215:ILE:HB	1.96	0.46
5:2:327:ARG:NH2	5:2:418:SER:O	2.49	0.46
6:7:258:ILE:N	6:7:271:GLN:O	2.38	0.46
10:F:73:SER:O	10:F:150:LYS:NZ	2.39	0.46
13:Y:11:DA:H1'	13:Y:12:DG:H5'	1.96	0.46
15:B:468:LEU:HD23	15:B:471:ARG:HD3	1.98	0.46
15:B:485:PRO:HB3	15:B:508:ILE:HG13	1.98	0.46
16:A:1342:ILE:HG23	16:A:1344:GLY:H	1.80	0.46
16:A:1663:LEU:HB3	16:A:1666:ASP:HB2	1.97	0.46
2:4:657:ALA:HA	2:4:662:ILE:HA	1.98	0.46
5:2:760:GLN:HA	5:2:763:LEU:HG	1.96	0.46
6:7:61:PRO:HG2	6:7:64:MET:HB2	1.97	0.46
9:E:173:GLU:O	9:E:176:ILE:HG13	2.16	0.46
15:B:271:ILE:HG12	15:B:284:LEU:HD21	1.97	0.46
16:A:1574:SER:O	16:A:1577:THR:OG1	2.28	0.46
16:A:1611:PRO:HB3	16:A:1660:ILE:HG23	1.98	0.46
3:5:549:ARG:NE	17:5:802:AGS:O2G	2.49	0.46
6:7:451:ARG:O	6:7:694:ARG:NH2	2.46	0.46
9:E:20:PHE:HA	9:E:72:VAL:HA	1.97	0.46
10:F:210:ASN:HA	10:F:218:MET:HG3	1.98	0.46
11:G:527:LEU:HD11	11:G:641:LEU:HD13	1.98	0.46
15:B:419:LYS:HD2	15:B:687:ILE:HD12	1.98	0.46
16:A:1491:PRO:HB3	16:A:1599:LYS:HE3	1.98	0.46
2:4:251:TYR:CE2	2:4:253:GLN:HB3	2.51	0.45
6:7:527:ASP:O	6:7:534:ARG:NH2	2.49	0.45
12:X:14:DC:H1'	12:X:15:DC:H5'	1.97	0.45
14:J:5:DT:H2'	14:J:6:DT:C5	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:362:LEU:HA	15:B:379:LEU:HA	1.98	0.45
2:4:518:LEU:HG	2:4:522:LEU:HD23	1.97	0.45
2:4:721:ALA:O	2:4:725:THR:OG1	2.22	0.45
2:4:722:LYS:HE2	6:7:661:VAL:HG11	1.99	0.45
3:5:423:SER:OG	17:5:801:AGS:O3G	2.33	0.45
6:7:550:LYS:HB2	6:7:553:ILE:HB	1.99	0.45
7:C:166:ARG:NH1	7:C:188:GLN:OE1	2.49	0.45
15:B:173:ILE:HB	15:B:531:ARG:HB2	1.98	0.45
1:3:409:GLY:HA3	1:3:549:VAL:HB	1.98	0.45
2:4:197:PHE:HB2	2:4:254:THR:HG21	1.97	0.45
3:5:535:SER:OG	3:5:538:ASP:OD2	2.35	0.45
6:7:457:CYS:SG	6:7:458:LEU:N	2.89	0.45
11:G:145:ASP:HA	11:G:146:GLY:HA2	1.74	0.45
15:B:541:ILE:HA	15:B:640:VAL:HB	1.98	0.45
16:A:1784:SER:O	16:A:1835:HIS:NE2	2.49	0.45
1:3:277:ILE:HD12	1:3:320:LEU:HD13	1.98	0.45
1:3:565:VAL:HG12	1:3:569:HIS:HE1	1.81	0.45
4:6:123:SER:HB2	4:6:135:VAL:HB	1.99	0.45
5:2:294:HIS:CE1	5:2:296:ARG:HH22	2.34	0.45
5:2:398:PRO:HB2	5:2:401:ARG:HH11	1.81	0.45
5:2:788:ARG:HH12	16:A:2069:ILE:HB	1.82	0.45
7:C:130:TYR:CG	10:F:193:LEU:HD22	2.52	0.45
11:G:429:THR:HA	11:G:432:LEU:HG	1.99	0.45
13:Y:16:DG:H1'	13:Y:17:DG:H5'	1.98	0.45
15:B:328:VAL:HG12	15:B:344:MET:HA	1.99	0.45
4:6:175:TYR:HA	4:6:178:LEU:HD13	1.98	0.45
11:G:38:ALA:HA	11:G:251:ILE:HD11	1.98	0.45
12:X:20:DT:H1'	12:X:21:DA:H5'	1.98	0.45
15:B:546:LEU:HD13	15:B:546:LEU:HA	1.82	0.45
3:5:155:HIS:O	3:5:298:TYR:HB3	2.16	0.45
4:6:609:THR:HG23	4:6:661:ILE:HD13	1.98	0.45
10:F:237:ASP:OD2	10:F:248:GLU:N	2.49	0.45
1:3:416:SER:HA	1:3:419:LEU:HD12	1.99	0.45
3:5:299:SER:HB3	3:5:327:TYR:CZ	2.52	0.45
3:5:489:ASP:OD1	5:2:632:SER:OG	2.35	0.45
4:6:390:LYS:HD3	5:2:401:ARG:HH21	1.82	0.45
5:2:208:ALA:HB1	5:2:274:VAL:HG21	1.98	0.45
13:Y:15:DT:H1'	13:Y:16:DG:H5'	1.99	0.45
16:A:1575:GLN:O	16:A:1578:THR:OG1	2.32	0.45
16:A:1714:ASN:C	16:A:1716:SER:H	2.24	0.45
2:4:716:ASN:O	2:4:720:LEU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:356:TRP:HZ3	4:6:358:LYS:HB2	1.82	0.45
5:2:633:LYS:NZ	14:J:5:DT:OP1	2.49	0.45
9:E:96:ASP:OD1	9:E:168:LYS:HB2	2.17	0.45
10:F:94:GLN:HA	10:F:97:LEU:HB3	1.99	0.45
12:X:2:DC:H1'	12:X:3:DA:H5'	1.99	0.45
2:4:345:ALA:HB2	2:4:365:ILE:HD13	1.99	0.44
3:5:552:MET:HE2	3:5:552:MET:HB3	1.82	0.44
3:5:585:ASN:O	3:5:589:GLU:HG2	2.17	0.44
9:E:85:MET:O	9:E:89:LYS:HG3	2.17	0.44
12:X:8:DC:H1'	12:X:9:DG:H5'	1.98	0.44
1:3:201:HIS:HA	1:3:243:THR:HA	1.99	0.44
2:4:398:LYS:HA	2:4:416:SER:HA	1.99	0.44
2:4:592:SER:HA	2:4:632:ASP:HB2	1.97	0.44
2:4:601:LEU:HA	2:4:620:ALA:HB3	1.98	0.44
8:D:134:PHE:HD2	8:D:137:PRO:HG3	1.82	0.44
11:G:89:VAL:O	11:G:130:ASN:ND2	2.49	0.44
13:Y:20:DG:H1'	13:Y:21:DC:H5'	1.99	0.44
16:A:1896:SER:HA	16:A:1898:LEU:HD23	1.99	0.44
5:2:384:ASN:OD1	5:2:384:ASN:N	2.49	0.44
6:7:133:ASP:H	6:7:136:ASP:HB2	1.81	0.44
6:7:715:GLU:OE2	6:7:718:ARG:NH1	2.35	0.44
10:F:220:ASP:HA	10:F:221:GLU:HA	1.80	0.44
15:B:318:HIS:HA	15:B:601:LYS:HD2	2.00	0.44
16:A:1733:ASP:HB3	16:A:1906:TRP:CD1	2.52	0.44
3:5:561:ASN:HB2	3:5:564:ARG:HB3	2.00	0.44
6:7:374:THR:OG1	6:7:375:TYR:N	2.51	0.44
7:C:4:ASP:OD1	7:C:4:ASP:N	2.48	0.44
12:X:4:DG:H1'	12:X:5:DC:H5'	1.99	0.44
3:5:627:VAL:HG11	15:B:276:GLY:HA2	1.98	0.44
6:7:398:GLU:HA	6:7:401:VAL:HB	1.99	0.44
9:E:72:VAL:HG12	9:E:74:LEU:H	1.83	0.44
9:E:165:PHE:O	9:E:168:LYS:HG2	2.18	0.44
12:X:12:DG:H1'	12:X:13:DG:H5'	1.99	0.44
16:A:1733:ASP:HB3	16:A:1906:TRP:HB2	1.99	0.44
2:4:729:LEU:HD23	6:7:652:MET:HE3	2.00	0.44
3:5:431:LYS:HB3	3:5:431:LYS:HE3	1.77	0.44
6:7:423:TYR:HB2	6:7:615:HIS:CD2	2.53	0.44
7:C:48:ARG:HA	7:C:51:THR:HB	1.99	0.44
8:D:194:GLU:O	8:D:198:ALA:HB2	2.15	0.44
9:E:85:MET:O	9:E:88:ILE:HG12	2.17	0.44
11:G:328:LEU:O	11:G:332:SER:OG	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:X:3:DA:H1'	12:X:4:DG:H5'	2.00	0.44
1:3:53:ALA:O	1:3:57:ASN:ND2	2.50	0.44
2:4:342:MET:HE1	2:4:386:HIS:HB2	2.00	0.44
5:2:297:ILE:N	5:2:455:SER:OG	2.47	0.44
8:D:19:ILE:O	8:D:22:ASN:ND2	2.51	0.44
9:E:20:PHE:CD2	9:E:24:ILE:HD13	2.52	0.44
10:F:137:LYS:O	10:F:141:ARG:HG3	2.17	0.44
12:X:5:DC:H1'	12:X:6:DC:H5'	1.99	0.44
3:5:610:CYS:SG	3:5:612:PRO:HD3	2.58	0.44
4:6:148:LEU:O	4:6:150:THR:N	2.51	0.44
4:6:534:ALA:HB3	4:6:544:LYS:HD3	1.99	0.44
6:7:517:ASP:HA	6:7:561:THR:HG22	2.00	0.44
7:C:125:HIS:CD2	15:B:361:ASN:HD22	2.35	0.44
14:J:6:DT:H1'	14:J:7:DT:C2	2.53	0.44
16:A:1739:LEU:O	16:A:1743:THR:OG1	2.20	0.44
16:A:1808:THR:O	16:A:1812:LEU:HB2	2.18	0.44
1:3:194:PRO:HA	1:3:252:ASP:HA	1.99	0.44
3:5:595:SER:OG	3:5:597:GLU:HG2	2.17	0.44
4:6:552:LEU:HD21	4:6:758:ALA:HB1	2.00	0.44
7:C:178:TYR:CE1	15:B:19:PRO:HG2	2.53	0.44
11:G:66:GLU:OE2	11:G:70:HIS:NE2	2.51	0.44
3:5:366:LEU:HA	3:5:369:ILE:HG22	1.98	0.43
4:6:746:PHE:HA	4:6:750:GLN:HE21	1.83	0.43
10:F:62:ASP:HA	10:F:65:LYS:HB3	2.00	0.43
15:B:399:PHE:HD2	15:B:675:TYR:HD2	1.66	0.43
16:A:1338:VAL:H	16:A:1349:ILE:HG22	1.82	0.43
16:A:2178:HIS:ND1	16:A:2179:CYS:O	2.51	0.43
1:3:206:THR:HB	1:3:208:ARG:HH21	1.83	0.43
2:4:592:SER:OG	2:4:593:GLY:N	2.51	0.43
4:6:398:THR:OG1	4:6:458:HIS:O	2.25	0.43
11:G:268:SER:O	11:G:272:LEU:HG	2.18	0.43
2:4:206:ARG:HA	2:4:209:LEU:HB3	1.99	0.43
2:4:818:GLU:HG3	2:4:820:GLU:H	1.83	0.43
6:7:526:PHE:HZ	6:7:534:ARG:HA	1.83	0.43
15:B:633:CYS:HA	15:B:634:PRO:HA	1.78	0.43
16:A:1939:TRP:HA	16:A:1942:LYS:HB2	1.99	0.43
1:3:194:PRO:O	6:7:372:THR:OG1	2.32	0.43
1:3:399:LEU:HD22	6:7:620:HIS:HE1	1.82	0.43
3:5:48:ASP:HA	3:5:51:ARG:HE	1.82	0.43
3:5:601:ARG:O	3:5:604:THR:OG1	2.31	0.43
4:6:460:ILE:HD12	4:6:460:ILE:HA	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:796:THR:HG22	4:6:798:ARG:H	1.83	0.43
6:7:517:ASP:HB2	6:7:560:ARG:HB2	2.00	0.43
8:D:56:ASP:HB3	10:F:57:GLN:HA	2.00	0.43
10:F:277:MET:HB3	10:F:277:MET:HE2	1.73	0.43
11:G:89:VAL:HB	11:G:90:ILE:HD12	2.00	0.43
11:G:637:LEU:O	11:G:641:LEU:HG	2.19	0.43
16:A:2158:LEU:HA	16:A:2158:LEU:HD23	1.76	0.43
1:3:183:GLU:OE1	1:3:183:GLU:N	2.51	0.43
3:5:170:SER:HB3	3:5:254:GLN:O	2.18	0.43
3:5:393:MET:HB3	3:5:665:LYS:HD2	2.00	0.43
5:2:523:VAL:HG21	5:2:776:PRO:HD2	2.01	0.43
9:E:112:ILE:HG23	9:E:113:MET:HE2	2.01	0.43
11:G:120:ILE:H	11:G:139:ILE:HB	1.82	0.43
15:B:172:VAL:HA	15:B:532:ILE:HA	2.00	0.43
16:A:1679:LYS:HD3	16:A:1682:LYS:HD2	2.00	0.43
16:A:1690:ASN:OD1	16:A:1690:ASN:N	2.52	0.43
2:4:804:LEU:HD21	2:4:828:LEU:HD12	2.00	0.43
4:6:108:GLY:O	4:6:112:ARG:HB2	2.18	0.43
8:D:21:GLU:OE1	10:F:135:ARG:NE	2.51	0.43
8:D:23:GLU:O	8:D:73:LEU:N	2.52	0.43
8:D:94:THR:HG22	8:D:96:LYS:HG2	2.01	0.43
16:A:1489:HIS:CE1	16:A:1599:LYS:HB2	2.53	0.43
1:3:92:LEU:HA	1:3:92:LEU:HD23	1.85	0.43
2:4:385:ILE:HG22	2:4:387:ASN:H	1.82	0.43
2:4:563:ASN:OD1	2:4:671:ILE:N	2.52	0.43
5:2:327:ARG:HH22	5:2:419:LYS:HA	1.84	0.43
8:D:163:LEU:HB3	8:D:189:MET:HE1	2.00	0.43
9:E:98:HIS:HA	9:E:102:SER:HB2	2.01	0.43
1:3:363:LEU:HD23	1:3:363:LEU:HA	1.84	0.43
1:3:559:ARG:O	1:3:562:SER:OG	2.25	0.43
2:4:425:ASP:OD2	4:6:277:ARG:NH2	2.49	0.43
3:5:469:MET:HE3	3:5:493:ILE:HD12	2.00	0.43
5:2:327:ARG:NH2	5:2:416:ASP:OD1	2.49	0.43
8:D:148:LEU:HA	8:D:151:ILE:HG12	2.00	0.43
15:B:480:THR:HA	15:B:522:ASN:HB3	2.00	0.43
16:A:1596:PHE:HA	16:A:1597:ILE:HA	1.73	0.43
2:4:574:LYS:HE3	2:4:708:VAL:HG21	2.00	0.43
15:B:421:LEU:O	15:B:425:ASN:ND2	2.52	0.43
15:B:643:ASP:OD2	15:B:646:SER:N	2.50	0.43
16:A:2141:LEU:HD23	16:A:2141:LEU:HA	1.87	0.43
16:A:2164:CYS:SG	16:A:2166:ARG:N	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:100:LEU:HB3	1:3:111:TRP:CH2	2.54	0.43
1:3:537:ASP:HA	1:3:540:LEU:HD13	2.01	0.43
3:5:169:THR:HA	3:5:256:LEU:HA	1.99	0.43
4:6:589:VAL:HG21	4:6:597:TYR:HB2	1.99	0.43
8:D:13:PRO:HB2	9:E:190:TRP:CD1	2.54	0.43
16:A:1917:PHE:HB2	16:A:1933:TYR:CE2	2.54	0.43
2:4:572:THR:HB	2:4:574:LYS:HG3	2.01	0.42
3:5:44:PHE:CE2	3:5:47:ARG:HB3	2.54	0.42
4:6:306:LYS:HD3	4:6:306:LYS:HA	1.69	0.42
5:2:232:ARG:O	5:2:283:TYR:OH	2.34	0.42
15:B:214:LYS:HB2	15:B:624:TRP:CE2	2.54	0.42
16:A:1322:TRP:HA	16:A:1340:VAL:HG12	2.00	0.42
16:A:1615:LEU:HB3	16:A:1616:SER:H	1.68	0.42
2:4:441:SER:HA	2:4:459:THR:HA	2.01	0.42
5:2:324:VAL:HG21	5:2:418:SER:HB2	2.00	0.42
5:2:567:THR:OG1	5:2:568:GLY:N	2.52	0.42
6:7:599:LEU:HD22	6:7:727:LEU:HD23	2.01	0.42
3:5:420:THR:HG21	3:5:556:VAL:HG11	2.01	0.42
6:7:581:LEU:HA	6:7:584:ILE:HD12	2.00	0.42
6:7:636:SER:HA	6:7:639:ARG:HE	1.85	0.42
7:C:157:PRO:HD2	8:D:14:GLU:OE1	2.19	0.42
1:3:100:LEU:HD23	1:3:100:LEU:HA	1.87	0.42
6:7:276:ARG:HA	6:7:276:ARG:HD3	1.82	0.42
1:3:376:HIS:HB2	1:3:735:PHE:CE2	2.54	0.42
1:3:409:GLY:O	1:3:415:LYS:NZ	2.45	0.42
2:4:443:PRO:HB3	2:4:457:TYR:CE1	2.54	0.42
3:5:579:ASN:HB2	3:5:582:ALA:HB3	2.01	0.42
3:5:622:LEU:HA	3:5:622:LEU:HD23	1.78	0.42
4:6:112:ARG:HH12	4:6:187:ARG:NH1	2.16	0.42
4:6:390:LYS:HD2	4:6:391:PRO:HD2	2.01	0.42
4:6:802:SER:HA	4:6:805:ARG:HG2	2.01	0.42
7:C:22:ARG:HB3	7:C:23:SER:HA	2.02	0.42
10:F:79:TYR:CE2	10:F:81:HIS:HB3	2.53	0.42
11:G:487:ARG:HG3	11:G:488:LYS:HG3	2.00	0.42
11:G:510:GLY:HA3	11:G:551:TRP:CH2	2.55	0.42
13:Y:14:DG:H1'	13:Y:15:DT:H5'	1.99	0.42
16:A:2173:ASP:OD1	16:A:2173:ASP:N	2.53	0.42
1:3:103:LEU:HD23	1:3:103:LEU:HA	1.88	0.42
3:5:48:ASP:OD1	3:5:51:ARG:NE	2.51	0.42
3:5:102:SER:O	3:5:105:SER:OG	2.35	0.42
3:5:471:LEU:HD23	3:5:471:LEU:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:533:LEU:HA	3:5:533:LEU:HD23	1.82	0.42
5:2:411:LEU:HB3	5:2:412:ALA:H	1.70	0.42
5:2:770:ALA:O	5:2:774:ILE:HG22	2.20	0.42
15:B:10:VAL:HG11	15:B:47:THR:HA	2.01	0.42
16:A:1723:ASN:HA	16:A:2060:HIS:NE2	2.35	0.42
16:A:1745:LEU:HB2	16:A:1897:TYR:CE2	2.54	0.42
4:6:171:SER:HA	4:6:287:LEU:HD13	2.02	0.42
4:6:279:ILE:HG21	4:6:452:ILE:HG21	2.01	0.42
4:6:412:LEU:HD22	4:6:449:THR:HG21	2.01	0.42
6:7:696:SER:HA	6:7:699:LEU:HD12	2.02	0.42
7:C:172:GLY:HA2	7:C:173:GLU:HA	1.79	0.42
10:F:147:ARG:O	10:F:151:ILE:HG12	2.19	0.42
11:G:15:ILE:O	11:G:19:SER:OG	2.23	0.42
14:J:4:DT:H6	14:J:4:DT:H2'	1.67	0.42
1:3:417:GLN:NE2	3:5:404:MET:HB2	2.32	0.42
2:4:450:GLN:CD	13:Y:4:DA:H5''	2.45	0.42
3:5:178:TYR:HA	3:5:193:THR:HA	2.01	0.42
3:5:666:LEU:HD23	3:5:666:LEU:HA	1.82	0.42
5:2:484:PHE:HZ	5:2:766:TYR:HD1	1.68	0.42
5:2:628:SER:HB3	5:2:641:GLN:HG2	2.01	0.42
10:F:200:LYS:HB2	10:F:201:TYR:CD2	2.54	0.42
11:G:620:VAL:HG22	11:G:632:ILE:HD13	2.01	0.42
15:B:686:GLU:HG2	15:B:688:TYR:H	1.84	0.42
16:A:1586:LEU:HD23	16:A:1586:LEU:HA	1.91	0.42
4:6:164:GLY:HA2	4:6:167:ALA:HB3	2.01	0.42
4:6:773:LEU:HD12	4:6:824:ILE:HD12	2.02	0.42
6:7:227:VAL:HA	6:7:230:ILE:HD12	2.02	0.42
6:7:550:LYS:HE2	6:7:553:ILE:HD13	2.02	0.42
6:7:661:VAL:O	6:7:665:ILE:HG12	2.20	0.42
10:F:200:LYS:H	10:F:201:TYR:HB2	1.84	0.42
11:G:525:TYR:HB2	11:G:566:PRO:HG2	2.01	0.42
1:3:477:LYS:HB3	3:5:491:VAL:HG21	2.01	0.42
3:5:167:ILE:H	3:5:258:LEU:HA	1.84	0.42
3:5:282:LEU:HD22	3:5:333:ILE:HG22	2.01	0.42
4:6:298:SER:O	5:2:404:ARG:NH1	2.53	0.42
4:6:736:MET:O	4:6:740:GLU:HB3	2.20	0.42
7:C:36:ILE:O	7:C:40:ILE:HG13	2.20	0.42
8:D:107:THR:HG23	8:D:108:HIS:ND1	2.35	0.42
10:F:224:TRP:O	10:F:280:GLU:N	2.53	0.42
16:A:1503:LYS:HE2	16:A:1505:TRP:HB2	2.01	0.42
2:4:284:ILE:HG13	2:4:290:ASP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:799:GLU:HA	2:4:802:ILE:HG12	2.02	0.41
5:2:231:ILE:HG23	5:2:279:THR:HG23	2.02	0.41
5:2:619:SER:OG	5:2:620:ILE:N	2.53	0.41
7:C:4:ASP:O	7:C:8:LYS:HG2	2.20	0.41
8:D:161:LYS:HA	9:E:133:GLN:NE2	2.33	0.41
13:Y:6:DC:H1'	13:Y:7:DG:H5'	2.02	0.41
15:B:433:ILE:HG13	15:B:482:ILE:HD12	2.01	0.41
16:A:1905:TYR:HB2	16:A:1920:LEU:HD13	2.00	0.41
1:3:282:LEU:HD23	1:3:282:LEU:HA	1.85	0.41
2:4:592:SER:HA	2:4:632:ASP:H	1.85	0.41
11:G:561:ASP:HA	11:G:562:LYS:HA	1.87	0.41
16:A:2071:GLU:HG2	16:A:2072:ILE:HG12	2.01	0.41
4:6:573:VAL:HA	4:6:712:PHE:O	2.21	0.41
4:6:648:ASP:O	4:6:652:ILE:HG12	2.19	0.41
4:6:702:THR:HG22	4:6:705:ILE:HG12	2.02	0.41
11:G:337:SER:O	11:G:341:SER:OG	2.25	0.41
16:A:1594:SER:HB3	16:A:1596:PHE:HE1	1.85	0.41
16:A:2189:LEU:HD12	16:A:2189:LEU:HA	1.90	0.41
1:3:347:ILE:HA	1:3:350:ILE:HD12	2.02	0.41
1:3:377:ILE:HG12	1:3:547:PHE:CE2	2.55	0.41
3:5:39:ARG:NH1	8:D:139:HIS:HA	2.35	0.41
3:5:138:ILE:HG23	3:5:332:GLY:HA2	2.03	0.41
3:5:353:GLU:HB3	3:5:357:PHE:CZ	2.55	0.41
3:5:631:LYS:HB3	3:5:631:LYS:HE3	1.87	0.41
4:6:517:LYS:HD2	4:6:517:LYS:HA	1.91	0.41
4:6:646:ILE:H	4:6:646:ILE:HG13	1.46	0.41
5:2:226:VAL:O	5:2:230:ARG:CB	2.68	0.41
5:2:576:LEU:HD23	5:2:576:LEU:HA	1.85	0.41
5:2:620:ILE:HG23	5:2:646:ILE:HD13	2.01	0.41
7:C:50:ASN:O	7:C:54:LEU:HG	2.21	0.41
11:G:61:ILE:HD12	11:G:61:ILE:H	1.85	0.41
16:A:1523:ILE:HG13	16:A:1526:SER:H	1.85	0.41
2:4:344:VAL:O	2:4:389:CYS:HB2	2.21	0.41
3:5:49:GLN:NE2	3:5:62:THR:OG1	2.54	0.41
4:6:119:LEU:HD11	4:6:188:VAL:HG21	2.03	0.41
4:6:393:ASP:OD1	4:6:394:ARG:N	2.54	0.41
8:D:166:SER:OG	10:F:278:ARG:NH2	2.51	0.41
16:A:1535:MET:O	16:A:1539:LYS:N	2.46	0.41
3:5:104:LEU:HA	8:D:154:ILE:HD13	2.02	0.41
3:5:388:ILE:HD11	3:5:425:LEU:HD21	2.02	0.41
4:6:303:GLU:N	4:6:354:LEU:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:309:ALA:HB3	6:7:337:GLY:H	1.84	0.41
6:7:689:LEU:HD12	6:7:689:LEU:HA	1.88	0.41
9:E:48:LEU:O	9:E:52:ARG:CB	2.61	0.41
10:F:196:ASP:HA	10:F:200:LYS:HD3	2.03	0.41
11:G:12:TYR:O	11:G:16:LEU:HG	2.20	0.41
1:3:553:ILE:H	1:3:553:ILE:HG13	1.73	0.41
2:4:505:ASP:OD1	2:4:505:ASP:N	2.54	0.41
15:B:271:ILE:HD13	15:B:305:VAL:HG12	2.03	0.41
2:4:777:MET:HE1	2:4:833:ILE:HD13	2.02	0.41
3:5:421:ALA:HB2	17:5:801:AGS:N3	2.36	0.41
4:6:298:SER:HG	4:6:358:LYS:H	1.66	0.41
4:6:631:ALA:O	4:6:676:THR:HG22	2.21	0.41
5:2:603:VAL:HG22	5:2:645:SER:HB2	2.02	0.41
5:2:806:THR:HG22	5:2:809:HIS:H	1.85	0.41
16:A:1489:HIS:NE2	16:A:1595:PRO:HA	2.36	0.41
2:4:382:MET:HE2	2:4:382:MET:HB3	1.82	0.41
3:5:486:ARG:NH2	3:5:488:GLU:OE2	2.47	0.41
3:5:526:ILE:H	3:5:526:ILE:HG13	1.65	0.41
4:6:364:ASN:ND2	4:6:394:ARG:HH12	2.19	0.41
4:6:559:THR:OG1	4:6:563:ILE:O	2.35	0.41
5:2:430:TYR:HD1	5:2:451:ILE:HG12	1.86	0.41
7:C:103:ASN:OD1	7:C:104:ASN:N	2.52	0.41
9:E:97:LEU:HG	9:E:131:ARG:HH22	1.85	0.41
10:F:74:PRO:HD2	10:F:279:TYR:CZ	2.56	0.41
10:F:284:ASP:OD1	10:F:285:LEU:N	2.53	0.41
11:G:494:ARG:HE	11:G:498:LEU:HD11	1.85	0.41
3:5:497:MET:HB2	3:5:497:MET:HE3	1.77	0.41
5:2:333:GLN:O	5:2:383:ARG:N	2.54	0.41
5:2:843:ASP:N	5:2:843:ASP:OD1	2.52	0.41
6:7:678:LYS:HG3	6:7:679:PHE:H	1.86	0.41
11:G:252:SER:OG	11:G:273:ASN:OD1	2.39	0.41
11:G:266:ASN:HB2	11:G:269:ASN:HB2	2.03	0.41
16:A:1731:VAL:HG22	16:A:1870:THR:HG22	2.03	0.41
3:5:65:MET:HA	3:5:68:LEU:HD12	2.02	0.40
3:5:571:HIS:CE1	3:5:575:ILE:HD11	2.56	0.40
4:6:767:LYS:C	4:6:770:ARG:HH21	2.29	0.40
5:2:567:THR:HG21	5:2:571:ALA:N	2.35	0.40
6:7:484:THR:OG1	6:7:485:GLY:N	2.55	0.40
8:D:52:LEU:HD12	8:D:52:LEU:HA	1.84	0.40
8:D:117:TRP:NE1	8:D:175:LEU:HB2	2.36	0.40
10:F:83:LEU:O	10:F:86:ARG:HG2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:206:LEU:HD23	10:F:206:LEU:HA	1.91	0.40
15:B:396:ASP:O	15:B:430:THR:OG1	2.38	0.40
1:3:679:ILE:HB	1:3:705:LEU:HD13	2.04	0.40
4:6:157:HIS:HA	4:6:160:MET:HG2	2.02	0.40
4:6:791:SER:HB3	4:6:793:TYR:CZ	2.56	0.40
6:7:615:HIS:O	6:7:619:VAL:HG23	2.20	0.40
8:D:175:LEU:HA	8:D:178:ILE:HD12	2.02	0.40
16:A:1335:VAL:HG22	16:A:1352:HIS:HB3	2.03	0.40
16:A:1513:VAL:HG23	16:A:1565:ASP:H	1.86	0.40
1:3:376:HIS:HB2	1:3:735:PHE:CD2	2.56	0.40
2:4:536:VAL:HG22	2:4:706:TYR:CE1	2.57	0.40
3:5:39:ARG:HH12	8:D:139:HIS:HA	1.85	0.40
4:6:280:ARG:H	4:6:283:LYS:HG3	1.87	0.40
6:7:573:ARG:HD3	6:7:602:ASP:HB3	2.03	0.40
8:D:118:ASN:OD1	8:D:118:ASN:N	2.46	0.40
8:D:158:LYS:O	8:D:161:LYS:HG2	2.21	0.40
10:F:72:CYS:SG	10:F:293:LEU:HB3	2.61	0.40
10:F:270:THR:H	10:F:275:TYR:HE2	1.70	0.40
16:A:1418:PHE:CD2	16:A:1426:VAL:HG22	2.57	0.40
16:A:1546:TYR:HB3	16:A:1549:LEU:HD12	2.02	0.40
3:5:414:LEU:HA	3:5:414:LEU:HD23	1.91	0.40
7:C:178:TYR:HE1	15:B:19:PRO:HG2	1.85	0.40
8:D:112:PHE:HB3	8:D:152:ARG:NH1	2.37	0.40
9:E:47:PRO:HD2	9:E:50:LEU:HD11	2.04	0.40
10:F:79:TYR:HA	10:F:147:ARG:HH22	1.86	0.40
11:G:328:LEU:HD23	11:G:328:LEU:HA	1.85	0.40
12:X:13:DG:H1'	12:X:14:DC:H5'	2.03	0.40
13:Y:1:DT:H1'	13:Y:2:DA:H5'	2.03	0.40
13:Y:4:DA:H1'	13:Y:5:DA:H5'	2.03	0.40
15:B:607:LEU:HD23	15:B:607:LEU:HA	1.81	0.40
16:A:1745:LEU:HA	16:A:1745:LEU:HD23	1.88	0.40
16:A:2189:LEU:HD12	16:A:2190:PRO:HD2	2.02	0.40
1:3:672:THR:OG1	1:3:721:VAL:O	2.32	0.40
2:4:315:ARG:O	6:7:341:ARG:NE	2.54	0.40
2:4:326:ILE:HG22	2:4:328:LEU:HG	2.04	0.40
5:2:538:ASN:HB2	5:2:678:ASP:H	1.86	0.40
5:2:606:ILE:HG22	5:2:609:PHE:HE1	1.86	0.40
5:2:792:ASP:O	5:2:796:GLU:HB2	2.21	0.40
6:7:73:ARG:HA	6:7:199:ARG:HH22	1.87	0.40
8:D:119:TRP:NE1	8:D:174:SER:HB2	2.36	0.40
16:A:1632:LEU:O	16:A:1636:VAL:N	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:2044:HIS:CD2	16:A:2048:LYS:HD2	2.57	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	3	542/971 (56%)	500 (92%)	40 (7%)	2 (0%)	30	67
2	4	569/933 (61%)	508 (89%)	60 (10%)	1 (0%)	43	77
3	5	598/775 (77%)	547 (92%)	51 (8%)	0	100	100
4	6	551/1017 (54%)	496 (90%)	55 (10%)	0	100	100
5	2	527/868 (61%)	483 (92%)	44 (8%)	0	100	100
6	7	588/845 (70%)	539 (92%)	48 (8%)	1 (0%)	43	77
7	C	188/208 (90%)	177 (94%)	10 (5%)	1 (0%)	24	63
8	D	177/213 (83%)	164 (93%)	10 (6%)	3 (2%)	7	34
9	E	151/194 (78%)	143 (95%)	8 (5%)	0	100	100
10	F	206/294 (70%)	184 (89%)	21 (10%)	1 (0%)	24	63
11	G	525/650 (81%)	478 (91%)	44 (8%)	3 (1%)	21	58
15	B	441/689 (64%)	390 (88%)	50 (11%)	1 (0%)	43	77
16	A	751/914 (82%)	553 (74%)	193 (26%)	5 (1%)	18	55
All	All	5814/8571 (68%)	5162 (89%)	634 (11%)	18 (0%)	37	72

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	4	374	ILE
8	D	54	THR

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Mol	Chain	Res	Type
8	D	113	SER
8	D	171	ASP
11	G	284	TYR
16	A	1657	ASN
11	G	602	LEU
1	3	173	ALA
1	3	175	HIS
10	F	171	LEU
16	A	1715	ASP
7	C	27	VAL
11	G	489	VAL
15	B	443	VAL
16	A	1668	MET
16	A	1875	PRO
16	A	2029	ASP
6	7	462	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	
1	3	458/835 (55%)	456 (100%)	2 (0%)	84	83
2	4	493/848 (58%)	490 (99%)	3 (1%)	78	81
3	5	488/688 (71%)	486 (100%)	2 (0%)	84	83
4	6	435/886 (49%)	433 (100%)	2 (0%)	81	82
5	2	435/770 (56%)	435 (100%)	0	100	100
6	7	524/753 (70%)	522 (100%)	2 (0%)	84	83
7	C	149/193 (77%)	149 (100%)	0	100	100
8	D	156/198 (79%)	155 (99%)	1 (1%)	78	81
9	E	135/173 (78%)	135 (100%)	0	100	100
10	F	194/279 (70%)	194 (100%)	0	100	100
11	G	443/586 (76%)	442 (100%)	1 (0%)	87	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	B	409/629 (65%)	408 (100%)	1 (0%)	87	86
16	A	624/837 (75%)	614 (98%)	10 (2%)	55	69
All	All	4943/7675 (64%)	4919 (100%)	24 (0%)	78	82

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3	320	LEU
1	3	553	ILE
2	4	442	ILE
2	4	636	LYS
2	4	692	ILE
3	5	265	VAL
3	5	573	ILE
4	6	140	ILE
4	6	306	LYS
6	7	418	ILE
6	7	476	ILE
8	D	118	ASN
11	G	33	CYS
15	B	11	LYS
16	A	1325	LEU
16	A	1362	LYS
16	A	1408	LEU
16	A	1592	LEU
16	A	1658	ILE
16	A	1686	VAL
16	A	1791	LEU
16	A	1795	LEU
16	A	1887	LYS
16	A	1902	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	3	29	GLN
1	3	57	ASN
1	3	417	GLN
1	3	492	GLN
1	3	532	ASN

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Mol	Chain	Res	Type
1	3	569	HIS
1	3	688	ASN
2	4	231	ASN
2	4	450	GLN
2	4	582	HIS
3	5	33	ASN
3	5	49	GLN
3	5	53	ASN
3	5	58	ASN
3	5	185	ASN
3	5	411	ASN
3	5	494	HIS
3	5	571	HIS
3	5	581	ASN
3	5	632	GLN
4	6	125	GLN
4	6	658	GLN
4	6	659	GLN
4	6	698	ASN
4	6	730	HIS
4	6	750	GLN
5	2	248	HIS
5	2	290	HIS
5	2	386	GLN
5	2	627	GLN
6	7	30	GLN
6	7	89	GLN
6	7	90	ASN
6	7	95	GLN
6	7	455	ASN
6	7	585	ASN
6	7	620	HIS
7	C	28	ASN
7	C	50	ASN
7	C	90	GLN
7	C	122	ASN
7	C	201	GLN
7	C	202	GLN
8	D	22	ASN
8	D	167	HIS
8	D	172	ASN
9	E	98	HIS

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Mol	Chain	Res	Type
9	E	133	GLN
10	F	186	HIS
11	G	22	HIS
11	G	138	GLN
11	G	249	ASN
11	G	273	ASN
11	G	395	ASN
15	B	48	ASN
15	B	189	GLN
15	B	361	ASN
15	B	553	HIS
15	B	609	GLN
16	A	1385	ASN
16	A	1609	GLN
16	A	1657	ASN
16	A	1703	ASN
16	A	1742	ASN
16	A	1865	GLN
16	A	2143	GLN
16	A	2168	HIS

5.3.3 RNA [i](#)

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
17	AGS	5	801	-	32,33,33	1.48	4 (12%)	45,52,52	1.30	4 (8%)
17	AGS	5	802	-	32,33,33	1.17	3 (9%)	45,52,52	1.51	7 (15%)

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
17	AGS	5	801	-	-	9/21/38/38	0/3/3/3
17	AGS	5	802	-	-	5/21/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	801	AGS	PB-O3A	-5.00	1.54	1.59
17	5	801	AGS	PA-O3A	-4.69	1.54	1.59
17	5	802	AGS	PB-O3B	-4.37	1.54	1.59
17	5	801	AGS	PB-O3B	-3.82	1.55	1.59
17	5	802	AGS	PA-O3A	-2.50	1.56	1.59
17	5	802	AGS	PB-O3A	-2.38	1.56	1.59
17	5	801	AGS	PG-S1G	2.24	1.95	1.90

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	5	801	AGS	PB-O3B-PG	-6.16	110.64	133.17
17	5	802	AGS	C4'-O4'-C1'	-5.10	98.21	109.47
17	5	802	AGS	PB-O3B-PG	-4.42	116.98	133.17
17	5	802	AGS	O4'-C1'-C2'	-3.76	98.58	106.62
17	5	802	AGS	C1'-N9-C8	-2.96	120.53	127.09
17	5	801	AGS	O3A-PB-O1B	-2.90	101.99	110.70
17	5	802	AGS	C2'-C1'-N9	2.63	119.84	113.30
17	5	802	AGS	C4-N9-C1'	2.61	132.73	126.63
17	5	801	AGS	O2A-PA-O1A	2.21	122.72	112.44
17	5	802	AGS	C3'-C2'-C1'	-2.16	97.38	101.46
17	5	801	AGS	C2'-C1'-N9	2.10	118.52	113.30

There are no chirality outliers.

All (14) torsion outliers are listed below:

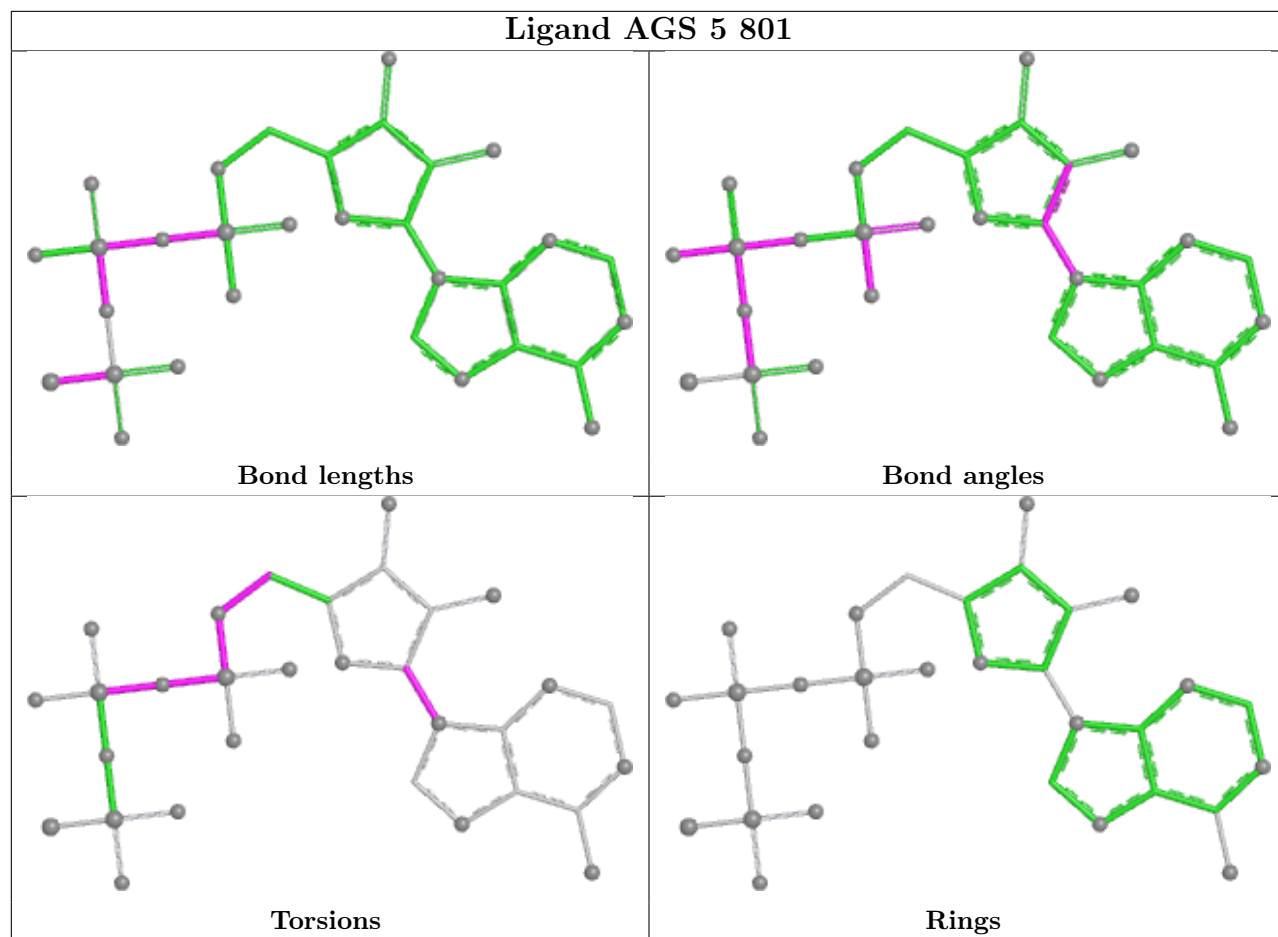
Mol	Chain	Res	Type	Atoms
17	5	801	AGS	C5'-O5'-PA-O1A
17	5	801	AGS	C5'-O5'-PA-O2A
17	5	801	AGS	C5'-O5'-PA-O3A
17	5	801	AGS	O4'-C1'-N9-C4
17	5	802	AGS	C5'-O5'-PA-O1A
17	5	802	AGS	C5'-O5'-PA-O2A
17	5	802	AGS	C5'-O5'-PA-O3A
17	5	802	AGS	C2'-C1'-N9-C8
17	5	802	AGS	C2'-C1'-N9-C4
17	5	801	AGS	O4'-C1'-N9-C8
17	5	801	AGS	PA-O3A-PB-O2B
17	5	801	AGS	C4'-C5'-O5'-PA
17	5	801	AGS	PA-O3A-PB-O1B
17	5	801	AGS	PB-O3A-PA-O1A

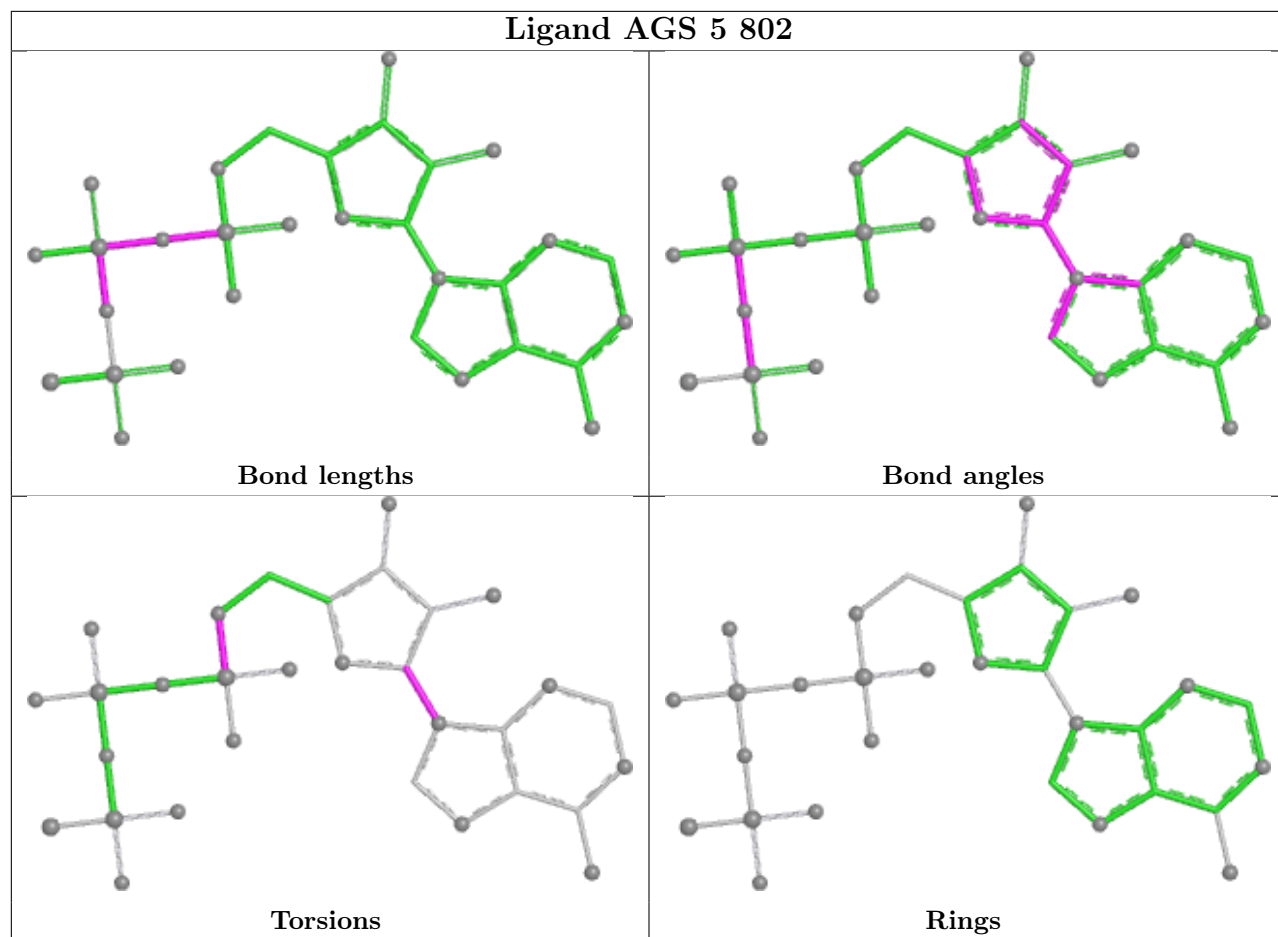
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	5	801	AGS	5	0
17	5	802	AGS	3	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
16	A	1
15	B	1
3	5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2060:HIS	C	2061:VAL	N	14.58
1	B	280:GLN	C	281:ASN	N	5.05
1	5	269:GLU	C	270:MET	N	1.09

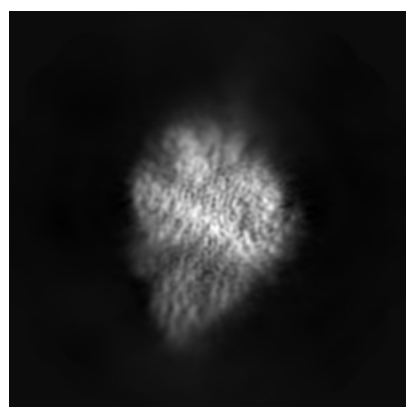
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0288. These allow visual inspection of the internal detail of the map and identification of artifacts.

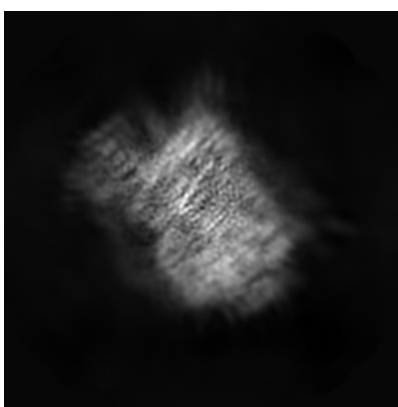
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

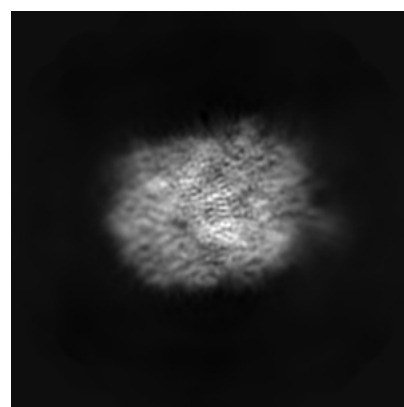
6.1.1 Primary map



X



Y

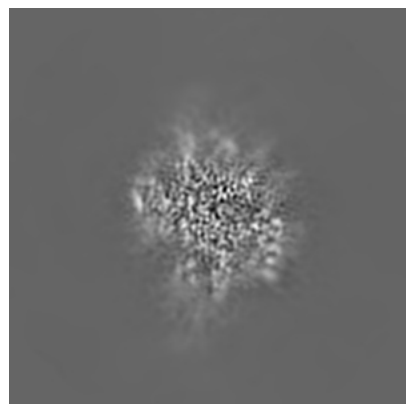


Z

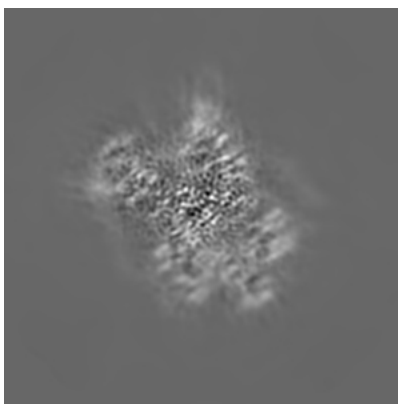
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

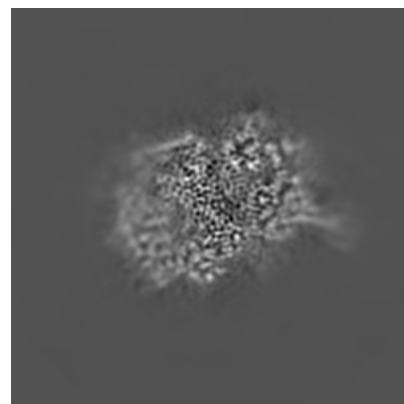
6.2.1 Primary map



X Index: 128



Y Index: 128

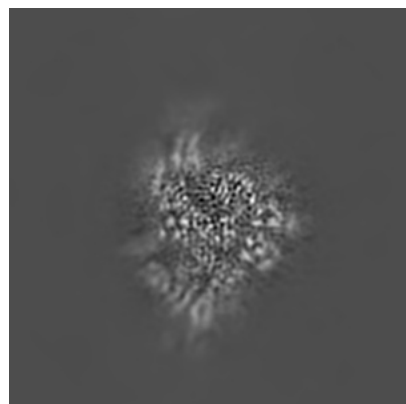


Z Index: 128

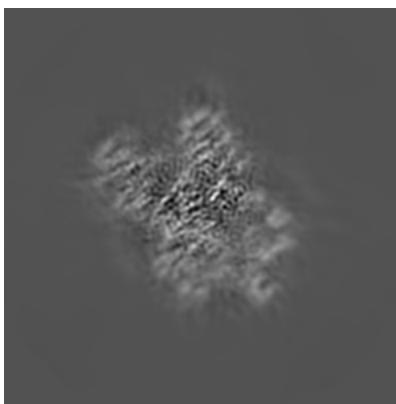
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

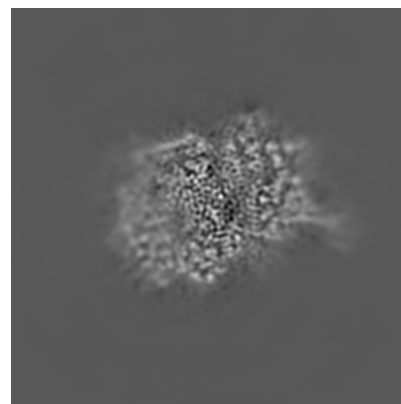
6.3.1 Primary map



X Index: 139



Y Index: 132

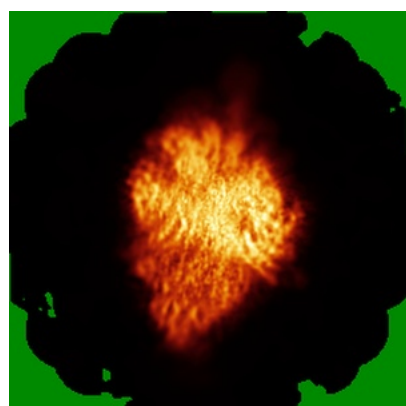


Z Index: 129

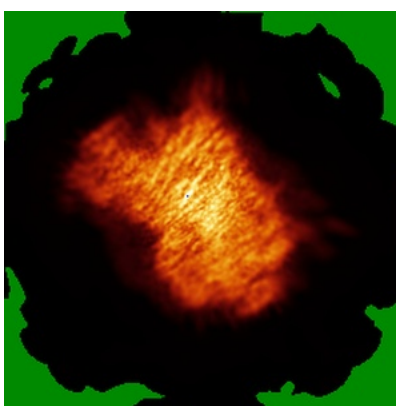
The images above show the largest variance slices of the map in three orthogonal directions.

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

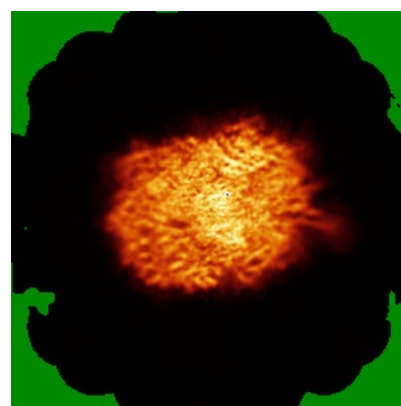
6.4.1 Primary map



X



Y

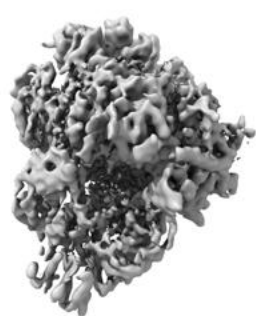


Z

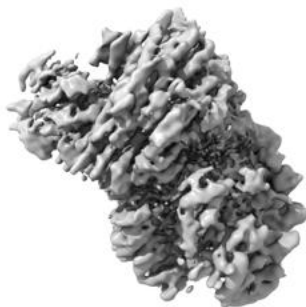
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

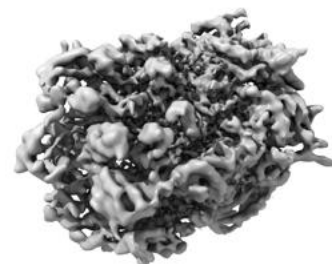
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

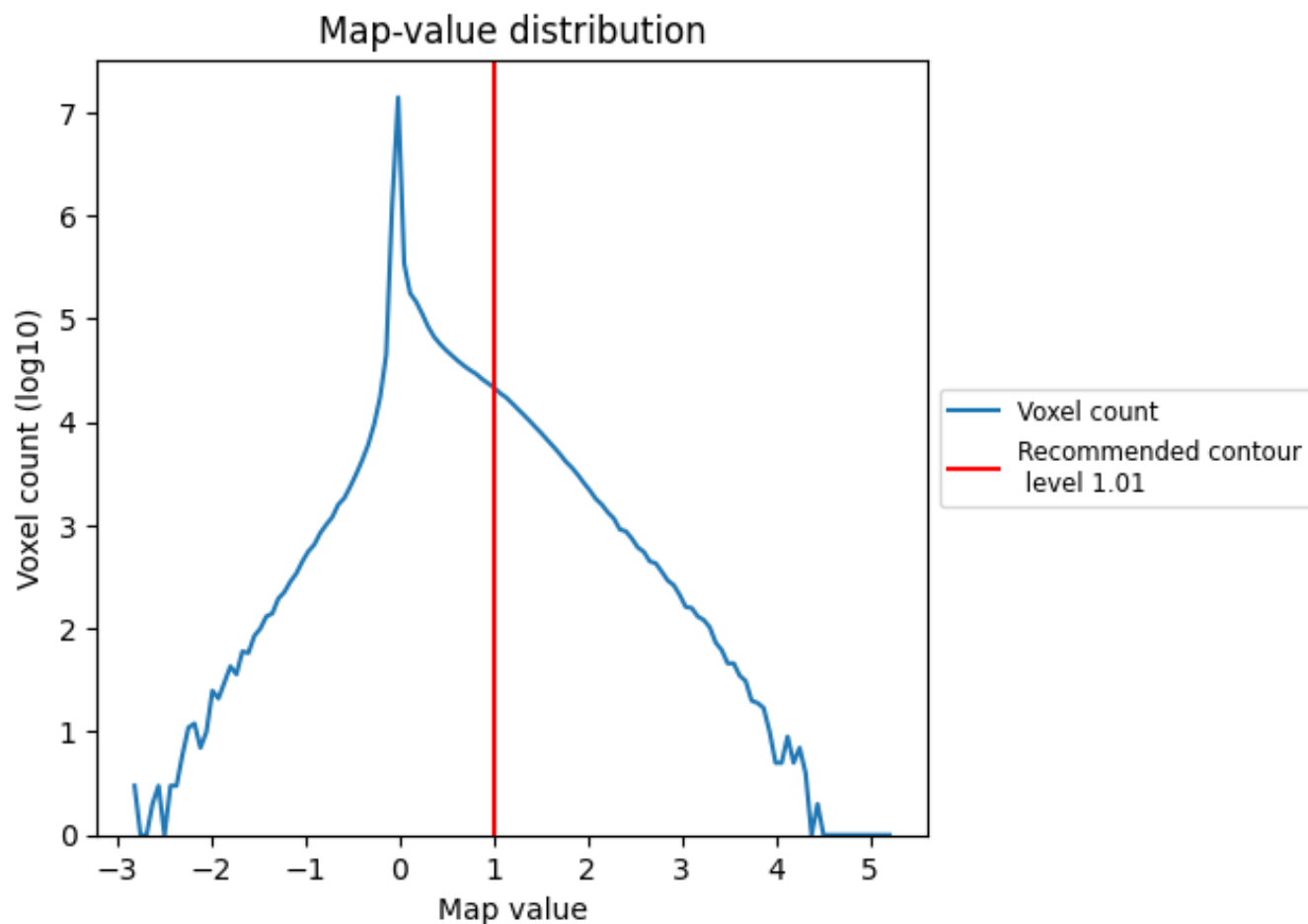
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

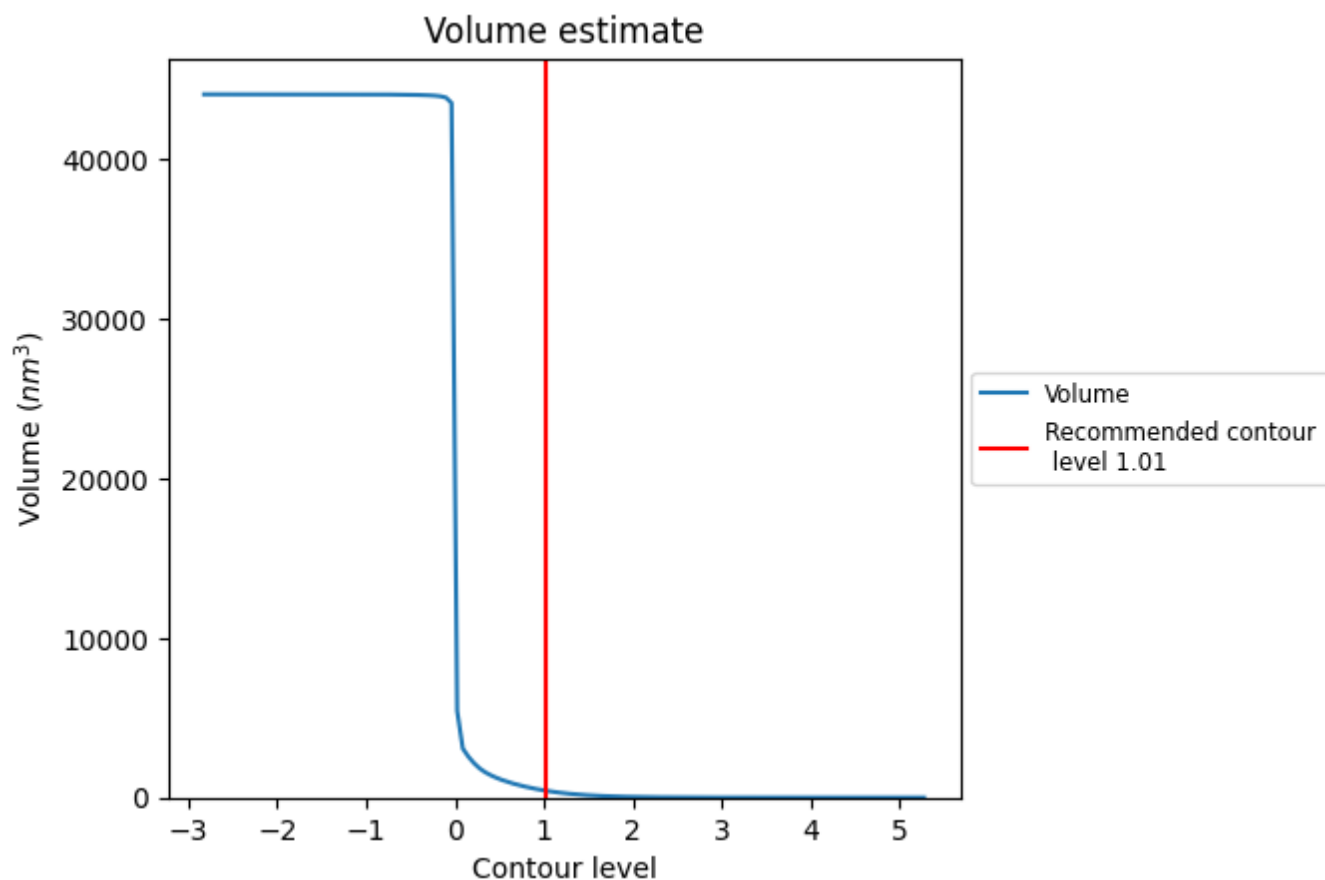
This section contains the results of statistical analysis of the map.

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.

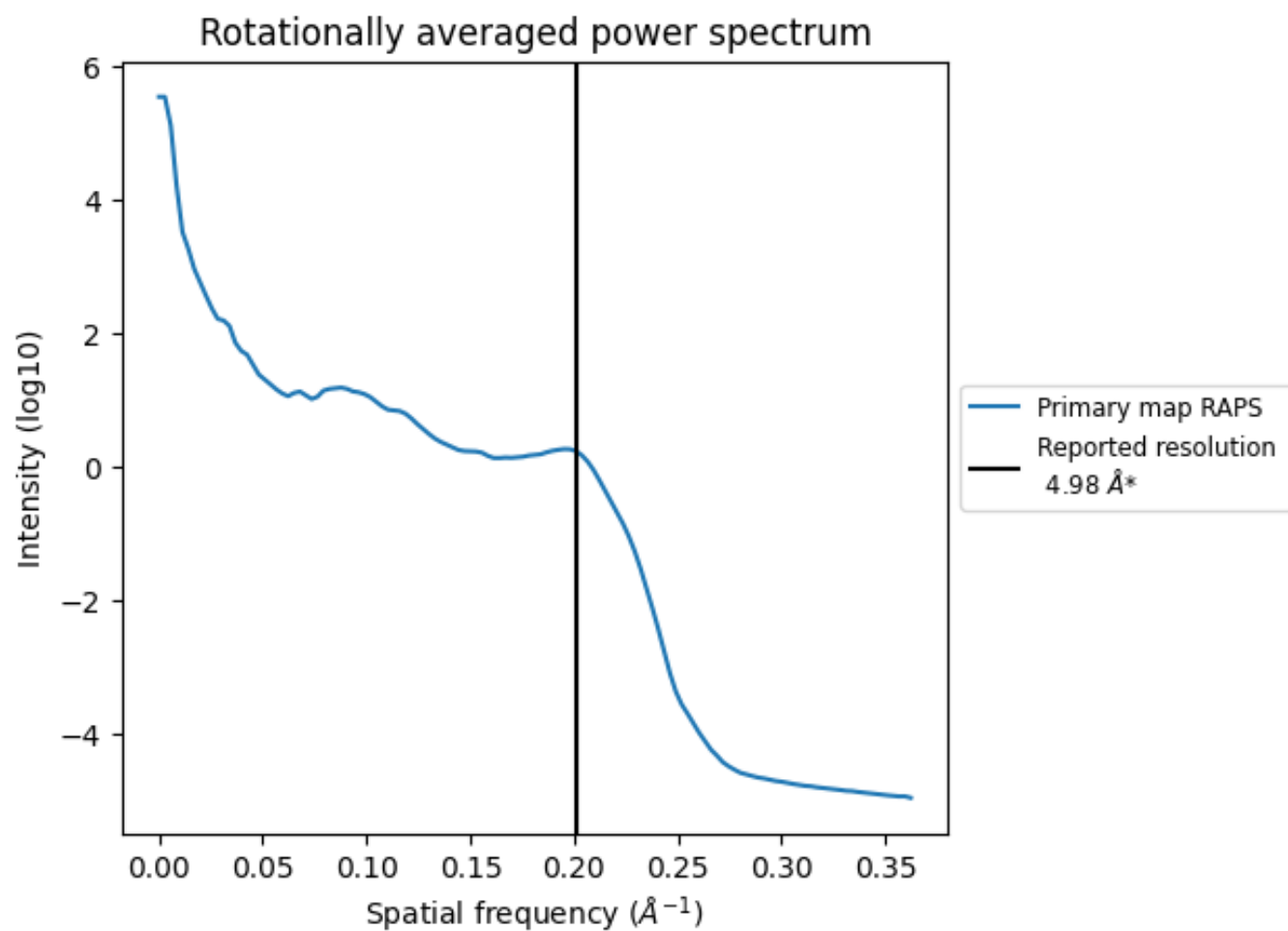
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 440 nm³; this corresponds to an approximate mass of 397 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 0.201 Å⁻¹

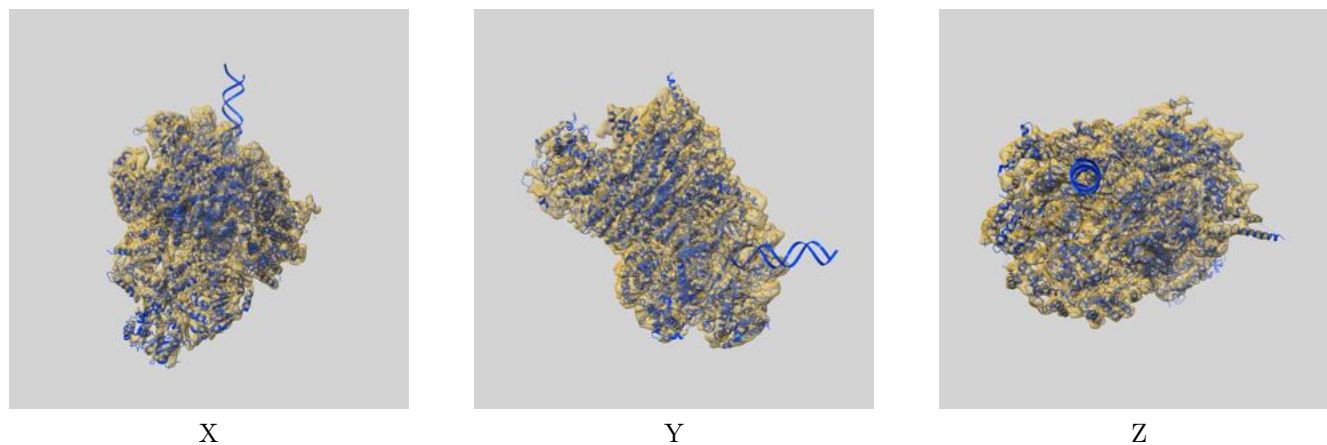
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

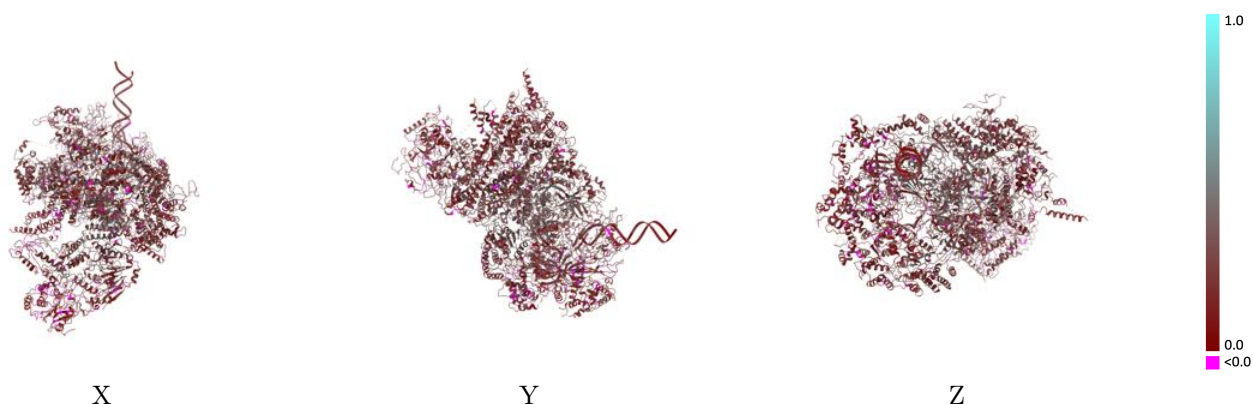
This section contains information regarding the fit between EMDB map EMD-0288 and PDB model 6HV9. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



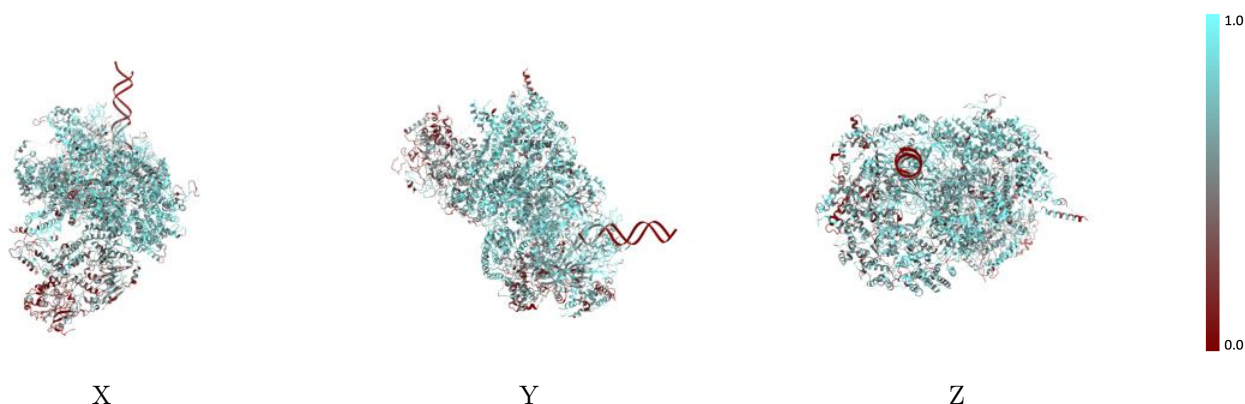
The images above show the 3D surface view of the map at the recommended contour level 1.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



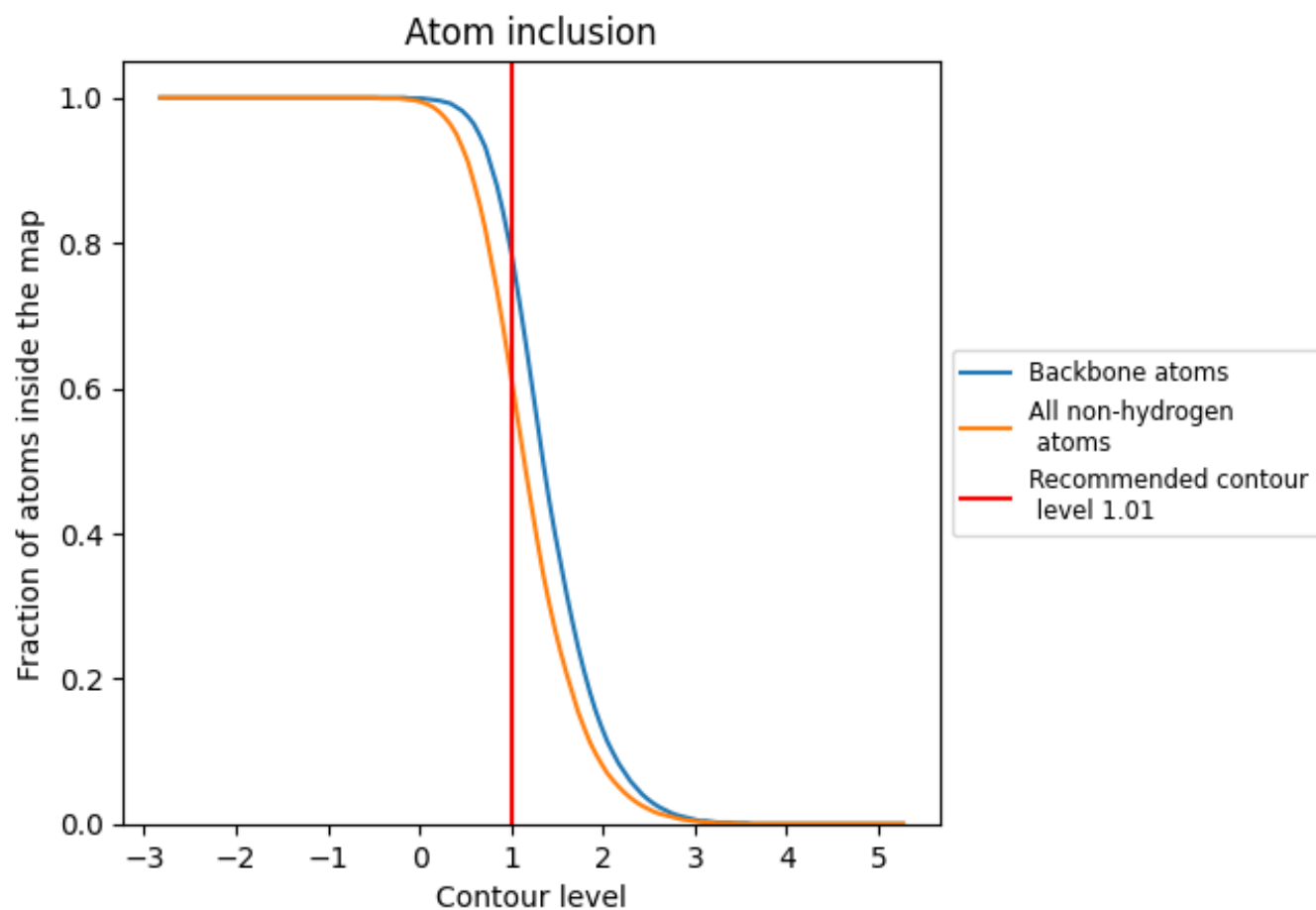
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 61% 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 (1.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6090	0.2310
2	0.6910	0.2780
3	0.7390	0.2870
4	0.5710	0.1860
5	0.6920	0.3050
6	0.6500	0.2140
7	0.5230	0.1890
A	0.4210	0.1710
B	0.5140	0.2290
C	0.7020	0.2280
D	0.7350	0.2480
E	0.7440	0.2690
F	0.6930	0.2300
G	0.6860	0.2410
J	0.5710	0.2480
X	0.1650	0.1690
Y	0.1520	0.1610

1.0

0.0

<0.0