



Full wwPDB EM Validation Report ⓘ

Jul 3, 2023 – 12:29 PM JST

PDB ID : 8IUE
EMDB ID : EMD-35719
Title : RNA polymerase III pre-initiation complex melting complex 1
Authors : Hou, H.; Jin, Q.; Ren, Y.; Wang, Q.; Xu, Y.
Deposited on : 2023-03-24
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:

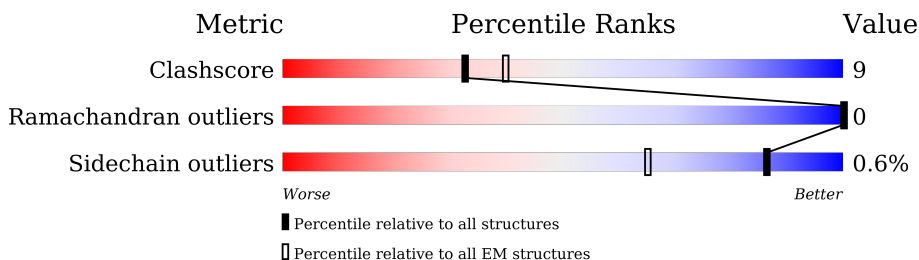
EMDB validation analysis : 0.0.1.dev50
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.34

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 4.10 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.



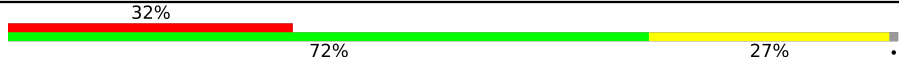







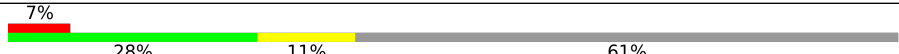

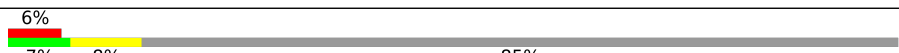
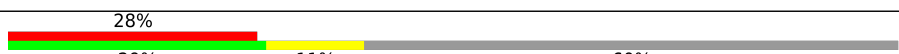



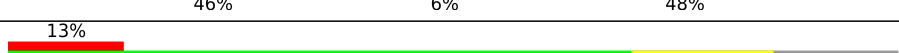

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1390	78% 21%
2	B	1133	74% 23%
3	C	346	79% 20%
4	D	148	14% 57% 26% 18%
5	E	210	6% 78% 21%
6	F	127	55% 5% 40%
7	G	204	5% 57% 25% 19%
8	H	150	8% 83% 15%

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Mol	Chain	Length	Quality of chain
9	I	108	
10	J	67	
11	K	133	
12	L	58	
13	M	708	
14	N	317	
15	O	534	
16	P	316	
17	Q	223	
18	X	464	
19	Y	464	
20	1	368	
21	3	411	
22	4	1469	
23	U	339	
24	V	419	
25	W	2624	

2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 57927 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 III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1378	10814	6850	1886	2005	73	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1105	8741	5538	1529	1605	69	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	343	2736	1723	488	514	11	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	122	985	614	172	196	3	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	209	1715	1083	300	324	8	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	76	610	392	103	110	5	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	166	1337	876	211	245	5	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	148	1186	750	194	237	5	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	107	848	525	157	153	13	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	24	ALA	SER	variant	UNP Q9Y2Y1

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	65	512	331	87	88	6	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	103	822	513	145	157	7	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	46	388	241	75	66	6	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	422	3382	2138	588	636	20	0	0

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	146	1128	710	191	221	6	0	0

There are 81 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	LYS	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	PHE	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	GLY	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	ARG	deletion	UNP P05423
N	?	-	ASN	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	THR	deletion	UNP P05423
N	?	-	ARG	deletion	UNP P05423
N	?	-	ASN	deletion	UNP P05423
N	?	-	MET	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	VAL	deletion	UNP P05423
N	?	-	GLN	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	HIS	deletion	UNP P05423
N	?	-	SER	deletion	UNP P05423
N	?	-	GLY	deletion	UNP P05423
N	?	-	TRP	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	PHE	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423

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Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	ASN	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	VAL	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	TRP	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	GLY	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	MET	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	VAL	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	ILE	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	VAL	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	VAL	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	ARG	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	MET	deletion	UNP P05423

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Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	LYS	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	ARG	deletion	UNP P05423

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	512	4075	2565	712	774	24	0	0

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	303	2403	1516	411	460	16	0	0

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	87	754	488	126	134	6	0	0

- Molecule 18 is a DNA chain called Human gene for U 6 RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
18	X	74	1517	727	263	453	74	0	0

- Molecule 19 is a DNA chain called DNA (74-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
19	Y	70	1437	686	271	410	70	0	0

- Molecule 20 is a protein called snRNA-activating protein complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	1	146	1233	804	212	209	8	0	0

- Molecule 21 is a protein called snRNA-activating protein complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	3	374	3037	1925	521	570	21	0	0

- Molecule 22 is a protein called snRNA-activating protein complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	4	365	3058	1921	573	555	9	0	0

- Molecule 23 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	U	176	1396	907	244	238	7	1	0

- Molecule 24 is a protein called Transcription factor IIIB 50 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	V	361	2853	1792	507	531	23	1	0

- Molecule 25 is a protein called Transcription factor TFIIB component B'' homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	W	111	943	606	163	170	4	0	0

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
26	A	2	Total	Zn	0
			2	2	
26	B	1	Total	Zn	0
			1	1	
26	I	2	Total	Zn	0
			2	2	

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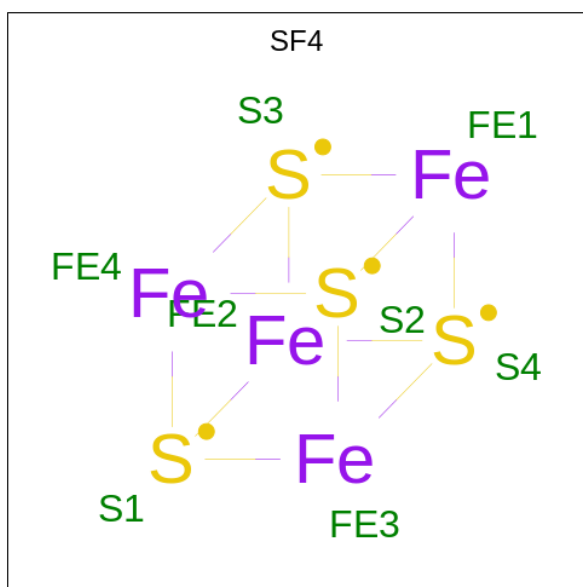
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Mol	Chain	Residues	Atoms		AltConf
26	J	1	Total	Zn	0
			1	1	
26	L	1	Total	Zn	0
			1	1	
26	V	1	Total	Zn	0
			1	1	

- Molecule 27 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
27	A	1	Total	Mg	0
			1	1	

- Molecule 28 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

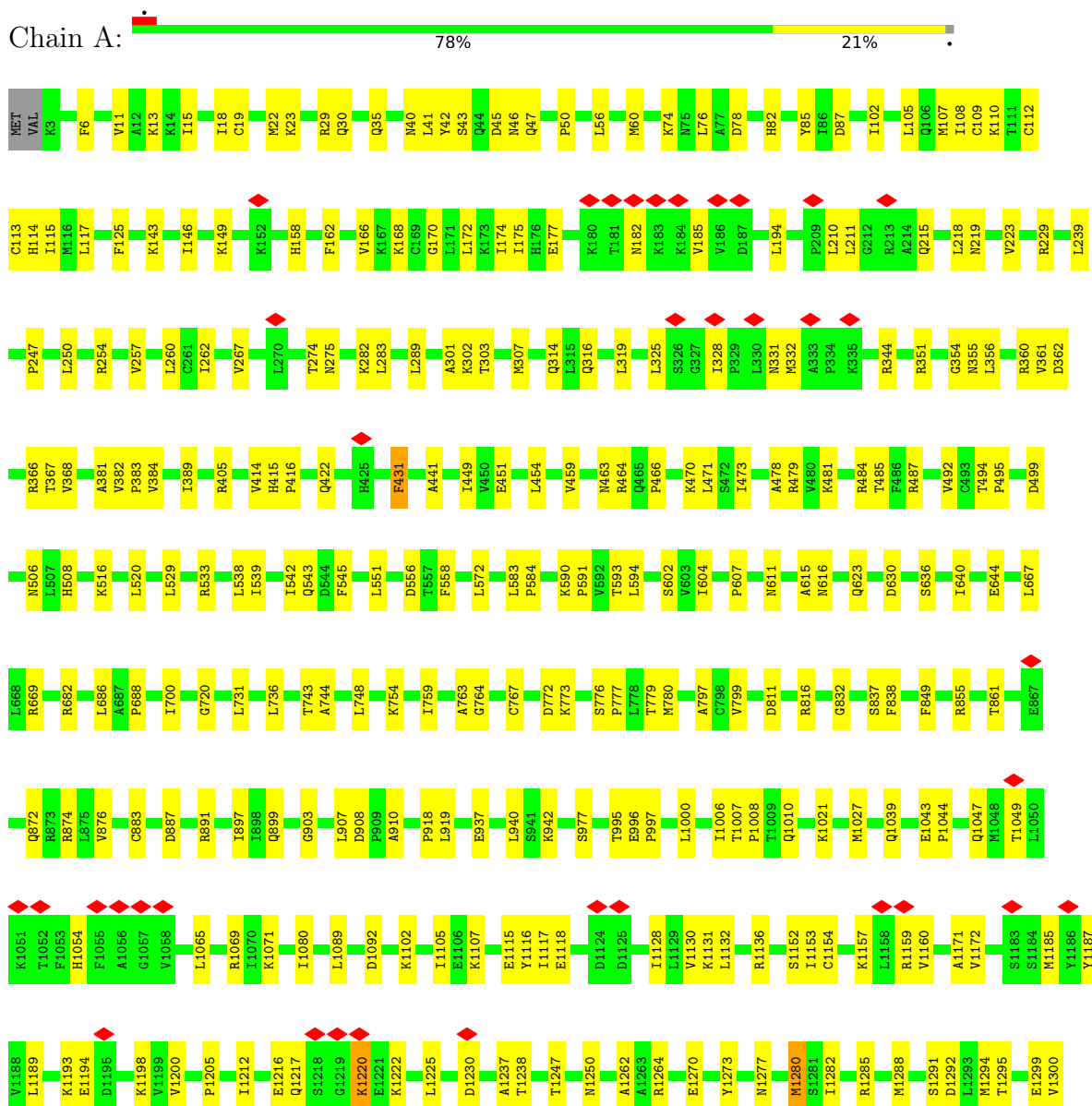


Mol	Chain	Residues	Atoms			AltConf
28	P	1	Total	Fe	S	0
			8	4	4	

3 Residue-property plots

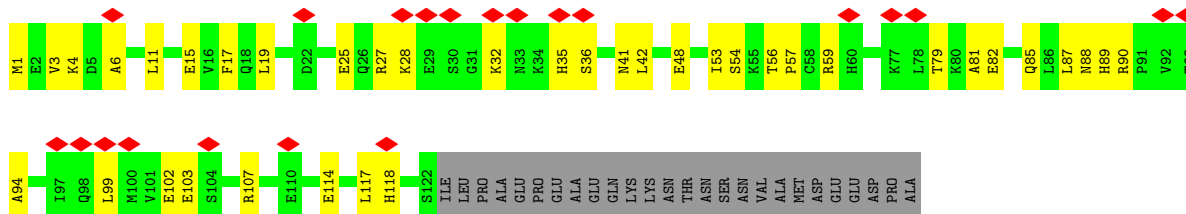
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 III subunit RPC1

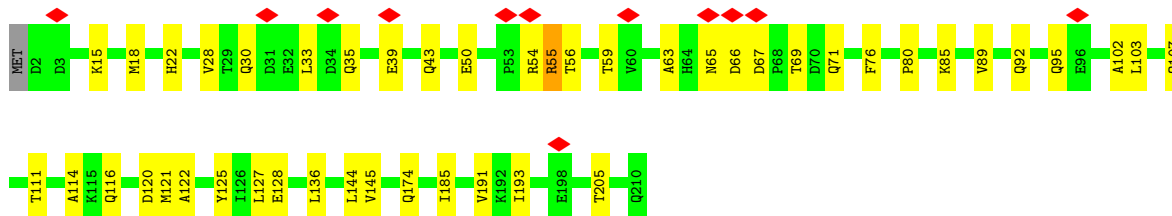
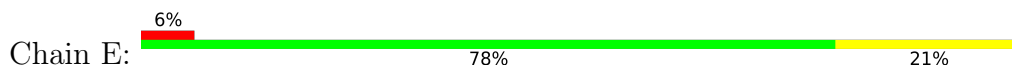




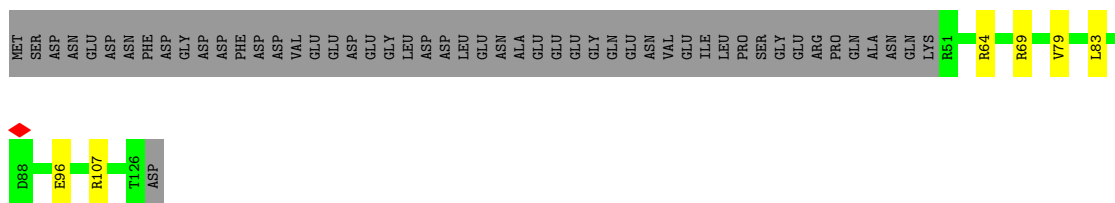
- Molecule 4: DNA-directed RNA polymerase III subunit RPC9



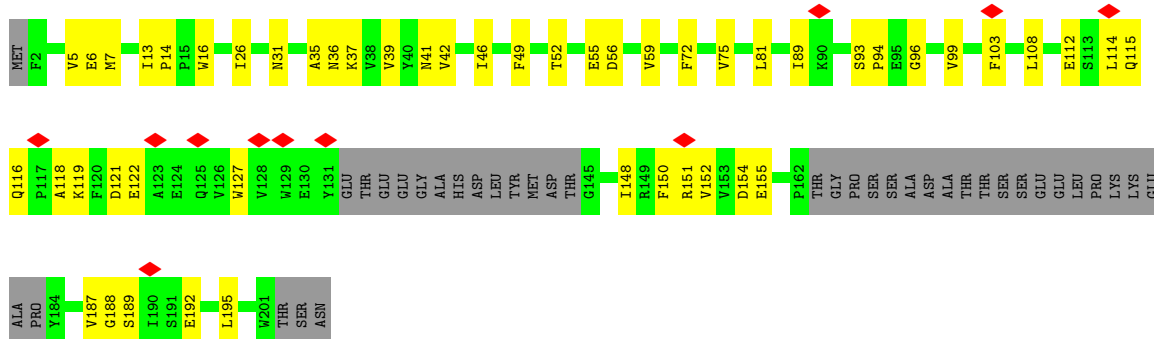
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



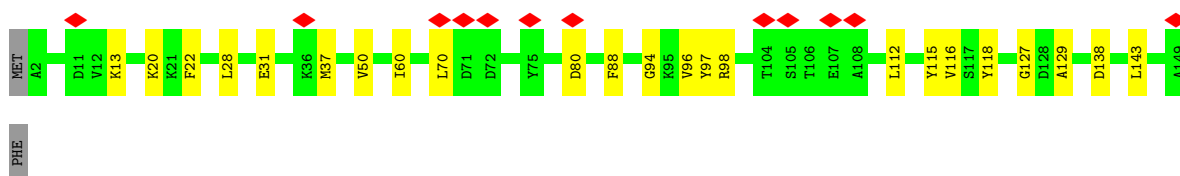
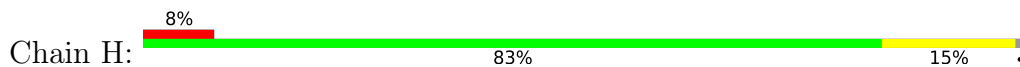
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



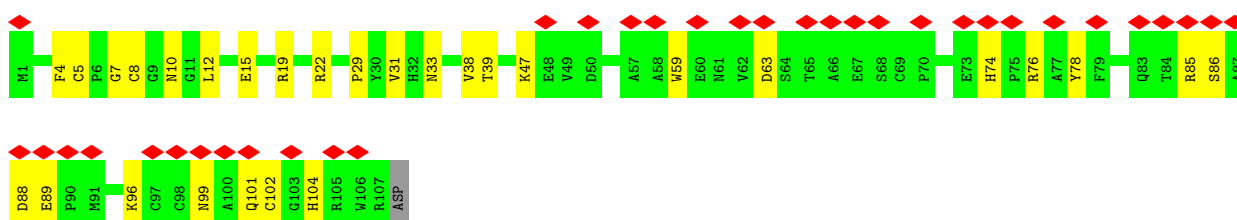
- Molecule 7: DNA-directed RNA polymerase III subunit RPC8



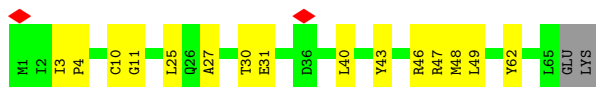
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



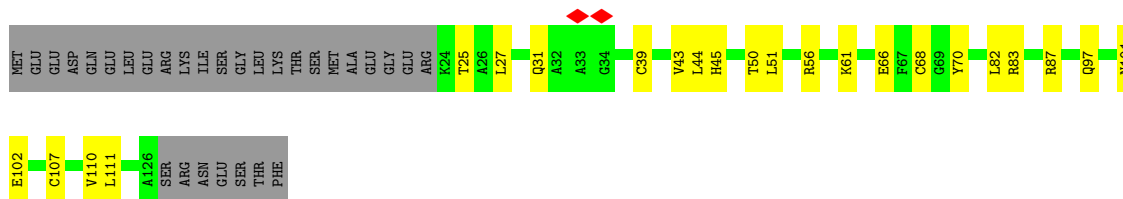
- Molecule 9: DNA-directed RNA polymerase III subunit RPC10



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

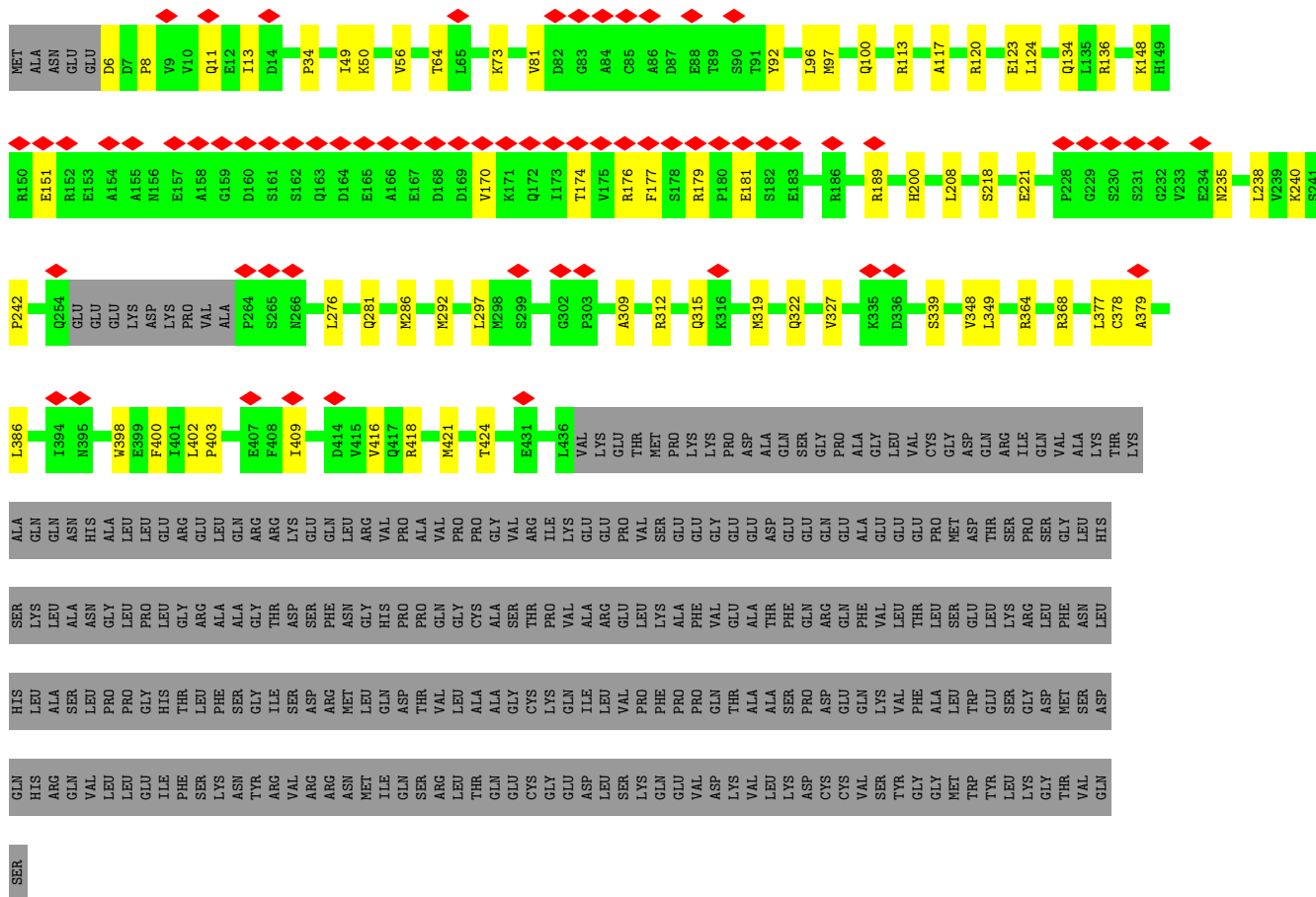


- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

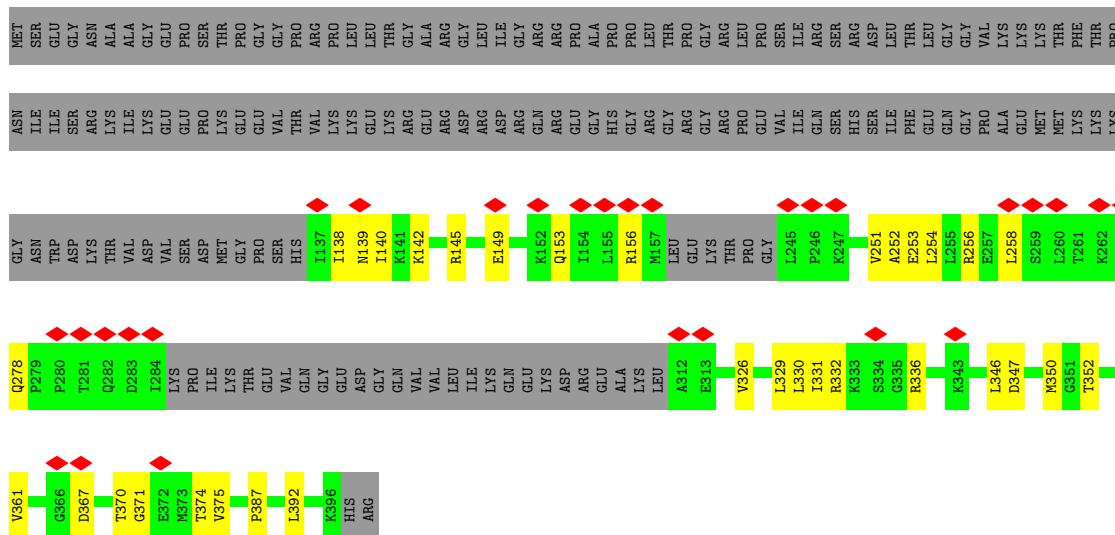
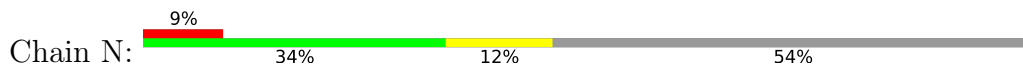


- Molecule 13: DNA-directed RNA polymerase III subunit RPC5

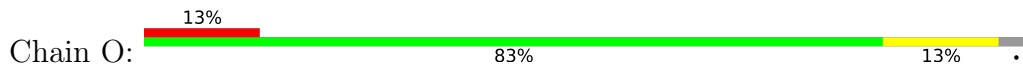


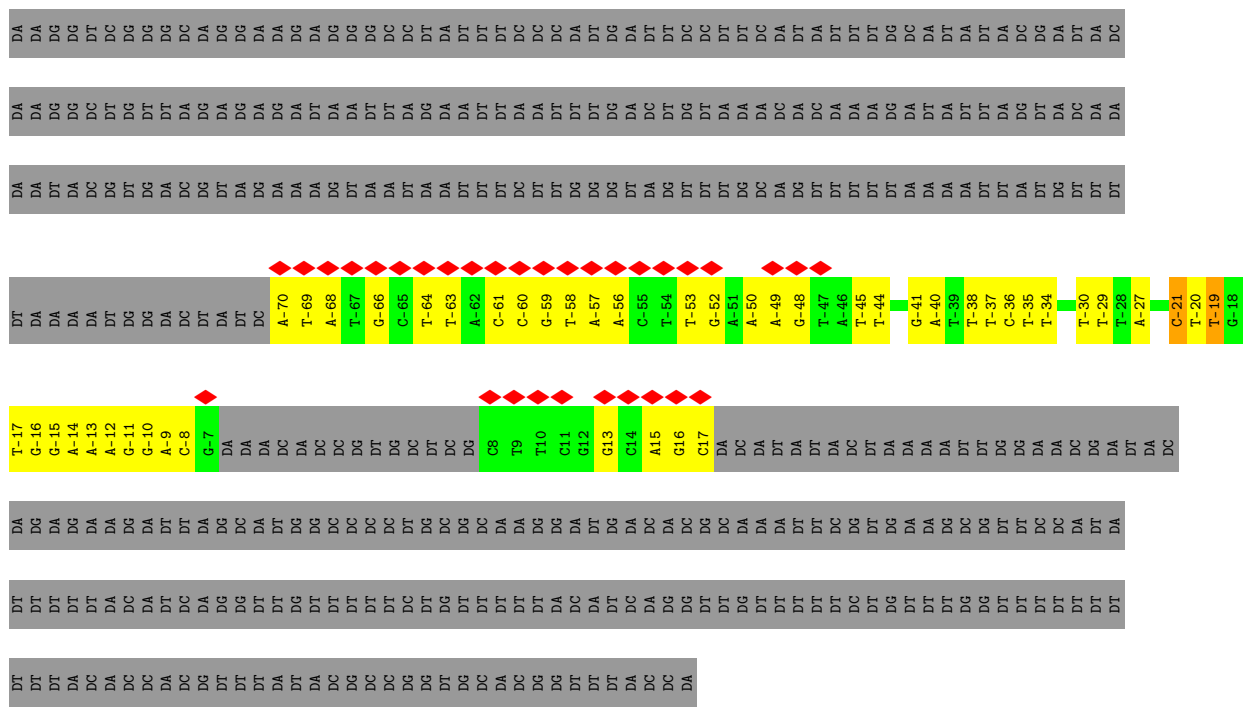


• Molecule 14: DNA-directed RNA polymerase III subunit RPC4

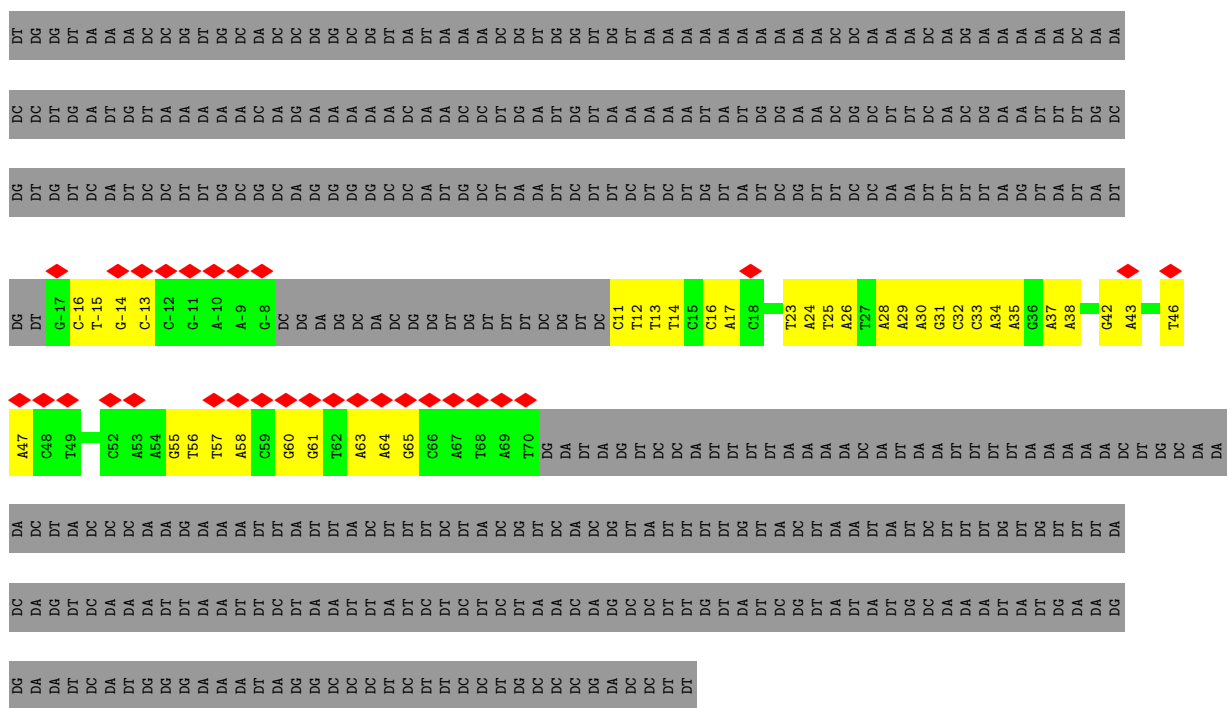


• Molecule 15: DNA-directed RNA polymerase III subunit RPC3





• Molecule 19: DNA (74-MER)



• Molecule 20: snRNA-activating protein complex subunit 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37656	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.184	Depositor
Minimum map value	-0.056	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.024	Depositor
Map size (Å)	426.88, 426.88, 426.88	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.334, 1.334, 1.334	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, MG, 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	A	0.24	0/11008	0.40	0/14842
2	B	0.24	0/8910	0.40	0/12018
3	C	0.24	0/2790	0.40	0/3782
4	D	0.23	0/997	0.39	0/1343
5	E	0.23	0/1745	0.40	0/2358
6	F	0.23	0/620	0.39	0/839
7	G	0.24	0/1374	0.42	0/1868
8	H	0.24	0/1207	0.43	0/1628
9	I	0.24	0/869	0.44	0/1174
10	J	0.23	0/521	0.37	0/703
11	K	0.23	0/837	0.41	0/1129
12	L	0.23	0/394	0.41	0/524
13	M	0.23	0/3455	0.38	0/4673
14	N	0.23	0/1137	0.44	0/1530
15	O	0.23	0/4141	0.39	0/5592
16	P	0.23	0/2446	0.37	0/3301
17	Q	0.24	0/777	0.39	0/1050
18	X	1.10	1/1697 (0.1%)	1.00	3/2616 (0.1%)
19	Y	0.47	0/1614	0.86	0/2485
20	1	0.24	0/1266	0.38	0/1708
21	3	0.24	0/3112	0.41	0/4206
22	4	0.23	0/3121	0.39	0/4181
23	U	0.24	0/1424	0.43	0/1918
24	V	0.23	0/2904	0.39	0/3941
25	W	0.24	0/967	0.38	0/1293
All	All	0.30	1/59333 (0.0%)	0.45	3/80702 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	X	-21	DC	O3'-P	-39.90	1.13	1.61

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	X	-21	DC	O3'-P-O5'	-8.67	87.53	104.00
18	X	-21	DC	P-O3'-C3'	-7.90	110.22	119.70
18	X	-19	DT	C1'-O4'-C4'	-5.64	104.46	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10814	0	11057	221	0
2	B	8741	0	8867	214	0
3	C	2736	0	2712	54	0
4	D	985	0	1006	33	0
5	E	1715	0	1733	38	0
6	F	610	0	642	6	0
7	G	1337	0	1306	46	0
8	H	1186	0	1147	16	0
9	I	848	0	811	47	0
10	J	512	0	525	13	0
11	K	822	0	810	18	0
12	L	388	0	395	19	0
13	M	3382	0	3376	56	0
14	N	1128	0	1181	33	0
15	O	4075	0	4149	49	0
16	P	2403	0	2409	46	0
17	Q	754	0	759	23	0
18	X	1517	0	844	61	0
19	Y	1437	0	789	32	0
20	1	1233	0	1231	35	0
21	3	3037	0	2911	80	0
22	4	3058	0	3064	68	0
23	U	1396	0	1490	14	0
24	V	2853	0	2892	53	0
25	W	943	0	924	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	A	2	0	0	0	0
26	B	1	0	0	0	0
26	I	2	0	0	0	0
26	J	1	0	0	0	0
26	L	1	0	0	0	0
26	V	1	0	0	0	0
27	A	1	0	0	0	0
28	P	8	0	0	1	0
All	All	57927	0	57030	1067	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 (1067) 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)
9:I:76:ARG:CD	9:I:99:ASN:HB2	1.23	1.60
2:B:741:VAL:CG2	2:B:1009:TYR:CE2	1.87	1.55
18:X:-21:DC:O3'	18:X:-20:DT:P	1.13	1.52
2:B:741:VAL:HG21	2:B:1009:TYR:CZ	1.36	1.52
9:I:76:ARG:CD	9:I:99:ASN:CB	1.99	1.38
18:X:-21:DC:C3'	18:X:-20:DT:P	2.09	1.38
2:B:741:VAL:CG1	2:B:1009:TYR:OH	1.73	1.36
2:B:741:VAL:CG2	2:B:1009:TYR:OH	1.74	1.35
2:B:741:VAL:HG21	2:B:1009:TYR:CE2	1.51	1.33
2:B:741:VAL:HG21	2:B:1009:TYR:OH	1.27	1.29
2:B:741:VAL:CG2	2:B:1009:TYR:CZ	2.03	1.25
2:B:741:VAL:HG11	2:B:1009:TYR:OH	1.27	1.25
9:I:76:ARG:HD3	9:I:99:ASN:CB	1.66	1.20
2:B:741:VAL:HG22	2:B:1009:TYR:CE2	1.71	1.17
4:D:81:ALA:HB2	17:Q:84:ILE:HD12	1.25	1.17
2:B:741:VAL:CB	2:B:1009:TYR:OH	1.93	1.15
9:I:76:ARG:HD2	9:I:99:ASN:HB2	1.27	1.15
21:3:373:PRO:HA	22:4:286:ASN:ND2	1.62	1.14
9:I:76:ARG:NE	9:I:99:ASN:CB	2.11	1.13
5:E:111:THR:HG21	18:X:16:DG:H5''	1.29	1.13
4:D:99:LEU:HD21	7:G:195:LEU:O	1.50	1.12
21:3:222:VAL:CG1	22:4:176:PHE:HE2	1.63	1.12
9:I:76:ARG:CZ	9:I:99:ASN:HB3	1.80	1.12
20:1:63:TRP:HE3	20:1:82:LEU:HD22	1.09	1.10
10:J:30:THR:HG22	10:J:31:GLU:H	1.15	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:15:MET:N	12:L:27:GLU:OE2	1.84	1.09
2:B:741:VAL:CG2	2:B:1009:TYR:HE2	1.37	1.08
9:I:76:ARG:NE	9:I:99:ASN:HB3	1.68	1.08
18:X:-21:DC:H4'	18:X:-20:DT:H5'	1.35	1.06
20:1:63:TRP:HE3	20:1:82:LEU:CD2	1.68	1.05
21:3:222:VAL:HG11	22:4:176:PHE:HE2	1.16	1.04
21:3:311:TYR:HB3	21:3:321:ILE:HD11	1.42	1.01
1:A:257:VAL:HG23	1:A:283:LEU:HD13	1.43	1.00
21:3:222:VAL:HG11	22:4:176:PHE:CE2	1.97	1.00
20:1:63:TRP:CE3	20:1:82:LEU:HD22	1.98	0.99
16:P:88:SER:O	16:P:91:GLN:NE2	1.98	0.97
4:D:99:LEU:CD2	7:G:195:LEU:O	2.11	0.97
12:L:15:MET:H	12:L:27:GLU:CD	1.68	0.96
4:D:81:ALA:HB2	17:Q:84:ILE:CD1	1.96	0.95
21:3:373:PRO:HA	22:4:286:ASN:HD21	1.18	0.94
9:I:76:ARG:HE	9:I:99:ASN:N	1.65	0.93
12:L:14:PRO:HA	12:L:27:GLU:OE2	1.70	0.92
16:P:88:SER:OG	16:P:91:GLN:OE1	1.86	0.92
3:C:133:THR:O	3:C:137:THR:HG22	1.71	0.91
9:I:76:ARG:HD3	9:I:99:ASN:HB2	0.90	0.90
18:X:-21:DC:HO3'	18:X:-20:DT:P	1.30	0.90
13:M:13:ILE:HD12	14:N:329:LEU:HD23	1.52	0.90
2:B:741:VAL:HG11	2:B:1009:TYR:HH	1.09	0.89
9:I:76:ARG:HE	9:I:99:ASN:H	1.17	0.88
22:4:424:TRP:CB	22:4:436:ASP:OD1	2.22	0.88
18:X:-21:DC:H3'	18:X:-20:DT:P	2.11	0.88
18:X:-21:DC:O3'	18:X:-20:DT:O5'	1.91	0.87
10:J:30:THR:HG22	10:J:31:GLU:N	1.88	0.87
16:P:90:ASN:OD1	16:P:91:GLN:OE1	1.93	0.87
20:1:63:TRP:CE3	20:1:82:LEU:CD2	2.56	0.86
2:B:741:VAL:HG23	2:B:1009:TYR:HE2	1.37	0.86
9:I:76:ARG:NE	9:I:99:ASN:N	2.22	0.86
21:3:222:VAL:CG1	22:4:176:PHE:CE2	2.55	0.84
21:3:188:TYR:HH	22:4:176:PHE:HD2	1.26	0.84
18:X:-21:DC:C4'	18:X:-20:DT:H5'	2.07	0.84
16:P:88:SER:HB3	16:P:91:GLN:HE22	1.42	0.83
1:A:60:MET:HE3	1:A:257:VAL:HG13	1.61	0.83
1:A:257:VAL:HG23	1:A:283:LEU:CD1	2.08	0.83
1:A:764:GLY:HA2	1:A:767:CYS:SG	2.19	0.82
18:X:-21:DC:C3'	18:X:-20:DT:OP1	2.28	0.81
18:X:-21:DC:H4'	18:X:-20:DT:C5'	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:X:-21:DC:H3'	18:X:-20:DT:OP1	1.80	0.80
21:3:319:HIS:O	21:3:321:ILE:HD12	1.81	0.80
22:4:424:TRP:HB3	22:4:436:ASP:OD1	1.80	0.80
4:D:99:LEU:HD21	7:G:195:LEU:C	2.01	0.79
10:J:30:THR:CG2	10:J:31:GLU:H	1.95	0.79
21:3:373:PRO:CA	22:4:286:ASN:HD21	1.95	0.79
15:O:106:ILE:O	15:O:110:LEU:HD13	1.82	0.79
1:A:776:SER:OG	1:A:777:PRO:HD3	1.84	0.78
5:E:56:THR:HG22	5:E:76:PHE:CE1	2.18	0.78
8:H:98:ARG:HB3	8:H:115:TYR:HB2	1.65	0.77
22:4:424:TRP:HB2	22:4:436:ASP:OD1	1.83	0.77
9:I:59:TRP:HZ2	9:I:96:LYS:HD3	1.49	0.77
2:B:679:GLN:HG2	2:B:681:PRO:HD2	1.67	0.76
21:3:221:CYS:O	21:3:224:ASP:OD1	2.03	0.76
18:X:-21:DC:O3'	18:X:-20:DT:C5'	2.35	0.75
21:3:188:TYR:OH	22:4:176:PHE:CD2	2.38	0.75
5:E:111:THR:HG21	18:X:16:DG:C5'	2.13	0.74
1:A:720:GLY:HA3	1:A:759:ILE:HD11	1.68	0.74
1:A:492:VAL:O	1:A:492:VAL:HG12	1.86	0.74
1:A:764:GLY:O	1:A:767:CYS:SG	2.45	0.74
24:V:282:TRP:O	24:V:286:LEU:HG	1.87	0.74
21:3:188:TYR:OH	22:4:176:PHE:HD2	1.68	0.73
21:3:311:TYR:CB	21:3:321:ILE:HD11	2.18	0.73
24:V:189:VAL:HG23	24:V:253:LEU:HD11	1.70	0.73
1:A:1044:PRO:HB3	1:A:1280:MET:HG3	1.70	0.72
1:A:1264:ARG:NH2	1:A:1288:MET:SD	2.63	0.72
1:A:1217:GLN:HA	9:I:101:GLN:HG2	1.72	0.71
7:G:114:LEU:HD11	7:G:192:GLU:H	1.55	0.71
16:P:142:VAL:HG21	16:P:167:TYR:HB3	1.72	0.71
3:C:49:PHE:HA	3:C:66:VAL:O	1.89	0.71
4:D:41:ASN:HB2	7:G:36:ASN:HD22	1.56	0.71
21:3:234:THR:HG23	21:3:234:THR:O	1.89	0.71
3:C:98:THR:O	3:C:98:THR:HG22	1.89	0.70
2:B:404:LYS:HD2	24:V:141:LEU:HA	1.74	0.70
21:3:386:MET:SD	22:4:317:TRP:NE1	2.63	0.70
1:A:494:THR:OG1	1:A:495:PRO:HD3	1.91	0.70
1:A:414:VAL:HG12	1:A:416:PRO:HD2	1.74	0.70
1:A:463:ASN:HB2	1:A:473:ILE:HG13	1.73	0.69
14:N:332:ARG:HB2	14:N:336:ARG:HB3	1.74	0.69
9:I:59:TRP:HZ2	9:I:96:LYS:CD	2.05	0.69
13:M:174:THR:HG23	13:M:174:THR:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:78:ARG:HE	11:K:50:THR:HG22	1.58	0.69
17:Q:80:GLU:HG2	17:Q:81:ARG:HD3	1.74	0.69
12:L:15:MET:N	12:L:27:GLU:CD	2.39	0.69
20:1:63:TRP:HB2	20:1:82:LEU:HD21	1.73	0.69
1:A:464:ARG:HG2	1:A:466:PRO:HD2	1.73	0.69
2:B:682:ARG:HD2	2:B:937:ARG:HB3	1.76	0.68
16:P:88:SER:HB3	16:P:91:GLN:NE2	2.09	0.68
2:B:715:PRO:HB2	2:B:734:PRO:HG2	1.75	0.68
2:B:785:GLN:NE2	24:V:96:TYR:OH	2.26	0.68
2:B:392:ILE:HD13	2:B:400:PHE:HB3	1.76	0.67
2:B:304:THR:O	2:B:304:THR:HG22	1.93	0.67
4:D:48:GLU:HB3	7:G:103:PHE:HB3	1.76	0.67
16:P:88:SER:CB	16:P:91:GLN:HE22	2.06	0.67
2:B:741:VAL:HG22	2:B:1009:TYR:CZ	2.03	0.67
4:D:17:PHE:HB2	4:D:53:ILE:HG21	1.76	0.67
9:I:78:TYR:HB3	9:I:96:LYS:HB3	1.77	0.67
5:E:80:PRO:HA	5:E:107:GLN:HB3	1.76	0.67
2:B:205:SER:HG	2:B:320:HIS:H	1.42	0.67
21:3:297:THR:HG22	21:3:298:PHE:N	2.10	0.67
12:L:15:MET:C	12:L:27:GLU:OE1	2.32	0.66
23:U:169:VAL:HG22	23:U:222:THR:HG22	1.78	0.66
2:B:725:ILE:HG23	2:B:730:PHE:HB3	1.76	0.66
15:O:349:THR:HG23	16:P:280:THR:HG21	1.79	0.65
16:P:210:PHE:HB3	16:P:269:LEU:HB3	1.77	0.65
3:C:236:LEU:HD13	3:C:305:HIS:CE1	2.31	0.65
1:A:485:THR:OG1	1:A:487:ARG:NH1	2.29	0.65
2:B:755:LEU:CD1	2:B:757:LEU:HD21	2.27	0.65
22:4:163:GLU:HA	22:4:166:ARG:HH21	1.62	0.65
2:B:178:ILE:HG12	2:B:437:THR:HG22	1.78	0.65
24:V:189:VAL:CG2	24:V:253:LEU:HD11	2.27	0.65
15:O:507:ASN:OD1	17:Q:62:GLN:NE2	2.29	0.65
1:A:23:LYS:HG3	2:B:1123:ILE:HG13	1.77	0.64
1:A:471:LEU:HD22	1:A:538:LEU:HD12	1.79	0.64
18:X:-38:DT:OP1	24:V:267:GLN:NE2	2.31	0.64
14:N:361:VAL:HG12	14:N:375:VAL:HA	1.80	0.64
10:J:27:ALA:O	13:M:368:ARG:NH2	2.30	0.64
13:M:170:VAL:HG21	16:P:66:LEU:HA	1.78	0.64
15:O:445:ASN:ND2	16:P:296:CYS:SG	2.71	0.64
1:A:1044:PRO:HG2	1:A:1282:ILE:HD11	1.79	0.64
2:B:85:PRO:HG3	2:B:138:ILE:HG13	1.79	0.64
1:A:604:ILE:HD11	1:A:686:LEU:HD13	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:3:313:HIS:O	21:3:317:CYS:HB3	1.98	0.64
18:X:-27:DA:H1'	23:U:169:VAL:HG11	1.80	0.64
13:M:117:ALA:HB2	14:N:269:LEU:HD22	1.79	0.63
21:3:100:LEU:HA	21:3:103:VAL:HG22	1.79	0.63
4:D:54:SER:O	4:D:59:ARG:NH1	2.32	0.63
12:L:14:PRO:CA	12:L:27:GLU:OE2	2.45	0.63
2:B:77:TYR:HA	2:B:117:ILE:HG22	1.80	0.63
2:B:915:ASP:OD1	3:C:78:ARG:NH2	2.31	0.63
21:3:268:ARG:HH12	22:4:167:GLU:HG3	1.64	0.63
1:A:42:TYR:HA	1:A:50:PRO:HA	1.81	0.63
4:D:82:GLU:HG3	4:D:107:ARG:HH12	1.63	0.63
5:E:59:THR:OG1	5:E:71:GLN:NE2	2.32	0.63
16:P:108:TRP:HB3	16:P:147:LYS:HD3	1.80	0.63
2:B:516:SER:HB2	13:M:113:ARG:HH12	1.64	0.63
9:I:76:ARG:NE	9:I:99:ASN:H	1.89	0.63
17:Q:86:ARG:HG2	17:Q:89:LYS:HG2	1.80	0.63
2:B:131:LEU:HD21	2:B:406:MET:HG3	1.80	0.63
1:A:470:LYS:HB3	1:A:1039:GLN:HE22	1.62	0.62
2:B:212:SER:HB2	2:B:227:HIS:HE2	1.64	0.62
13:M:49:ILE:HB	13:M:56:VAL:HG23	1.80	0.62
5:E:102:ALA:HB3	5:E:127:LEU:HG	1.82	0.62
8:H:20:LYS:NZ	8:H:22:PHE:O	2.29	0.62
20:1:147:ARG:HD3	21:3:199:LYS:HG2	1.80	0.62
22:4:286:ASN:OD1	22:4:287:SER:N	2.33	0.62
24:V:283:LEU:HD23	24:V:286:LEU:HD12	1.81	0.62
25:W:325:ILE:HG22	25:W:337:ILE:HD13	1.80	0.62
9:I:59:TRP:CZ2	9:I:96:LYS:HE2	2.34	0.62
9:I:76:ARG:NE	9:I:99:ASN:CA	2.61	0.62
8:H:112:LEU:HD13	8:H:129:ALA:HB2	1.81	0.62
4:D:102:GLU:O	4:D:107:ARG:NH2	2.33	0.62
21:3:184:VAL:CG2	21:3:321:ILE:HG23	2.30	0.61
21:3:390:ASP:HA	22:4:315:LEU:HD22	1.82	0.61
20:1:130:ARG:O	20:1:133:ARG:NH2	2.29	0.61
13:M:409:ILE:HG23	13:M:416:VAL:HG21	1.81	0.61
22:4:416:VAL:HG22	22:4:443:TYR:HE1	1.66	0.61
1:A:19:CYS:HB2	2:B:1125:ARG:HB2	1.82	0.61
23:U:168:ILE:HB	23:U:224:ALA:HB3	1.81	0.61
11:K:66:GLU:HG2	11:K:87:ARG:HG2	1.83	0.61
1:A:257:VAL:CG2	1:A:283:LEU:HD13	2.25	0.61
1:A:481:LYS:HB2	1:A:487:ARG:HH21	1.65	0.61
2:B:750:ASP:HA	2:B:754:ALA:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:819:GLU:HG3	12:L:49:THR:HG21	1.82	0.60
1:A:361:VAL:HG12	2:B:1072:SER:HB3	1.82	0.60
1:A:1047:GLN:O	9:I:85:ARG:NH2	2.34	0.60
7:G:115:GLN:NE2	7:G:192:GLU:O	2.34	0.60
2:B:128:ARG:HH12	2:B:131:LEU:HD13	1.66	0.60
7:G:94:PRO:HA	7:G:121:ASP:HB2	1.83	0.60
15:O:258:ARG:HD3	16:P:276:ILE:HG12	1.83	0.60
12:L:39:CYS:SG	12:L:40:GLY:N	2.75	0.60
1:A:590:LYS:NZ	8:H:88:PHE:O	2.35	0.60
21:3:324:THR:HG23	21:3:325:ASP:N	2.17	0.60
23:U:204:ILE:HG13	23:U:207:PRO:HD2	1.84	0.60
2:B:396:ARG:HE	2:B:398:ALA:HB3	1.65	0.60
2:B:128:ARG:NH2	25:W:287:SER:OG	2.35	0.60
9:I:5:CYS:HB2	9:I:12:LEU:HD21	1.84	0.60
1:A:46:ASN:OD1	1:A:47:GLN:OE1	2.19	0.59
1:A:174:ILE:HG23	1:A:218:LEU:HB2	1.83	0.59
3:C:23:ASN:O	3:C:303:ARG:NH2	2.35	0.59
3:C:235:LEU:HB2	3:C:301:ARG:HH11	1.68	0.59
15:O:147:THR:HG22	15:O:150:ARG:HH22	1.65	0.59
18:X:-66:DG:H5''	22:4:456:TRP:HE1	1.66	0.59
21:3:158:GLU:HB3	22:4:366:VAL:HG23	1.83	0.59
1:A:1185:MET:HG2	1:A:1187:TYR:H	1.66	0.59
3:C:326:ILE:HG21	11:K:111:LEU:HB2	1.82	0.59
19:Y:25:DT:H2''	19:Y:26:DA:H5'	1.82	0.59
21:3:216:ARG:NH2	21:3:248:LYS:O	2.32	0.59
1:A:855:ARG:NH2	2:B:481:PRO:O	2.34	0.59
18:X:-21:DC:O3'	18:X:-20:DT:H5'	2.01	0.59
2:B:751:ILE:O	2:B:930:ASN:ND2	2.36	0.59
21:3:411:ASN:OD1	22:4:374:ARG:NH2	2.35	0.59
3:C:28:ASP:O	11:K:61:LYS:NZ	2.34	0.59
16:P:217:TRP:NE1	16:P:230:LEU:O	2.35	0.59
1:A:995:THR:HG22	1:A:997:PRO:HD2	1.85	0.59
1:A:1340:VAL:HA	1:A:1345:GLU:HG3	1.84	0.59
20:1:67:LEU:HB3	20:1:69:PRO:HD2	1.84	0.59
2:B:722:THR:HG23	2:B:962:THR:HA	1.83	0.59
2:B:986:LYS:O	3:C:285:ARG:NH2	2.35	0.59
18:X:-17:DT:H5'	24:V:111:LEU:HD23	1.83	0.59
21:3:234:THR:HG23	21:3:237:GLN:HB2	1.83	0.59
1:A:891:ARG:HG2	1:A:897:ILE:HG12	1.84	0.59
2:B:394:LYS:HZ2	19:Y:14:DT:H71	1.67	0.59
20:1:83:TYR:OH	21:3:101:ARG:NH1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:3:150:CYS:HB2	21:3:153:GLU:HB2	1.84	0.59
1:A:172:LEU:HD23	1:A:314:GLN:HB3	1.85	0.58
4:D:79:THR:OG1	17:Q:85:GLU:O	2.20	0.58
4:D:87:LEU:O	4:D:90:ARG:NH1	2.35	0.58
21:3:86:VAL:HG12	21:3:91:ASP:HB2	1.84	0.58
1:A:861:THR:HG21	9:I:86:SER:H	1.68	0.58
4:D:4:LYS:HB2	7:G:6:GLU:HB2	1.84	0.58
2:B:526:LEU:HD12	2:B:527:CYS:O	2.04	0.58
4:D:41:ASN:ND2	7:G:35:ALA:O	2.37	0.58
13:M:117:ALA:HB1	13:M:124:LEU:HD11	1.86	0.58
1:A:1368:ARG:HH22	7:G:56:ASP:HA	1.68	0.58
1:A:102:ILE:HG12	1:A:174:ILE:HD13	1.85	0.58
2:B:750:ASP:O	2:B:930:ASN:ND2	2.36	0.58
1:A:463:ASN:HB2	1:A:473:ILE:CG1	2.33	0.58
1:A:1360:PHE:O	6:F:64:ARG:NH1	2.36	0.58
2:B:394:LYS:HG3	2:B:394:LYS:O	2.04	0.58
1:A:125:PHE:HZ	1:A:149:LYS:HD2	1.68	0.58
1:A:344:ARG:HH21	1:A:351:ARG:HH21	1.52	0.58
2:B:594:ARG:NH2	2:B:663:THR:OG1	2.35	0.58
2:B:1079:VAL:HB	2:B:1128:LEU:HD11	1.85	0.58
24:V:173:VAL:HG21	24:V:208:VAL:HG21	1.85	0.58
3:C:266:GLU:OE2	3:C:271:LYS:NZ	2.34	0.58
18:X:-29:DT:H5'	18:X:-29:DT:C6	2.38	0.58
1:A:351:ARG:HD3	1:A:355:ASN:HD22	1.69	0.57
2:B:113:ILE:HD11	2:B:136:MET:HG2	1.86	0.57
13:M:218:SER:HA	14:N:374:THR:HG23	1.86	0.57
2:B:313:LEU:HD23	2:B:317:ILE:HD12	1.86	0.57
20:1:133:ARG:NH1	21:3:58:ALA:O	2.35	0.57
1:A:6:PHE:HA	7:G:37:LYS:HE3	1.87	0.57
1:A:1194:GLU:O	1:A:1198:LYS:NZ	2.37	0.57
2:B:254:MET:HA	2:B:528:GLY:HA3	1.87	0.57
2:B:755:LEU:HD13	2:B:927:ILE:HG23	1.86	0.57
9:I:76:ARG:NH1	9:I:99:ASN:HB3	2.19	0.57
15:O:176:PRO:HA	17:Q:108:ARG:HE	1.69	0.57
16:P:284:ARG:HD3	17:Q:48:LEU:HA	1.87	0.57
18:X:-70:DA:H2''	18:X:-69:DT:C4	2.40	0.57
18:X:-16:DG:H2''	18:X:-15:DG:C8	2.38	0.57
21:3:347:HIS:O	21:3:411:ASN:ND2	2.34	0.57
13:M:50:LYS:NZ	13:M:200:HIS:O	2.37	0.57
22:4:354:ASP:OD1	22:4:390:ARG:NH1	2.37	0.57
12:L:15:MET:N	12:L:27:GLU:OE1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1132:LEU:HB3	1:A:1171:ALA:HB1	1.86	0.57
1:A:422:GLN:HB3	1:A:449:ILE:HB	1.87	0.57
2:B:755:LEU:CD1	2:B:757:LEU:CD2	2.83	0.57
9:I:15:GLU:OE1	9:I:22:ARG:NH1	2.37	0.57
10:J:25:LEU:O	13:M:368:ARG:NH2	2.35	0.57
2:B:341:ARG:NH2	2:B:582:CYS:SG	2.71	0.57
3:C:155:ASP:HB3	13:M:348:VAL:HG21	1.86	0.57
5:E:56:THR:HG22	5:E:56:THR:O	2.04	0.57
15:O:508:LYS:HD2	16:P:314:LEU:HD23	1.85	0.57
2:B:781:ARG:NH2	2:B:785:GLN:OE1	2.38	0.56
2:B:396:ARG:HG2	2:B:398:ALA:H	1.69	0.56
3:C:86:THR:HG21	3:C:227:PRO:HB3	1.87	0.56
1:A:899:GLN:NE2	1:A:1292:ASP:OD2	2.29	0.56
1:A:1247:THR:HG22	5:E:144:LEU:HD11	1.87	0.56
1:A:1273:TYR:O	1:A:1277:ASN:ND2	2.28	0.56
2:B:634:ASP:OD1	2:B:635:VAL:N	2.35	0.56
5:E:59:THR:O	5:E:71:GLN:NE2	2.34	0.56
8:H:28:LEU:HD21	8:H:50:VAL:HG21	1.87	0.56
10:J:3:ILE:HD12	10:J:4:PRO:HD2	1.87	0.56
11:K:97:GLN:O	11:K:101:ASN:ND2	2.35	0.56
19:Y:16:DC:H2''	19:Y:17:DA:C8	2.40	0.56
1:A:431:PHE:N	24:V:32:GLY:O	2.36	0.56
1:A:1294:MET:HG3	1:A:1295:THR:HG23	1.87	0.56
2:B:712:LEU:HD21	2:B:737:GLN:HG3	1.87	0.56
3:C:115:ILE:HG22	3:C:117:ALA:H	1.70	0.56
20:1:67:LEU:O	20:1:75:ARG:NH1	2.36	0.56
14:N:145:ARG:NH1	14:N:153:GLN:OE1	2.38	0.56
18:X:-70:DA:H2''	18:X:-69:DT:C5	2.41	0.56
2:B:524:ASN:O	13:M:134:GLN:NE2	2.39	0.56
2:B:526:LEU:CD1	2:B:527:CYS:O	2.53	0.56
9:I:85:ARG:NH1	9:I:88:ASP:OD2	2.38	0.56
1:A:29:ARG:HH21	1:A:254:ARG:HH21	1.53	0.56
2:B:779:LEU:O	2:B:878:ALA:HA	2.06	0.56
18:X:-61:DC:N4	22:4:441:ASP:OD2	2.39	0.56
1:A:533:ARG:NH1	1:A:1043:GLU:OE1	2.39	0.56
5:E:56:THR:HG22	5:E:76:PHE:CD1	2.39	0.56
15:O:164:PRO:HD3	15:O:181:VAL:HG22	1.86	0.56
23:U:243:LYS:HG3	24:V:389:ILE:HG21	1.87	0.56
23:U:317:VAL:HG12	23:U:320:GLU:HG3	1.87	0.56
1:A:175:ILE:HD11	1:A:215:GLN:HB2	1.88	0.56
1:A:542:ILE:HG13	1:A:543:GLN:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:149:ASN:ND2	3:C:151:HIS:O	2.38	0.56
14:N:350:MET:SD	14:N:350:MET:N	2.79	0.56
1:A:1368:ARG:NH1	7:G:55:GLU:O	2.38	0.56
5:E:85:LYS:HD2	18:X:17:DC:H3'	1.88	0.56
12:L:19:CYS:SG	12:L:23:HIS:N	2.79	0.56
16:P:252:ILE:HG12	16:P:268:LYS:HG2	1.88	0.56
25:W:335:ILE:O	25:W:339:ASN:ND2	2.38	0.56
2:B:408:GLN:OE1	24:V:82:VAL:HA	2.06	0.55
7:G:187:VAL:HG23	7:G:188:GLY:N	2.20	0.55
11:K:50:THR:OG1	11:K:51:LEU:N	2.39	0.55
19:Y:55:DG:H2'	22:4:388:ILE:HD13	1.88	0.55
2:B:483:ASP:OD2	2:B:495:ASN:ND2	2.39	0.55
21:3:311:TYR:CB	21:3:321:ILE:CD1	2.85	0.55
2:B:528:GLY:HA2	2:B:531:LEU:HD23	1.87	0.55
4:D:99:LEU:HD22	7:G:195:LEU:O	2.03	0.55
21:3:407:PRO:HG3	22:4:176:PHE:CZ	2.42	0.55
22:4:405:ALA:HB1	22:4:408:GLU:HB3	1.87	0.55
24:V:294:VAL:HA	24:V:297:ILE:HG13	1.88	0.55
1:A:381:ALA:HB3	1:A:487:ARG:HB2	1.88	0.55
1:A:838:PHE:O	2:B:677:HIS:ND1	2.33	0.55
2:B:549:ILE:HG12	2:B:555:LEU:HD22	1.86	0.55
9:I:76:ARG:CD	9:I:99:ASN:CA	2.81	0.55
1:A:105:LEU:HD21	1:A:223:VAL:HG23	1.87	0.55
15:O:255:VAL:HG21	15:O:267:VAL:HG11	1.89	0.55
21:3:311:TYR:HB3	21:3:321:ILE:CD1	2.27	0.55
21:3:407:PRO:HG3	22:4:176:PHE:HZ	1.71	0.55
22:4:182:THR:HG1	22:4:275:ARG:HH12	1.52	0.55
6:F:69:ARG:NE	6:F:96:GLU:OE1	2.39	0.55
2:B:755:LEU:HD11	2:B:757:LEU:HD21	1.89	0.55
18:X:-12:DA:H2''	18:X:-11:DG:C8	2.42	0.55
1:A:1328:LEU:HD13	2:B:1117:LEU:HD11	1.89	0.55
2:B:401:ASP:OD1	2:B:401:ASP:N	2.40	0.55
2:B:75:LEU:HD11	2:B:117:ILE:HD12	1.89	0.54
21:3:343:LEU:HD22	21:3:346:LYS:HE2	1.88	0.54
1:A:492:VAL:O	1:A:492:VAL:CG1	2.54	0.54
20:1:123:ALA:HB1	21:3:90:LEU:HD13	1.88	0.54
2:B:1023:ARG:NH2	2:B:1027:PRO:O	2.40	0.54
1:A:669:ARG:NH2	1:A:910:ALA:O	2.40	0.54
2:B:180:ILE:HB	2:B:455:ILE:HG12	1.89	0.54
2:B:1028:ARG:NH1	2:B:1072:SER:O	2.40	0.54
13:M:34:PRO:HA	14:N:356:PHE:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:4:269:ILE:HG23	24:V:295:LYS:HB2	1.89	0.54
22:4:346:ARG:HE	22:4:381:GLY:HA3	1.72	0.54
1:A:76:LEU:O	2:B:1033:ARG:NH2	2.41	0.54
1:A:872:GLN:HE22	1:A:1039:GLN:HA	1.73	0.54
2:B:307:GLU:OE1	2:B:310:ARG:NH1	2.41	0.54
5:E:111:THR:CG2	18:X:16:DG:OP2	2.56	0.54
5:E:116:GLN:NE2	5:E:120:ASP:OD2	2.38	0.54
19:Y:23:DT:H2''	19:Y:24:DA:H5''	1.87	0.54
12:L:16:ILE:HG23	12:L:27:GLU:OE1	2.07	0.54
14:N:254:LEU:HD11	14:N:329:LEU:HD21	1.89	0.54
1:A:1089:LEU:HD11	1:A:1225:LEU:HD21	1.89	0.54
2:B:607:THR:HG1	2:B:610:HIS:HD1	1.55	0.54
20:1:98:ARG:NH2	21:3:325:ASP:OD1	2.40	0.54
11:K:66:GLU:OE2	11:K:87:ARG:NH1	2.41	0.54
19:Y:11:DC:H1'	19:Y:12:DT:C4	2.43	0.54
19:Y:64:DA:H2''	19:Y:65:DG:C8	2.42	0.54
9:I:7:GLY:O	13:M:100:GLN:NE2	2.40	0.54
9:I:8:CYS:SG	9:I:10:ASN:ND2	2.80	0.54
1:A:60:MET:CE	1:A:257:VAL:HG13	2.36	0.54
18:X:-19:DT:O2	24:V:110:ARG:NH2	2.40	0.54
24:V:224:PRO:HD3	25:W:291:TYR:HE1	1.72	0.54
3:C:91:LYS:HB2	3:C:213:HIS:HB2	1.90	0.53
1:A:366:ARG:NH1	1:A:506:ASN:OD1	2.41	0.53
2:B:176:LYS:HE2	2:B:439:VAL:HG22	1.91	0.53
13:M:64:THR:HG21	13:M:96:LEU:HD13	1.91	0.53
13:M:421:MET:O	13:M:424:THR:OG1	2.25	0.53
22:4:203:ARG:NH1	22:4:260:SER:O	2.41	0.53
1:A:113:CYS:SG	1:A:229:ARG:NH1	2.82	0.53
1:A:908:ASP:HA	1:A:1027:MET:SD	2.49	0.53
16:P:142:VAL:HG23	16:P:170:GLN:HA	1.91	0.53
3:C:98:THR:O	3:C:98:THR:CG2	2.57	0.53
4:D:27:ARG:HH21	4:D:36:SER:HB3	1.74	0.53
1:A:887:ASP:OD2	1:A:891:ARG:NH2	2.42	0.53
2:B:990:THR:HA	2:B:997:PRO:HA	1.91	0.53
3:C:157:SER:HB3	13:M:377:LEU:HA	1.91	0.53
7:G:187:VAL:HG23	7:G:188:GLY:H	1.72	0.53
22:4:264:GLU:O	22:4:268:ASN:ND2	2.34	0.53
24:V:212:ASN:HD22	24:V:217:VAL:HG21	1.73	0.53
1:A:1237:ALA:HB1	5:E:136:LEU:HD12	1.90	0.52
1:A:405:ARG:NH1	1:A:441:ALA:O	2.42	0.52
2:B:139:MET:HE2	2:B:169:PHE:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:406:MET:O	2:B:408:GLN:OE1	2.27	0.52
20:1:78:ALA:O	20:1:82:LEU:HD13	2.09	0.52
22:4:383:ASP:OD1	22:4:386:GLN:NE2	2.42	0.52
1:A:1007:THR:HG23	1:A:1010:GLN:H	1.75	0.52
2:B:702:ARG:NH2	2:B:867:GLU:OE2	2.36	0.52
4:D:94:ALA:HB2	4:D:117:LEU:HD11	1.91	0.52
19:Y:64:DA:H2''	19:Y:65:DG:N7	2.24	0.52
13:M:181:GLU:OE1	13:M:189:ARG:NH2	2.43	0.52
2:B:394:LYS:HZ2	19:Y:14:DT:C7	2.22	0.52
20:1:133:ARG:HH11	21:3:59:GLY:HA3	1.74	0.52
1:A:499:ASP:OD1	1:A:499:ASP:N	2.39	0.52
1:A:1230:ASP:OD1	1:A:1250:ASN:ND2	2.34	0.52
18:X:-16:DG:N2	19:Y:17:DA:N3	2.58	0.52
20:1:21:THR:OG1	20:1:73:GLN:NE2	2.42	0.52
21:3:297:THR:CG2	21:3:298:PHE:N	2.73	0.52
1:A:367:THR:HG22	1:A:368:VAL:N	2.24	0.52
2:B:391:VAL:HG13	2:B:395:GLN:HG3	1.92	0.52
7:G:41:ASN:H	7:G:155:GLU:HG2	1.74	0.52
13:M:11:GLN:HE22	14:N:258:LEU:HD22	1.73	0.52
1:A:816:ARG:NH2	2:B:639:ASN:O	2.42	0.52
3:C:40:TRP:NE1	11:K:102:GLU:OE2	2.42	0.52
13:M:6:ASP:HB2	14:N:332:ARG:HB3	1.91	0.52
22:4:366:VAL:HG13	22:4:366:VAL:O	2.10	0.52
1:A:383:PRO:HB3	1:A:484:ARG:HA	1.91	0.52
1:A:583:LEU:HD12	1:A:584:PRO:HD2	1.92	0.52
5:E:193:ILE:HB	5:E:205:THR:HG23	1.92	0.52
14:N:336:ARG:NH1	14:N:347:ASP:OD1	2.43	0.52
1:A:1069:ARG:HH21	1:A:1270:GLU:HG2	1.75	0.51
2:B:395:GLN:HB3	2:B:396:ARG:HD3	1.92	0.51
2:B:1023:ARG:NH1	2:B:1042:ASP:O	2.42	0.51
3:C:236:LEU:CD1	3:C:305:HIS:CE1	2.93	0.51
7:G:93:SER:OG	7:G:96:GLY:O	2.24	0.51
16:P:309:TYR:OH	17:Q:39:PRO:O	2.22	0.51
1:A:1185:MET:SD	1:A:1185:MET:N	2.83	0.51
4:D:25:GLU:HA	4:D:28:LYS:HG2	1.91	0.51
21:3:369:ASP:OD1	21:3:370:SER:N	2.43	0.51
22:4:295:GLN:O	22:4:328:ARG:NH1	2.43	0.51
1:A:764:GLY:CA	1:A:767:CYS:SG	2.95	0.51
3:C:109:ARG:NH2	3:C:198:LEU:O	2.42	0.51
18:X:-17:DT:H2''	18:X:-16:DG:C8	2.46	0.51
25:W:276:VAL:O	25:W:276:VAL:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:ARG:HG2	2:B:1046:ARG:HB2	1.93	0.51
2:B:1021:HIS:NE2	2:B:1043:GLY:O	2.32	0.51
4:D:114:GLU:O	4:D:118:HIS:ND1	2.32	0.51
7:G:151:ARG:HH21	7:G:189:SER:HB2	1.75	0.51
1:A:108:ILE:HA	1:A:115:ILE:HA	1.93	0.51
1:A:117:LEU:HD21	1:A:125:PHE:HD2	1.76	0.51
1:A:1152:SER:OG	1:A:1200:VAL:O	2.28	0.51
2:B:206:SER:HB2	2:B:211:LYS:HG2	1.93	0.51
2:B:674:TYR:HB3	2:B:677:HIS:HD2	1.74	0.51
10:J:10:CYS:SG	10:J:11:GLY:N	2.84	0.51
18:X:-16:DG:OP2	24:V:68:SER:OG	2.25	0.51
24:V:263:SER:O	24:V:266:LEU:HB3	2.11	0.51
1:A:1105:ILE:HG22	1:A:1238:THR:HG21	1.93	0.51
2:B:20:ILE:HD12	2:B:21:PRO:HD2	1.93	0.51
3:C:263:GLU:OE2	3:C:274:ARG:NH1	2.39	0.51
13:M:170:VAL:CG2	16:P:66:LEU:HA	2.41	0.51
15:O:404:MET:HG2	15:O:426:VAL:HG22	1.93	0.51
2:B:121:ARG:HE	2:B:126:ILE:HG13	1.75	0.51
2:B:649:THR:HG22	2:B:649:THR:O	2.11	0.51
2:B:772:TYR:HB3	2:B:884:LEU:HD11	1.93	0.51
1:A:56:LEU:HA	1:A:260:LEU:HD21	1.91	0.51
2:B:869:VAL:HG22	2:B:883:MET:HG3	1.92	0.51
2:B:1050:MET:SD	2:B:1050:MET:N	2.70	0.51
8:H:70:LEU:HD23	8:H:70:LEU:H	1.76	0.51
2:B:622:GLU:OE2	2:B:626:HIS:NE2	2.44	0.50
3:C:96:ASN:HA	12:L:48:ARG:HD3	1.93	0.50
3:C:264:VAL:HB	3:C:271:LYS:HD2	1.93	0.50
1:A:177:GLU:HG2	1:A:215:GLN:HG3	1.92	0.50
1:A:731:LEU:HB2	1:A:736:LEU:HD22	1.93	0.50
21:3:156:VAL:HG12	21:3:156:VAL:O	2.11	0.50
2:B:807:GLU:HG2	12:L:51:ARG:HH12	1.75	0.50
1:A:356:LEU:HD11	2:B:1113:LEU:HD22	1.92	0.50
1:A:590:LYS:HB3	1:A:591:PRO:HD3	1.93	0.50
1:A:942:LYS:HG3	1:A:977:SER:HB2	1.93	0.50
1:A:1363:LEU:HD11	6:F:107:ARG:HD2	1.92	0.50
3:C:287:ILE:HG12	3:C:297:VAL:HG21	1.93	0.50
18:X:-30:DT:H2'	18:X:-29:DT:H72	1.92	0.50
1:A:35:GLN:NE2	1:A:87:ASP:OD2	2.44	0.50
1:A:301:ALA:O	15:O:396:TYR:OH	2.25	0.50
1:A:903:GLY:HA3	1:A:1285:ARG:HG2	1.92	0.50
18:X:-57:DA:H2''	18:X:-56:DA:N7	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Y:42:DG:H2''	19:Y:43:DA:C8	2.47	0.50
24:V:15:LEU:HD12	24:V:26:LEU:HD22	1.93	0.50
24:V:222:PRO:O	24:V:226:ILE:HG12	2.12	0.50
2:B:563:ARG:NH2	2:B:637:GLU:OE2	2.39	0.50
16:P:279:PRO:O	16:P:284:ARG:NH1	2.40	0.50
22:4:194:LYS:HB3	24:V:286:LEU:HD23	1.93	0.50
2:B:181:GLN:HE21	2:B:436:VAL:HG13	1.77	0.50
2:B:790:VAL:HG23	2:B:790:VAL:O	2.11	0.50
5:E:95:GLN:OE1	5:E:125:TYR:OH	2.21	0.50
16:P:113:ARG:HH12	19:Y:13:DT:H4'	1.77	0.50
1:A:1117:ILE:HG12	1:A:1130:VAL:HG13	1.94	0.50
9:I:76:ARG:CD	9:I:99:ASN:N	2.72	0.50
18:X:-60:DC:H2'	18:X:-59:DG:N2	2.27	0.50
1:A:471:LEU:HB3	1:A:495:PRO:HB3	1.93	0.50
1:A:572:LEU:HD13	11:K:83:ARG:HD2	1.94	0.50
13:M:221:GLU:HB3	14:N:374:THR:HG21	1.93	0.50
16:P:211:ALA:N	16:P:270:TYR:O	2.42	0.50
20:1:114:LEU:HD13	20:1:122:ALA:HB1	1.94	0.50
21:3:360:TYR:HE1	22:4:381:GLY:H	1.59	0.50
21:3:373:PRO:C	22:4:286:ASN:HD21	2.15	0.50
23:U:235:ARG:NH1	24:V:382:GLU:O	2.41	0.50
1:A:700:ILE:HG21	2:B:947:LEU:HD22	1.93	0.49
1:A:940:LEU:HD21	1:A:1008:PRO:HD3	1.94	0.49
2:B:1021:HIS:HB2	2:B:1039:ARG:HE	1.77	0.49
1:A:593:THR:HB	3:C:32:ASN:HA	1.94	0.49
1:A:772:ASP:OD1	1:A:773:LYS:N	2.46	0.49
2:B:83:GLY:O	2:B:144:ASN:ND2	2.42	0.49
15:O:447:ILE:HG23	15:O:450:ARG:HH12	1.77	0.49
1:A:262:ILE:HD11	2:B:1115:GLN:HB3	1.93	0.49
1:A:1049:THR:HG22	9:I:85:ARG:HE	1.77	0.49
1:A:1131:LYS:HE2	1:A:1172:VAL:HG22	1.94	0.49
2:B:168:TYR:HB3	2:B:177:VAL:HG22	1.93	0.49
2:B:394:LYS:NZ	19:Y:14:DT:C7	2.75	0.49
2:B:716:GLN:NE2	10:J:48:MET:SD	2.86	0.49
2:B:989:VAL:HG21	2:B:1002:ILE:HB	1.95	0.49
5:E:43:GLN:HB3	5:E:55:ARG:HH21	1.77	0.49
9:I:38:VAL:O	9:I:38:VAL:HG23	2.12	0.49
21:3:230:GLU:OE1	21:3:232:SER:N	2.42	0.49
22:4:265:LYS:HG2	22:4:269:ILE:HD12	1.93	0.49
9:I:76:ARG:HD2	9:I:99:ASN:CA	2.41	0.49
15:O:159:ARG:NH2	15:O:189:LEU:O	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:120:LEU:HB2	19:Y:14:DT:P	2.51	0.49
21:3:204:MET:HG2	21:3:343:LEU:HG	1.93	0.49
1:A:210:LEU:HG	15:O:411:LYS:HA	1.94	0.49
1:A:918:PRO:HB2	1:A:919:LEU:HD12	1.94	0.49
2:B:563:ARG:HA	2:B:568:ILE:HB	1.95	0.49
18:X:-14:DA:H2'	18:X:-13:DA:H8	1.77	0.49
21:3:216:ARG:HE	21:3:250:ALA:HB3	1.77	0.49
1:A:811:ASP:OD1	1:A:811:ASP:N	2.45	0.49
1:A:1374:LYS:HE3	7:G:52:THR:HG22	1.93	0.49
2:B:139:MET:CE	2:B:169:PHE:CE1	2.96	0.49
21:3:311:TYR:N	21:3:321:ILE:CD1	2.76	0.49
1:A:1069:ARG:HH12	1:A:1080:ILE:HD12	1.78	0.49
2:B:900:ARG:NH2	2:B:945:GLU:OE2	2.40	0.49
5:E:50:GLU:OE2	5:E:56:THR:OG1	2.31	0.49
20:1:15:LEU:HD22	20:1:74:ILE:HD12	1.95	0.49
1:A:459:VAL:HG21	1:A:520:LEU:HB2	1.94	0.49
1:A:996:GLU:HB3	1:A:997:PRO:HD3	1.94	0.49
5:E:185:ILE:HD13	5:E:191:VAL:HG11	1.95	0.49
7:G:115:GLN:HE21	7:G:192:GLU:HG3	1.77	0.49
13:M:176:ARG:HE	13:M:177:PHE:H	1.61	0.49
22:4:508:ARG:HH11	22:4:511:ARG:HH21	1.59	0.49
24:V:15:LEU:H	24:V:15:LEU:HD23	1.77	0.49
1:A:1118:GLU:OE1	9:I:39:THR:OG1	2.27	0.49
2:B:192:GLU:HA	2:B:351:VAL:HG13	1.95	0.49
15:O:507:ASN:HB3	17:Q:58:LEU:HD13	1.95	0.49
19:Y:-15:DT:H2''	19:Y:-14:DG:C8	2.48	0.49
24:V:276:MET:HB3	24:V:307:LEU:HD13	1.93	0.49
1:A:459:VAL:HB	1:A:516:LYS:HG3	1.95	0.48
2:B:823:ASN:OD1	2:B:824:LYS:N	2.44	0.48
13:M:276:LEU:O	13:M:281:GLN:NE2	2.46	0.48
1:A:41:LEU:HB2	24:V:58:SER:HB2	1.95	0.48
7:G:46:ILE:HB	7:G:75:VAL:HG23	1.94	0.48
16:P:88:SER:OG	16:P:90:ASN:OD1	2.29	0.48
21:3:319:HIS:O	21:3:321:ILE:CD1	2.57	0.48
1:A:247:PRO:HA	1:A:250:LEU:HD13	1.94	0.48
18:X:-17:DT:H2''	18:X:-16:DG:N7	2.28	0.48
22:4:474:GLY:H	22:4:479:ILE:HD11	1.78	0.48
24:V:214:THR:HA	24:V:312:PHE:HZ	1.78	0.48
1:A:30:GLN:NE2	2:B:1094:TYR:O	2.47	0.48
2:B:214:THR:HG22	2:B:227:HIS:HD2	1.76	0.48
2:B:753:ASP:OD2	2:B:937:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:511:ALA:HB2	17:Q:58:LEU:HD21	1.94	0.48
1:A:275:ASN:HB3	24:V:50:LEU:HB3	1.95	0.48
1:A:602:SER:HB2	1:A:644:GLU:HA	1.95	0.48
1:A:780:MET:HE1	2:B:932:HIS:HA	1.96	0.48
1:A:1264:ARG:HG3	1:A:1291:SER:HB2	1.94	0.48
21:3:184:VAL:HG23	21:3:321:ILE:HG23	1.94	0.48
22:4:371:PRO:HB2	22:4:374:ARG:HG2	1.94	0.48
1:A:143:LYS:HB2	1:A:239:LEU:HG	1.95	0.48
2:B:516:SER:O	13:M:113:ARG:NH2	2.39	0.48
21:3:179:GLU:HB3	21:3:329:VAL:HB	1.96	0.48
1:A:354:GLY:HA2	2:B:1046:ARG:HH22	1.77	0.48
2:B:539:VAL:HG12	2:B:583:VAL:HB	1.95	0.48
6:F:107:ARG:NH1	7:G:56:ASP:OD2	2.47	0.48
2:B:898:SER:HB3	2:B:1010:GLN:HG3	1.94	0.48
18:X:-36:DC:H2'	18:X:-35:DT:C6	2.49	0.48
22:4:483:LEU:HB3	22:4:486:ARG:HB2	1.96	0.48
8:H:80:ASP:OD1	8:H:80:ASP:N	2.47	0.48
15:O:381:GLU:OE2	15:O:392:LYS:NZ	2.36	0.48
18:X:-58:DT:H2''	18:X:-57:DA:C8	2.48	0.48
1:A:22:MET:SD	1:A:22:MET:N	2.87	0.48
1:A:166:VAL:HG12	1:A:174:ILE:HD11	1.96	0.48
4:D:85:GLN:O	4:D:89:HIS:ND1	2.44	0.48
8:H:94:GLY:HA3	8:H:118:TYR:HD1	1.79	0.48
16:P:18:ILE:O	16:P:21:ARG:HG3	2.14	0.48
1:A:937:GLU:OE1	1:A:1007:THR:OG1	2.22	0.47
1:A:997:PRO:HB2	1:A:1000:LEU:HG	1.96	0.47
2:B:106:ASP:OD1	2:B:882:LYS:NZ	2.39	0.47
4:D:1:MET:SD	4:D:1:MET:N	2.81	0.47
22:4:435:SER:H	22:4:438:GLN:HE21	1.62	0.47
1:A:303:THR:OG1	15:O:377:GLN:OE1	2.29	0.47
2:B:916:MET:HE3	2:B:925:PRO:HG2	1.95	0.47
3:C:296:VAL:HG23	3:C:297:VAL:HG13	1.94	0.47
7:G:96:GLY:HA2	7:G:112:GLU:HG2	1.95	0.47
13:M:174:THR:O	13:M:174:THR:CG2	2.60	0.47
13:M:339:SER:HB2	13:M:349:LEU:HD11	1.95	0.47
19:Y:46:DT:H2''	19:Y:47:DA:H5''	1.95	0.47
19:Y:63:DA:H2''	19:Y:64:DA:C8	2.48	0.47
21:3:390:ASP:OD1	21:3:394:ASN:N	2.45	0.47
22:4:373:ARG:HH11	22:4:384:SER:HB2	1.80	0.47
24:V:20:HIS:CG	24:V:21:TYR:H	2.32	0.47
2:B:300:GLY:N	2:B:304:THR:OG1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:108:TRP:HD1	16:P:147:LYS:HB2	1.80	0.47
4:D:11:LEU:HD12	4:D:15:GLU:HB2	1.97	0.47
5:E:111:THR:CG2	18:X:16:DG:P	3.03	0.47
13:M:134:GLN:OE1	13:M:136:ARG:NH2	2.47	0.47
16:P:161:VAL:HG23	16:P:162:THR:HG22	1.96	0.47
20:1:4:PRO:HB2	20:1:7:LEU:HD13	1.96	0.47
20:1:130:ARG:HH12	21:3:55:LEU:HD11	1.80	0.47
21:3:234:THR:O	21:3:234:THR:CG2	2.59	0.47
24:V:76:VAL:HG22	24:V:118:VAL:HG13	1.96	0.47
1:A:799:VAL:HG23	1:A:837:SER:HA	1.95	0.47
2:B:554:LYS:NZ	14:N:347:ASP:OD2	2.47	0.47
2:B:793:PRO:HB2	2:B:802:PRO:HB3	1.96	0.47
5:E:121:MET:SD	5:E:122:ALA:N	2.88	0.47
13:M:364:ARG:HH22	13:M:403:PRO:HA	1.80	0.47
15:O:337:ASN:HB3	15:O:340:LYS:HE2	1.95	0.47
16:P:158:ASP:HB3	16:P:161:VAL:HG22	1.96	0.47
22:4:303:GLU:N	22:4:303:GLU:OE1	2.47	0.47
24:V:109:ALA:O	24:V:114:LYS:NZ	2.46	0.47
2:B:106:ASP:HA	2:B:173:GLY:HA3	1.97	0.47
2:B:235:PRO:HD2	2:B:238:ILE:HD12	1.97	0.47
2:B:304:THR:O	2:B:304:THR:CG2	2.62	0.47
5:E:30:GLN:HA	5:E:33:LEU:HD12	1.96	0.47
11:K:39:CYS:SG	11:K:83:ARG:NE	2.87	0.47
13:M:6:ASP:OD1	13:M:6:ASP:N	2.46	0.47
18:X:15:DA:H2''	18:X:16:DG:O5'	2.14	0.47
1:A:60:MET:HA	1:A:82:HIS:HB2	1.97	0.47
3:C:86:THR:HA	3:C:119:PRO:HB3	1.97	0.47
5:E:63:ALA:HB3	5:E:67:ASP:H	1.78	0.47
14:N:254:LEU:CD1	14:N:329:LEU:HD21	2.44	0.47
14:N:367:ASP:HB3	14:N:370:THR:HB	1.97	0.47
21:3:234:THR:CG2	21:3:237:GLN:HB2	2.45	0.47
1:A:1363:LEU:HD11	6:F:107:ARG:HH11	1.80	0.47
2:B:287:ILE:O	2:B:291:VAL:HG23	2.15	0.47
5:E:15:LYS:O	5:E:18:MET:HG3	2.15	0.47
13:M:322:GLN:HE22	13:M:364:ARG:HA	1.79	0.47
1:A:1089:LEU:HD21	1:A:1225:LEU:HD11	1.96	0.47
2:B:23:VAL:HG23	2:B:26:LYS:HB2	1.97	0.47
3:C:144:VAL:HG21	3:C:168:VAL:HG13	1.97	0.47
4:D:53:ILE:O	4:D:56:THR:OG1	2.27	0.47
7:G:116:GLN:HE22	7:G:118:ALA:HB3	1.79	0.47
15:O:271:LEU:O	15:O:275:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:109:SER:HB2	16:P:150:TYR:HE2	1.79	0.47
22:4:297:TRP:HZ2	22:4:333:CYS:HB2	1.79	0.47
1:A:87:ASP:OD1	1:A:254:ARG:NE	2.48	0.47
1:A:508:HIS:HB3	2:B:1067:ARG:HH11	1.80	0.47
2:B:506:MET:SD	2:B:569:ASN:ND2	2.88	0.47
2:B:817:PRO:HG3	2:B:869:VAL:HG23	1.96	0.47
3:C:238:ASP:OD1	3:C:238:ASP:N	2.48	0.47
9:I:22:ARG:HE	9:I:31:VAL:HG11	1.79	0.47
18:X:-9:DA:H2''	18:X:-8:DC:C6	2.50	0.47
1:A:182:ASN:ND2	1:A:185:VAL:O	2.47	0.46
9:I:76:ARG:HD2	9:I:99:ASN:N	2.31	0.46
13:M:92:TYR:CZ	13:M:97:MET:HG2	2.50	0.46
19:Y:11:DC:H2''	19:Y:12:DT:H72	1.97	0.46
1:A:35:GLN:HB2	1:A:85:TYR:CZ	2.50	0.46
1:A:940:LEU:HB2	1:A:1006:ILE:HG23	1.98	0.46
2:B:300:GLY:HA3	2:B:304:THR:OG1	2.16	0.46
2:B:1041:ARG:HH21	24:V:44:PHE:HD1	1.63	0.46
7:G:7:MET:HB3	7:G:72:PHE:CE2	2.51	0.46
7:G:89:ILE:HG21	7:G:127:TRP:CD1	2.51	0.46
13:M:11:GLN:HB2	14:N:331:ILE:HD13	1.97	0.46
15:O:445:ASN:ND2	28:P:401:SF4:S1	2.87	0.46
18:X:-11:DG:C2	18:X:-10:DG:C6	3.04	0.46
24:V:294:VAL:HG23	24:V:297:ILE:HD12	1.97	0.46
1:A:832:GLY:HA2	1:A:849:PHE:CD2	2.50	0.46
1:A:883:CYS:HB2	1:A:1355:ILE:HG22	1.97	0.46
15:O:36:LEU:HD21	15:O:47:LEU:HD11	1.97	0.46
15:O:274:SER:OG	15:O:285:THR:OG1	2.31	0.46
21:3:175:ILE:HG12	21:3:337:ARG:HB2	1.96	0.46
1:A:41:LEU:HD12	24:V:53:VAL:HG11	1.98	0.46
9:I:19:ARG:HH21	9:I:33:ASN:HD22	1.63	0.46
16:P:276:ILE:HG22	16:P:277:ILE:HG23	1.97	0.46
22:4:399:LEU:HA	22:4:433:GLY:HA2	1.97	0.46
22:4:434:ARG:HB3	22:4:439:CYS:SG	2.56	0.46
1:A:194:LEU:HD22	1:A:211:LEU:HG	1.98	0.46
1:A:382:VAL:N	1:A:479:ARG:O	2.42	0.46
1:A:630:ASP:OD2	8:H:97:TYR:OH	2.30	0.46
1:A:1299:GLU:OE1	5:E:174:GLN:NE2	2.49	0.46
9:I:29:PRO:HA	13:M:73:LYS:HD3	1.97	0.46
9:I:59:TRP:CZ2	9:I:96:LYS:CD	2.93	0.46
13:M:386:LEU:HD13	13:M:398:TRP:NE1	2.30	0.46
14:N:251:VAL:HG13	14:N:252:ALA:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:88:TYR:O	15:O:92:ILE:HG12	2.15	0.46
18:X:-41:DG:H2''	18:X:-40:DA:C8	2.50	0.46
20:1:67:LEU:C	20:1:75:ARG:HH12	2.18	0.46
2:B:755:LEU:HD13	2:B:757:LEU:CD2	2.46	0.46
13:M:120:ARG:HB2	13:M:123:GLU:HG2	1.98	0.46
23:U:268[A]:ILE:HD13	23:U:332:LEU:HD22	1.96	0.46
23:U:268[B]:ILE:HD13	23:U:332:LEU:HD22	1.96	0.46
2:B:207:THR:HG23	2:B:210:LYS:H	1.81	0.46
11:K:27:LEU:HG	11:K:43:VAL:HB	1.97	0.46
17:Q:83:ASP:OD1	17:Q:83:ASP:N	2.48	0.46
18:X:-58:DT:H2''	18:X:-57:DA:N7	2.31	0.46
20:1:71:THR:O	20:1:75:ARG:HG3	2.15	0.46
24:V:257:ASP:OD1	24:V:257:ASP:N	2.49	0.46
3:C:79:ILE:HD13	3:C:83:GLU:HG3	1.98	0.46
3:C:287:ILE:HD11	3:C:293:LEU:HB3	1.97	0.46
12:L:14:PRO:C	12:L:27:GLU:OE2	2.50	0.46
15:O:265:GLU:OE1	15:O:268:ARG:NH1	2.49	0.46
19:Y:56:DT:H5''	21:3:146:ILE:HD11	1.98	0.46
22:4:256:ASN:H	22:4:259:ASP:HB2	1.81	0.46
2:B:803:ILE:HG13	2:B:806:HIS:H	1.81	0.46
21:3:224:ASP:HA	21:3:314:GLN:HE22	1.81	0.46
21:3:297:THR:HG22	21:3:298:PHE:H	1.78	0.46
5:E:22:HIS:HB2	5:E:28:VAL:HG21	1.98	0.46
9:I:76:ARG:HD2	9:I:99:ASN:CB	2.04	0.46
3:C:144:VAL:HG11	3:C:168:VAL:HG22	1.98	0.45
3:C:166:HIS:CD2	3:C:167:LYS:HG3	2.50	0.45
14:N:139:ASN:O	14:N:142:LYS:NZ	2.43	0.45
16:P:19:GLU:HB3	16:P:57:LEU:HD21	1.97	0.45
17:Q:33:LYS:HD2	17:Q:34:PRO:HD2	1.97	0.45
19:Y:-14:DG:H2''	19:Y:-13:DC:C6	2.52	0.45
24:V:280:LEU:HD12	24:V:283:LEU:HD12	1.98	0.45
1:A:1291:SER:O	1:A:1295:THR:OG1	2.27	0.45
2:B:160:GLU:O	10:J:62:TYR:OH	2.23	0.45
8:H:60:ILE:HD11	8:H:143:LEU:HD12	1.98	0.45
14:N:251:VAL:HG23	14:N:331:ILE:CG2	2.46	0.45
15:O:104:GLU:OE2	17:Q:56:TYR:OH	2.33	0.45
18:X:-10:DG:H2''	18:X:-9:DA:C8	2.51	0.45
19:Y:-16:DC:H2'	19:Y:-15:DT:C5	2.51	0.45
19:Y:28:DA:H1'	19:Y:29:DA:C5	2.52	0.45
22:4:157:VAL:HG13	22:4:158:GLY:N	2.31	0.45
2:B:686:GLN:HE22	2:B:1010:GLN:HE22	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:94:GLY:HA3	8:H:118:TYR:CD1	2.51	0.45
16:P:195:ALA:O	16:P:198:SER:OG	2.34	0.45
22:4:473:VAL:HB	22:4:475:HIS:CD2	2.52	0.45
1:A:23:LYS:HE3	2:B:1123:ILE:HG21	1.99	0.45
1:A:743:THR:OG1	1:A:744:ALA:N	2.48	0.45
2:B:406:MET:O	2:B:408:GLN:CD	2.54	0.45
2:B:1069:MET:HG3	2:B:1107:PRO:HG3	1.99	0.45
12:L:25:GLU:N	12:L:25:GLU:OE1	2.50	0.45
18:X:-35:DT:H2'	18:X:-34:DT:C6	2.52	0.45
2:B:80:ILE:HG22	2:B:115:VAL:HG23	1.98	0.45
2:B:250:GLU:OE2	2:B:329:ARG:NH1	2.50	0.45
11:K:25:THR:O	11:K:45:HIS:ND1	2.45	0.45
25:W:344:GLU:HB3	25:W:352:ILE:HD11	1.99	0.45
1:A:1355:ILE:HD11	2:B:1056:ILE:HG23	1.98	0.45
5:E:111:THR:HG23	18:X:16:DG:OP2	2.17	0.45
1:A:41:LEU:HB3	1:A:56:LEU:HD12	1.98	0.45
1:A:43:SER:OG	1:A:45:ASP:OD2	2.25	0.45
1:A:1216:GLU:O	9:I:101:GLN:NE2	2.49	0.45
12:L:16:ILE:HG13	12:L:47:LYS:HD3	1.98	0.45
16:P:216:VAL:HG21	16:P:239:LEU:HD11	1.99	0.45
21:3:161:SER:HA	21:3:164:ILE:HG12	1.99	0.45
1:A:168:LYS:NZ	1:A:170:GLY:O	2.49	0.45
1:A:616:ASN:HA	1:A:640:ILE:O	2.17	0.45
1:A:1220:LYS:HZ2	1:A:1222:LYS:HD3	1.81	0.45
2:B:245:VAL:HG23	2:B:250:GLU:OE1	2.16	0.45
9:I:63:ASP:OD1	9:I:63:ASP:N	2.46	0.45
13:M:177:PHE:CD1	16:P:94:LEU:HD21	2.52	0.45
16:P:313:TRP:HZ2	17:Q:48:LEU:HD11	1.81	0.45
18:X:-69:DT:H2''	18:X:-68:DA:N7	2.31	0.45
20:1:28:ASP:OD1	20:1:29:PHE:N	2.49	0.45
21:3:324:THR:CG2	21:3:325:ASP:N	2.80	0.45
2:B:314:ALA:HA	2:B:328:PHE:HE2	1.82	0.45
2:B:451:MET:HA	2:B:454:ARG:HG3	1.98	0.45
10:J:40:LEU:HD11	10:J:49:LEU:HD12	1.99	0.45
15:O:398:MET:HG2	15:O:403:PHE:HB2	1.98	0.45
16:P:239:LEU:HD23	16:P:242:LEU:HD12	1.99	0.45
17:Q:42:ASP:OD1	17:Q:42:ASP:N	2.50	0.45
22:4:457:ASN:HD22	22:4:459:LYS:H	1.65	0.45
25:W:332:ARG:HH21	25:W:336:GLU:HB3	1.81	0.45
13:M:235:ASN:HD22	14:N:326:VAL:HG12	1.81	0.45
1:A:907:LEU:HD13	1:A:918:PRO:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1128:ILE:HG13	1:A:1189:LEU:HD22	1.99	0.44
1:A:1291:SER:HA	1:A:1294:MET:HG2	1.99	0.44
3:C:86:THR:OG1	3:C:225:PHE:O	2.30	0.44
9:I:74:HIS:ND1	9:I:76:ARG:NH1	2.65	0.44
15:O:106:ILE:O	15:O:110:LEU:CD1	2.59	0.44
15:O:267:VAL:O	15:O:270:MET:HG3	2.17	0.44
2:B:190:ILE:HG21	2:B:354:ARG:HE	1.81	0.44
7:G:13:ILE:HD11	7:G:26:ILE:HD11	1.99	0.44
13:M:238:LEU:HD23	14:N:277:GLY:HA3	1.99	0.44
15:O:361:ARG:HH21	15:O:386:ILE:HG23	1.82	0.44
17:Q:53:GLY:O	17:Q:57:MET:HG2	2.17	0.44
2:B:739:ALA:HB3	2:B:1009:TYR:CD2	2.53	0.44
6:F:79:VAL:HG11	6:F:83:LEU:HD23	1.98	0.44
8:H:13:LYS:HZ3	8:H:31:GLU:HB3	1.82	0.44
14:N:253:GLU:O	14:N:256:ARG:HG3	2.17	0.44
19:Y:32:DC:H2''	19:Y:33:DC:C5	2.51	0.44
21:3:188:TYR:HB2	21:3:319:HIS:ND1	2.33	0.44
21:3:405:VAL:HG23	21:3:405:VAL:O	2.16	0.44
1:A:325:LEU:HB2	1:A:328:ILE:HG13	1.98	0.44
1:A:545:PHE:HE1	1:A:688:PRO:HG3	1.82	0.44
1:A:1102:LYS:HD2	1:A:1212:ILE:HD11	1.99	0.44
3:C:133:THR:OG1	3:C:136:ASP:OD1	2.33	0.44
4:D:42:LEU:HD11	7:G:31:ASN:HB3	1.98	0.44
7:G:115:GLN:H	7:G:119:LYS:HZ2	1.66	0.44
19:Y:37:DA:H2''	19:Y:38:DA:C8	2.53	0.44
23:U:263:ASP:HA	23:U:309:LYS:HA	1.99	0.44
1:A:731:LEU:HD23	1:A:748:LEU:HD22	2.00	0.44
1:A:1102:LYS:HB2	1:A:1212:ILE:HD11	2.00	0.44
1:A:1107:LYS:HD3	1:A:1205:PRO:HA	2.00	0.44
1:A:1159:ARG:HH21	18:X:13:DG:H2'	1.82	0.44
20:1:52:ASN:OD1	20:1:95:GLN:NE2	2.50	0.44
21:3:87:ALA:HA	21:3:91:ASP:HB3	1.98	0.44
22:4:194:LYS:HB3	24:V:286:LEU:CD2	2.48	0.44
1:A:463:ASN:HB2	1:A:473:ILE:CD1	2.48	0.44
2:B:528:GLY:O	2:B:531:LEU:HB2	2.18	0.44
24:V:124:ILE:O	24:V:128:GLN:HG2	2.18	0.44
24:V:261:PRO:O	24:V:264:SER:OG	2.23	0.44
2:B:376:LEU:HB3	2:B:411:ILE:HD12	1.99	0.44
4:D:88:ASN:O	4:D:90:ARG:NH2	2.50	0.44
15:O:36:LEU:HD12	15:O:54:LEU:HD12	1.99	0.44
15:O:82:VAL:O	15:O:85:MET:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Y:34:DA:H2''	19:Y:35:DA:C8	2.52	0.44
1:A:384:VAL:HG13	1:A:415:HIS:CD2	2.53	0.44
2:B:89:GLU:OE1	12:L:42:ARG:NE	2.49	0.44
21:3:49:GLU:OE1	21:3:49:GLU:N	2.50	0.44
21:3:140:ARG:HG3	21:3:144:ILE:HB	1.99	0.44
2:B:240:PHE:HE1	2:B:254:MET:HE1	1.83	0.44
22:4:253:LEU:HD12	22:4:254:LEU:HD12	2.00	0.44
2:B:392:ILE:N	2:B:393:PRO:HD2	2.33	0.43
2:B:394:LYS:NZ	19:Y:14:DT:H73	2.33	0.43
2:B:505:ASP:OD1	2:B:505:ASP:N	2.51	0.43
2:B:530:GLU:HG2	14:N:352:THR:HB	2.00	0.43
3:C:49:PHE:HE1	3:C:68:ILE:HB	1.82	0.43
15:O:127:ASP:O	15:O:130:THR:OG1	2.36	0.43
19:Y:30:DA:H2'	19:Y:31:DG:C8	2.52	0.43
1:A:74:LYS:HB3	1:A:78:ASP:HB2	1.99	0.43
1:A:473:ILE:HG23	1:A:473:ILE:O	2.18	0.43
2:B:357:TYR:CE2	2:B:475:GLN:HG2	2.53	0.43
20:1:80:TYR:CZ	20:1:125:ILE:HG13	2.53	0.43
21:3:281:HIS:CE1	24:V:187:PRO:HG2	2.53	0.43
23:U:187:ALA:O	24:V:394:ARG:NH1	2.51	0.43
1:A:267:VAL:HA	1:A:274:THR:HG22	2.01	0.43
1:A:623:GLN:HG2	1:A:636:SER:HB2	2.01	0.43
13:M:286:MET:HB3	13:M:327:VAL:HB	1.99	0.43
18:X:-64:DT:H2''	18:X:-63:DT:C6	2.54	0.43
19:Y:60:DG:H2''	19:Y:61:DG:C8	2.53	0.43
20:1:26:PHE:N	20:1:121:ASP:OD2	2.47	0.43
20:1:41:ILE:HD11	21:3:133:ARG:HD3	2.00	0.43
20:1:59:LEU:HB3	20:1:97:ILE:HG22	1.99	0.43
22:4:219:GLN:HA	22:4:222:VAL:HG12	2.00	0.43
1:A:876:VAL:HG11	2:B:1053:ASP:HB3	2.00	0.43
1:A:1262:ALA:HB2	5:E:145:VAL:HG22	1.99	0.43
2:B:67:SER:HA	2:B:385:LYS:HE3	2.01	0.43
2:B:763:ASP:HB3	3:C:222:HIS:CE1	2.54	0.43
3:C:291:GLU:HA	3:C:294:LYS:HE2	2.00	0.43
13:M:8:PRO:HG3	14:N:330:LEU:HD23	2.00	0.43
2:B:233:ASP:N	2:B:233:ASP:OD1	2.51	0.43
10:J:43:TYR:HA	10:J:46:ARG:HD3	2.01	0.43
18:X:-21:DC:C3'	18:X:-20:DT:H5'	2.48	0.43
21:3:407:PRO:CG	22:4:176:PHE:HZ	2.32	0.43
2:B:207:THR:HG23	2:B:209:GLU:H	1.82	0.43
2:B:903:GLN:OE1	2:B:937:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:67:ASP:OD2	5:E:69:THR:OG1	2.35	0.43
13:M:13:ILE:HB	14:N:329:LEU:HB3	2.01	0.43
13:M:242:PRO:HB3	14:N:392:LEU:HD22	2.01	0.43
13:M:400:PHE:HD2	13:M:402:LEU:H	1.67	0.43
7:G:59:VAL:O	7:G:59:VAL:HG13	2.18	0.43
7:G:108:LEU:HD13	7:G:148:ILE:HG21	2.01	0.43
21:3:297:THR:CG2	21:3:298:PHE:H	2.31	0.43
1:A:40:ASN:HB3	24:V:58:SER:O	2.18	0.43
1:A:307:MET:HG3	15:O:422:TYR:CE1	2.53	0.43
2:B:115:VAL:HG12	2:B:131:LEU:O	2.19	0.43
2:B:122:GLY:O	2:B:123:SER:OG	2.33	0.43
2:B:577:ASN:O	2:B:581:ARG:N	2.51	0.43
3:C:155:ASP:N	3:C:155:ASP:OD1	2.47	0.43
16:P:92:GLU:OE2	16:P:133:LYS:NZ	2.38	0.43
18:X:-50:DA:H5'	21:3:350:TRP:HE1	1.83	0.43
24:V:238:GLN:HB3	24:V:242:ARG:HD2	2.01	0.43
1:A:529:LEU:HA	1:A:539:ILE:HD13	2.01	0.43
1:A:669:ARG:O	1:A:1021:LYS:NZ	2.52	0.43
1:A:1319:ALA:O	1:A:1324:THR:HG22	2.19	0.43
1:A:1332:ALA:HB2	2:B:1122:ILE:HG23	2.01	0.43
2:B:82:VAL:HG23	2:B:144:ASN:HD21	1.84	0.43
5:E:111:THR:OG1	5:E:114:ALA:CB	2.66	0.43
7:G:115:GLN:HG3	7:G:116:GLN:HG3	2.01	0.43
7:G:154:ASP:OD1	7:G:154:ASP:N	2.50	0.43
15:O:252:VAL:HG22	15:O:267:VAL:HG13	2.01	0.43
24:V:281:ALA:O	24:V:284:ARG:HG2	2.19	0.43
24:V:283:LEU:HD22	24:V:288:LEU:HD11	2.01	0.43
2:B:946:LEU:HD22	2:B:1003:TYR:CE2	2.54	0.43
2:B:946:LEU:HD22	2:B:1003:TYR:CZ	2.54	0.43
9:I:59:TRP:CZ2	9:I:96:LYS:CE	3.02	0.43
1:A:275:ASN:HA	24:V:52:GLU:HA	2.00	0.42
1:A:289:LEU:HD11	1:A:316:GLN:HG3	2.01	0.42
2:B:40:VAL:O	2:B:40:VAL:HG22	2.19	0.42
2:B:695:GLY:HA3	2:B:735:ALA:HA	1.99	0.42
2:B:751:ILE:HG22	2:B:752:GLU:HG3	2.00	0.42
2:B:993:ILE:O	3:C:74:ASN:ND2	2.52	0.42
3:C:9:GLU:OE2	3:C:298:ARG:NH1	2.52	0.42
4:D:6:ALA:HA	7:G:5:VAL:HG22	2.01	0.42
11:K:56:ARG:HG2	11:K:68:CYS:SG	2.59	0.42
16:P:310:MET:HE1	16:P:313:TRP:CZ3	2.53	0.42
20:1:66:PHE:O	20:1:75:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:VAL:HG13	2:B:245:VAL:O	2.19	0.42
2:B:901:HIS:NE2	2:B:945:GLU:OE1	2.48	0.42
17:Q:88:SER:HA	17:Q:91:TYR:HD2	1.83	0.42
18:X:-11:DG:H2''	18:X:-10:DG:C8	2.53	0.42
20:1:48:ASN:ND2	20:1:49:LEU:H	2.17	0.42
24:V:132:PRO:HG2	24:V:175:THR:HG21	2.00	0.42
2:B:91:PHE:O	24:V:175:THR:HG22	2.19	0.42
3:C:151:HIS:O	3:C:151:HIS:ND1	2.52	0.42
15:O:193:LEU:HD21	15:O:230:ASP:HB3	2.01	0.42
15:O:481:GLU:HA	15:O:484:LEU:HD23	2.02	0.42
22:4:372:TYR:CE1	22:4:388:ILE:HG23	2.54	0.42
1:A:331:ASN:OD1	1:A:332:MET:N	2.51	0.42
3:C:290:ASN:O	3:C:294:LYS:HG3	2.20	0.42
5:E:35:GLN:NE2	5:E:39:GLU:OE1	2.53	0.42
5:E:103:LEU:HG	5:E:128:GLU:HB2	2.01	0.42
12:L:15:MET:O	12:L:27:GLU:OE1	2.37	0.42
16:P:90:ASN:OD1	16:P:91:GLN:N	2.51	0.42
20:1:75:ARG:NH2	20:1:106:GLU:OE1	2.51	0.42
2:B:531:LEU:HD11	2:B:538:LEU:HD21	2.01	0.42
7:G:114:LEU:H	7:G:119:LYS:HZ3	1.67	0.42
15:O:47:LEU:HG	15:O:51:LYS:HE3	2.02	0.42
21:3:316:ASP:HB3	22:4:165:THR:HG22	2.01	0.42
22:4:312:HIS:CE1	22:4:315:LEU:HB2	2.55	0.42
1:A:763:ALA:HB1	1:A:797:ALA:HB1	2.02	0.42
4:D:57:PRO:HB2	4:D:90:ARG:HE	1.84	0.42
3:C:120:ARG:NH1	3:C:324:GLU:OE2	2.42	0.42
4:D:103:GLU:O	4:D:107:ARG:NE	2.52	0.42
11:K:31:GLN:HB3	11:K:39:CYS:HB3	2.01	0.42
13:M:148:LYS:O	13:M:151:GLU:HG2	2.20	0.42
13:M:368:ARG:HD3	13:M:398:TRP:CH2	2.55	0.42
15:O:195:LEU:HD23	15:O:195:LEU:H	1.83	0.42
2:B:744:MET:SD	2:B:746:TYR:HB2	2.60	0.42
4:D:19:LEU:HD22	7:G:49:PHE:HD1	1.85	0.42
7:G:39:VAL:HB	7:G:42:VAL:HB	2.02	0.42
11:K:107:CYS:HA	11:K:110:VAL:HG12	2.01	0.42
12:L:35:ARG:NH1	12:L:36:CYS:H	2.17	0.42
13:M:81:VAL:HG11	13:M:92:TYR:HE2	1.83	0.42
13:M:292:MET:HG2	13:M:297:LEU:HD13	2.02	0.42
15:O:80:SER:O	15:O:84:ARG:HG2	2.19	0.42
16:P:65:LEU:HD11	16:P:72:LEU:HD22	2.01	0.42
18:X:-45:DT:H2''	18:X:-44:DT:C5	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Y:13:DT:H2''	19:Y:14:DT:C6	2.54	0.42
1:A:282:LYS:HZ1	1:A:319:LEU:HB2	1.84	0.42
1:A:1054:HIS:CD2	1:A:1065:LEU:HD12	2.55	0.42
5:E:111:THR:CG2	18:X:16:DG:H5''	2.21	0.42
15:O:477:THR:HG23	15:O:477:THR:O	2.20	0.42
18:X:-69:DT:H6	18:X:-69:DT:H2'	1.70	0.42
1:A:109:CYS:N	1:A:114:HIS:O	2.40	0.42
1:A:177:GLU:HA	1:A:215:GLN:HB3	2.00	0.42
5:E:65:ASN:OD1	5:E:66:ASP:N	2.53	0.42
5:E:111:THR:HG22	18:X:16:DG:P	2.60	0.42
13:M:179:ARG:HD3	16:P:117:ASN:HD22	1.85	0.42
14:N:346:LEU:HD22	14:N:387:PRO:HA	2.02	0.42
18:X:-49:DA:H2''	18:X:-48:DG:C8	2.55	0.42
1:A:558:PHE:HB3	1:A:594:LEU:HD13	2.02	0.41
2:B:87:VAL:HG22	2:B:89:GLU:H	1.85	0.41
5:E:56:THR:CG2	5:E:76:PHE:CD1	3.03	0.41
1:A:367:THR:CG2	1:A:368:VAL:N	2.83	0.41
2:B:682:ARG:NH2	9:I:89:GLU:OE2	2.50	0.41
13:M:378:CYS:SG	13:M:379:ALA:N	2.93	0.41
15:O:92:ILE:HD11	15:O:111:LEU:HD12	2.02	0.41
1:A:604:ILE:HD12	1:A:682:ARG:HB3	2.03	0.41
2:B:252:VAL:HG21	9:I:4:PHE:HZ	1.85	0.41
2:B:508:ASP:HB3	2:B:541:LEU:HD21	2.01	0.41
7:G:115:GLN:HG3	7:G:116:GLN:H	1.85	0.41
22:4:424:TRP:HA	22:4:427:ILE:HD13	2.02	0.41
24:V:86:PRO:HD2	24:V:89:PHE:CD2	2.55	0.41
1:A:1136:ARG:NH2	9:I:47:LYS:O	2.28	0.41
1:A:1157:LYS:O	1:A:1160:VAL:HG23	2.21	0.41
16:P:38:ILE:HG22	16:P:50:ARG:HD2	2.01	0.41
1:A:551:LEU:HD21	1:A:779:THR:HG21	2.03	0.41
1:A:604:ILE:HG23	1:A:682:ARG:HB2	2.02	0.41
1:A:615:ALA:HB2	1:A:667:LEU:HD21	2.03	0.41
1:A:1193:LYS:HE3	1:A:1193:LYS:HB3	1.85	0.41
2:B:1032:THR:HG23	2:B:1032:THR:O	2.21	0.41
3:C:188:GLY:O	3:C:191:ARG:NH1	2.44	0.41
4:D:3:VAL:HG21	7:G:42:VAL:HG21	2.02	0.41
7:G:122:GLU:OE1	7:G:122:GLU:N	2.53	0.41
20:1:124:TYR:HE1	21:3:86:VAL:HG21	1.86	0.41
23:U:242:GLN:HG3	23:U:248:ALA:HB3	2.03	0.41
1:A:454:LEU:HD21	1:A:478:ALA:HB1	2.02	0.41
1:A:1295:THR:HG22	1:A:1300:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1344:SER:OG	1:A:1345:GLU:OE1	2.39	0.41
2:B:137:PRO:HG2	2:B:419:ILE:HD12	2.01	0.41
7:G:150:PHE:CZ	7:G:188:GLY:HA3	2.55	0.41
22:4:361:VAL:HG21	22:4:391:TRP:CE2	2.56	0.41
1:A:107:MET:HE1	1:A:146:ILE:HG22	2.02	0.41
1:A:607:PRO:HD2	1:A:611:ASN:HD22	1.86	0.41
2:B:738:ASN:O	10:J:47:ARG:NH1	2.54	0.41
13:M:208:LEU:HD22	14:N:371:GLY:N	2.36	0.41
13:M:315:GLN:HE22	13:M:418:ARG:NH2	2.19	0.41
17:Q:89:LYS:O	17:Q:93:LYS:N	2.54	0.41
19:Y:57:DT:H2''	19:Y:58:DA:C8	2.55	0.41
20:1:63:TRP:CB	20:1:82:LEU:HD21	2.47	0.41
21:3:310:LEU:HD11	21:3:318:GLU:HB2	2.02	0.41
24:V:309:ARG:HB3	24:V:313:ARG:NH1	2.36	0.41
1:A:874:ARG:HH22	1:A:1071:LYS:HG3	1.86	0.41
2:B:131:LEU:HD12	2:B:132:PRO:HD2	2.03	0.41
2:B:738:ASN:HB2	10:J:47:ARG:HD3	2.02	0.41
2:B:974:GLU:HA	2:B:977:VAL:HG12	2.01	0.41
7:G:116:GLN:O	7:G:118:ALA:N	2.47	0.41
23:U:208:ARG:HE	25:W:345:GLU:HB3	1.86	0.41
24:V:207:LEU:HD23	24:V:301:LEU:HD21	2.02	0.41
1:A:219:ASN:OD1	1:A:219:ASN:N	2.54	0.41
1:A:254:ARG:HH22	16:P:295:ASP:CG	2.24	0.41
1:A:1092:ASP:HB2	1:A:1222:LYS:HB2	2.01	0.41
2:B:171:VAL:O	2:B:174:VAL:HG22	2.21	0.41
2:B:357:TYR:HB2	2:B:474:SER:HB3	2.03	0.41
3:C:139:GLN:HB3	3:C:211:LEU:HD11	2.03	0.41
3:C:249:ALA:HB1	3:C:293:LEU:HD11	2.03	0.41
4:D:81:ALA:CB	17:Q:84:ILE:CD1	2.84	0.41
5:E:102:ALA:O	5:E:127:LEU:HA	2.21	0.41
13:M:309:ALA:HA	13:M:312:ARG:HG2	2.03	0.41
16:P:137:LYS:NZ	16:P:157:PRO:HD3	2.36	0.41
16:P:284:ARG:HG2	17:Q:46:VAL:HB	2.02	0.41
18:X:-57:DA:H2''	18:X:-56:DA:C5	2.56	0.41
18:X:-29:DT:H6	18:X:-29:DT:H2'	1.70	0.41
21:3:196:LYS:HG2	21:3:197:GLU:H	1.86	0.41
21:3:310:LEU:HD22	22:4:153:LYS:H	1.85	0.41
22:4:216:HIS:O	22:4:219:GLN:HG3	2.21	0.41
1:A:556:ASP:OD1	8:H:22:PHE:HB3	2.21	0.41
2:B:177:VAL:HG21	2:B:440:LEU:HD13	2.03	0.41
2:B:633:LEU:HD11	2:B:656:HIS:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:740:THR:HG22	2:B:925:PRO:HB3	2.03	0.41
2:B:986:LYS:HB3	2:B:1001:TYR:HB2	2.03	0.41
3:C:68:ILE:HD12	3:C:68:ILE:HA	1.98	0.41
4:D:32:LYS:HB2	4:D:35:HIS:HB2	2.03	0.41
7:G:89:ILE:HD13	7:G:99:VAL:HB	2.04	0.41
11:K:70:TYR:HB3	11:K:82:LEU:HD13	2.03	0.41
14:N:149:GLU:OE2	14:N:355:SER:OG	2.34	0.41
15:O:65:TYR:OH	17:Q:105:ARG:O	2.25	0.41
15:O:409:ILE:HG13	15:O:421:PHE:HB2	2.02	0.41
20:1:29:PHE:CZ	20:1:77:GLY:HA2	2.56	0.41
1:A:11:VAL:HG11	1:A:13:LYS:HE3	2.03	0.40
1:A:15:ILE:HD11	1:A:18:ILE:HG12	2.03	0.40
1:A:112:CYS:O	1:A:114:HIS:ND1	2.43	0.40
1:A:389:ILE:HG12	24:V:21:TYR:CD1	2.57	0.40
8:H:96:VAL:O	8:H:138:ASP:N	2.54	0.40
19:Y:13:DT:H6	19:Y:13:DT:H2'	1.71	0.40
22:4:200:ARG:HA	22:4:200:ARG:HD2	1.90	0.40
1:A:302:LYS:HA	15:O:377:GLN:HE22	1.86	0.40
1:A:1117:ILE:HG23	1:A:1130:VAL:HG22	2.01	0.40
2:B:915:ASP:HA	3:C:78:ARG:HH12	1.86	0.40
5:E:89:VAL:O	5:E:92:GLN:HG3	2.21	0.40
7:G:81:LEU:HD22	7:G:152:VAL:HA	2.03	0.40
8:H:37:MET:SD	8:H:127:GLY:HA3	2.61	0.40
14:N:138:ILE:HG22	14:N:140:ILE:H	1.86	0.40
15:O:85:MET:HA	15:O:88:TYR:CE1	2.55	0.40
1:A:451:GLU:OE2	2:B:1025:ARG:NH2	2.50	0.40
1:A:754:LYS:HE3	1:A:754:LYS:HB3	1.90	0.40
2:B:136:MET:HE1	2:B:415:MET:HG3	2.03	0.40
2:B:613:GLU:HB3	2:B:618:TYR:HB2	2.03	0.40
3:C:49:PHE:CZ	11:K:110:VAL:HG23	2.57	0.40
3:C:64:ASP:OD2	3:C:279:ARG:NH1	2.54	0.40
7:G:14:PRO:HB2	7:G:16:TRP:CD1	2.57	0.40
1:A:109:CYS:SG	1:A:110:LYS:N	2.94	0.40
1:A:158:HIS:O	15:O:533:ARG:NH2	2.47	0.40
2:B:284:LEU:HB3	2:B:306:ILE:HG23	2.03	0.40
2:B:596:TYR:HB3	2:B:656:HIS:HB3	2.03	0.40
2:B:668:CYS:SG	2:B:691:LYS:NZ	2.83	0.40
2:B:749:TYR:CD1	2:B:909:LEU:HD22	2.56	0.40
8:H:96:VAL:HA	8:H:116:VAL:HG22	2.03	0.40
9:I:19:ARG:HH21	9:I:33:ASN:ND2	2.20	0.40
9:I:102:CYS:HB3	9:I:104:HIS:CE1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:514:ILE:HD11	17:Q:61:LYS:HD2	2.04	0.40
18:X:-53:DT:H2"	18:X:-52:DG:C8	2.57	0.40
19:Y:28:DA:H2	23:U:259:VAL:HG21	1.87	0.40
21:3:158:GLU:HG2	22:4:366:VAL:HA	2.03	0.40
1:A:1115:GLU:HG3	1:A:1116:TYR:CD2	2.57	0.40
1:A:1153:ILE:HG22	1:A:1154:CYS:H	1.86	0.40
2:B:633:LEU:HD11	2:B:656:HIS:CD2	2.56	0.40
2:B:761:SER:OG	2:B:926:ASP:OD1	2.34	0.40
2:B:880:LEU:HD21	2:B:882:LYS:HE3	2.04	0.40
2:B:954:LEU:HD12	2:B:976:LEU:HD23	2.03	0.40
3:C:336:PHE:HE1	11:K:44:LEU:HD22	1.86	0.40
13:M:240:LYS:HE3	14:N:278:GLN:HB2	2.03	0.40
14:N:253:GLU:OE2	14:N:256:ARG:NH2	2.40	0.40
18:X:-37:DT:H2"	18:X:-36:DC:C6	2.57	0.40
20:1:91:CYS:SG	20:1:93:PRO:HD2	2.62	0.40
21:3:155:PHE:CE1	22:4:366:VAL:HG11	2.57	0.40
24:V:134:THR:HG23	24:V:137:ALA:H	1.86	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	1376/1390 (99%)	1342 (98%)	34 (2%)	0	100	100
2	B	1101/1133 (97%)	1072 (97%)	29 (3%)	0	100	100
3	C	341/346 (99%)	336 (98%)	5 (2%)	0	100	100
4	D	120/148 (81%)	115 (96%)	5 (4%)	0	100	100
5	E	207/210 (99%)	205 (99%)	2 (1%)	0	100	100
6	F	74/127 (58%)	73 (99%)	1 (1%)	0	100	100
7	G	160/204 (78%)	151 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	146/150 (97%)	146 (100%)	0	0	100	100
9	I	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
10	J	63/67 (94%)	61 (97%)	2 (3%)	0	100	100
11	K	101/133 (76%)	100 (99%)	1 (1%)	0	100	100
12	L	44/58 (76%)	42 (96%)	2 (4%)	0	100	100
13	M	418/708 (59%)	403 (96%)	15 (4%)	0	100	100
14	N	140/317 (44%)	140 (100%)	0	0	100	100
15	O	508/534 (95%)	497 (98%)	11 (2%)	0	100	100
16	P	301/316 (95%)	295 (98%)	6 (2%)	0	100	100
17	Q	85/223 (38%)	82 (96%)	3 (4%)	0	100	100
20	1	144/368 (39%)	142 (99%)	2 (1%)	0	100	100
21	3	368/411 (90%)	356 (97%)	12 (3%)	0	100	100
22	4	363/1469 (25%)	350 (96%)	13 (4%)	0	100	100
23	U	175/339 (52%)	173 (99%)	2 (1%)	0	100	100
24	V	358/419 (85%)	349 (98%)	9 (2%)	0	100	100
25	W	109/2624 (4%)	105 (96%)	4 (4%)	0	100	100
All	All	6807/11802 (58%)	6636 (98%)	171 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1200/1212 (99%)	1195 (100%)	5 (0%)	91	94
2	B	964/988 (98%)	961 (100%)	3 (0%)	92	95
3	C	299/302 (99%)	298 (100%)	1 (0%)	92	95
4	D	114/136 (84%)	114 (100%)	0	100	100
5	E	191/192 (100%)	189 (99%)	2 (1%)	76	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	66/111 (60%)	66 (100%)	0	100	100
7	G	149/181 (82%)	149 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	92/93 (99%)	92 (100%)	0	100	100
10	J	53/56 (95%)	53 (100%)	0	100	100
11	K	92/119 (77%)	92 (100%)	0	100	100
12	L	43/55 (78%)	42 (98%)	1 (2%)	50	70
13	M	377/622 (61%)	376 (100%)	1 (0%)	92	95
14	N	131/276 (48%)	130 (99%)	1 (1%)	81	88
15	O	458/476 (96%)	455 (99%)	3 (1%)	84	90
16	P	269/280 (96%)	269 (100%)	0	100	100
17	Q	84/195 (43%)	82 (98%)	2 (2%)	49	69
20	1	130/334 (39%)	129 (99%)	1 (1%)	81	88
21	3	330/356 (93%)	320 (97%)	10 (3%)	41	64
22	4	321/1213 (26%)	318 (99%)	3 (1%)	78	87
23	U	152/293 (52%)	152 (100%)	0	100	100
24	V	325/365 (89%)	323 (99%)	2 (1%)	86	92
25	W	102/2381 (4%)	101 (99%)	1 (1%)	76	85
All	All	6071/10367 (59%)	6035 (99%)	36 (1%)	86	92

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	PHE
1	A	362	ASP
1	A	431	PHE
1	A	1220	LYS
1	A	1280	MET
2	B	396	ARG
2	B	407	ARG
2	B	1050	MET
3	C	163	TYR
5	E	54	ARG
5	E	55	ARG
12	L	41	TYR
13	M	319	MET

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Mol	Chain	Res	Type
14	N	156	ARG
15	O	133	MET
15	O	137	LYS
15	O	455	LYS
17	Q	70	ARG
17	Q	81	ARG
20	1	26	PHE
21	3	47	PHE
21	3	51	TRP
21	3	83	ASP
21	3	89	ASP
21	3	148	ARG
21	3	167	LYS
21	3	313	HIS
21	3	340	TYR
21	3	355	PHE
21	3	386	MET
22	4	166	ARG
22	4	177	GLU
22	4	461	GLU
24	V	52	GLU
24	V	381	ASP
25	W	309	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	355	ASN
1	A	423	GLN
1	A	528	ASN
1	A	820	HIS
1	A	872	GLN
1	A	1039	GLN
1	A	1217	GLN
2	B	181	GLN
2	B	260	HIS
2	B	395	GLN
2	B	608	ASN
2	B	1010	GLN
3	C	127	GLN
3	C	160	ASN

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Mol	Chain	Res	Type
3	C	305	HIS
3	C	344	GLN
4	D	26	GLN
4	D	43	ASN
4	D	61	GLN
5	E	71	GLN
5	E	108	GLN
7	G	23	ASN
7	G	36	ASN
7	G	115	GLN
7	G	116	GLN
7	G	125	GLN
9	I	104	HIS
13	M	315	GLN
14	N	282	GLN
15	O	286	GLN
15	O	402	ASN
15	O	445	ASN
15	O	465	GLN
15	O	497	GLN
16	P	117	ASN
16	P	182	GLN
20	1	48	ASN
20	1	52	ASN
20	1	95	GLN
20	1	111	GLN
20	1	116	ASN
21	3	202	GLN
21	3	226	GLN
21	3	314	GLN
22	4	171	GLN
22	4	229	GLN
22	4	243	GLN
22	4	312	HIS
22	4	438	GLN
22	4	457	ASN
23	U	164	GLN
23	U	166	GLN
23	U	278	GLN
24	V	129	HIS
24	V	206	GLN
24	V	212	ASN

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Mol	Chain	Res	Type
25	W	327	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
28	SF4	P	401	-	0,12,12	-	-	-		

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
28	SF4	P	401	-	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	P	401	SF4	1	0

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
18	X	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	-21:DC	O3'	-20:DT	P	1.13

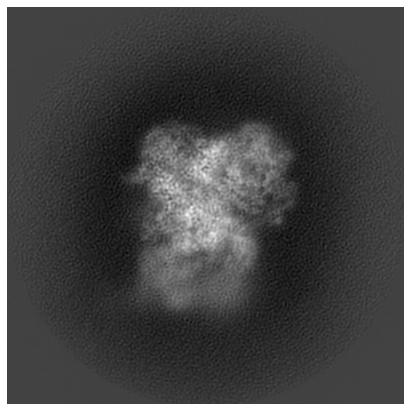
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35719. These allow visual inspection of the internal detail of the map and identification of artifacts.

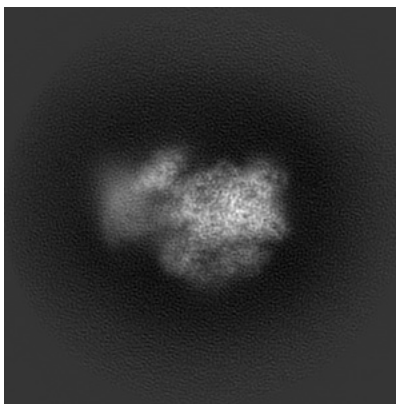
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

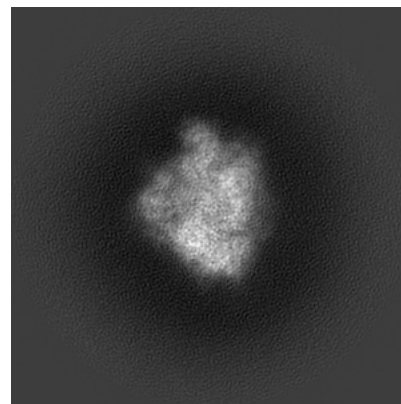
6.1.1 Primary map



X

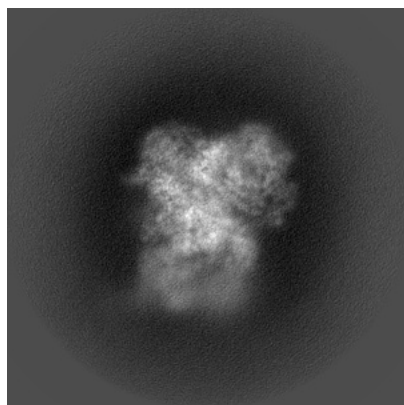


Y

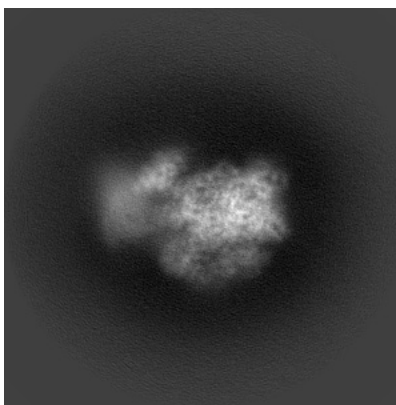


Z

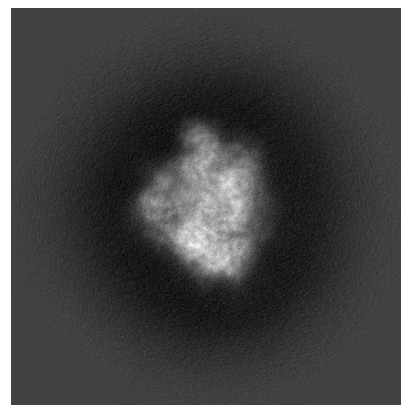
6.1.2 Raw map



X



Y

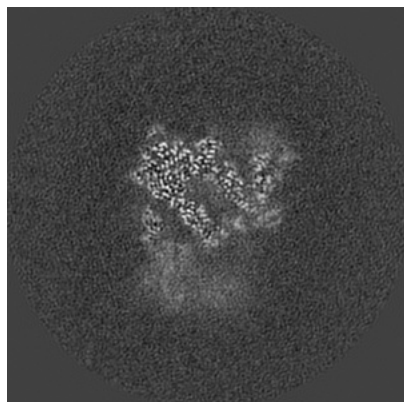


Z

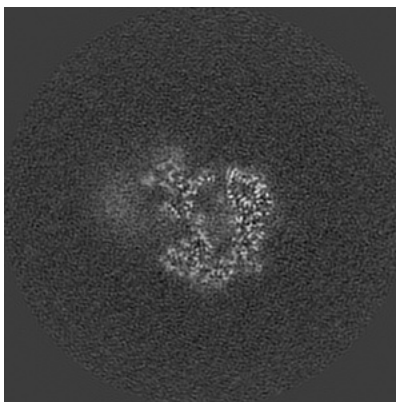
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

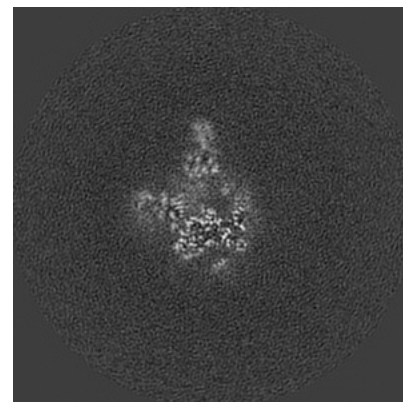
6.2.1 Primary map



X Index: 160

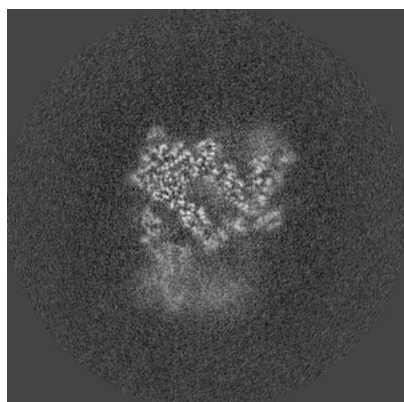


Y Index: 160

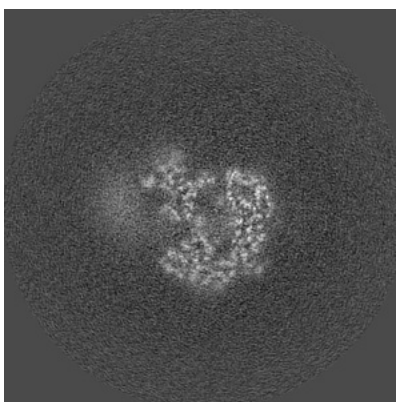


Z Index: 160

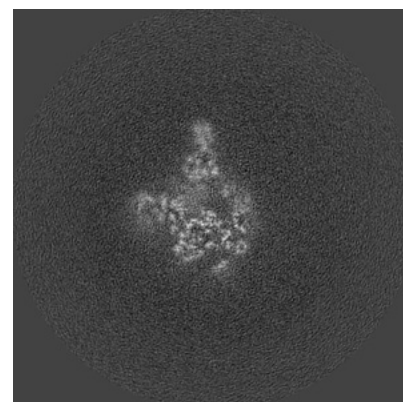
6.2.2 Raw map



X Index: 160



Y Index: 160

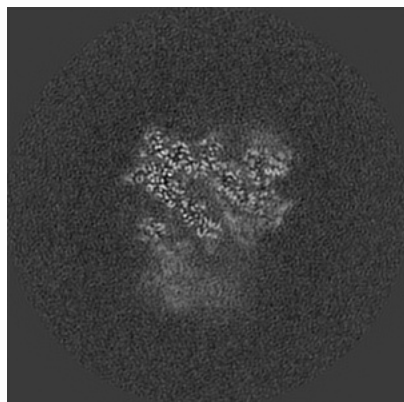


Z Index: 160

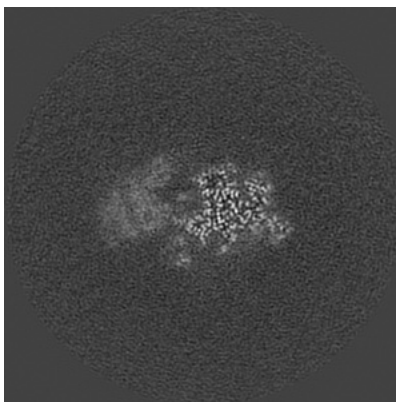
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

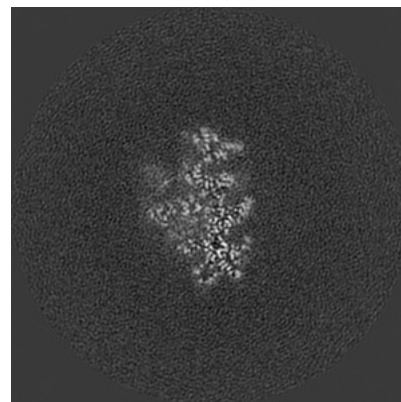
6.3.1 Primary map



X Index: 156

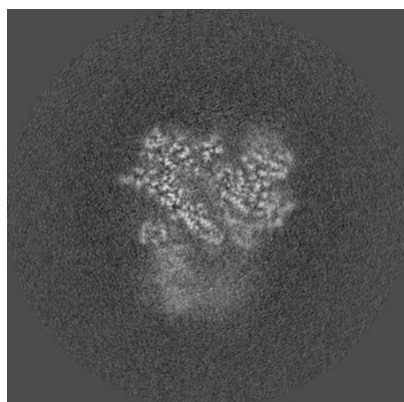


Y Index: 130

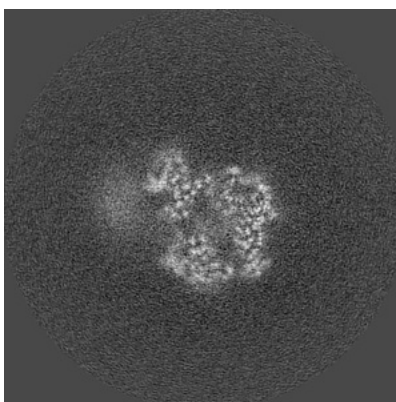


Z Index: 186

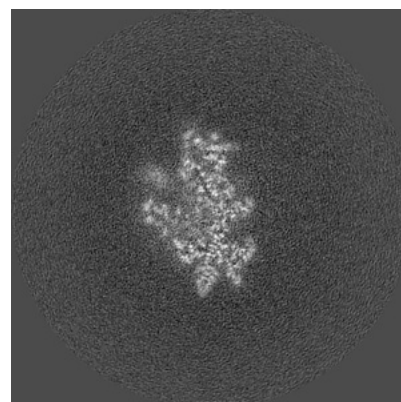
6.3.2 Raw map



X Index: 154



Y Index: 164

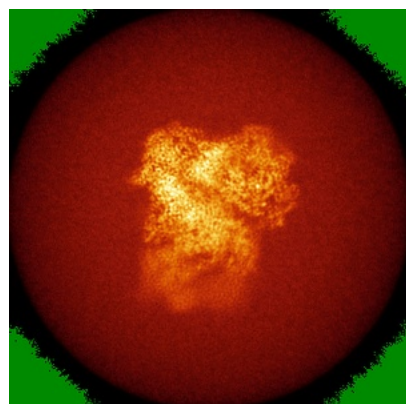


Z Index: 182

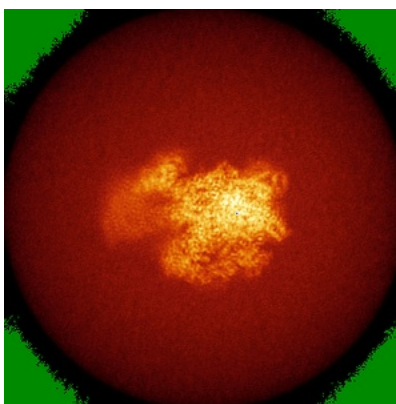
The images above show the largest variance slices of the map in three orthogonal directions.

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

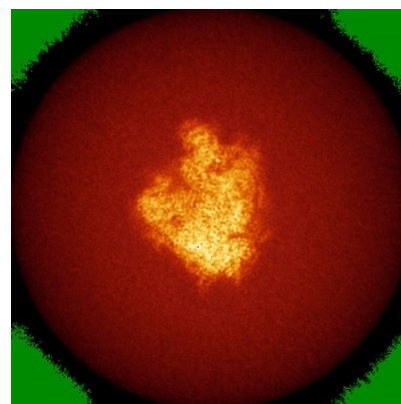
6.4.1 Primary map



X

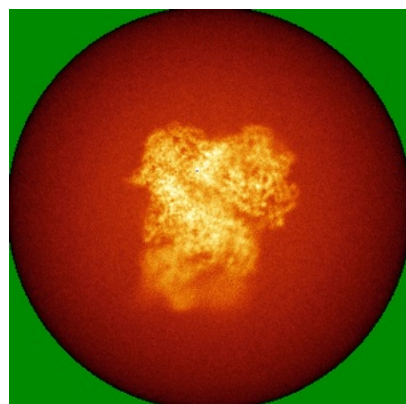


Y

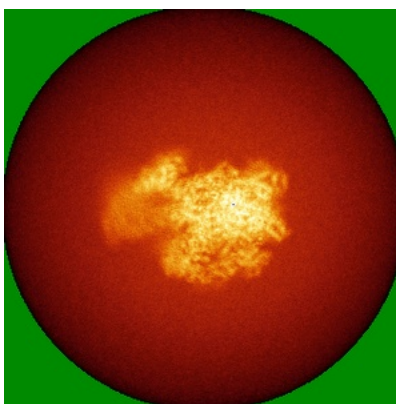


Z

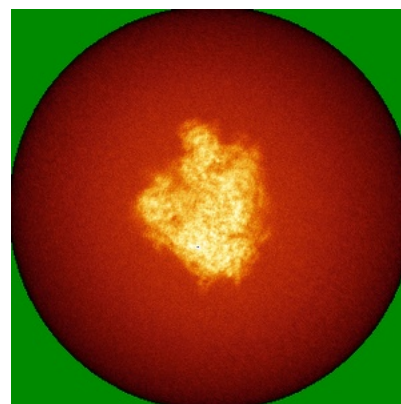
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.024. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

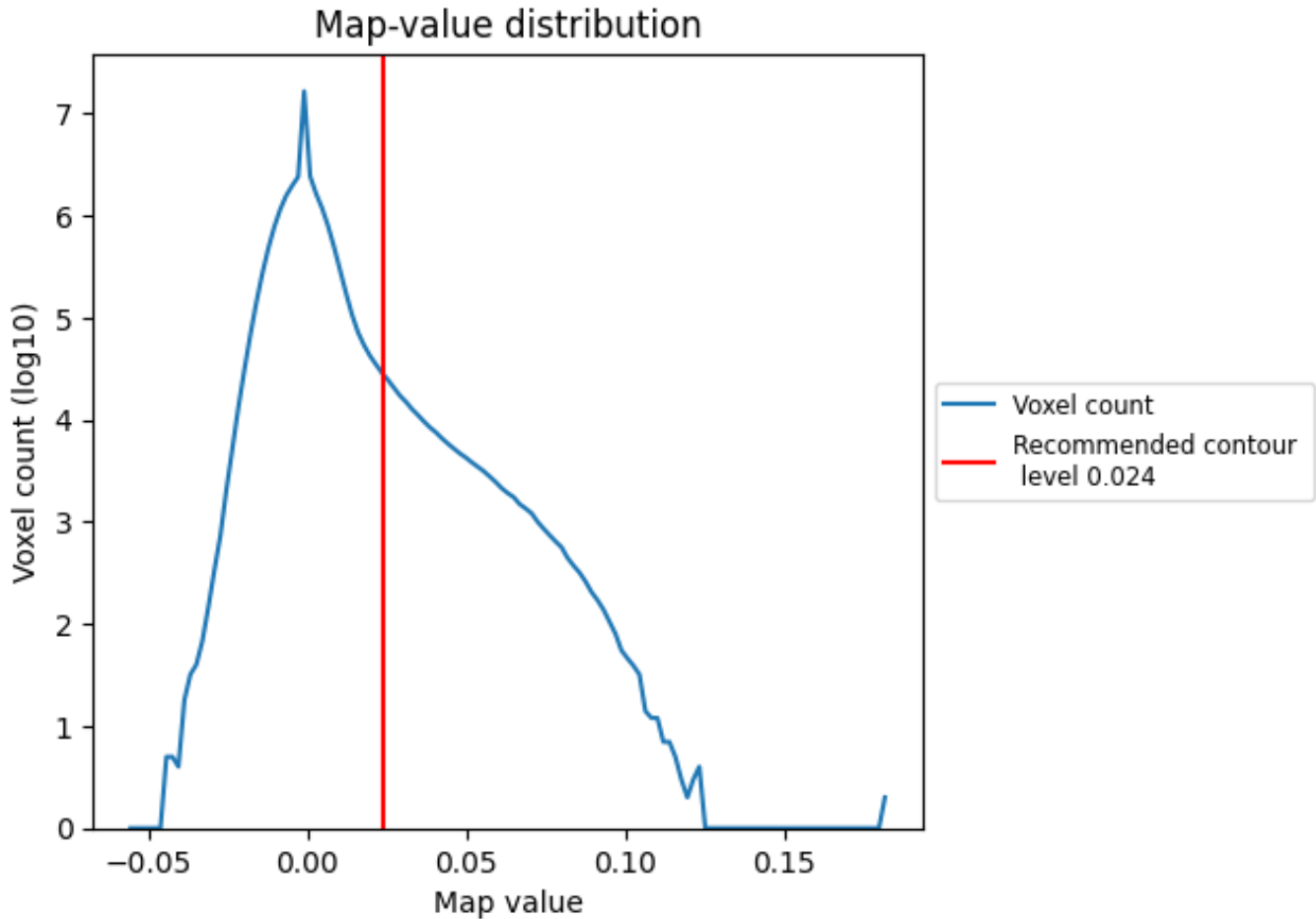
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

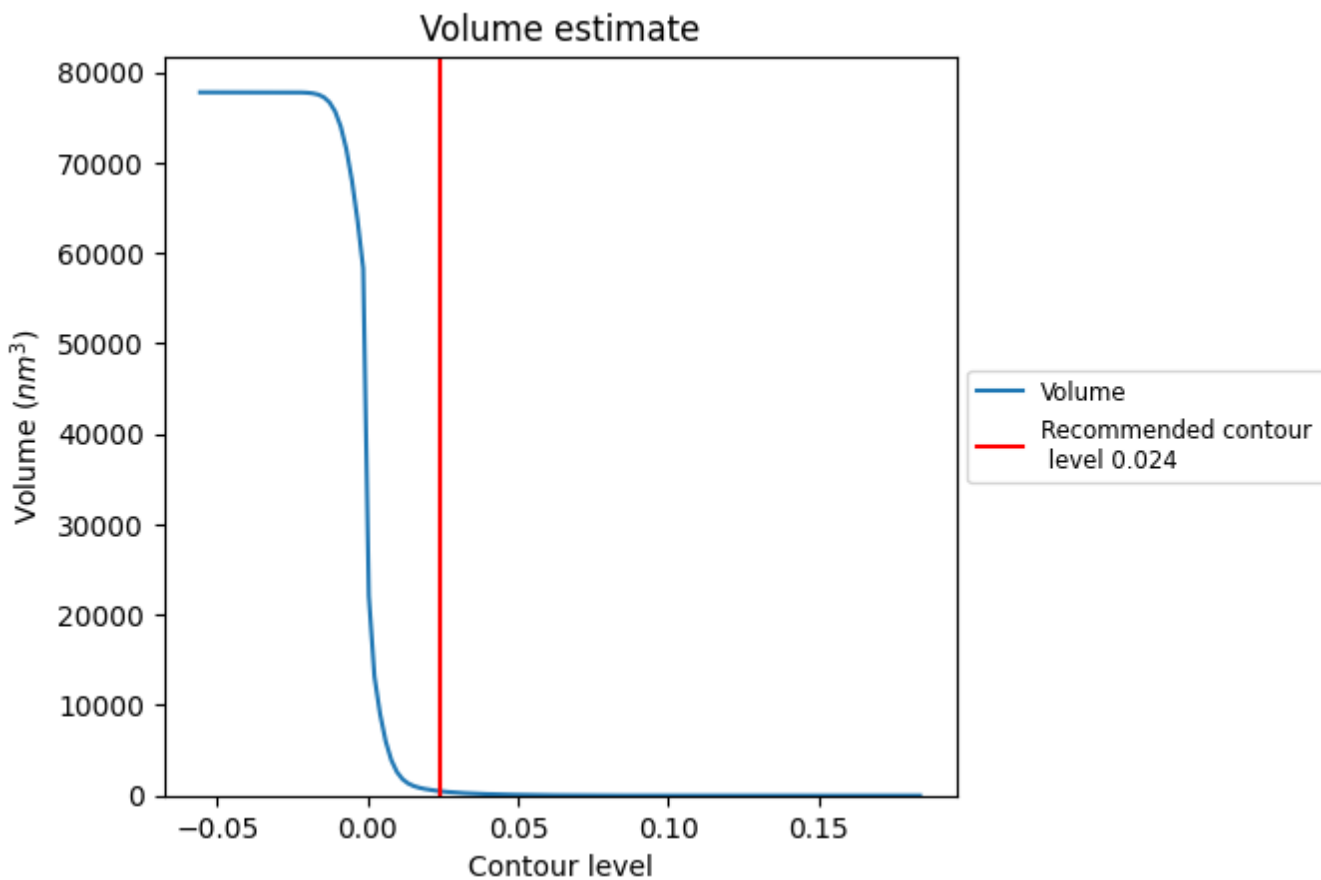
This section contains the results of statistical analysis of the map.

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.

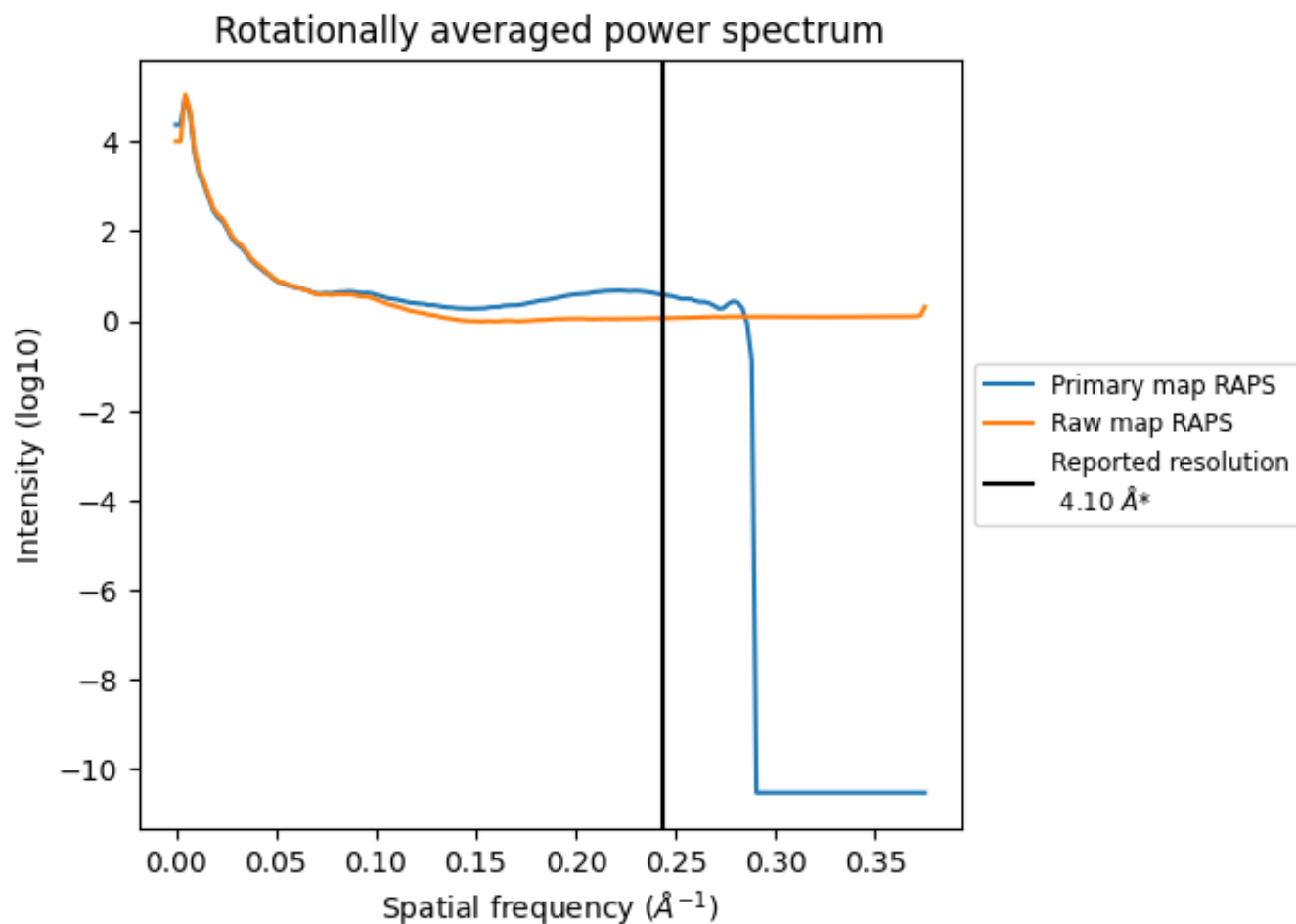
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 491 nm³; this corresponds to an approximate mass of 443 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 [i](#)

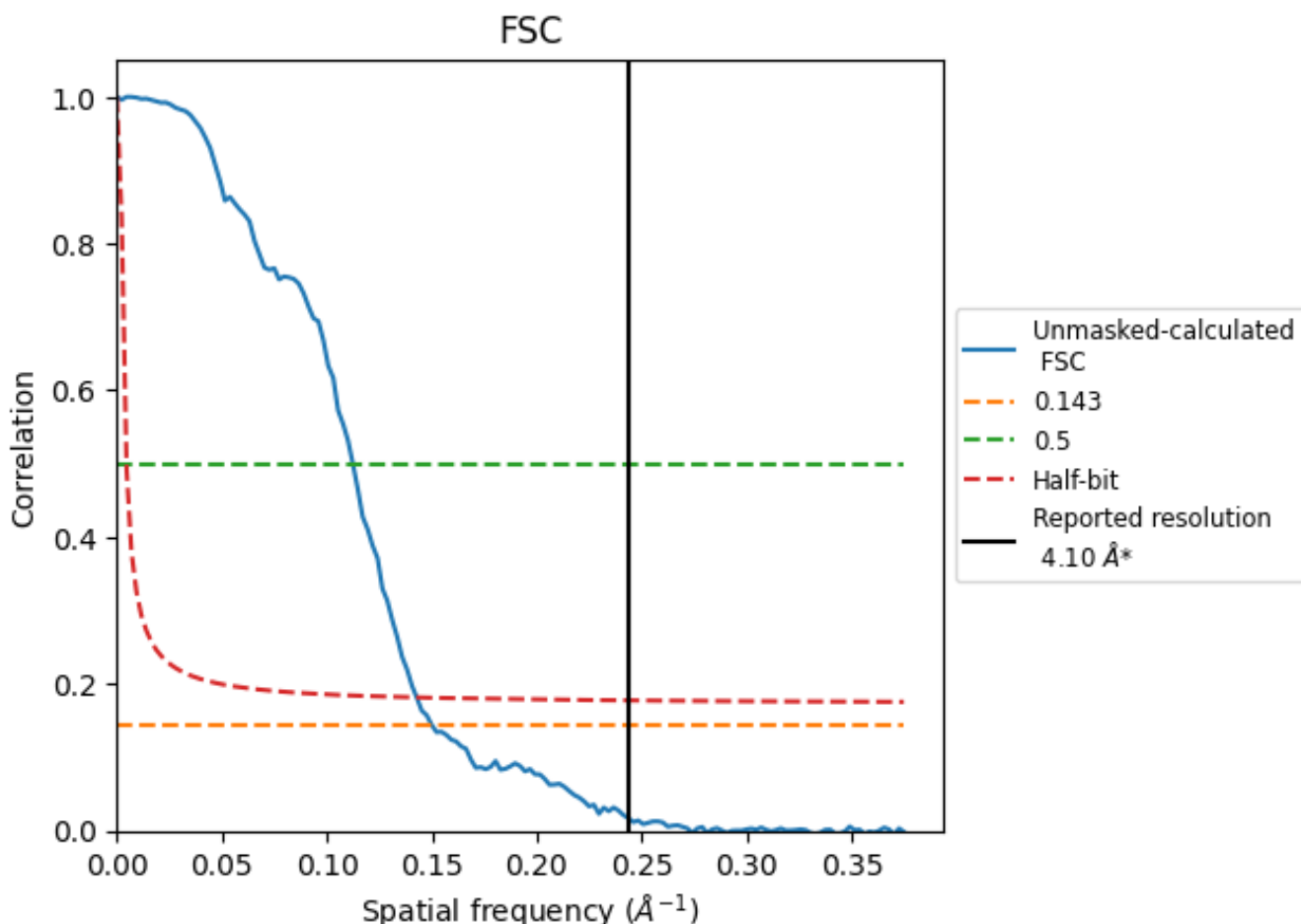


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.244 \AA^{-1}

8.2 Resolution estimates [i](#)

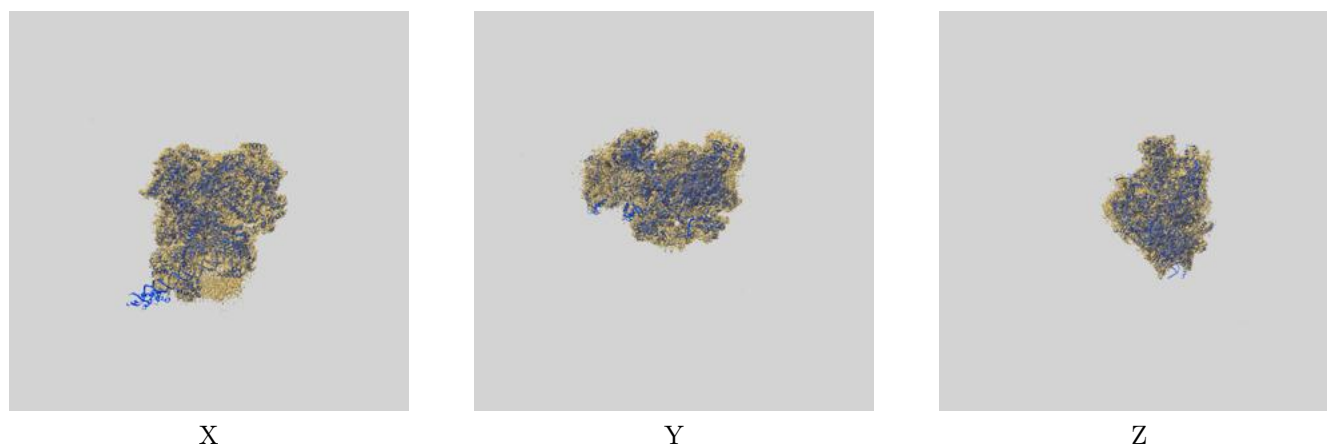
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.66	8.89	7.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.66 differs from the reported value 4.1 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35719 and PDB model 8IUE. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



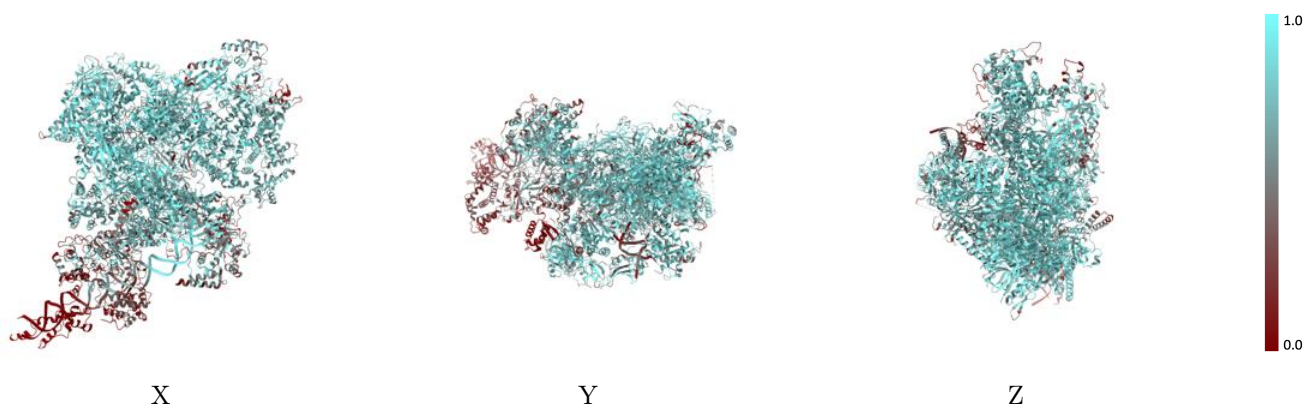
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



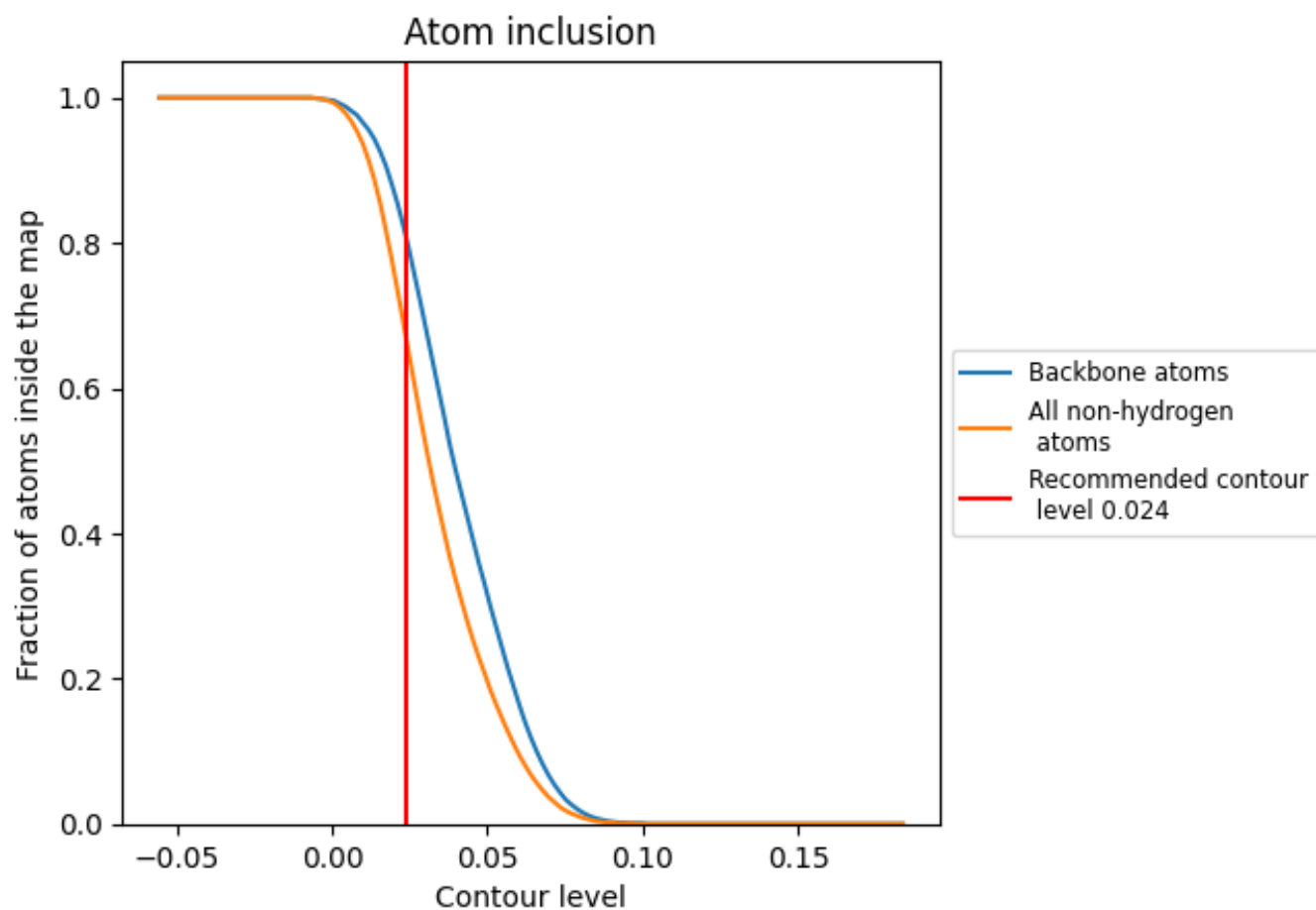
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.024).





















































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 66% 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 (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6640	 0.2910
1	 0.2820	 0.0650
3	 0.3490	 0.0760
4	 0.2470	 0.0710
A	 0.8020	 0.3840
B	 0.8210	 0.4140
C	 0.8060	 0.4180
D	 0.6290	 0.2170
E	 0.7260	 0.3030
F	 0.8490	 0.4310
G	 0.7610	 0.2970
H	 0.7430	 0.3900
I	 0.5820	 0.2510
J	 0.8360	 0.4250
K	 0.8050	 0.4080
L	 0.8120	 0.3960
M	 0.6600	 0.2980
N	 0.6300	 0.2830
O	 0.6900	 0.3000
P	 0.4530	 0.1740
Q	 0.6580	 0.2710
U	 0.6290	 0.2020
V	 0.6670	 0.2600
W	 0.5160	 0.1200
X	 0.4920	 0.1070
Y	 0.5000	 0.1160

