



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 03:25 AM UTC

PDB ID : 7PKS / pdb_00007pks
EMDB ID : EMD-13479
Title : Structural basis of Integrator-mediated transcription regulation
Authors : Fianu, I.; Chen, Y.; Dienemann, C.; Cramer, P.
Deposited on : 2021-08-26
Resolution : 3.60 Å(reported)
Based on initial models : 3DW8, 6GML, 7CUN, 7BFP

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

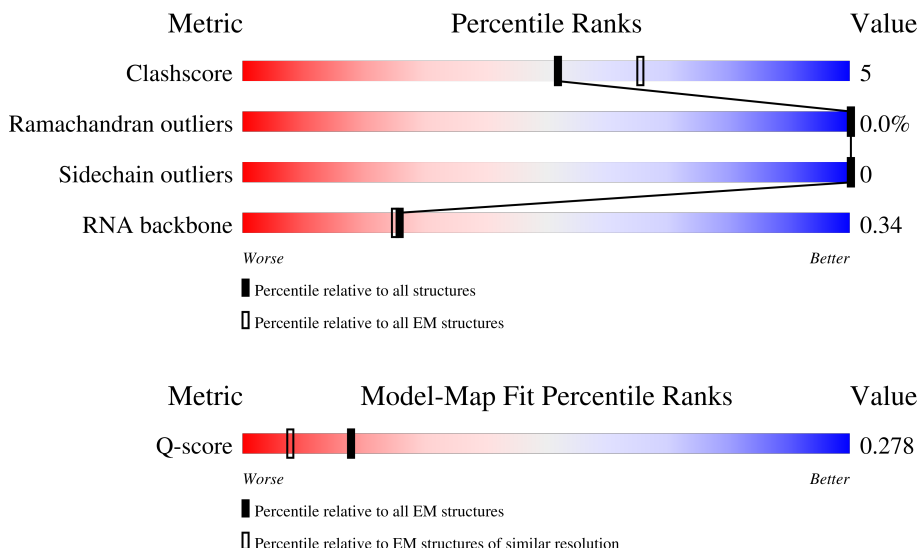
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	1970	
2	B	1174	
3	C	275	

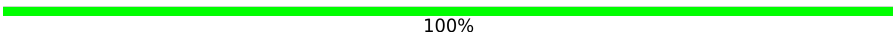
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Mol	Chain	Length	Quality of chain
4	D	142	
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	13	
14	N	48	
15	P	17	
16	T	48	
17	U	528	
18	V	614	
19	W	616	
20	X	22	
21	Z	1087	
22	a	2190	
23	b	1204	
24	d	963	
25	e	1019	
26	f	887	
27	g	962	
28	h	995	

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Mol	Chain	Length	Quality of chain
29	i	658	 71% 13% 16%
30	k	600	 66% 10% 24%
31	p	589	 79% 19% .
32	q	309	 78% 16% 6%
33	u	27	 100%

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 101147 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1392	Total	C	N	O	S	0	0
			11012	6933	1973	2037	69		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	THR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	TYR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	THR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1112	Total	C	N	O	S	0	0
			8901	5634	1560	1643	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	261	Total	C	N	O	S	0	0
			2096	1314	360	416	6		

- Molecule 4 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	126	Total	C	N	O	S	0	0
			975	613	166	192	4		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	78	Total	C	N	O	S	0	0
			627	401	106	115	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1316	858	208	242	8		

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

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	117	Total	C	N	O	S	0	0
			944	584	166	183	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 11 is a protein called RNA_pol_L_2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			383	238	72	67	6		

- Molecule 13 is a protein called RPBI C-terminal domain peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	13	Total	C	N	O	0	0
			95	60	13	22		

- Molecule 14 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	24	Total	C	N	O	P	0	0
			489	234	90	141	24		

- Molecule 15 is a RNA chain called TAR RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	17	Total	C	N	O	P	0	0
			361	162	66	116	17		

- Molecule 16 is a DNA chain called DNA Template.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	33	Total	C	N	O	P	0	0
			682	325	122	202	33		

- Molecule 17 is a protein called Negative elongation factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	183	Total	C	N	O	S	0	0
			1398	889	238	264	7		

- Molecule 18 is a protein called Negative elongation factor B.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	V	451	Total	C	N	O	0	0
			2040	1102	466	472		

- Molecule 19 is a protein called Negative elongation factor C/D.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	508	Total	C	N	O	S	0	0
			3854	2468	654	713	19		

- Molecule 20 is a protein called Negative elongation factor E.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	X	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 21 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	273	Total	C	N	O	S	0	0
			2174	1369	392	402	11		

- Molecule 22 is a protein called Integrator complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	a	1227	Total	C	N	O	S	0	0
			8337	5233	1513	1550	41		

- Molecule 23 is a protein called Integrator complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	b	1047	Total	C	N	O	S	0	0
			7926	5085	1332	1447	62		

- Molecule 24 is a protein called Integrator complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	d	820	Total	C	N	O	S	0	0
			6410	4090	1093	1193	34		

- Molecule 25 is a protein called Integrator complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	e	649	Total	C	N	O	S	0	0
			4671	2973	857	824	17		

- Molecule 26 is a protein called Integrator complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	f	536	Total	C	N	O	S	0	0
			4075	2617	692	743	23		

- Molecule 27 is a protein called Integrator complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	g	886	Total	C	N	O	S	0	0
			6710	4250	1163	1257	40		

- Molecule 28 is a protein called Integrator complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	h	887	Total	C	N	O	S	0	0
			6749	4332	1156	1223	38		

- Molecule 29 is a protein called Integrator complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	i	550	Total	C	N	O	S	0	0
			4249	2741	689	788	31		

- Molecule 30 is a protein called Integrator complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	k	458	Total	C	N	O	S	0	0
			3336	2143	575	593	25		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	487	GLU	ASP	conflict	UNP Q5TA45

- Molecule 31 is a protein called Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	p	575	Total	C	N	O	S	0	0
			4388	2795	748	818	27		

- Molecule 32 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	q	290	Total	C	N	O	S	0	0
			2322	1467	403	437	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	88	ASN	ASP	conflict	UNP P67775

- Molecule 33 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	u	27	Total	C	N	O	0	0
			144	89	28	27		

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 35 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
35	A	2	Total	Zn	0
			2	2	
35	B	1	Total	Zn	0
			1	1	
35	C	1	Total	Zn	0
			1	1	
35	I	2	Total	Zn	0
			2	2	
35	J	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
35	L	1	Total 1	Zn 1	0
35	k	2	Total 2	Zn 2	0

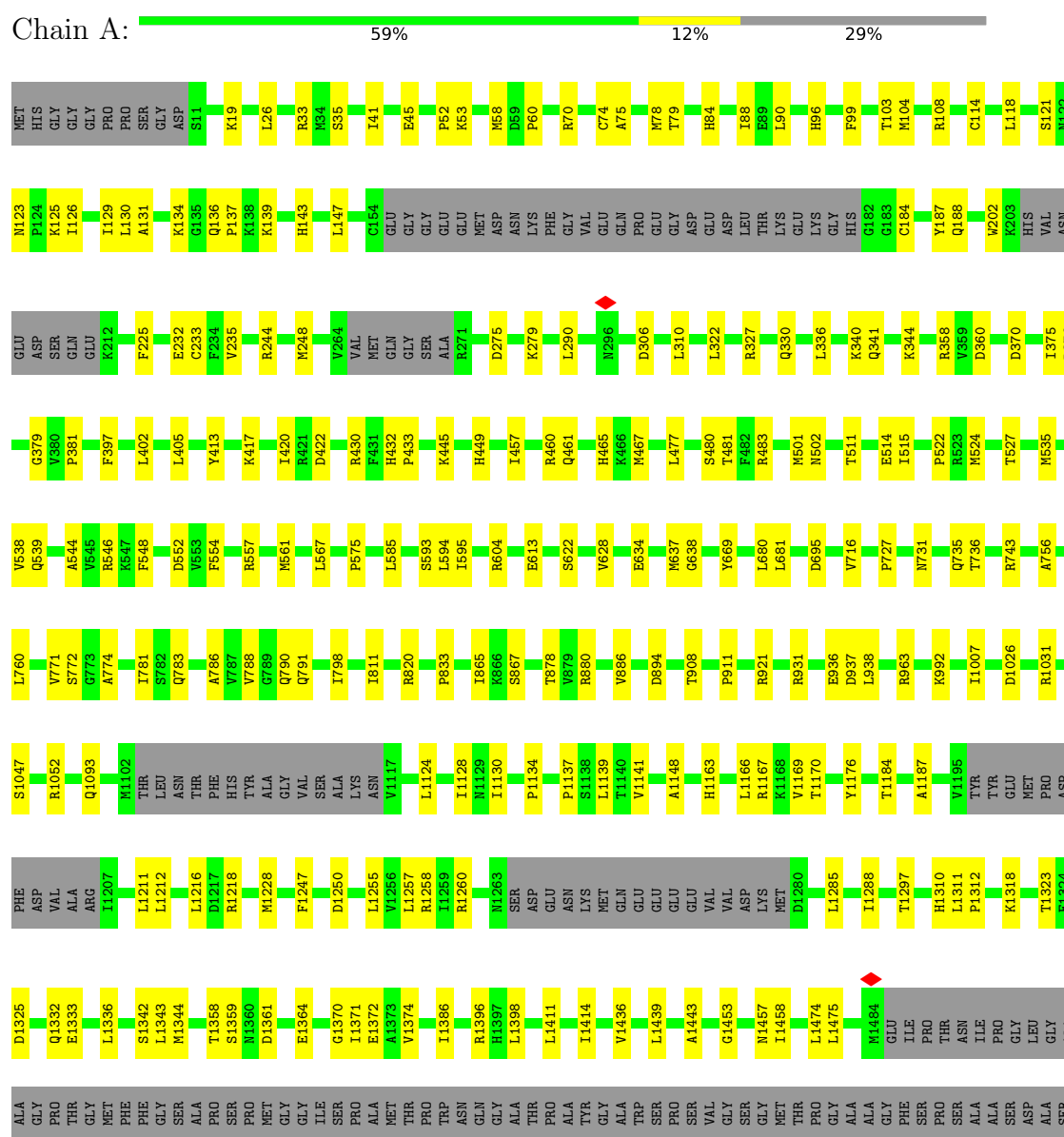
- Molecule 36 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

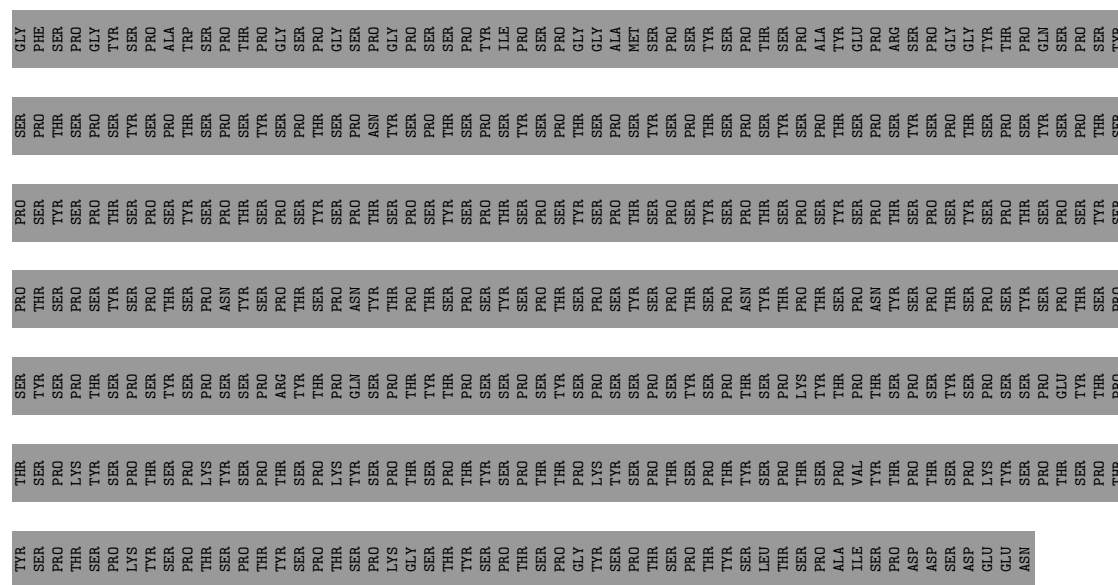
Mol	Chain	Residues	Atoms		AltConf
36	q	2	Total 2	Mn 2	0

3 Residue-property plots

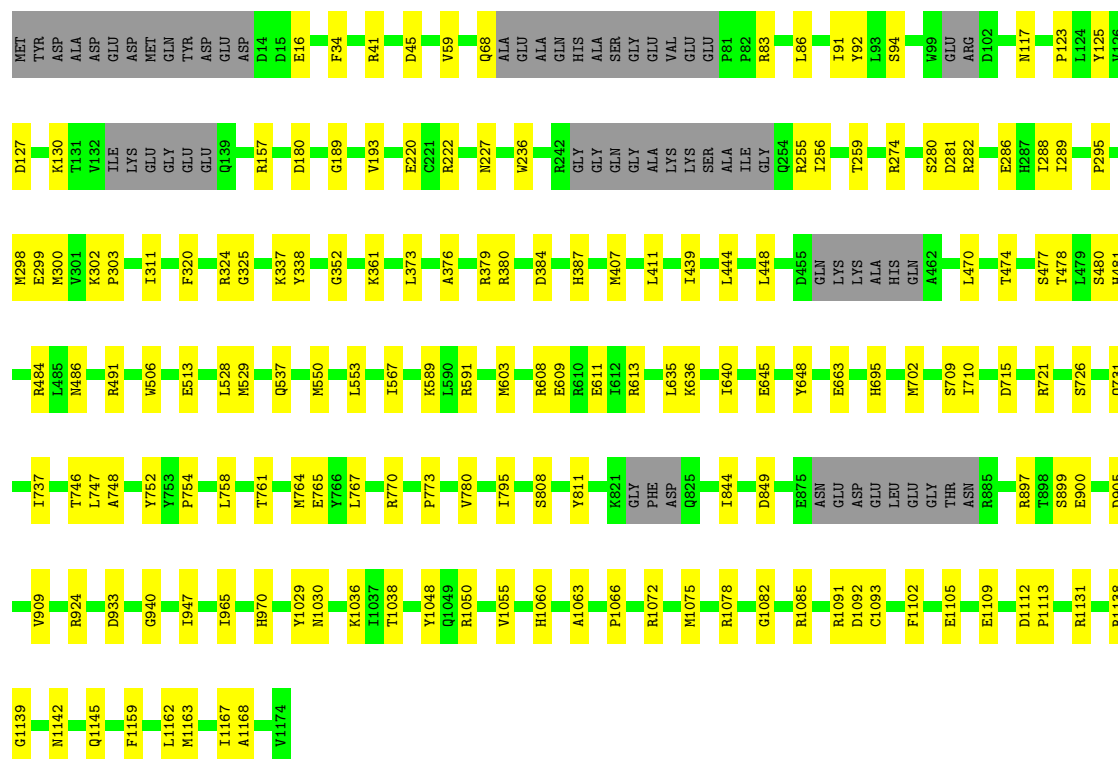
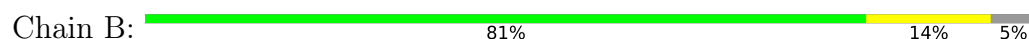
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: DNA-directed RNA polymerase subunit

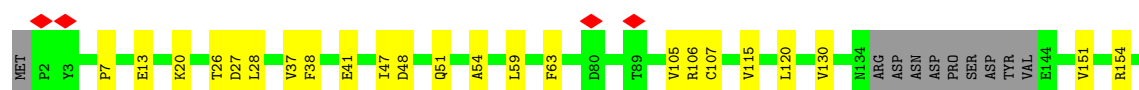
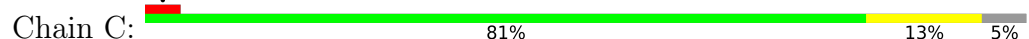




- Molecule 2: DNA-directed RNA polymerase subunit beta

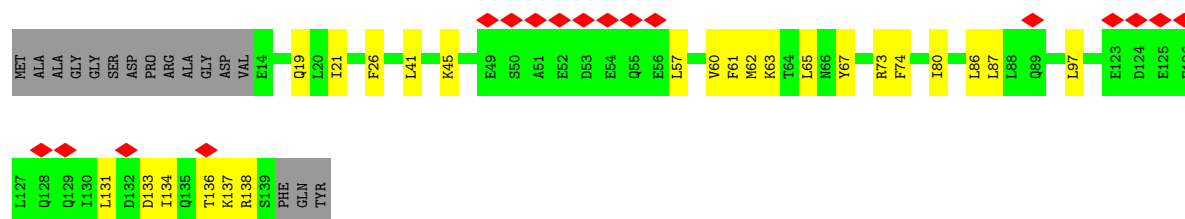


- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

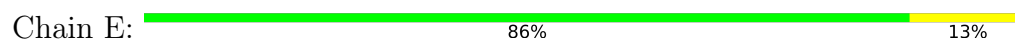




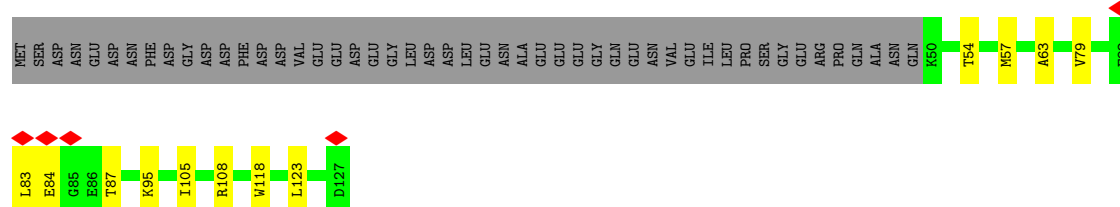
• Molecule 4: RNA polymerase II subunit D



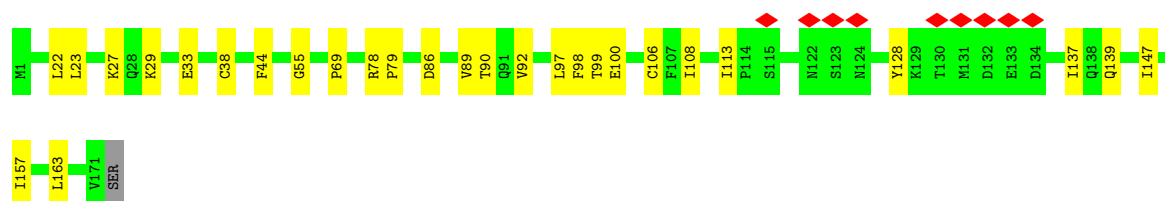
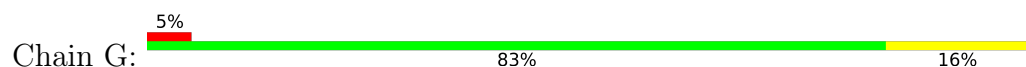
• Molecule 5: DNA-directed RNA polymerase II subunit E



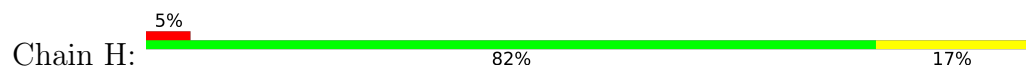
• Molecule 6: DNA-directed RNA polymerase II subunit F



• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

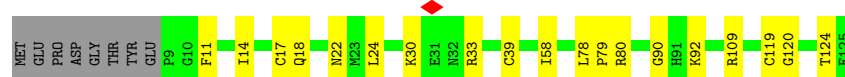
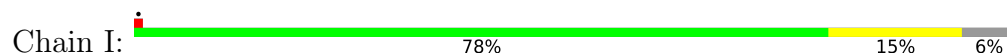


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

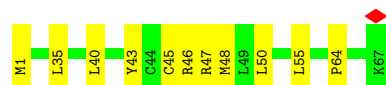
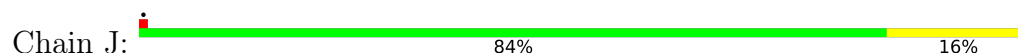




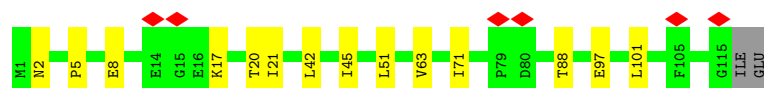
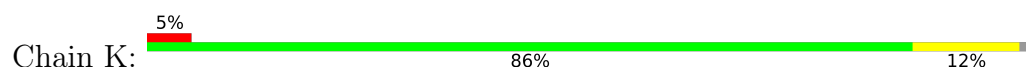
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



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



- Molecule 11: RNA_pol_L_2 domain-containing protein



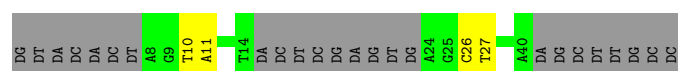
- Molecule 12: RNA polymerase II subunit K



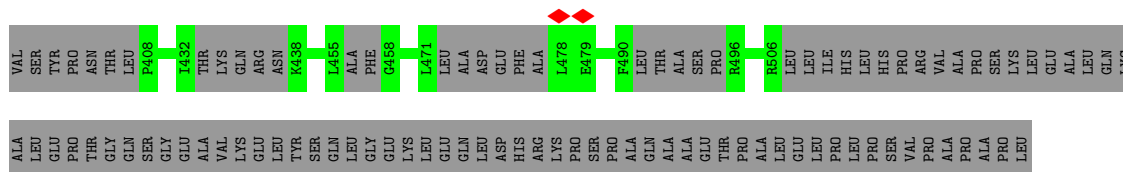
- Molecule 13: RPBI C-terminal domain peptide



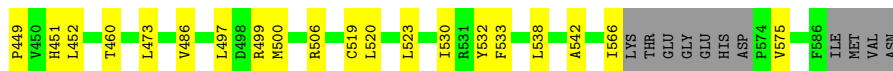
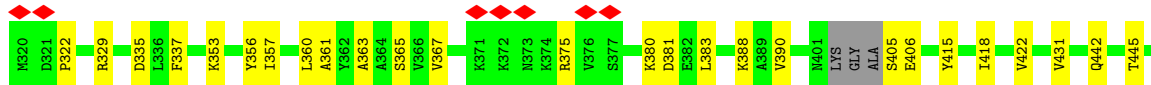
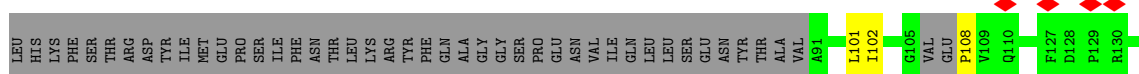
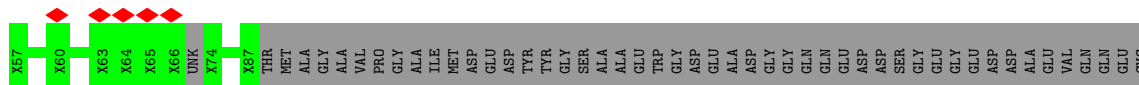
- Molecule 14: Non-template DNA



- Molecule 15: TAR RNA



- Molecule 19: Negative elongation factor C/D

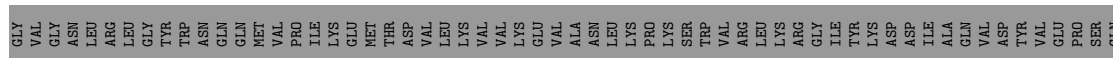
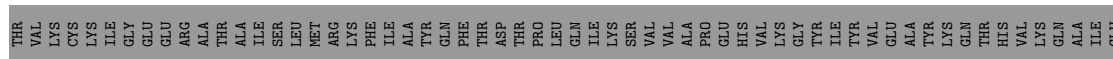
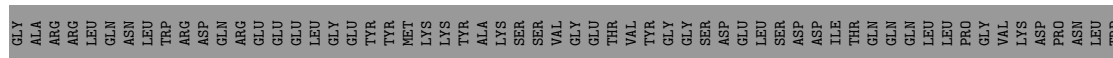
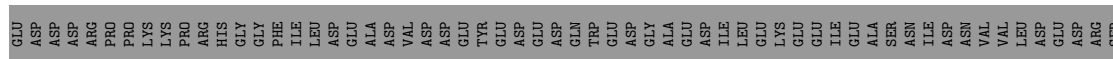


- Molecule 20: Negative elongation factor E

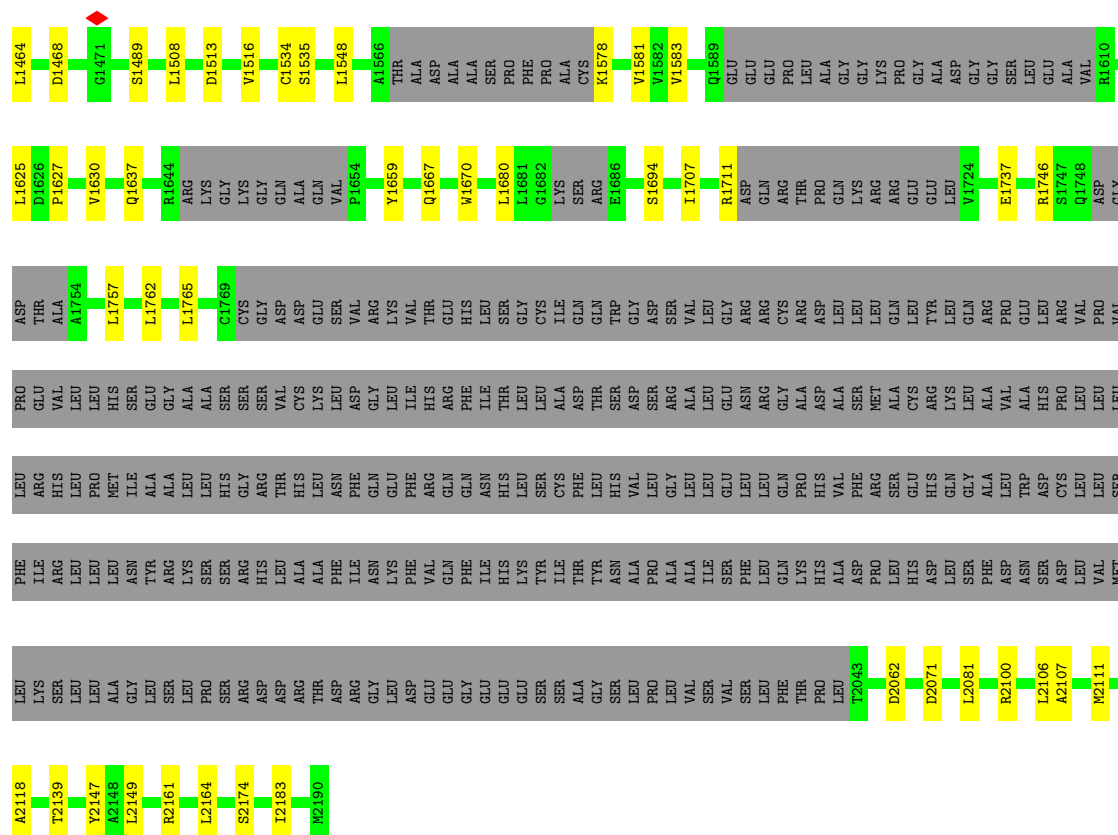


There are no outlier residues recorded for this chain.

- Molecule 21: Transcription elongation factor SPT5

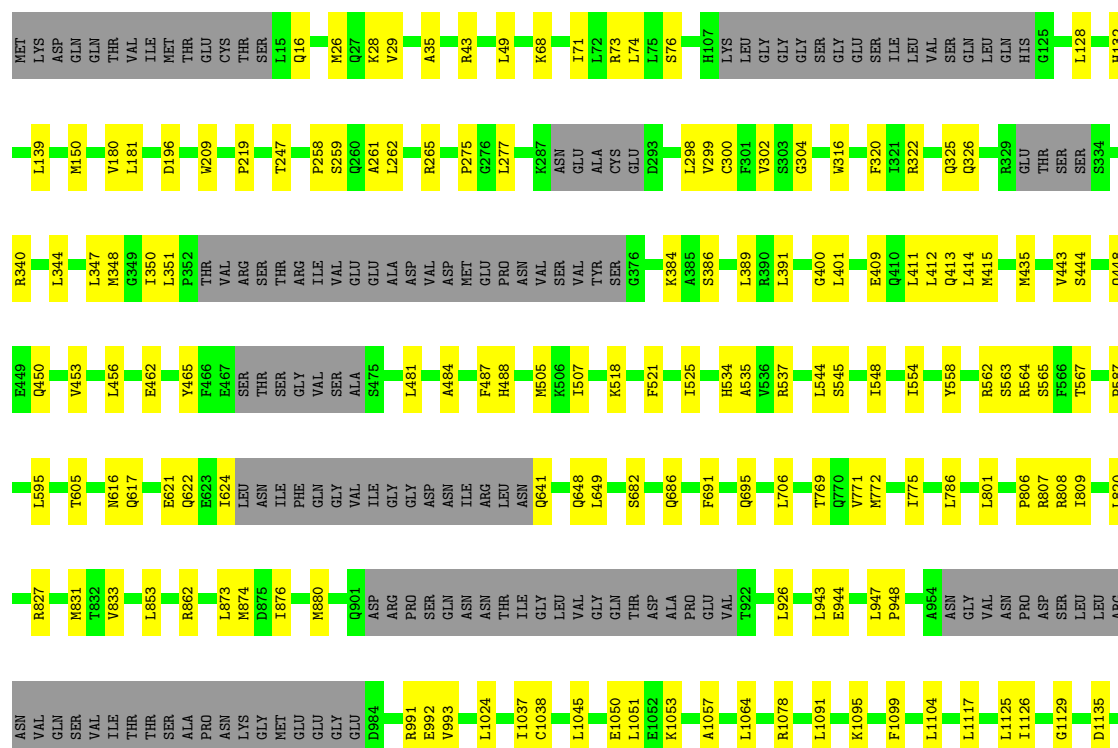






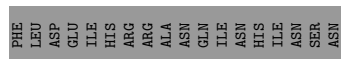
• Molecule 23: Integrator complex subunit 2

Chain b: 74% 13% 13%

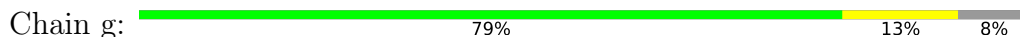


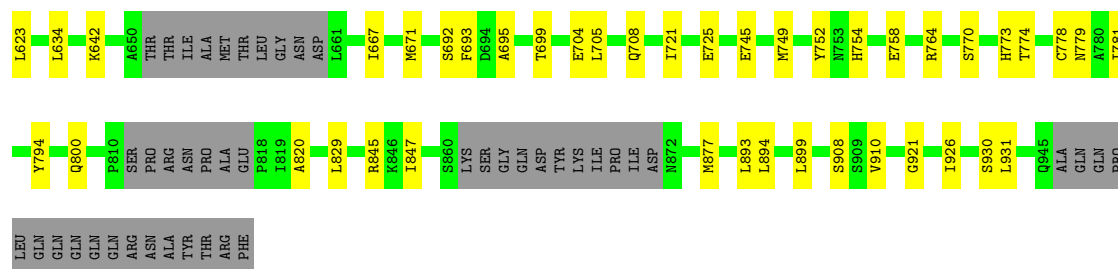


- Molecule 26: Integrator complex subunit 6



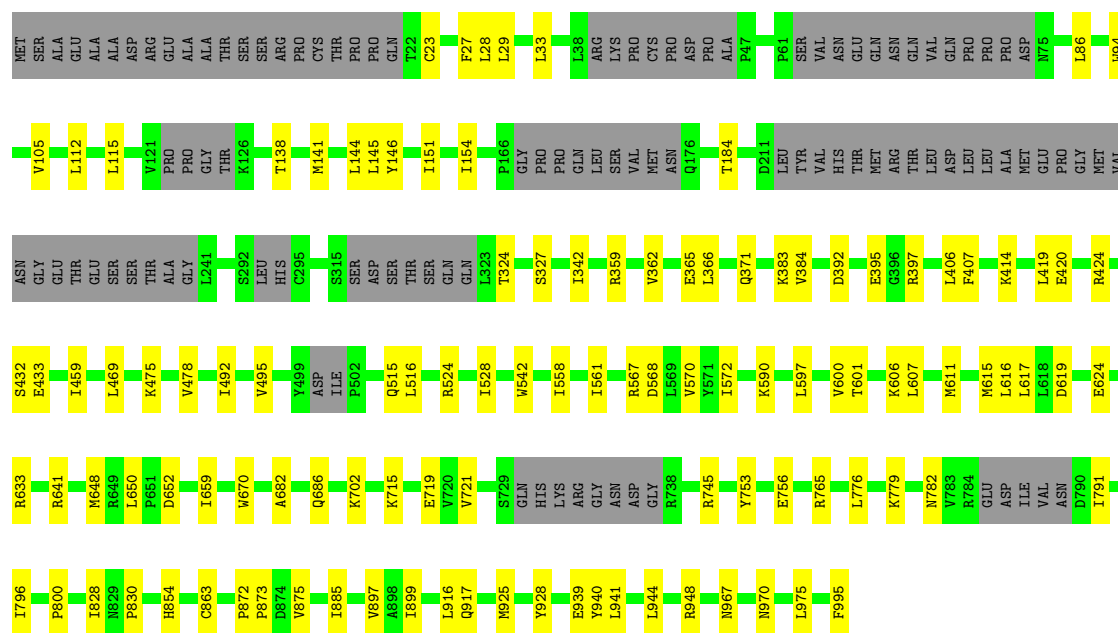
● Molecule 27: Integrator complex subunit 7





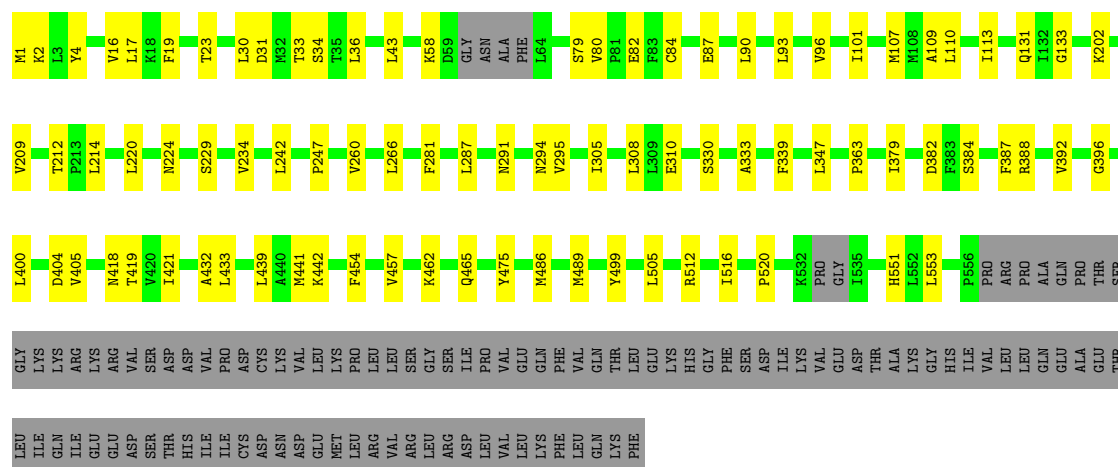
• Molecule 28: Integrator complex subunit 8

Chain h: 78% 11% 11%



• Molecule 29: Integrator complex subunit 9

Chain i: 71% 13% 16%



There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	614283	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.18	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.203	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.19	0/11210	0.39	0/15130
2	B	0.21	0/9076	0.41	0/12250
3	C	0.23	0/2139	0.35	0/2906
4	D	0.18	0/988	0.50	0/1333
5	E	0.17	0/1752	0.37	0/2366
6	F	0.20	0/637	0.37	0/859
7	G	0.16	0/1347	0.40	0/1833
8	H	0.19	0/1207	0.33	0/1628
9	I	0.20	0/967	0.49	0/1309
10	J	0.21	0/542	0.43	0/730
11	K	0.23	0/939	0.41	0/1271
12	L	0.31	0/389	0.51	0/517
13	M	0.14	0/100	0.25	0/139
14	N	0.18	0/547	0.37	0/838
15	P	0.16	0/403	0.35	0/625
16	T	0.19	0/764	0.41	0/1179
17	U	0.18	0/1422	0.44	0/1933
18	V	0.13	0/1912	0.38	0/2453
19	W	0.16	0/3812	0.43	0/5186
21	Z	0.13	0/2206	0.33	0/2968
22	a	0.18	0/8430	0.48	1/11494 (0.0%)
23	b	0.19	0/8065	0.44	0/10992
24	d	0.18	0/6535	0.42	0/8877
25	e	0.19	0/4775	0.41	0/6511
26	f	0.19	0/4179	0.42	0/5705
27	g	0.20	0/6817	0.43	0/9246
28	h	0.19	0/6867	0.42	3/9329 (0.0%)
29	i	0.21	0/4360	0.42	0/5957
30	k	0.18	0/3408	0.41	0/4632
31	p	0.19	0/4460	0.47	0/6064
32	q	0.19	0/2378	0.41	2/3228 (0.1%)
33	u	0.21	0/15	0.24	0/20

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.19	0/102648	0.42	6/139508 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
22	a	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	h	469	LEU	CA-C-N	5.71	132.45	121.54
28	h	469	LEU	C-N-CA	5.71	132.45	121.54
32	q	88	ASN	CA-C-N	5.45	131.95	121.54
32	q	88	ASN	C-N-CA	5.45	131.95	121.54
28	h	719	GLU	N-CA-CB	5.07	117.67	110.16
22	a	1737	GLU	N-CA-CB	5.01	118.57	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	a	1033	LEU	Peptide

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	11012	0	11159	152	0
2	B	8901	0	8923	106	0
3	C	2096	0	2040	25	0
4	D	975	0	929	16	0
5	E	1721	0	1737	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	627	0	657	9	0
7	G	1316	0	1288	18	0
8	H	1186	0	1147	18	0
9	I	944	0	868	12	0
10	J	533	0	553	7	0
11	K	920	0	942	11	0
12	L	383	0	382	7	0
13	M	95	0	82	1	0
14	N	489	0	272	2	0
15	P	361	0	185	9	0
16	T	682	0	375	3	0
17	U	1398	0	1441	22	0
18	V	2040	0	847	5	0
19	W	3854	0	3702	49	0
20	X	110	0	24	0	0
21	Z	2174	0	2201	23	0
22	a	8337	0	7272	85	0
23	b	7926	0	7935	104	0
24	d	6410	0	6434	65	0
25	e	4671	0	4484	44	0
26	f	4075	0	3933	38	0
27	g	6710	0	6654	85	0
28	h	6749	0	6609	72	0
29	i	4249	0	4208	50	0
30	k	3336	0	3128	41	0
31	p	4388	0	4454	67	0
32	q	2322	0	2215	33	0
33	u	144	0	39	0	0
34	A	1	0	0	0	0
35	A	2	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	I	2	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	k	2	0	0	0	0
36	q	2	0	0	0	0
All	All	101147	0	97119	1074	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 5.

All (1074) 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)
30:k:177:GLY:O	30:k:203:GLU:OE2	1.64	1.14
30:k:177:GLY:O	30:k:203:GLU:CD	1.95	1.09
24:d:41:ILE:O	24:d:45:LYS:HB2	1.83	0.78
23:b:128:LEU:O	23:b:132:HIS:HB2	1.85	0.75
30:k:177:GLY:O	30:k:203:GLU:CG	2.35	0.74
4:D:57:LEU:HD22	4:D:61:PHE:HB2	1.70	0.74
27:g:908:SER:HB2	27:g:921:GLY:HA3	1.72	0.71
6:F:57:MET:HB2	6:F:123:LEU:HB3	1.74	0.70
32:q:156:THR:HG22	32:q:166:LEU:HD13	1.73	0.70
17:U:38:ILE:HA	17:U:41:ILE:HG12	1.72	0.69
30:k:70:HIS:CE1	30:k:157:HIS:NE2	2.60	0.69
23:b:617:GLN:O	23:b:621:GLU:HB3	1.94	0.68
24:d:849:ALA:HB3	24:d:892:LEU:HB3	1.76	0.68
19:W:146:LEU:O	19:W:150:ILE:HB	1.93	0.68
29:i:101:ILE:HD13	29:i:107:MET:HG3	1.76	0.68
1:A:99:PHE:HB3	1:A:248:MET:HE3	1.77	0.67
28:h:590:LYS:HG3	28:h:615:MET:HE1	1.76	0.67
24:d:453:LEU:HB3	24:d:488:GLU:HG3	1.77	0.67
18:V:52:ASP:HA	18:V:56:THR:HB	1.77	0.66
22:a:1667:GLN:HG3	23:b:808:ARG:HB2	1.76	0.66
25:e:394:LEU:O	25:e:398:ALA:HB3	1.96	0.66
22:a:2111:MET:HE3	22:a:2118:ALA:HA	1.78	0.65
17:U:180:GLN:NE2	17:U:184:GLU:OE2	2.29	0.65
24:d:866:LEU:HB3	24:d:910:GLU:HB3	1.79	0.65
3:C:154:ARG:HD3	10:J:64:PRO:HD3	1.78	0.65
1:A:743:ARG:HG2	19:W:442:GLN:HE21	1.62	0.65
22:a:1711:ARG:HH11	23:b:991:ARG:HH22	1.45	0.64
22:a:1680:LEU:HD21	22:a:1694:SER:HB3	1.79	0.64
2:B:1029:TYR:HA	2:B:1036:LYS:HA	1.80	0.64
2:B:709:SER:HB2	2:B:767:LEU:HD11	1.79	0.64
27:g:774:THR:O	27:g:778:CYS:HB2	1.97	0.64
27:g:695:ALA:HB1	27:g:699:THR:HB	1.81	0.63
29:i:419:THR:HG22	29:i:442:LYS:HB2	1.79	0.63
1:A:460:ARG:HB2	1:A:501:MET:HE3	1.79	0.63
1:A:413:TYR:O	1:A:449:HIS:ND1	2.32	0.63
23:b:1104:LEU:HB3	23:b:1192:THR:HG21	1.80	0.63
28:h:29:LEU:HD13	31:p:41:ALA:HB2	1.80	0.63
30:k:284:PRO:HA	30:k:291:ARG:HD3	1.79	0.63
3:C:193:ARG:NH2	3:C:218:ALA:O	2.33	0.62
23:b:649:LEU:HB3	23:b:706:LEU:HD21	1.80	0.62
24:d:452:VAL:HG13	24:d:467:LEU:HD11	1.82	0.62
23:b:682:SER:O	23:b:686:GLN:NE2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:1125:LEU:HD13	23:b:1193:VAL:HG12	1.82	0.62
30:k:177:GLY:O	30:k:203:GLU:HG3	1.99	0.62
1:A:1343:LEU:HD21	1:A:1359:SER:HB2	1.81	0.62
22:a:1746:ARG:HG3	22:a:1757:LEU:HD22	1.82	0.61
24:d:687:LEU:HD11	27:g:704:GLU:HG2	1.81	0.61
1:A:233:CYS:SG	1:A:244:ARG:NH1	2.73	0.61
25:e:833:PRO:HA	25:e:951:ARG:HD2	1.81	0.61
31:p:323:MET:HE2	31:p:356:LEU:HD11	1.80	0.61
28:h:682:ALA:O	28:h:686:GLN:NE2	2.34	0.61
2:B:899:SER:OG	2:B:1078:ARG:NH1	2.34	0.61
3:C:260:GLN:HE22	11:K:88:THR:HG23	1.64	0.61
29:i:439:LEU:HD13	29:i:441:MET:HB3	1.83	0.61
29:i:209:VAL:HG12	29:i:229:SER:HB2	1.81	0.61
31:p:17:ILE:HD11	31:p:38:ILE:HG13	1.82	0.61
1:A:467:MET:HE2	1:A:524:MET:HB3	1.81	0.61
2:B:761:THR:H	2:B:764:MET:HE3	1.65	0.60
27:g:820:ALA:HB1	27:g:931:LEU:HD22	1.83	0.60
1:A:75:ALA:O	2:B:1131:ARG:NH1	2.32	0.60
22:a:974:TYR:HA	22:a:977:ARG:HD2	1.82	0.60
1:A:136:GLN:HE21	1:A:139:LYS:HD2	1.67	0.60
2:B:236:TRP:HB2	2:B:259:THR:HB	1.83	0.60
24:d:74:ARG:NH1	24:d:113:ASP:OD2	2.34	0.60
31:p:48:ARG:NH1	31:p:80:VAL:O	2.35	0.60
2:B:281:ASP:HB2	9:I:22:ASN:HA	1.83	0.60
28:h:721:VAL:HG21	28:h:776:LEU:HD21	1.82	0.60
1:A:139:LYS:O	1:A:143:HIS:ND1	2.34	0.60
23:b:622:GLN:HE22	23:b:648:GLN:HA	1.65	0.60
5:E:9:ARG:HG3	5:E:136:LEU:HD21	1.84	0.59
1:A:511:THR:HG21	2:B:1105:GLU:HG2	1.84	0.59
23:b:624:ILE:HD11	23:b:641:GLN:HA	1.83	0.59
1:A:1344:MET:HE2	5:E:134:GLU:HA	1.83	0.59
22:a:1534:CYS:SG	22:a:1535:SER:N	2.76	0.59
23:b:481:LEU:HD11	23:b:535:ALA:HA	1.84	0.59
25:e:632:CYS:O	25:e:676:ARG:NH2	2.34	0.59
31:p:572:ASP:OD2	32:q:110:ARG:NH1	2.35	0.59
9:I:119:CYS:SG	9:I:120:GLY:N	2.75	0.59
24:d:475:ASN:OD1	24:d:513:ARG:NH1	2.36	0.59
1:A:74:CYS:SG	1:A:84:HIS:CE1	2.84	0.58
2:B:780:VAL:HG21	2:B:1048:TYR:HE2	1.68	0.58
17:U:139:LEU:HD13	19:W:267:ARG:HH21	1.67	0.58
29:i:462:LYS:O	29:i:465:GLN:NE2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1091:ARG:HD2	22:a:1165:LEU:HD22	1.83	0.58
30:k:203:GLU:HG2	30:k:414:HIS:HB3	1.84	0.58
22:a:1513:ASP:HB3	22:a:1516:VAL:HB	1.86	0.58
27:g:800:GLN:NE2	27:g:845:ARG:O	2.36	0.58
30:k:93:THR:HG22	30:k:95:PRO:HD2	1.84	0.58
2:B:611:GLU:OE1	2:B:613:ARG:NH1	2.36	0.58
29:i:31:ASP:HB3	29:i:84:CYS:HB3	1.85	0.58
1:A:1166:LEU:HA	1:A:1169:VAL:HG12	1.86	0.58
2:B:748:ALA:HB3	2:B:811:TYR:HB2	1.86	0.58
31:p:254:ASP:O	31:p:260:ARG:NH1	2.34	0.58
27:g:183:MET:HG3	27:g:197:LEU:HD21	1.84	0.58
30:k:6:VAL:HG22	30:k:22:VAL:HG22	1.86	0.58
27:g:594:LEU:O	27:g:598:HIS:ND1	2.36	0.58
30:k:143:GLN:NE2	30:k:149:GLU:OE1	2.35	0.58
32:q:202:ASP:OD1	32:q:239:ARG:NH2	2.36	0.58
23:b:558:TYR:OH	23:b:562:ARG:NH2	2.36	0.58
31:p:277:GLU:HA	31:p:280:LYS:HE3	1.84	0.58
24:d:464:ARG:NH1	24:d:499:ASP:OD2	2.37	0.57
27:g:180:ILE:HD12	27:g:197:LEU:HD11	1.86	0.57
27:g:464:GLY:HA2	27:g:467:MET:HE2	1.86	0.57
27:g:540:ASP:HB3	27:g:573:GLN:HG3	1.86	0.57
1:A:340:LYS:HG3	1:A:1436:VAL:HG21	1.85	0.57
19:W:217:GLU:HA	19:W:220:LEU:HD12	1.86	0.57
23:b:772:MET:HE1	23:b:808:ARG:HG2	1.85	0.57
31:p:522:LEU:HD12	31:p:551:LEU:HD22	1.86	0.57
1:A:322:LEU:O	1:A:327:ARG:NH2	2.37	0.57
2:B:529:MET:HG3	2:B:702:MET:HE2	1.86	0.57
27:g:829:LEU:HD23	27:g:894:LEU:HD13	1.85	0.57
4:D:86:LEU:HD21	4:D:137:LYS:HZ1	1.69	0.57
21:Z:450:ILE:HG21	21:Z:468:LEU:HD11	1.86	0.57
24:d:155:ALA:HB2	24:d:173:LEU:HD23	1.85	0.57
5:E:38:GLU:HA	5:E:41:LYS:HD3	1.87	0.57
12:L:19:CYS:HA	12:L:44:MET:HG2	1.86	0.57
23:b:806:PRO:HD2	23:b:809:ILE:HD12	1.85	0.57
1:A:727:PRO:HA	1:A:736:THR:HG21	1.86	0.57
1:A:931:ARG:NH1	1:A:936:GLU:OE1	2.38	0.57
23:b:49:LEU:HD22	23:b:71:ILE:HD11	1.86	0.57
22:a:1044:SER:HA	22:a:1047:ALA:HB3	1.86	0.57
22:a:1630:VAL:HG22	22:a:1637:GLN:HB3	1.85	0.57
1:A:90:LEU:HD12	1:A:310:LEU:HD21	1.86	0.57
2:B:227:ASN:ND2	2:B:537:GLN:OE1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:18:MET:HE1	5:E:60:VAL:HG11	1.86	0.57
28:h:324:THR:HG23	28:h:327:SER:H	1.70	0.57
28:h:782:ASN:ND2	28:h:791:ILE:O	2.35	0.57
30:k:35:MET:HG2	30:k:75:GLY:HA3	1.85	0.57
32:q:121:ARG:NH1	32:q:188:GLU:OE1	2.35	0.57
3:C:7:PRO:HB2	11:K:101:LEU:HD13	1.87	0.57
9:I:30:LYS:HA	9:I:33:ARG:HH22	1.70	0.57
23:b:150:MET:HE3	23:b:196:ASP:HB3	1.86	0.57
1:A:1218:ARG:NH2	1:A:1250:ASP:O	2.38	0.57
27:g:260:LEU:O	27:g:269:LYS:NZ	2.36	0.57
31:p:260:ARG:NH2	31:p:295:GLU:OE2	2.38	0.57
27:g:198:ILE:HG22	27:g:237:THR:HG21	1.86	0.56
30:k:457:SER:HB3	30:k:493:VAL:HG12	1.87	0.56
25:e:823:ASP:OD2	25:e:824:ALA:N	2.38	0.56
5:E:107:GLN:HA	5:E:132:GLN:HB2	1.86	0.56
22:a:1170:MET:HA	22:a:1173:LEU:HD23	1.87	0.56
23:b:299:VAL:HG23	23:b:391:LEU:HD22	1.87	0.56
24:d:144:ASN:HB3	24:d:147:ILE:HG12	1.87	0.56
29:i:23:THR:HB	29:i:96:VAL:HA	1.87	0.56
32:q:239:ARG:HH12	32:q:242:GLN:HB2	1.69	0.56
23:b:389:LEU:HD22	23:b:435:MET:HE1	1.87	0.56
25:e:890:GLU:OE2	25:e:940:ARG:NE	2.34	0.56
5:E:163:TYR:HB2	5:E:165:LEU:HD22	1.88	0.56
27:g:374:CYS:SG	27:g:375:GLN:N	2.78	0.56
2:B:92:TYR:HB2	2:B:125:TYR:HB2	1.86	0.56
2:B:905:ASP:HB2	2:B:924:ARG:HB2	1.86	0.56
24:d:525:LEU:HD12	24:d:551:ILE:HD11	1.88	0.56
27:g:198:ILE:HD12	27:g:221:LEU:HD21	1.88	0.56
1:A:1176:TYR:HB2	1:A:1211:LEU:HD21	1.88	0.56
24:d:40:HIS:HB2	24:d:75:ILE:HD13	1.87	0.56
32:q:61:GLN:NE2	32:q:64:ASP:OD2	2.38	0.56
8:H:59:VAL:HB	8:H:144:LEU:HB2	1.87	0.56
23:b:35:ALA:HA	23:b:74:LEU:HD13	1.88	0.56
25:e:910:LEU:HG	25:e:914:MET:HE2	1.87	0.56
32:q:294:ARG:O	32:q:295:ARG:NE	2.33	0.56
1:A:341:GLN:HG3	1:A:344:LYS:HE2	1.87	0.56
7:G:113:ILE:HD12	7:G:163:LEU:HB3	1.88	0.56
22:a:2161:ARG:NH2	25:e:562:HIS:O	2.38	0.56
23:b:544:LEU:HA	23:b:548:ILE:HD12	1.87	0.56
1:A:1310:HIS:HA	19:W:486:VAL:HG21	1.86	0.55
3:C:59:LEU:HD12	3:C:151:VAL:HG23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:U:17:LEU:HB2	17:U:52:VAL:HG23	1.86	0.55
19:W:431:VAL:HG13	19:W:451:HIS:HB3	1.89	0.55
27:g:399:GLN:NE2	27:g:440:SER:O	2.38	0.55
1:A:911:PRO:O	1:A:963:ARG:NH2	2.35	0.55
10:J:47:ARG:NH1	10:J:48:MET:SD	2.79	0.55
27:g:218:LEU:HD23	27:g:221:LEU:HD23	1.88	0.55
4:D:60:VAL:HA	4:D:63:LYS:HE3	1.88	0.55
23:b:322:ARG:O	23:b:326:GLN:NE2	2.39	0.55
25:e:588:GLY:HA2	25:e:592:PRO:HG2	1.88	0.55
25:e:824:ALA:HB1	25:e:827:ALA:HB2	1.87	0.55
32:q:83:MET:HE3	32:q:240:ALA:HB2	1.88	0.55
1:A:420:ILE:HB	1:A:445:LYS:HB2	1.89	0.55
28:h:419:LEU:HD21	28:h:459:ILE:HG23	1.88	0.55
17:U:96:ILE:HG12	17:U:106:LEU:HD23	1.89	0.55
27:g:899:LEU:HA	27:g:930:SER:HB2	1.87	0.55
6:F:84:GLU:OE1	6:F:95:LYS:NZ	2.39	0.55
24:d:449:LEU:HD22	24:d:476:VAL:HG21	1.89	0.55
27:g:705:LEU:O	27:g:752:TYR:OH	2.24	0.55
28:h:561:ILE:HB	28:h:567:ARG:HB2	1.89	0.55
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.89	0.55
26:f:65:GLY:H	26:f:68:GLU:HG3	1.72	0.55
4:D:67:TYR:OH	7:G:100:GLU:O	2.24	0.55
30:k:70:HIS:HE1	30:k:157:HIS:NE2	2.01	0.55
2:B:780:VAL:HG22	2:B:965:ILE:HB	1.89	0.55
22:a:987:ARG:NH1	22:a:1056:MET:O	2.39	0.55
28:h:885:ILE:HG23	28:h:897:VAL:HG13	1.89	0.55
1:A:358:ARG:HA	2:B:1085:ARG:HA	1.89	0.54
15:P:39:A:H2'	15:P:40:A:C8	2.42	0.54
22:a:1124:PHE:HE2	22:a:1173:LEU:HD21	1.73	0.54
23:b:833:VAL:HG11	23:b:853:LEU:HD21	1.89	0.54
2:B:645:GLU:HB2	2:B:648:TYR:HB2	1.88	0.54
6:F:57:MET:HG3	6:F:123:LEU:HD13	1.88	0.54
22:a:2062:ASP:OD1	28:h:745:ARG:NH2	2.41	0.54
28:h:112:LEU:HD23	28:h:146:TYR:HA	1.89	0.54
24:d:827:PRO:HD3	24:d:847:VAL:HA	1.88	0.54
17:U:143:TYR:OH	19:W:335:ASP:OD1	2.26	0.54
23:b:409:GLU:OE1	23:b:448:GLN:NE2	2.40	0.54
27:g:293:GLN:NE2	27:g:343:ASP:OD2	2.39	0.54
31:p:138:GLY:O	31:p:144:ARG:NH1	2.40	0.54
8:H:66:GLU:N	8:H:66:GLU:OE1	2.41	0.54
17:U:76:MET:HE2	17:U:101:PRO:HG2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:16:GLN:O	23:b:209:TRP:NE1	2.41	0.54
23:b:304:GLY:HA3	27:g:605:THR:HG23	1.90	0.54
31:p:537:ARG:NE	31:p:570:ASP:OD2	2.39	0.54
2:B:1142:ASN:HD21	2:B:1145:GLN:HB2	1.73	0.54
25:e:881:LEU:HD23	25:e:910:LEU:HD13	1.89	0.54
26:f:386:TYR:HB2	26:f:390:LEU:HD23	1.89	0.54
1:A:397:PHE:HB3	6:F:87:THR:HG23	1.90	0.54
2:B:41:ARG:O	2:B:45:ASP:HB2	2.08	0.54
2:B:780:VAL:HG21	2:B:1048:TYR:CE2	2.43	0.54
2:B:754:PRO:HB2	2:B:773:PRO:HG2	1.90	0.53
8:H:69:THR:OG1	8:H:81:ARG:NH2	2.41	0.53
22:a:1088:ASP:OD1	22:a:1091:ARG:NH1	2.40	0.53
21:Z:705:LEU:HG	21:Z:724:VAL:HG21	1.91	0.53
25:e:474:LEU:HD23	25:e:477:LEU:HD12	1.91	0.53
1:A:1386:ILE:HD12	1:A:1398:LEU:HD21	1.91	0.53
3:C:48:ASP:OD1	3:C:175:LYS:NZ	2.38	0.53
17:U:48:LEU:O	17:U:53:LYS:NZ	2.41	0.53
2:B:721:ARG:NH2	2:B:940:GLY:O	2.37	0.53
21:Z:479:LYS:HD3	21:Z:521:CYS:HB2	1.90	0.53
30:k:198:ASN:O	30:k:409:SER:OG	2.26	0.53
31:p:300:ALA:O	31:p:304:HIS:ND1	2.41	0.53
1:A:461:GLN:OE1	1:A:502:ASN:ND2	2.41	0.53
3:C:106:ARG:NH1	3:C:107:CYS:O	2.41	0.53
10:J:1:MET:HA	10:J:55:LEU:HB2	1.88	0.53
17:U:144:LEU:HD21	19:W:329:ARG:HD3	1.90	0.53
19:W:452:LEU:HB3	19:W:499:ARG:HD2	1.90	0.53
24:d:883:ARG:HE	24:d:893:ILE:HD12	1.73	0.53
32:q:67:GLU:HB2	32:q:292:ALA:HB2	1.89	0.53
1:A:867:SER:HB3	1:A:1414:ILE:HG23	1.91	0.53
23:b:534:HIS:HA	23:b:537:ARG:HE	1.73	0.53
23:b:876:ILE:HG22	23:b:880:MET:HE2	1.90	0.53
23:b:943:LEU:HB3	23:b:1024:LEU:HD13	1.90	0.53
25:e:934:LEU:HD11	25:e:999:LEU:HD11	1.90	0.53
28:h:542:TRP:HA	28:h:572:ILE:HD11	1.90	0.53
28:h:779:LYS:HD3	28:h:796:ILE:HG12	1.91	0.53
19:W:381:ASP:OD1	19:W:381:ASP:N	2.41	0.53
26:f:160:GLU:OE1	26:f:303:SER:OG	2.25	0.53
29:i:454:PHE:HA	29:i:457:VAL:HG12	1.91	0.53
1:A:760:LEU:HD11	1:A:781:ILE:HG21	1.91	0.53
15:P:38:G:H2'	15:P:39:A:C8	2.43	0.53
23:b:505:MET:HE3	23:b:507:ILE:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:p:432:GLY:HA2	31:p:472:LYS:HE3	1.91	0.53
1:A:790:GLN:NE2	1:A:791:GLN:O	2.42	0.53
22:a:2107:ALA:O	22:a:2111:MET:HG3	2.08	0.53
28:h:28:LEU:HD22	31:p:16:LEU:HD21	1.90	0.53
29:i:516:ILE:HG13	29:i:551:HIS:HB2	1.91	0.53
31:p:361:THR:HG23	31:p:365:LEU:HD12	1.91	0.53
2:B:298:MET:HB3	9:I:14:ILE:HG12	1.90	0.52
11:K:17:LYS:HE2	11:K:20:THR:HG22	1.91	0.52
23:b:1050:GLU:HB2	23:b:1053:LYS:HG2	1.91	0.52
27:g:754:HIS:NE2	27:g:758:GLU:OE2	2.42	0.52
32:q:276:MET:HE2	32:q:278:LEU:HD21	1.91	0.52
3:C:13:GLU:HB3	3:C:20:LYS:HB3	1.89	0.52
22:a:1457:LEU:HD11	22:a:1489:SER:HB3	1.91	0.52
26:f:583:PRO:O	26:f:585:ALA:N	2.42	0.52
27:g:593:SER:O	27:g:597:TYR:HB2	2.08	0.52
1:A:552:ASP:HB2	8:H:24:ARG:HB2	1.91	0.52
2:B:765:GLU:OE2	2:B:770:ARG:NH2	2.41	0.52
23:b:139:LEU:HA	23:b:181:LEU:HD21	1.90	0.52
1:A:593:SER:HB3	1:A:634:GLU:HB2	1.91	0.52
1:A:783:GLN:HG2	1:A:788:VAL:HA	1.91	0.52
2:B:274:ARG:NH1	2:B:311:ILE:O	2.43	0.52
9:I:90:GLY:O	9:I:92:LYS:NZ	2.38	0.52
21:Z:501:ILE:HD11	21:Z:510:GLU:HB3	1.91	0.52
25:e:953:HIS:O	25:e:959:LYS:NZ	2.42	0.52
1:A:798:ILE:O	1:A:820:ARG:NH1	2.43	0.52
22:a:1067:LEU:HD11	22:a:1116:VAL:HG22	1.92	0.52
23:b:450:GLN:HA	23:b:453:VAL:HG22	1.91	0.52
27:g:472:MET:HE1	27:g:512:VAL:HG23	1.92	0.52
28:h:342:ILE:HD13	28:h:383:LYS:HD3	1.91	0.52
1:A:567:LEU:HD21	1:A:595:ILE:HG12	1.90	0.52
19:W:329:ARG:NH1	19:W:363:ALA:O	2.42	0.52
26:f:17:ARG:O	28:h:967:ASN:ND2	2.43	0.52
2:B:256:ILE:HD11	2:B:373:LEU:HD21	1.91	0.52
2:B:591:ARG:NH2	2:B:663:GLU:OE1	2.43	0.52
7:G:38:CYS:HB2	7:G:44:PHE:HD2	1.74	0.52
11:K:63:VAL:HG22	11:K:71:ILE:HG22	1.90	0.52
12:L:56:ASP:OD1	21:Z:738:SER:OG	2.23	0.52
19:W:538:LEU:HD12	19:W:575:VAL:HG12	1.91	0.52
22:a:1059:ASP:OD2	22:a:1061:GLN:NE2	2.40	0.52
2:B:295:PRO:HB2	9:I:11:PHE:HB3	1.91	0.52
17:U:96:ILE:HA	17:U:107:ASN:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1627:PRO:HB2	23:b:806:PRO:HG2	1.92	0.52
23:b:262:LEU:HD12	23:b:265:ARG:HH21	1.74	0.52
23:b:325:GLN:NE2	23:b:400:GLY:O	2.41	0.52
28:h:715:LYS:HD2	28:h:800:PRO:HG3	1.91	0.52
1:A:45:GLU:OE2	1:A:53:LYS:NZ	2.41	0.52
1:A:1026:ASP:O	1:A:1031:ARG:NH1	2.43	0.52
2:B:1066:PRO:HB2	2:B:1075:MET:HE2	1.91	0.52
4:D:74:PHE:HD2	4:D:80:ILE:HG13	1.75	0.52
32:q:121:ARG:NH2	32:q:148:ASP:OD1	2.43	0.52
2:B:352:GLY:O	2:B:361:LYS:NZ	2.38	0.52
28:h:23:CYS:SG	31:p:34:LYS:NZ	2.80	0.52
29:i:247:PRO:HA	29:i:347:LEU:HA	1.92	0.52
30:k:497:GLN:HA	30:k:500:LYS:HG2	1.92	0.52
31:p:87:HIS:HA	31:p:90:LEU:HD23	1.92	0.52
31:p:176:ASP:OD1	31:p:178:THR:OG1	2.27	0.52
19:W:102:ILE:HG12	19:W:108:PRO:HA	1.92	0.51
22:a:1051:GLN:HG2	22:a:1089:VAL:HG21	1.92	0.51
22:a:1171:VAL:HA	22:a:1174:LEU:HG	1.92	0.51
22:a:1244:LEU:HD11	22:a:1264:PHE:HD1	1.75	0.51
28:h:94:TRP:HB3	28:h:145:LEU:HD11	1.92	0.51
1:A:370:ASP:HB2	1:A:483:ARG:HB3	1.93	0.51
30:k:267:PHE:HA	30:k:322:PHE:HB2	1.92	0.51
1:A:114:CYS:SG	1:A:184:CYS:HB3	2.50	0.51
1:A:1453:GLY:O	1:A:1457:ASN:ND2	2.43	0.51
28:h:86:LEU:HD11	28:h:115:LEU:HB2	1.93	0.51
23:b:73:ARG:O	23:b:76:SER:OG	2.27	0.51
28:h:917:GLN:NE2	28:h:940:TYR:OH	2.44	0.51
3:C:51:GLN:OE1	3:C:162:ARG:NH1	2.43	0.51
8:H:95:LYS:HB3	8:H:140:ARG:HD3	1.92	0.51
23:b:801:LEU:HD21	23:b:873:LEU:HD22	1.92	0.51
29:i:87:GLU:OE2	29:i:90:LEU:N	2.43	0.51
5:E:26:TYR:HA	5:E:64:HIS:HA	1.93	0.51
23:b:564:ARG:HH22	23:b:567:THR:HG21	1.76	0.51
26:f:104:LEU:HD13	26:f:459:LEU:HB3	1.93	0.51
26:f:351:TYR:HB3	26:f:364:PRO:HA	1.92	0.51
31:p:451:LEU:HD11	31:p:466:LEU:HD11	1.92	0.51
32:q:184:ASP:O	32:q:187:GLN:NE2	2.43	0.51
1:A:379:GLY:HA3	1:A:477:LEU:HD12	1.91	0.51
2:B:710:ILE:HA	2:B:764:MET:HE2	1.92	0.51
19:W:519:CYS:HA	19:W:523:LEU:HB2	1.93	0.51
31:p:245:MET:HE2	31:p:282:ASP:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:259:LEU:HD22	11:K:42:LEU:HD21	1.92	0.51
22:a:1167:VAL:HA	22:a:1170:MET:HG3	1.91	0.51
23:b:28:LYS:HE3	27:g:584:SER:HB2	1.92	0.51
28:h:779:LYS:NZ	28:h:796:ILE:O	2.44	0.51
29:i:1:MET:HE2	29:i:2:LYS:HE3	1.92	0.51
2:B:1038:THR:HA	3:C:195:THR:HA	1.93	0.51
22:a:1258:MET:HA	22:a:1261:LEU:HG	1.92	0.51
25:e:397:GLN:HA	25:e:472:PRO:HD2	1.92	0.51
25:e:591:GLY:HA2	28:h:492:ILE:HD13	1.92	0.51
31:p:408:ILE:HA	31:p:411:LEU:HD23	1.91	0.51
4:D:131:LEU:HA	4:D:134:ILE:HG22	1.93	0.50
24:d:80:TYR:OH	24:d:121:GLU:OE1	2.28	0.50
24:d:83:GLU:HG3	24:d:85:ASP:H	1.76	0.50
24:d:392:ILE:HG13	24:d:427:VAL:HG22	1.94	0.50
24:d:678:LEU:O	24:d:739:ARG:NH2	2.44	0.50
30:k:184:ASP:O	30:k:287:ASN:ND2	2.44	0.50
22:a:1269:VAL:HG13	22:a:1273:PRO:HB3	1.92	0.50
30:k:32:ASP:OD2	30:k:175:TYR:OH	2.24	0.50
1:A:52:PRO:HG3	1:A:58:MET:HE3	1.92	0.50
5:E:71:GLN:HB2	5:E:99:ILE:HG12	1.94	0.50
30:k:178:ASP:HA	30:k:203:GLU:OE1	2.12	0.50
1:A:467:MET:HE1	1:A:527:THR:HA	1.94	0.50
1:A:535:MET:O	1:A:669:TYR:OH	2.25	0.50
1:A:538:VAL:HG12	1:A:539:GLN:H	1.76	0.50
22:a:2111:MET:HE1	22:a:2147:TYR:CE1	2.46	0.50
24:d:419:MET:HG3	30:k:215:ARG:HH12	1.76	0.50
27:g:692:SER:OG	27:g:693:PHE:N	2.44	0.50
4:D:62:MET:HA	4:D:65:LEU:HB3	1.93	0.50
25:e:768:ASN:HB3	25:e:771:GLU:HG2	1.93	0.50
29:i:400:LEU:HD22	29:i:432:ALA:HB1	1.93	0.50
16:T:38:DT:H2"	16:T:39:DA:H5"	1.94	0.50
24:d:472:CYS:O	24:d:513:ARG:NH2	2.45	0.50
1:A:546:ARG:HD3	1:A:772:SER:HB3	1.93	0.50
2:B:808:SER:OG	2:B:1050:ARG:NH1	2.45	0.50
31:p:547:ILE:HG13	31:p:551:LEU:HD23	1.94	0.50
17:U:17:LEU:HB3	17:U:55:LYS:HD2	1.93	0.50
25:e:638:ALA:HB3	28:h:830:PRO:HD2	1.94	0.50
26:f:322:LEU:HD21	26:f:382:MET:HE1	1.94	0.50
23:b:1038:CYS:HB2	23:b:1064:LEU:HD11	1.93	0.50
24:d:798:ILE:O	24:d:802:MET:HB3	2.12	0.50
27:g:80:ARG:HB3	27:g:121:ILE:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:79:VAL:HG11	6:F:83:LEU:HD21	1.94	0.49
29:i:220:LEU:HA	29:i:247:PRO:HB3	1.92	0.49
31:p:156:PRO:HG3	31:p:195:VAL:HG21	1.94	0.49
31:p:379:GLU:O	31:p:383:ASN:ND2	2.45	0.49
14:N:26:DC:H2'	14:N:27:DT:C6	2.46	0.49
24:d:917:TYR:O	24:d:943:GLU:N	2.45	0.49
26:f:106:THR:HG23	26:f:108:ILE:HG12	1.93	0.49
28:h:392:ASP:OD1	28:h:397:ARG:NH1	2.41	0.49
28:h:753:TYR:HB2	28:h:756:GLU:HG3	1.93	0.49
31:p:271:GLN:HG3	31:p:279:THR:HG21	1.93	0.49
31:p:489:MET:HB2	31:p:501:THR:HB	1.94	0.49
1:A:637:MET:HB3	8:H:122:LEU:HD21	1.93	0.49
17:U:24:TRP:O	17:U:55:LYS:NZ	2.44	0.49
30:k:199:LEU:HD11	30:k:411:LEU:HB2	1.94	0.49
15:P:35:A:OP1	15:P:36:G:N2	2.45	0.49
29:i:486:MET:HA	29:i:489:MET:HE3	1.93	0.49
9:I:24:LEU:HD23	9:I:39:CYS:HB2	1.94	0.49
32:q:292:ALA:O	32:q:294:ARG:NH1	2.42	0.49
1:A:460:ARG:NH2	15:P:46:U:O2'	2.45	0.49
1:A:880:ARG:HG2	1:A:886:VAL:HA	1.94	0.49
22:a:1365:PHE:HZ	22:a:1405:VAL:HG13	1.78	0.49
28:h:652:ASP:OD1	28:h:652:ASP:N	2.46	0.49
19:W:497:LEU:HD21	19:W:533:PHE:HB2	1.93	0.49
22:a:1627:PRO:O	22:a:1667:GLN:NE2	2.38	0.49
23:b:262:LEU:HG	27:g:598:HIS:NE2	2.28	0.49
25:e:966:ARG:NH1	28:h:371:GLN:O	2.46	0.49
27:g:473:GLU:OE2	27:g:476:LYS:NZ	2.39	0.49
12:L:22:CYS:SG	12:L:24:THR:OG1	2.61	0.49
21:Z:546:THR:OG1	30:k:113:ASP:OD1	2.30	0.49
22:a:1241:PRO:HG3	22:a:1268:ALA:HB1	1.95	0.49
24:d:414:ASP:OD2	24:d:414:ASP:N	2.45	0.49
2:B:1109:GLU:HA	2:B:1113:PRO:HG3	1.94	0.49
3:C:38:PHE:HE1	3:C:245:VAL:HA	1.77	0.49
5:E:44:PHE:HB3	5:E:53:PRO:HB3	1.95	0.49
23:b:484:ALA:O	23:b:488:HIS:ND1	2.38	0.49
31:p:105:ARG:HD3	31:p:142:THR:HB	1.95	0.49
1:A:552:ASP:O	8:H:24:ARG:NH1	2.45	0.49
2:B:59:VAL:HG21	2:B:91:ILE:HD11	1.95	0.49
2:B:407:MET:HE1	2:B:444:LEU:HB2	1.95	0.49
7:G:128:TYR:HB2	7:G:137:ILE:HB	1.95	0.49
19:W:497:LEU:HD23	19:W:532:TYR:HD2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:344:LEU:HG	23:b:348:MET:HE1	1.95	0.49
26:f:293:GLN:HA	26:f:449:SER:HB2	1.95	0.49
27:g:597:TYR:CE2	27:g:621:VAL:HG13	2.48	0.49
2:B:193:VAL:HG21	2:B:470:LEU:HD13	1.95	0.48
19:W:405:SER:OG	19:W:406:GLU:N	2.43	0.48
21:Z:539:LEU:HD11	21:Z:547:VAL:HB	1.95	0.48
24:d:567:ASP:OD1	24:d:567:ASP:N	2.45	0.48
25:e:586:GLN:NE2	25:e:631:ILE:O	2.41	0.48
29:i:379:ILE:HD11	29:i:404:ASP:HB3	1.94	0.48
32:q:120:SER:OG	32:q:188:GLU:OE2	2.24	0.48
19:W:357:ILE:HD12	19:W:390:VAL:HG12	1.95	0.48
19:W:361:ALA:O	19:W:365:SER:CB	2.60	0.48
28:h:29:LEU:HD11	31:p:38:ILE:HD13	1.94	0.48
28:h:607:LEU:HD12	28:h:611:MET:HE1	1.95	0.48
29:i:234:VAL:HG13	29:i:260:VAL:HG13	1.94	0.48
31:p:160:SER:HA	31:p:163:LYS:HB2	1.95	0.48
1:A:546:ARG:HD2	1:A:771:VAL:HG23	1.95	0.48
1:A:1167:ARG:HD3	9:I:58:ILE:HD11	1.95	0.48
23:b:443:VAL:HG23	23:b:444:SER:H	1.77	0.48
25:e:500:HIS:HB3	28:h:495:VAL:HG21	1.95	0.48
25:e:575:LEU:HD11	25:e:613:LEU:HD13	1.95	0.48
27:g:300:LEU:HD22	27:g:347:LEU:HD13	1.95	0.48
2:B:1060:HIS:NE2	2:B:1082:GLY:O	2.39	0.48
23:b:26:MET:HG3	23:b:219:PRO:HG3	1.95	0.48
26:f:111:TYR:HH	26:f:158:THR:HG1	1.59	0.48
27:g:192:ASP:OD1	27:g:192:ASP:N	2.46	0.48
19:W:473:LEU:HD13	19:W:500:MET:HG3	1.95	0.48
24:d:824:ILE:HD12	24:d:827:PRO:HG2	1.96	0.48
26:f:283:TRP:NE1	26:f:323:PRO:O	2.35	0.48
1:A:575:PRO:HG3	1:A:594:LEU:HD11	1.95	0.48
2:B:663:GLU:OE2	2:B:695:HIS:NE2	2.35	0.48
22:a:1190:LEU:HG	22:a:1230:ARG:HE	1.78	0.48
26:f:49:ARG:NH2	26:f:121:GLU:OE2	2.47	0.48
28:h:407:PHE:HE1	28:h:414:LYS:HB3	1.78	0.48
1:A:539:GLN:HA	1:A:774:ALA:HB1	1.95	0.48
1:A:756:ALA:HB2	1:A:786:ALA:HB2	1.96	0.48
2:B:758:LEU:HD21	10:J:47:ARG:HB2	1.96	0.48
4:D:73:ARG:NH2	7:G:86:ASP:OD2	2.46	0.48
22:a:760:TYR:O	22:a:762:THR:N	2.45	0.48
22:a:998:LEU:HD13	22:a:1028:TRP:HE1	1.77	0.48
22:a:1383:LEU:HD13	22:a:1402:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1746:ARG:HE	22:a:1757:LEU:HD13	1.78	0.48
27:g:482:ALA:O	27:g:486:GLN:NE2	2.46	0.48
28:h:420:GLU:OE2	28:h:424:ARG:NH2	2.46	0.48
28:h:542:TRP:N	28:h:568:ASP:OD1	2.47	0.48
30:k:250:ILE:HD11	30:k:299:MET:HB3	1.96	0.48
1:A:402:LEU:HD23	1:A:405:LEU:HD12	1.95	0.48
4:D:134:ILE:HA	4:D:137:LYS:HG2	1.95	0.48
12:L:35:ARG:NH1	12:L:40:GLY:O	2.46	0.48
23:b:1045:LEU:HG	23:b:1057:ALA:HB2	1.96	0.48
24:d:791:LYS:HG2	24:d:792:PRO:HD2	1.96	0.48
26:f:88:LEU:HD21	26:f:196:ILE:HD13	1.94	0.48
19:W:337:PHE:HE2	19:W:360:LEU:HD22	1.79	0.48
21:Z:469:ARG:NH2	21:Z:497:GLU:O	2.47	0.48
24:d:299:ARG:NE	24:d:385:ASP:OD2	2.47	0.48
27:g:581:GLU:OE2	27:g:779:ASN:ND2	2.47	0.48
30:k:17:ARG:HB2	30:k:36:HIS:HB2	1.96	0.48
22:a:1248:VAL:HG11	22:a:1286:MET:HE1	1.94	0.48
27:g:155:VAL:HG11	27:g:193:LEU:HD11	1.95	0.48
27:g:353:TYR:OH	27:g:385:ASP:OD1	2.26	0.48
4:D:87:LEU:HD13	4:D:97:LEU:HG	1.96	0.47
24:d:556:LYS:HE3	24:d:557:THR:HG23	1.96	0.47
27:g:540:ASP:N	27:g:540:ASP:OD1	2.45	0.47
28:h:432:SER:OG	28:h:433:GLU:N	2.47	0.47
28:h:917:GLN:O	28:h:948:ARG:NH2	2.38	0.47
30:k:178:ASP:HA	30:k:203:GLU:CD	2.39	0.47
1:A:557:ARG:HG2	1:A:561:MET:HE3	1.95	0.47
2:B:480:SER:OG	2:B:484:ARG:NH2	2.45	0.47
18:V:293:GLY:HA3	18:V:360:PHE:H	1.79	0.47
5:E:82:VAL:HB	5:E:110:MET:HG2	1.95	0.47
27:g:699:THR:HG21	27:g:794:TYR:HB3	1.96	0.47
31:p:301:ALA:HA	31:p:304:HIS:HD1	1.80	0.47
7:G:92:VAL:HG22	7:G:97:LEU:HD13	1.97	0.47
11:K:42:LEU:HD12	11:K:45:ILE:HD11	1.96	0.47
17:U:141:CYS:HA	17:U:144:LEU:HG	1.95	0.47
23:b:691:PHE:O	23:b:695:GLN:OE1	2.31	0.47
28:h:27:PHE:HA	28:h:33:LEU:HD11	1.97	0.47
30:k:213:SER:OG	30:k:214:LYS:N	2.47	0.47
30:k:250:ILE:HD11	30:k:299:MET:HE2	1.96	0.47
1:A:129:ILE:HD11	1:A:147:LEU:HD13	1.95	0.47
22:a:2149:LEU:HD21	22:a:2183:ILE:HG21	1.97	0.47
23:b:563:SER:OG	23:b:565:SER:OG	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:h:916:LEU:HD22	28:h:941:LEU:HD21	1.95	0.47
1:A:41:ILE:HB	1:A:88:ILE:HG12	1.96	0.47
27:g:383:GLU:HG2	27:g:426:LEU:HD13	1.97	0.47
28:h:624:GLU:OE1	28:h:765:ARG:NH2	2.46	0.47
29:i:79:SER:OG	29:i:80:VAL:N	2.47	0.47
31:p:206:ILE:HA	31:p:209:PHE:HB3	1.96	0.47
31:p:362:ILE:HD12	31:p:399:GLN:HG2	1.97	0.47
31:p:444:ASN:HA	31:p:447:CYS:HB2	1.96	0.47
1:A:131:ALA:HA	1:A:134:LYS:HE2	1.96	0.47
1:A:422:ASP:OD1	1:A:422:ASP:N	2.47	0.47
1:A:1361:ASP:HB3	1:A:1364:GLU:HG2	1.97	0.47
2:B:157:ARG:NH1	2:B:180:ASP:O	2.48	0.47
2:B:255:ARG:HG2	2:B:303:PRO:HB2	1.95	0.47
2:B:513:GLU:HG3	2:B:726:SER:HB3	1.96	0.47
3:C:47:ILE:HA	3:C:165:ALA:HA	1.97	0.47
4:D:19:GLN:HB2	4:D:21:ILE:HG12	1.97	0.47
15:P:38:G:H2'	15:P:39:A:H8	1.79	0.47
21:Z:551:VAL:HG12	21:Z:635:MET:HG3	1.97	0.47
22:a:1035:ARG:HH21	22:a:1037:PRO:HG2	1.79	0.47
22:a:1046:THR:HG22	22:a:1050:LEU:HD23	1.97	0.47
22:a:1317:ASP:OD1	22:a:1317:ASP:N	2.45	0.47
23:b:29:VAL:HG21	27:g:642:LYS:HD2	1.96	0.47
23:b:1051:LEU:HD21	23:b:1099:PHE:HB2	1.95	0.47
24:d:842:VAL:HG21	29:i:43:LEU:HD23	1.96	0.47
25:e:882:LEU:HD11	25:e:943:LEU:HB3	1.97	0.47
28:h:366:LEU:HD12	28:h:384:VAL:HG11	1.97	0.47
30:k:203:GLU:HG2	30:k:414:HIS:CB	2.45	0.47
32:q:36:LYS:O	32:q:40:THR:OG1	2.25	0.47
32:q:64:ASP:HB3	32:q:263:PRO:HD2	1.97	0.47
1:A:1371:ILE:HA	1:A:1374:VAL:HG12	1.96	0.47
10:J:35:LEU:HD11	10:J:50:LEU:HD13	1.97	0.47
21:Z:451:MET:HB2	21:Z:460:MET:HE2	1.97	0.47
24:d:208:ASP:HB3	24:d:211:VAL:HG23	1.97	0.47
1:A:716:VAL:HG22	19:W:445:THR:HG21	1.97	0.47
8:H:97:TYR:CZ	8:H:115:TYR:HB3	2.50	0.47
26:f:29:LYS:HE2	26:f:80:LEU:HB2	1.96	0.47
23:b:247:THR:HA	23:b:277:LEU:HD12	1.96	0.47
23:b:300:CYS:HB3	27:g:603:SER:HA	1.97	0.47
28:h:395:GLU:OE1	28:h:397:ARG:NH2	2.37	0.47
2:B:379:ARG:O	2:B:608:ARG:NH2	2.48	0.46
22:a:1241:PRO:HA	22:a:1244:LEU:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1762:LEU:HD23	22:a:1765:LEU:HD21	1.96	0.46
25:e:370:SER:HB3	25:e:431:VAL:HG21	1.96	0.46
29:i:101:ILE:HD11	29:i:110:LEU:HD13	1.96	0.46
2:B:384:ASP:HB3	2:B:387:HIS:HB2	1.97	0.46
24:d:869:ASP:HA	27:g:877:MET:HE3	1.96	0.46
29:i:93:LEU:HD13	29:i:113:ILE:HG23	1.98	0.46
29:i:294:ASN:H	29:i:418:ASN:HA	1.80	0.46
1:A:1093:GLN:HE22	2:B:1093:CYS:HA	1.80	0.46
2:B:94:SER:HB3	2:B:123:PRO:HD2	1.96	0.46
2:B:752:TYR:HB3	3:C:63:PHE:HE1	1.80	0.46
29:i:131:GLN:HB3	29:i:339:PHE:CE1	2.50	0.46
29:i:266:LEU:HB2	29:i:475:TYR:CZ	2.50	0.46
2:B:34:PHE:HZ	2:B:528:LEU:HB3	1.80	0.46
2:B:68:GLN:HB3	2:B:83:ARG:HG3	1.97	0.46
4:D:26:PHE:HE2	7:G:78:ARG:HH12	1.62	0.46
16:T:14:DG:H2'	16:T:15:DA:C8	2.50	0.46
22:a:1051:GLN:HB3	22:a:1089:VAL:HG11	1.97	0.46
22:a:1288:HIS:HE1	23:b:68:LYS:HG2	1.80	0.46
25:e:507:SER:HB2	25:e:542:LEU:HD21	1.98	0.46
26:f:99:LEU:HD13	26:f:166:GLN:HG2	1.97	0.46
26:f:287:GLU:OE2	26:f:301:ARG:NH1	2.48	0.46
27:g:104:VAL:HG21	27:g:133:ILE:HG21	1.97	0.46
28:h:141:MET:HA	28:h:144:LEU:HG	1.97	0.46
29:i:396:GLY:HA3	29:i:405:VAL:HB	1.97	0.46
11:K:5:PRO:HG2	11:K:8:GLU:HG3	1.97	0.46
24:d:868:PRO:HB2	27:g:893:LEU:HB2	1.97	0.46
26:f:587:MET:SD	32:q:249:ASN:ND2	2.83	0.46
29:i:202:LYS:HA	29:i:212:THR:HG22	1.97	0.46
31:p:357:GLY:O	31:p:361:THR:OG1	2.28	0.46
1:A:1163:HIS:NE2	1:A:1297:THR:OG1	2.38	0.46
26:f:25:LEU:HG	26:f:29:LYS:HE3	1.96	0.46
29:i:295:VAL:HB	29:i:392:VAL:HG22	1.98	0.46
31:p:526:LEU:HD21	31:p:559:GLU:HB3	1.98	0.46
1:A:921:ARG:O	1:A:1052:ARG:NH1	2.41	0.46
2:B:474:THR:HG23	2:B:477:SER:H	1.79	0.46
19:W:305:LEU:HD12	19:W:356:TYR:HE1	1.81	0.46
21:Z:554:GLU:OE1	21:Z:557:THR:OG1	2.33	0.46
24:d:233:ILE:HD11	24:d:255:LEU:HD11	1.98	0.46
31:p:293:ASP:O	31:p:299:ARG:NH1	2.42	0.46
1:A:52:PRO:HB2	1:A:60:PRO:HD3	1.98	0.46
2:B:280:SER:OG	2:B:281:ASP:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:28:LYS:NZ	27:g:584:SER:O	2.37	0.46
27:g:634:LEU:HD23	27:g:781:ILE:HD11	1.97	0.46
27:g:725:GLU:HA	27:g:764:ARG:HH21	1.81	0.46
1:A:1141:VAL:HB	1:A:1336:LEU:HB2	1.97	0.46
26:f:63:LYS:HB3	26:f:76:GLU:HG2	1.98	0.46
28:h:516:LEU:HB2	28:h:528:ILE:HG21	1.97	0.46
31:p:100:GLU:O	31:p:105:ARG:NH1	2.49	0.46
1:A:26:LEU:HG	2:B:1168:ALA:HB2	1.98	0.46
1:A:731:ASN:HB2	1:A:735:GLN:HB2	1.98	0.46
2:B:300:MET:HE1	2:B:376:ALA:HB3	1.97	0.46
17:U:106:LEU:HD22	19:W:283:LEU:HD11	1.97	0.46
24:d:745:ASP:OD1	24:d:746:PRO:HD3	2.15	0.46
27:g:597:TYR:HE2	27:g:621:VAL:HG13	1.81	0.46
30:k:16:GLY:HA2	30:k:72:ASP:HB2	1.97	0.46
31:p:487:LEU:O	31:p:490:SER:OG	2.32	0.46
1:A:628:VAL:HA	1:A:638:GLY:HA3	1.98	0.45
1:A:992:LYS:HA	1:A:992:LYS:HD3	1.79	0.45
5:E:5:GLU:OE2	5:E:9:ARG:NH2	2.49	0.45
19:W:380:LYS:HD2	19:W:383:LEU:HD13	1.98	0.45
19:W:520:LEU:HD13	19:W:530:ILE:HG21	1.97	0.45
21:Z:438:GLY:HA3	21:Z:452:PRO:HB2	1.98	0.45
31:p:316:ASP:OD1	31:p:316:ASP:N	2.50	0.45
1:A:604:ARG:HD2	1:A:604:ARG:HA	1.83	0.45
1:A:1285:LEU:HD13	1:A:1288:ILE:HD11	1.99	0.45
2:B:16:GLU:OE2	2:B:636:LYS:NZ	2.36	0.45
2:B:849:ASP:HB3	12:L:15:MET:HE1	1.98	0.45
5:E:80:PRO:HA	5:E:107:GLN:HB2	1.97	0.45
23:b:521:PHE:HA	23:b:525:ILE:HB	1.97	0.45
24:d:440:ASN:OD1	24:d:441:ASN:N	2.49	0.45
28:h:606:LYS:NZ	28:h:652:ASP:O	2.50	0.45
28:h:872:PRO:HA	28:h:873:PRO:HD3	1.88	0.45
1:A:894:ASP:OD2	1:A:1396:ARG:NH2	2.49	0.45
2:B:486:ASN:OD1	2:B:491:ARG:NH2	2.50	0.45
24:d:118:LEU:HD11	24:d:130:LEU:HB3	1.98	0.45
1:A:1216:LEU:HB2	1:A:1255:LEU:HB3	1.97	0.45
2:B:746:THR:HG22	2:B:747:LEU:HD23	1.97	0.45
8:H:28:LEU:HD21	8:H:50:VAL:HG11	1.97	0.45
23:b:350:ILE:HD13	23:b:384:LYS:HG2	1.98	0.45
23:b:1142:ASP:OD1	23:b:1142:ASP:N	2.47	0.45
27:g:847:ILE:HG23	27:g:910:VAL:HG13	1.97	0.45
1:A:279:LYS:HE3	1:A:336:LEU:HD22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1358:THR:OG1	1:A:1359:SER:N	2.49	0.45
2:B:127:ASP:OD1	2:B:127:ASP:N	2.49	0.45
2:B:288:ILE:HG22	2:B:289:ILE:HG13	1.97	0.45
8:H:16:ASP:OD1	8:H:27:ARG:N	2.43	0.45
21:Z:440:ILE:HG23	21:Z:450:ILE:HD11	1.98	0.45
21:Z:479:LYS:NZ	21:Z:523:GLU:O	2.39	0.45
24:d:219:MET:SD	24:d:233:ILE:HD12	2.56	0.45
28:h:419:LEU:HD11	28:h:459:ILE:HA	1.98	0.45
1:A:118:LEU:HD11	1:A:188:GLN:HG3	1.98	0.45
1:A:375:ILE:HB	1:A:535:MET:HE1	1.97	0.45
22:a:997:VAL:HG23	22:a:998:LEU:HD12	1.97	0.45
22:a:1625:LEU:O	23:b:769:THR:OG1	2.31	0.45
23:b:874:MET:HG3	23:b:993:VAL:HG22	1.99	0.45
28:h:617:LEU:HD22	28:h:659:ILE:HG12	1.99	0.45
28:h:624:GLU:OE2	28:h:670:TRP:NE1	2.45	0.45
29:i:499:TYR:HB3	29:i:505:LEU:HD11	1.99	0.45
32:q:54:VAL:HG12	32:q:83:MET:HE2	1.99	0.45
2:B:635:LEU:HD21	2:B:640:ILE:HD11	1.98	0.45
15:P:39:A:H2'	15:P:40:A:H8	1.81	0.45
23:b:258:PRO:HA	23:b:261:ALA:HB2	1.99	0.45
27:g:493:LEU:O	27:g:497:ILE:HG12	2.15	0.45
18:V:41:LEU:O	18:V:43:SER:N	2.45	0.45
18:V:47:ALA:HB2	19:W:155:TRP:HH2	1.82	0.45
23:b:259:SER:HB2	27:g:591:ALA:HB1	1.99	0.45
23:b:340:ARG:HD3	23:b:401:LEU:HD11	1.99	0.45
28:h:925:MET:SD	28:h:925:MET:N	2.90	0.45
31:p:176:ASP:O	31:p:182:ARG:NH1	2.39	0.45
31:p:498:ARG:HE	31:p:536:VAL:HG21	1.81	0.45
1:A:104:MET:HE2	1:A:108:ARG:HH12	1.82	0.45
1:A:1474:LEU:HB2	6:F:105:ILE:HB	1.99	0.45
19:W:228:ALA:HA	19:W:231:VAL:HG22	1.98	0.45
19:W:361:ALA:O	19:W:365:SER:HB2	2.17	0.45
28:h:899:ILE:HD11	28:h:928:TYR:HB3	1.99	0.45
29:i:242:LEU:HD23	29:i:242:LEU:HA	1.86	0.45
30:k:456:ILE:HD13	30:k:492:LEU:HB3	1.98	0.45
31:p:414:ASP:O	31:p:420:ARG:NH1	2.48	0.45
32:q:264:ASN:HB2	32:q:291:PRO:HG3	1.99	0.45
1:A:360:ASP:HB3	2:B:1063:ALA:O	2.17	0.45
2:B:470:LEU:HA	2:B:481:HIS:HD1	1.82	0.45
19:W:264:GLU:HA	19:W:267:ARG:HG2	1.97	0.45
29:i:287:LEU:O	29:i:291:ASN:ND2	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:p:535:ASN:HA	31:p:538:PHE:CE2	2.52	0.45
32:q:6:PHE:N	32:q:9:GLU:OE1	2.50	0.45
1:A:376:ASP:HB3	1:A:522:PRO:HD3	1.99	0.44
1:A:554:PHE:HB3	1:A:585:LEU:HG	1.98	0.44
1:A:1247:PHE:HB3	1:A:1257:LEU:HG	1.98	0.44
1:A:1258:ARG:HH21	1:A:1260:ARG:HH21	1.64	0.44
8:H:96:VAL:HA	8:H:116:VAL:HA	1.99	0.44
13:M:1620:PRO:HB3	23:b:1037:ILE:HD13	1.99	0.44
24:d:65:GLU:O	24:d:69:VAL:N	2.46	0.44
24:d:388:TYR:HA	24:d:391:ARG:HE	1.82	0.44
27:g:261:LYS:HE2	27:g:261:LYS:HB2	1.79	0.44
28:h:105:VAL:HB	28:h:184:THR:HG22	1.97	0.44
28:h:515:GLN:OE1	28:h:524:ARG:NH2	2.49	0.44
29:i:281:PHE:HD1	29:i:421:ILE:HG21	1.81	0.44
31:p:120:SER:O	31:p:124:LEU:N	2.43	0.44
1:A:695:ASP:N	1:A:695:ASP:OD1	2.48	0.44
2:B:337:LYS:HD3	2:B:337:LYS:HA	1.81	0.44
2:B:1112:ASP:OD1	2:B:1112:ASP:N	2.49	0.44
3:C:54:ALA:HB3	3:C:160:ARG:HG3	1.99	0.44
21:Z:542:LEU:HD22	21:Z:570:VAL:HG11	2.00	0.44
22:a:954:LEU:O	22:a:958:LEU:HB2	2.17	0.44
22:a:992:LYS:O	22:a:995:SER:OG	2.33	0.44
24:d:913:LEU:HB2	24:d:949:SER:HB3	1.99	0.44
25:e:496:PHE:O	25:e:500:HIS:HB2	2.17	0.44
31:p:92:PRO:O	31:p:96:LEU:HD12	2.17	0.44
31:p:350:MET:HE2	31:p:388:LEU:HA	2.00	0.44
9:I:17:CYS:SG	9:I:18:GLN:N	2.91	0.44
22:a:1670:TRP:NE1	23:b:992:GLU:OE2	2.43	0.44
25:e:801:ALA:HB2	28:h:406:LEU:HD23	1.99	0.44
28:h:138:THR:HA	28:h:141:MET:HE2	1.99	0.44
29:i:330:SER:HB3	29:i:333:ALA:HB2	2.00	0.44
1:A:19:LYS:HE2	1:A:19:LYS:HB3	1.88	0.44
8:H:90:TYR:HB3	8:H:145:MET:HB2	1.99	0.44
19:W:353:LYS:O	19:W:357:ILE:HG12	2.18	0.44
24:d:917:TYR:HE2	24:d:946:ILE:HG23	1.81	0.44
26:f:100:ASN:OD1	26:f:166:GLN:NE2	2.45	0.44
31:p:42:LEU:HB3	31:p:46:ARG:HB2	1.99	0.44
31:p:256:SER:HB3	31:p:259:VAL:HG12	1.99	0.44
1:A:1312:PRO:HG2	1:A:1318:LYS:HG2	1.99	0.44
2:B:411:LEU:HA	2:B:439:ILE:HD11	1.99	0.44
3:C:193:ARG:HA	3:C:193:ARG:HD3	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:133:ASP:O	4:D:136:THR:OG1	2.30	0.44
25:e:1007:GLN:HB3	25:e:1009:PRO:HD2	2.00	0.44
32:q:117:ASN:HB2	32:q:200:TRP:CE2	2.52	0.44
1:A:79:THR:O	2:B:1072:ARG:NH1	2.48	0.44
1:A:1128:ILE:HG22	1:A:1414:ILE:HB	2.00	0.44
7:G:79:PRO:HG2	7:G:157:ILE:HG21	2.00	0.44
22:a:1464:LEU:O	22:a:1468:ASP:N	2.50	0.44
24:d:950:LYS:HD2	24:d:951:PRO:HD2	1.99	0.44
25:e:963:GLN:HE22	25:e:966:ARG:HH12	1.66	0.44
27:g:30:ASP:CG	27:g:34:ARG:HH12	2.26	0.44
29:i:382:ASP:N	29:i:382:ASP:OD1	2.51	0.44
1:A:70:ARG:HA	1:A:70:ARG:HD3	1.84	0.44
17:U:143:TYR:HD2	19:W:422:VAL:HG23	1.83	0.44
22:a:1315:ARG:HH21	22:a:1318:SER:HA	1.82	0.44
23:b:28:LYS:HZ3	27:g:588:SER:HB2	1.82	0.44
26:f:115:ARG:NH1	26:f:302:THR:O	2.50	0.44
27:g:246:LEU:HD12	27:g:247:VAL:HG13	1.99	0.44
28:h:600:VAL:HG21	28:h:611:MET:HE2	2.00	0.44
30:k:101:PRO:HG3	30:k:130:MET:HG3	2.00	0.44
31:p:359:ASP:OD1	31:p:359:ASP:N	2.50	0.44
32:q:73:GLY:O	32:q:80:TYR:OH	2.33	0.44
2:B:117:ASN:HA	2:B:189:GLY:HA3	2.00	0.44
8:H:96:VAL:HB	8:H:116:VAL:HG22	1.99	0.44
8:H:103:GLU:HB3	8:H:109:ALA:HB2	2.00	0.44
12:L:17:TYR:HB3	12:L:44:MET:HB3	2.00	0.44
19:W:322:PRO:O	19:W:375:ARG:NH2	2.40	0.44
23:b:1140:THR:HG23	25:e:698:HIS:HD2	1.83	0.44
24:d:621:VAL:HA	24:d:635:LEU:HD21	1.99	0.44
26:f:601:LEU:HB3	31:p:297:GLU:HG3	1.99	0.44
27:g:671:MET:HG3	27:g:721:ILE:HG21	2.00	0.44
28:h:151:ILE:HA	28:h:154:ILE:HG22	2.00	0.44
29:i:433:LEU:HD12	29:i:439:LEU:HD21	1.99	0.44
30:k:153:TYR:N	30:k:163:MET:O	2.48	0.44
1:A:865:ILE:HG12	2:B:1092:ASP:HB3	2.00	0.44
2:B:470:LEU:HD11	2:B:478:THR:HG23	2.00	0.44
17:U:29:ILE:HG12	17:U:59:GLY:HA3	1.99	0.44
22:a:1036:LEU:HD23	22:a:1037:PRO:HD3	1.99	0.44
22:a:1244:LEU:HD22	22:a:1265:LEU:HB3	1.98	0.44
22:a:1360:ASP:OD1	22:a:1360:ASP:N	2.51	0.44
23:b:564:ARG:HE	23:b:605:THR:HG21	1.83	0.44
24:d:608:ASP:OD1	24:d:608:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:f:56:GLU:OE1	26:f:63:LYS:NZ	2.39	0.44
1:A:480:SER:HB3	11:K:2:ASN:HD22	1.82	0.43
1:A:1228:MET:SD	1:A:1247:PHE:HB2	2.58	0.43
2:B:550:MET:HG3	2:B:567:ILE:HD12	2.00	0.43
2:B:589:LYS:HB2	2:B:589:LYS:HE3	1.79	0.43
21:Z:580:ASP:OD1	21:Z:580:ASP:N	2.50	0.43
23:b:347:LEU:HD22	23:b:414:LEU:HD22	2.01	0.43
23:b:545:SER:HB2	23:b:587:PRO:HB2	1.99	0.43
27:g:33:LEU:HD12	27:g:34:ARG:HD3	2.00	0.43
27:g:189:THR:HG23	27:g:193:LEU:HD22	2.00	0.43
29:i:33:THR:HA	29:i:36:LEU:HD23	2.00	0.43
31:p:26:GLN:O	31:p:30:ASN:ND2	2.47	0.43
2:B:844:ILE:HD13	21:Z:707:GLY:HA2	1.99	0.43
19:W:190:SER:HA	19:W:194:ALA:HB3	2.00	0.43
19:W:460:THR:HA	19:W:506:ARG:HD3	2.00	0.43
22:a:1020:THR:O	22:a:1024:GLN:N	2.47	0.43
24:d:685:LEU:HB3	27:g:708:GLN:HG2	1.99	0.43
27:g:413:LEU:HA	27:g:416:MET:HG2	2.00	0.43
32:q:39:LEU:HD22	32:q:154:PRO:HD3	1.99	0.43
1:A:514:GLU:HA	6:F:63:ALA:HB1	2.00	0.43
14:N:10:DT:O2	14:N:11:DA:N6	2.50	0.43
19:W:310:ILE:HD13	19:W:356:TYR:CZ	2.54	0.43
23:b:926:LEU:HD22	26:f:563:LEU:HD13	2.01	0.43
23:b:1091:LEU:HD22	23:b:1095:LYS:HB3	2.00	0.43
24:d:681:VAL:O	24:d:739:ARG:NH2	2.42	0.43
27:g:119:ARG:NH1	27:g:154:GLU:OE1	2.52	0.43
27:g:667:ILE:O	27:g:671:MET:HG2	2.19	0.43
29:i:34:SER:OG	29:i:82:GLU:O	2.35	0.43
29:i:305:ILE:HA	29:i:308:LEU:HG	2.01	0.43
31:p:45:GLU:HG3	31:p:48:ARG:HH21	1.82	0.43
6:F:108:ARG:HD2	6:F:118:TRP:CD1	2.53	0.43
7:G:23:LEU:O	7:G:27:LYS:HG3	2.19	0.43
7:G:97:LEU:HD23	7:G:108:ILE:HD13	1.99	0.43
19:W:361:ALA:O	19:W:365:SER:OG	2.32	0.43
28:h:590:LYS:NZ	28:h:619:ASP:OD1	2.49	0.43
1:A:136:GLN:HA	1:A:137:PRO:HD3	1.79	0.43
1:A:1184:THR:HG23	1:A:1187:ALA:H	1.82	0.43
2:B:407:MET:HE1	2:B:444:LEU:HD13	1.99	0.43
22:a:1386:GLU:OE2	22:a:1389:ARG:NH1	2.52	0.43
26:f:15:ASN:ND2	26:f:82:ALA:O	2.47	0.43
27:g:173:ALA:HA	27:g:176:ILE:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:g:598:HIS:HA	27:g:601:ILE:HG22	2.00	0.43
30:k:77:LEU:HD21	30:k:90:ILE:HG21	1.99	0.43
1:A:457:ILE:HD11	1:A:515:ILE:HD12	2.01	0.43
1:A:1311:LEU:HD22	1:A:1332:GLN:HG2	1.98	0.43
2:B:933:ASP:OD2	2:B:1050:ARG:NH2	2.45	0.43
3:C:27:ASP:OD1	3:C:28:LEU:N	2.49	0.43
31:p:504:CYS:O	31:p:508:LEU:HB2	2.17	0.43
1:A:1323:THR:OG1	1:A:1325:ASP:OD1	2.31	0.43
7:G:90:THR:HA	7:G:139:GLN:HG3	2.00	0.43
17:U:138:PRO:HD3	19:W:256:SER:HB2	2.01	0.43
22:a:1659:TYR:CZ	27:g:227:SER:HB2	2.54	0.43
26:f:604:LEU:HD21	31:p:262:MET:HE1	2.00	0.43
27:g:745:GLU:O	27:g:749:MET:HG2	2.19	0.43
1:A:35:SER:O	2:B:1138:ARG:NH2	2.52	0.43
1:A:539:GLN:HB3	2:B:970:HIS:CG	2.54	0.43
1:A:1372:GLU:HG3	5:E:193:ILE:HG21	2.01	0.43
2:B:380:ARG:HD3	2:B:609:GLU:HG2	2.01	0.43
5:E:81:LYS:HE2	5:E:81:LYS:HB2	1.80	0.43
7:G:79:PRO:HB3	7:G:147:ILE:HD12	2.01	0.43
9:I:78:LEU:O	9:I:80:ARG:NH1	2.45	0.43
22:a:1256:SER:O	22:a:1259:SER:OG	2.24	0.43
23:b:302:VAL:HG23	23:b:391:LEU:HD11	2.00	0.43
24:d:707:MET:HE3	24:d:707:MET:HB2	1.90	0.43
28:h:702:LYS:HE3	28:h:702:LYS:HB2	1.85	0.43
1:A:1124:LEU:O	1:A:1128:ILE:HG12	2.18	0.43
2:B:909:VAL:HG12	12:L:34:ILE:HG13	2.01	0.43
3:C:59:LEU:HD13	3:C:63:PHE:CE2	2.53	0.43
3:C:105:VAL:HG11	3:C:115:VAL:HG22	2.01	0.43
7:G:55:GLY:HA3	7:G:69:PRO:HG2	2.01	0.43
8:H:112:LEU:HD23	8:H:112:LEU:HA	1.90	0.43
17:U:74:ALA:O	17:U:78:ILE:HG12	2.19	0.43
24:d:720:VAL:HG13	24:d:721:ILE:HD12	2.01	0.43
23:b:456:LEU:HD13	23:b:521:PHE:HE1	1.84	0.43
24:d:474:THR:O	24:d:513:ARG:NH2	2.47	0.43
24:d:838:THR:HG21	29:i:387:PHE:HD2	1.84	0.43
30:k:7:THR:HG21	30:k:50:TYR:CZ	2.54	0.43
31:p:572:ASP:OD1	31:p:573:VAL:N	2.51	0.43
1:A:1212:LEU:HB2	1:A:1285:LEU:HD12	2.00	0.42
2:B:320:PHE:O	2:B:324:ARG:NH1	2.49	0.42
23:b:462:GLU:OE1	23:b:465:TYR:N	2.52	0.42
24:d:877:PRO:HB3	24:d:894:THR:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:p:288:GLN:HG3	31:p:325:GLN:HB3	2.00	0.42
1:A:1134:PRO:HG2	1:A:1137:PRO:HB3	2.00	0.42
1:A:1439:LEU:HD13	2:B:1162:LEU:HD21	2.01	0.42
1:A:1458:ILE:HD13	2:B:1091:ARG:HD2	2.00	0.42
19:W:566:ILE:HG23	19:W:575:VAL:HG21	2.01	0.42
24:d:851:LEU:HB2	24:d:890:HIS:HB2	2.01	0.42
26:f:57:GLU:O	26:f:61:ALA:N	2.52	0.42
26:f:235:PHE:HB3	26:f:309:PHE:HE2	1.85	0.42
1:A:232:GLU:HA	1:A:235:VAL:HG22	2.01	0.42
1:A:544:ALA:O	1:A:548:PHE:N	2.52	0.42
24:d:505:LYS:HE3	24:d:505:LYS:HB3	1.73	0.42
26:f:458:LYS:O	26:f:462:GLN:HG3	2.19	0.42
29:i:512:ARG:HA	30:k:458:LEU:HB2	2.02	0.42
1:A:417:LYS:HE2	1:A:430:ARG:HH11	1.82	0.42
1:A:1311:LEU:H	19:W:486:VAL:HG11	1.84	0.42
1:A:1370:GLY:HA2	5:E:178:PRO:HD2	2.01	0.42
3:C:26:THR:OG1	11:K:97:GLU:OE2	2.36	0.42
4:D:134:ILE:O	4:D:138:ARG:HG3	2.20	0.42
22:a:1219:LEU:O	22:a:1223:MET:HG3	2.19	0.42
23:b:43:ARG:HH12	23:b:180:VAL:HG21	1.84	0.42
23:b:389:LEU:HB3	23:b:435:MET:HE1	2.00	0.42
23:b:1191:ARG:O	23:b:1195:GLU:HG3	2.19	0.42
29:i:17:LEU:HG	29:i:19:PHE:HB2	2.01	0.42
29:i:58:LYS:HE2	29:i:58:LYS:HB2	1.91	0.42
29:i:214:LEU:O	29:i:224:ASN:N	2.50	0.42
31:p:467:LYS:HG3	31:p:511:VAL:HG11	2.02	0.42
1:A:130:LEU:HD21	1:A:235:VAL:HG12	2.01	0.42
17:U:122:GLY:HA2	17:U:125:ARG:HG2	2.01	0.42
18:V:73:LEU:HD22	19:W:101:LEU:HD21	2.00	0.42
23:b:827:ARG:O	23:b:831:MET:HG3	2.19	0.42
24:d:107:PRO:HG3	24:d:140:LYS:HD3	2.01	0.42
25:e:685:LEU:HD21	25:e:808:ALA:HB2	2.02	0.42
27:g:393:LEU:HD23	27:g:412:ALA:HB2	2.00	0.42
28:h:362:VAL:HA	28:h:365:GLU:HG2	2.00	0.42
28:h:863:CYS:SG	28:h:875:VAL:HG21	2.60	0.42
29:i:388:ARG:HA	29:i:388:ARG:HD3	1.81	0.42
32:q:223:ASP:OD1	32:q:223:ASP:N	2.53	0.42
2:B:731:GLN:NE2	15:P:44:A:O3'	2.51	0.42
6:F:54:THR:O	6:F:108:ARG:NH1	2.42	0.42
22:a:1035:ARG:NE	22:a:1037:PRO:O	2.49	0.42
22:a:1313:PRO:HA	22:a:1314:PRO:HD3	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1508:LEU:HD21	22:a:1548:LEU:HD23	2.01	0.42
22:a:1583:VAL:HG21	22:a:1625:LEU:HD21	2.01	0.42
23:b:386:SER:OG	27:g:556:GLU:OE1	2.37	0.42
28:h:558:ILE:HD11	28:h:570:VAL:HG12	2.01	0.42
28:h:597:LEU:O	28:h:601:THR:HG23	2.19	0.42
29:i:4:TYR:HB2	29:i:16:VAL:HB	2.01	0.42
1:A:187:TYR:HE2	1:A:202:TRP:HB3	1.84	0.42
1:A:1130:ILE:HG13	1:A:1411:LEU:HB3	2.01	0.42
11:K:51:LEU:HD23	11:K:51:LEU:HA	1.84	0.42
21:Z:613:GLU:H	21:Z:625:HIS:H	1.67	0.42
23:b:554:ILE:HG13	23:b:595:LEU:HD22	2.01	0.42
27:g:623:LEU:HD23	27:g:623:LEU:HA	1.92	0.42
28:h:917:GLN:HA	28:h:944:LEU:HD21	2.02	0.42
31:p:386:SER:O	31:p:426:TYR:OH	2.26	0.42
1:A:96:HIS:HB3	1:A:99:PHE:HB2	2.02	0.42
1:A:330:GLN:HG3	1:A:336:LEU:HD11	2.01	0.42
1:A:908:THR:HG1	1:A:1047:SER:HG	1.67	0.42
8:H:128:ASP:N	8:H:128:ASP:OD1	2.53	0.42
21:Z:542:LEU:HA	21:Z:575:VAL:HG12	2.01	0.42
22:a:2100:ARG:HE	22:a:2139:THR:HG21	1.84	0.42
23:b:1145:PRO:HG3	23:b:1183:VAL:HG13	2.02	0.42
25:e:550:LEU:HD12	25:e:554:PHE:CZ	2.55	0.42
26:f:319:ILE:HG21	26:f:394:ASP:HB2	2.02	0.42
27:g:194:LYS:O	27:g:198:ILE:HG12	2.19	0.42
31:p:381:ARG:HA	31:p:384:ILE:HG22	2.01	0.42
32:q:237:VAL:HB	32:q:256:VAL:HG22	2.02	0.42
1:A:381:PRO:HB3	1:A:480:SER:HA	2.02	0.42
1:A:1148:ALA:HB1	1:A:1333:GLU:HB2	2.02	0.42
2:B:299:GLU:HA	2:B:302:LYS:HG2	2.02	0.42
2:B:603:MET:HE3	2:B:603:MET:HB2	1.92	0.42
23:b:275:PRO:HG2	23:b:320:PHE:HB2	2.01	0.42
29:i:30:LEU:HD13	29:i:109:ALA:HB2	2.01	0.42
32:q:100:LEU:HD23	32:q:100:LEU:HA	1.83	0.42
1:A:481:THR:HG22	2:B:1055:VAL:HG21	2.02	0.42
1:A:681:LEU:HD22	2:B:1030:ASN:HD21	1.85	0.42
3:C:130:VAL:HG11	3:C:237:GLY:HA3	2.02	0.42
4:D:41:LEU:HD22	4:D:61:PHE:CE1	2.55	0.42
17:U:115:PRO:HA	17:U:118:GLN:HG3	2.01	0.42
21:Z:420:PHE:HB3	21:Z:440:ILE:HD13	2.01	0.42
23:b:412:LEU:HD11	23:b:443:VAL:HG12	2.01	0.42
23:b:487:PHE:O	23:b:518:LYS:NZ	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:e:389:ASN:O	25:e:393:HIS:ND1	2.53	0.42
25:e:816:LEU:HD11	25:e:860:LEU:HB3	2.01	0.42
31:p:330:ILE:HD13	31:p:333:LEU:HD12	2.02	0.42
2:B:897:ARG:HB2	2:B:900:GLU:HG3	2.02	0.41
3:C:120:LEU:HD23	3:C:120:LEU:HA	1.87	0.41
22:a:949:GLN:HB3	22:a:950:LEU:H	1.64	0.41
22:a:1373:ARG:HH12	22:a:1377:LEU:HD11	1.83	0.41
22:a:1437:ARG:HH11	27:g:353:TYR:HA	1.85	0.41
23:b:298:LEU:O	23:b:302:VAL:HG22	2.19	0.41
24:d:882:PHE:CE1	24:d:892:LEU:HD13	2.55	0.41
26:f:404:PRO:HG2	26:f:409:ARG:HH21	1.85	0.41
31:p:375:ASP:O	31:p:381:ARG:NH1	2.45	0.41
32:q:121:ARG:N	32:q:188:GLU:OE2	2.41	0.41
32:q:203:PRO:HD3	32:q:239:ARG:NE	2.35	0.41
1:A:33:ARG:HG3	2:B:1139:GLY:HA2	2.01	0.41
1:A:275:ASP:HB2	1:A:336:LEU:HG	2.02	0.41
1:A:878:THR:HG21	1:A:880:ARG:HE	1.84	0.41
1:A:1139:LEU:HD11	1:A:1342:SER:H	1.85	0.41
19:W:212:ILE:HD11	19:W:220:LEU:HA	2.01	0.41
19:W:307:PRO:HA	19:W:310:ILE:HG12	2.02	0.41
28:h:854:HIS:CD2	28:h:995:PHE:HB3	2.54	0.41
29:i:310:GLU:HG3	29:i:363:PRO:HG3	2.02	0.41
29:i:520:PRO:HG2	30:k:449:SER:HB2	2.03	0.41
30:k:68:HIS:HB3	30:k:161:ALA:HA	2.02	0.41
30:k:252:LEU:HD23	30:k:252:LEU:HA	1.86	0.41
31:p:264:ALA:HB2	31:p:290:LEU:HD13	2.01	0.41
32:q:28:VAL:HG11	32:q:142:VAL:HG23	2.02	0.41
2:B:448:LEU:HD23	2:B:448:LEU:HA	1.93	0.41
19:W:388:LYS:HB3	19:W:388:LYS:HE2	1.88	0.41
22:a:1029:LEU:HD21	22:a:1065:ALA:HB1	2.01	0.41
24:d:799:LEU:HA	24:d:802:MET:HG2	2.02	0.41
27:g:180:ILE:HG23	27:g:197:LEU:HG	2.02	0.41
32:q:186:LEU:HD12	32:q:186:LEU:HA	1.84	0.41
1:A:432:HIS:HA	1:A:433:PRO:HD3	1.93	0.41
2:B:553:LEU:HD23	2:B:553:LEU:HA	1.91	0.41
21:Z:444:ASP:HB3	21:Z:448:ILE:HA	2.02	0.41
22:a:2081:LEU:HD21	22:a:2106:LEU:HD12	2.02	0.41
23:b:944:GLU:OE1	25:e:729:LEU:N	2.45	0.41
26:f:35:PHE:HB2	26:f:220:LEU:HD22	2.00	0.41
27:g:176:ILE:O	27:g:180:ILE:HG12	2.20	0.41
27:g:725:GLU:HA	27:g:764:ARG:HE	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:GLU:OE2	2:B:1102:PHE:N	2.45	0.41
1:A:1170:THR:HA	1:A:1216:LEU:HA	2.03	0.41
9:I:109:ARG:HD3	9:I:124:THR:HG21	2.01	0.41
19:W:449:PRO:HD2	19:W:452:LEU:HD12	2.01	0.41
23:b:1078:ARG:HG2	23:b:1117:LEU:HD21	2.03	0.41
23:b:1135:ASP:O	23:b:1141:ARG:NH2	2.50	0.41
23:b:1140:THR:HG23	25:e:698:HIS:CD2	2.55	0.41
26:f:223:LEU:HD23	26:f:223:LEU:HA	1.92	0.41
27:g:110:VAL:HG13	27:g:122:THR:HG21	2.02	0.41
27:g:435:LEU:HD11	27:g:471:LEU:HG	2.02	0.41
27:g:512:VAL:O	27:g:516:GLN:HG3	2.21	0.41
28:h:359:ARG:HA	28:h:362:VAL:HG12	2.03	0.41
31:p:303:SER:HA	31:p:306:VAL:HG23	2.02	0.41
1:A:613:GLU:OE2	1:A:622:SER:OG	2.29	0.41
2:B:282:ARG:O	2:B:286:GLU:HB2	2.21	0.41
8:H:91:VAL:HG22	8:H:144:LEU:HD13	2.02	0.41
8:H:98:ARG:HB3	8:H:115:TYR:HB2	2.02	0.41
17:U:151:THR:HG21	19:W:367:VAL:HG13	2.03	0.41
21:Z:450:ILE:HG23	21:Z:452:PRO:HD3	2.02	0.41
22:a:1025:GLY:O	22:a:1029:LEU:HB2	2.21	0.41
24:d:121:GLU:OE2	24:d:123:SER:N	2.46	0.41
24:d:270:ILE:HG22	24:d:272:SER:H	1.84	0.41
26:f:101:LEU:HD12	26:f:467:SER:HA	2.02	0.41
26:f:131:GLY:HA3	26:f:174:ARG:HE	1.86	0.41
28:h:633:ARG:HE	28:h:633:ARG:HB3	1.65	0.41
1:A:894:ASP:HB3	5:E:200:ALA:HB2	2.01	0.41
2:B:795:ILE:HG12	2:B:947:ILE:HG22	2.03	0.41
7:G:99:THR:OG1	7:G:106:CYS:O	2.37	0.41
22:a:972:LEU:HD23	22:a:972:LEU:HA	1.89	0.41
22:a:2071:ASP:HA	22:a:2106:LEU:HD11	2.03	0.41
23:b:275:PRO:HG3	23:b:316:TRP:CE2	2.56	0.41
23:b:415:MET:HE1	23:b:435:MET:SD	2.61	0.41
23:b:943:LEU:HD23	23:b:943:LEU:HA	1.93	0.41
23:b:1129:GLY:HA2	23:b:1189:ILE:HD13	2.02	0.41
24:d:580:LEU:HD12	24:d:583:LEU:HD12	2.02	0.41
24:d:628:ASP:OD1	24:d:628:ASP:N	2.51	0.41
27:g:770:SER:HB3	27:g:773:HIS:CG	2.56	0.41
27:g:829:LEU:HD11	27:g:926:ILE:HD11	2.02	0.41
28:h:475:LYS:HA	28:h:478:VAL:HG22	2.01	0.41
28:h:648:MET:HE2	28:h:650:LEU:HB2	2.02	0.41
29:i:553:LEU:HD23	29:i:553:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:q:94:VAL:O	32:q:98:THR:OG1	2.33	0.41
22:a:1387:LEU:HD21	22:a:1442:TYR:HB2	2.02	0.41
22:a:2174:SER:HB3	23:b:1126:ILE:HG13	2.01	0.41
23:b:786:LEU:HD23	23:b:820:LEU:HG	2.02	0.41
25:e:760:PRO:HA	25:e:761:PRO:HD3	1.90	0.41
30:k:27:LYS:HD2	30:k:148:LEU:HB2	2.03	0.41
31:p:397:ILE:HD12	31:p:397:ILE:HA	1.94	0.41
1:A:121:SER:HA	1:A:126:ILE:HG13	2.02	0.41
1:A:465:HIS:CD2	1:A:467:MET:HB2	2.55	0.41
1:A:538:VAL:HG12	1:A:539:GLN:HG3	2.02	0.41
1:A:1475:LEU:HD21	7:G:22:LEU:HD11	2.03	0.41
2:B:86:LEU:HD21	2:B:130:LYS:HD3	2.01	0.41
15:P:41:C:H2'	15:P:42:C:C6	2.56	0.41
22:a:975:PHE:HE2	22:a:994:LEU:HB2	1.86	0.41
22:a:1245:LEU:HD13	22:a:1280:ILE:HG23	2.03	0.41
22:a:1255:VAL:HA	22:a:1258:MET:HG2	2.03	0.41
22:a:1578:LYS:HE3	22:a:1581:VAL:HG21	2.02	0.41
22:a:2164:LEU:HD11	23:b:1190:GLU:HG2	2.03	0.41
24:d:838:THR:OG1	29:i:384:SER:O	2.24	0.41
25:e:471:VAL:HG12	25:e:474:LEU:H	1.86	0.41
27:g:426:LEU:HD23	27:g:426:LEU:H	1.84	0.41
27:g:493:LEU:HA	27:g:496:VAL:HG12	2.03	0.41
30:k:146:ASP:OD1	30:k:146:ASP:N	2.50	0.41
31:p:275:GLY:O	31:p:279:THR:HG23	2.21	0.41
31:p:467:LYS:HE2	31:p:467:LYS:HB3	1.89	0.41
1:A:290:LEU:HD22	1:A:306:ASP:HB3	2.03	0.41
2:B:220:GLU:OE2	2:B:222:ARG:NH1	2.54	0.41
23:b:351:LEU:HD11	23:b:413:GLN:HB3	2.02	0.41
23:b:771:VAL:O	23:b:775:ILE:HG12	2.21	0.41
25:e:648:VAL:HG12	25:e:691:LEU:HD12	2.02	0.41
25:e:927:MET:SD	25:e:942:LEU:HB3	2.61	0.41
28:h:970:ASN:HB2	28:h:975:LEU:HG	2.03	0.41
29:i:107:MET:HE2	29:i:133:GLY:HA3	2.03	0.41
1:A:539:GLN:HB3	2:B:970:HIS:CD2	2.56	0.40
1:A:1007:ILE:HD12	1:A:1007:ILE:HA	1.93	0.40
5:E:194:ILE:HG12	5:E:204:ILE:HG12	2.03	0.40
10:J:43:TYR:HA	10:J:46:ARG:HB2	2.03	0.40
19:W:415:TYR:HD1	19:W:418:ILE:HD12	1.85	0.40
22:a:1044:SER:HB2	22:a:1048:LEU:HD23	2.03	0.40
24:d:321:LEU:HD23	24:d:321:LEU:HA	1.92	0.40
24:d:809:LEU:HD23	24:d:809:LEU:HA	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:f:111:TYR:OH	26:f:158:THR:OG1	2.28	0.40
28:h:616:LEU:HD13	28:h:641:ARG:HB3	2.03	0.40
32:q:239:ARG:NH2	32:q:241:HIS:HB3	2.35	0.40
2:B:715:ASP:OD1	2:B:715:ASP:N	2.53	0.40
2:B:737:ILE:HD12	2:B:737:ILE:HA	1.94	0.40
5:E:88:LYS:HD2	5:E:88:LYS:HA	1.73	0.40
10:J:40:LEU:HD22	10:J:45:CYS:HB3	2.03	0.40
15:P:37:G:H2'	15:P:38:G:C8	2.56	0.40
16:T:37:DG:H2''	16:T:38:DT:C6	2.56	0.40
17:U:166:LYS:HB3	19:W:542:ALA:HB2	2.03	0.40
22:a:1020:THR:HB	22:a:1023:LEU:HB3	2.03	0.40
23:b:862:ARG:HG2	25:e:733:ARG:HA	2.03	0.40
25:e:488:THR:HG22	25:e:534:LEU:HD13	2.03	0.40
27:g:68:LEU:HD23	27:g:68:LEU:HA	1.93	0.40
27:g:367:LEU:HD23	27:g:367:LEU:HA	1.97	0.40
28:h:828:ILE:HD13	28:h:828:ILE:HA	1.93	0.40
30:k:204:SER:O	30:k:415:GLY:HA3	2.21	0.40
31:p:67:LEU:HD21	31:p:103:VAL:HG13	2.02	0.40
1:A:103:THR:HG23	1:A:225:PHE:HE2	1.86	0.40
1:A:544:ALA:HB2	1:A:680:LEU:HD22	2.03	0.40
1:A:811:ILE:HD12	9:I:79:PRO:HB3	2.03	0.40
1:A:937:ASP:OD1	1:A:938:LEU:N	2.55	0.40
1:A:1443:ALA:HB2	2:B:1167:ILE:HG23	2.04	0.40
2:B:325:GLY:HA3	2:B:338:TYR:HE2	1.85	0.40
2:B:1159:PHE:O	2:B:1163:MET:HG3	2.21	0.40
3:C:37:VAL:HG13	3:C:41:GLU:HB2	2.02	0.40
3:C:266:GLU:HG2	11:K:21:ILE:HG12	2.02	0.40
4:D:45:LYS:HE3	4:D:61:PHE:CE2	2.56	0.40
7:G:90:THR:OG1	7:G:98:PHE:O	2.38	0.40
21:Z:543:ASP:OD1	21:Z:543:ASP:N	2.53	0.40
22:a:1707:ILE:HG23	23:b:991:ARG:HG2	2.03	0.40
25:e:392:VAL:HG11	25:e:441:LEU:HB3	2.03	0.40
7:G:89:VAL:HG13	7:G:97:LEU:HD11	2.03	0.40
23:b:616:ASN:HB2	23:b:617:GLN:H	1.70	0.40
23:b:807:ARG:NH2	23:b:992:GLU:OE1	2.53	0.40
25:e:384:LEU:HD23	25:e:384:LEU:HA	1.95	0.40
25:e:467:PRO:HA	25:e:468:PRO:HD3	1.99	0.40
26:f:86:THR:OG1	28:h:939:GLU:OE2	2.40	0.40
27:g:392:SER:HA	27:g:395:VAL:HG22	2.02	0.40
32:q:88:ASN:ND2	32:q:123:ILE:HG22	2.35	0.40
1:A:78:MET:O	2:B:1072:ARG:NH2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ASN:HB3	1:A:125:LYS:HG2	2.04	0.40
1:A:833:PRO:HB2	2:B:506:TRP:HH2	1.86	0.40
7:G:29:LYS:O	7:G:33:GLU:HG2	2.21	0.40
19:W:163:ALA:HA	19:W:172:LEU:HD13	2.03	0.40
22:a:979:LEU:HA	22:a:987:ARG:HG2	2.03	0.40
23:b:411:LEU:HG	23:b:415:MET:HE2	2.02	0.40
23:b:947:LEU:HA	23:b:948:PRO:HD3	1.97	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	1378/1970 (70%)	1351 (98%)	27 (2%)	0	100	100
2	B	1096/1174 (93%)	1066 (97%)	30 (3%)	0	100	100
3	C	257/275 (94%)	252 (98%)	5 (2%)	0	100	100
4	D	124/142 (87%)	119 (96%)	5 (4%)	0	100	100
5	E	207/210 (99%)	202 (98%)	5 (2%)	0	100	100
6	F	76/127 (60%)	76 (100%)	0	0	100	100
7	G	169/172 (98%)	155 (92%)	14 (8%)	0	100	100
8	H	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
9	I	115/125 (92%)	109 (95%)	6 (5%)	0	100	100
10	J	65/67 (97%)	65 (100%)	0	0	100	100
11	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
12	L	44/58 (76%)	39 (89%)	5 (11%)	0	100	100
13	M	11/13 (85%)	11 (100%)	0	0	100	100
17	U	181/528 (34%)	174 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	V	400/614 (65%)	366 (92%)	34 (8%)	0	100	100
19	W	476/616 (77%)	455 (96%)	21 (4%)	0	100	100
21	Z	265/1087 (24%)	250 (94%)	15 (6%)	0	100	100
22	a	1177/2190 (54%)	1103 (94%)	69 (6%)	5 (0%)	30	61
23	b	1027/1204 (85%)	977 (95%)	50 (5%)	0	100	100
24	d	810/963 (84%)	784 (97%)	26 (3%)	0	100	100
25	e	633/1019 (62%)	609 (96%)	24 (4%)	0	100	100
26	f	524/887 (59%)	506 (97%)	18 (3%)	0	100	100
27	g	876/962 (91%)	842 (96%)	34 (4%)	0	100	100
28	h	865/995 (87%)	825 (95%)	40 (5%)	0	100	100
29	i	544/658 (83%)	516 (95%)	28 (5%)	0	100	100
30	k	448/600 (75%)	423 (94%)	25 (6%)	0	100	100
31	p	571/589 (97%)	556 (97%)	15 (3%)	0	100	100
32	q	288/309 (93%)	276 (96%)	12 (4%)	0	100	100
33	u	1/27 (4%)	1 (100%)	0	0	100	100
All	All	12887/17848 (72%)	12361 (96%)	521 (4%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	a	631	PRO
22	a	761	PRO
22	a	415	LYS
22	a	1215	LEU
22	a	752	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1223/1749 (70%)	1223 (100%)	0	100	100
2	B	978/1027 (95%)	978 (100%)	0	100	100
3	C	238/252 (94%)	238 (100%)	0	100	100
4	D	101/126 (80%)	101 (100%)	0	100	100
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	68/111 (61%)	68 (100%)	0	100	100
7	G	141/153 (92%)	141 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	104/112 (93%)	104 (100%)	0	100	100
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	42/55 (76%)	42 (100%)	0	100	100
13	M	13/13 (100%)	13 (100%)	0	100	100
17	U	155/451 (34%)	155 (100%)	0	100	100
18	V	49/515 (10%)	49 (100%)	0	100	100
19	W	398/514 (77%)	398 (100%)	0	100	100
21	Z	243/940 (26%)	243 (100%)	0	100	100
22	a	684/1907 (36%)	684 (100%)	0	100	100
23	b	859/1072 (80%)	859 (100%)	0	100	100
24	d	704/845 (83%)	704 (100%)	0	100	100
25	e	444/812 (55%)	444 (100%)	0	100	100
26	f	431/796 (54%)	431 (100%)	0	100	100
27	g	719/840 (86%)	719 (100%)	0	100	100
28	h	700/896 (78%)	700 (100%)	0	100	100
29	i	482/600 (80%)	482 (100%)	0	100	100
30	k	317/520 (61%)	317 (100%)	0	100	100
31	p	480/512 (94%)	480 (100%)	0	100	100
32	q	251/274 (92%)	251 (100%)	0	100	100
33	u	1/1 (100%)	1 (100%)	0	100	100
All	All	10305/15578 (66%)	10305 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	GLN
1	A	296	ASN
1	A	504	HIS
1	A	740	GLN
1	A	780	ASN
1	A	792	ASN
1	A	1077	ASN
1	A	1093	GLN
2	B	143	GLN
2	B	254	GLN
2	B	315	ASN
2	B	420	GLN
2	B	525	ASN
2	B	842	HIS
2	B	1007	ASN
2	B	1101	GLN
2	B	1120	ASN
2	B	1160	GLN
3	C	83	GLN
3	C	111	GLN
3	C	260	GLN
4	D	47	GLN
4	D	48	ASN
9	I	46	GLN
9	I	118	HIS
17	U	46	HIS
18	V	62	HIS
19	W	95	ASN
19	W	112	GLN
19	W	358	HIS
19	W	442	GLN
19	W	585	ASN
21	Z	421	GLN
21	Z	748	GLN
22	a	2132	GLN
22	a	2170	GLN
23	b	27	GLN
23	b	410	GLN
23	b	622	GLN
23	b	695	GLN
23	b	700	GLN
23	b	799	GLN

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Mol	Chain	Res	Type
23	b	814	ASN
23	b	837	GLN
23	b	1002	HIS
24	d	54	GLN
24	d	129	GLN
24	d	168	ASN
24	d	172	GLN
24	d	403	GLN
24	d	468	HIS
24	d	492	ASN
24	d	699	GLN
25	e	452	HIS
25	e	537	GLN
25	e	769	GLN
25	e	836	HIS
25	e	993	HIS
26	f	110	ASN
26	f	141	GLN
26	f	145	HIS
26	f	378	ASN
27	g	274	GLN
27	g	384	GLN
27	g	428	GLN
27	g	515	GLN
27	g	538	ASN
27	g	633	GLN
27	g	779	ASN
27	g	837	HIS
27	g	903	ASN
28	h	330	HIS
28	h	609	GLN
28	h	613	ASN
28	h	673	ASN
28	h	854	HIS
28	h	902	GLN
28	h	919	GLN
28	h	963	GLN
28	h	988	GLN
29	i	142	ASN
29	i	246	HIS
29	i	334	ASN
29	i	437	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	i	465	GLN
30	k	28	ASN
30	k	94	HIS
30	k	198	ASN
31	p	127	HIS
32	q	162	GLN
32	q	288	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	16/17 (94%)	6 (37%)	1 (6%)

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	31	A
15	P	33	C
15	P	34	U
15	P	36	G
15	P	37	G
15	P	39	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	38	G

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 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

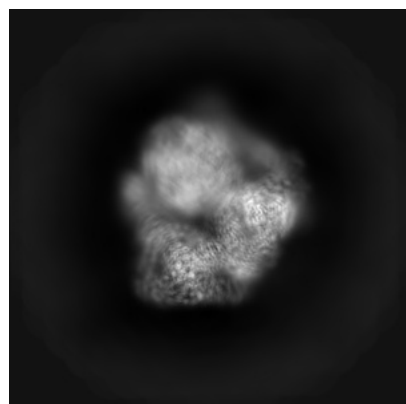
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13479. These allow visual inspection of the internal detail of the map and identification of artifacts.

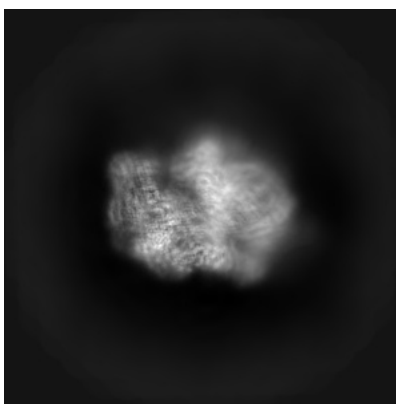
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

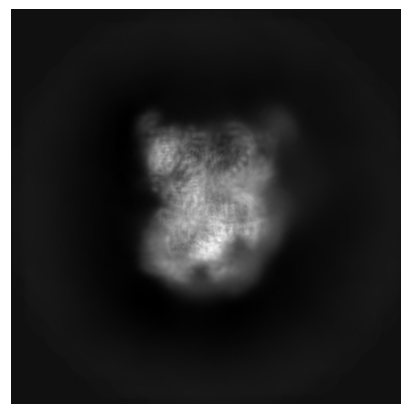
6.1.1 Primary map



X

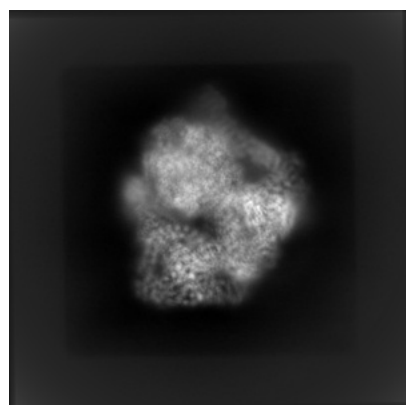


Y

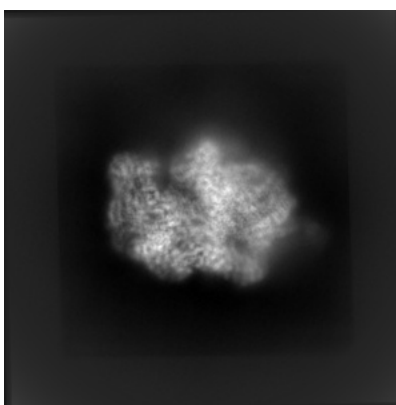


Z

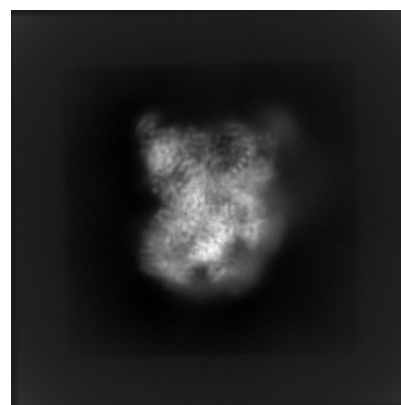
6.1.2 Raw map



X



Y

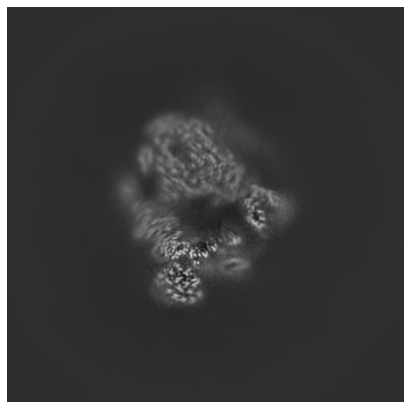


Z

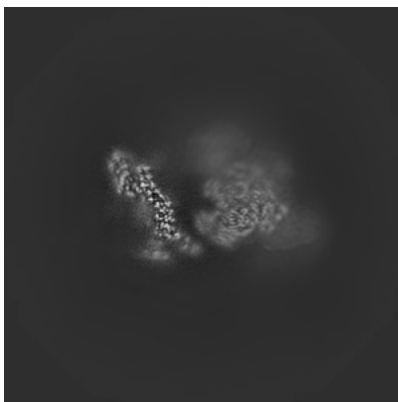
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

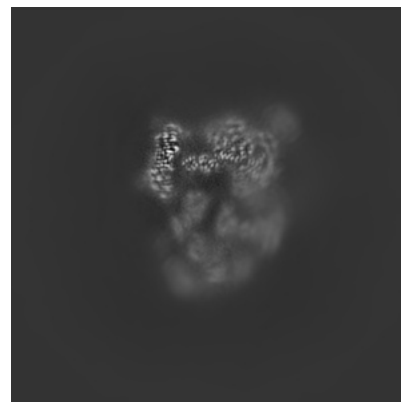
6.2.1 Primary map



X Index: 240

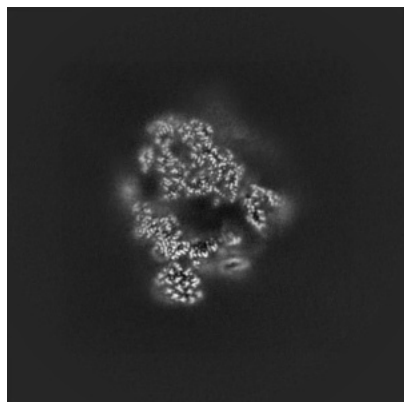


Y Index: 240

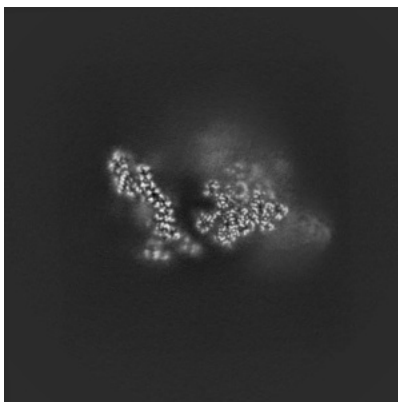


Z Index: 240

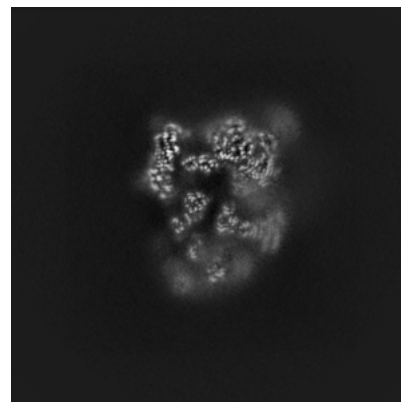
6.2.2 Raw map



X Index: 240



Y Index: 240

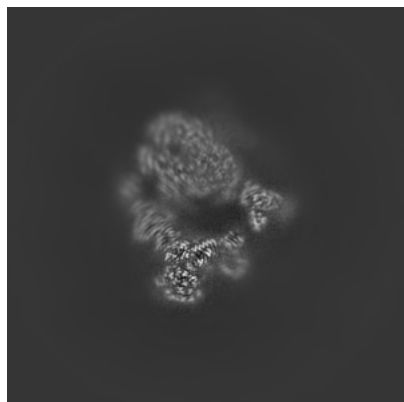


Z Index: 240

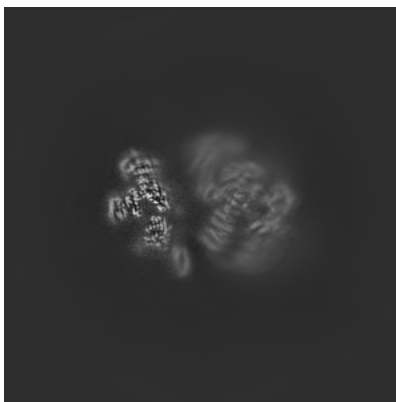
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

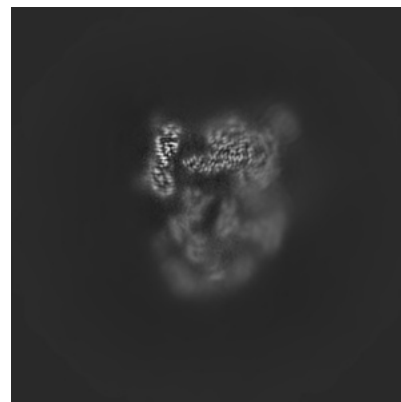
6.3.1 Primary map



X Index: 244

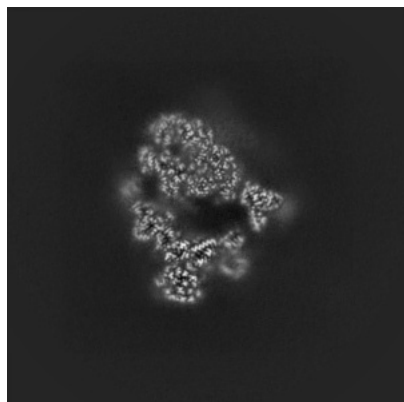


Y Index: 211

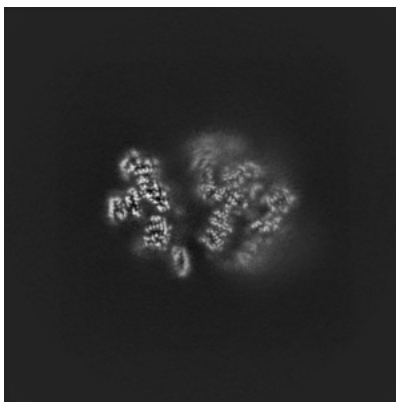


Z Index: 243

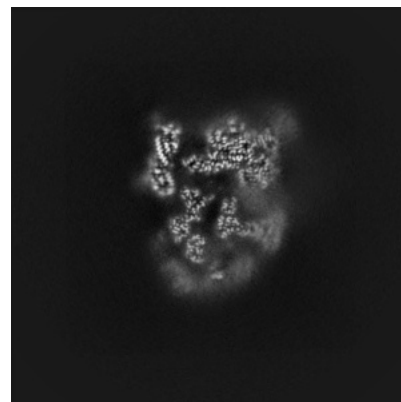
6.3.2 Raw map



X Index: 244



Y Index: 211

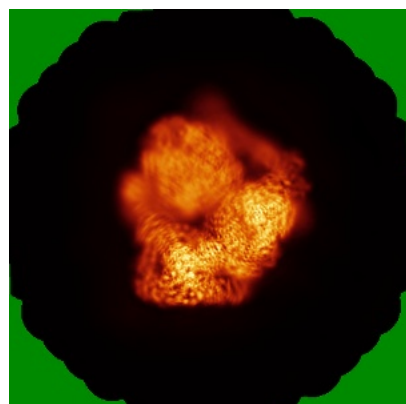


Z Index: 244

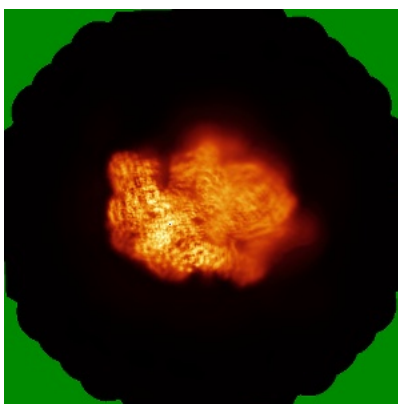
The images above show the largest variance slices of the map in three orthogonal directions.

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

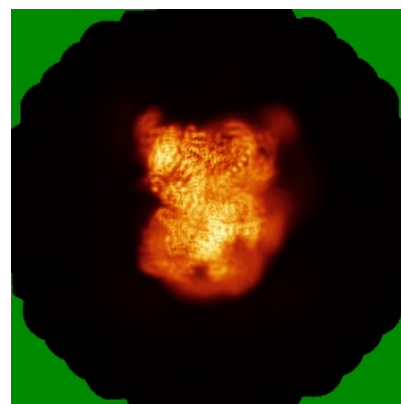
6.4.1 Primary map



X

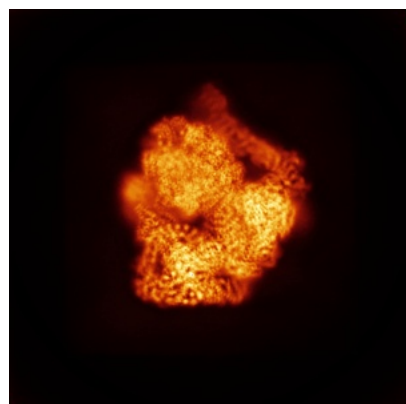


Y

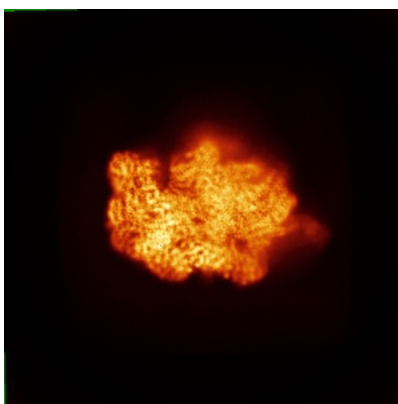


Z

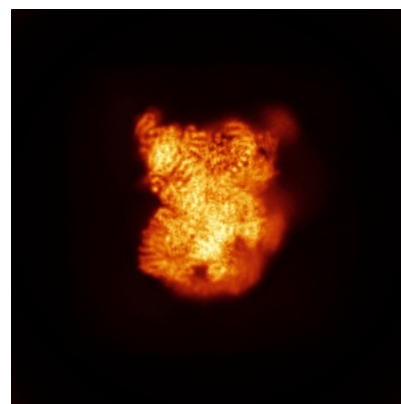
6.4.2 Raw map



X



Y

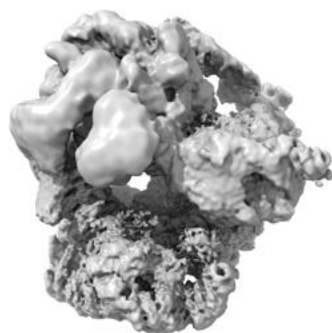


Z

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 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

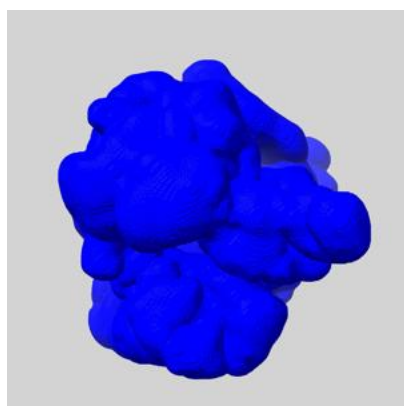
6.6 Mask visualisation [i](#)

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

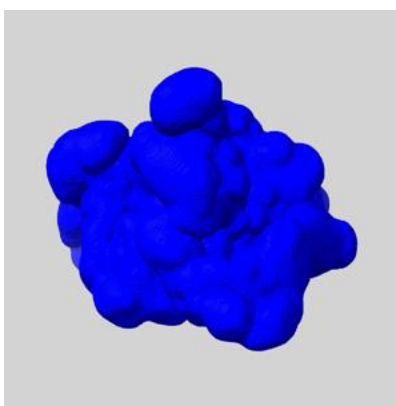
A mask typically either:

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

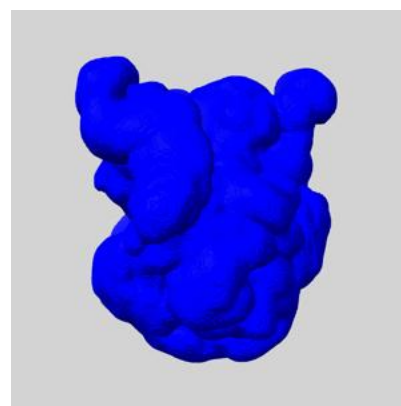
6.6.1 emd_13479_msk_1.map [i](#)



X



Y

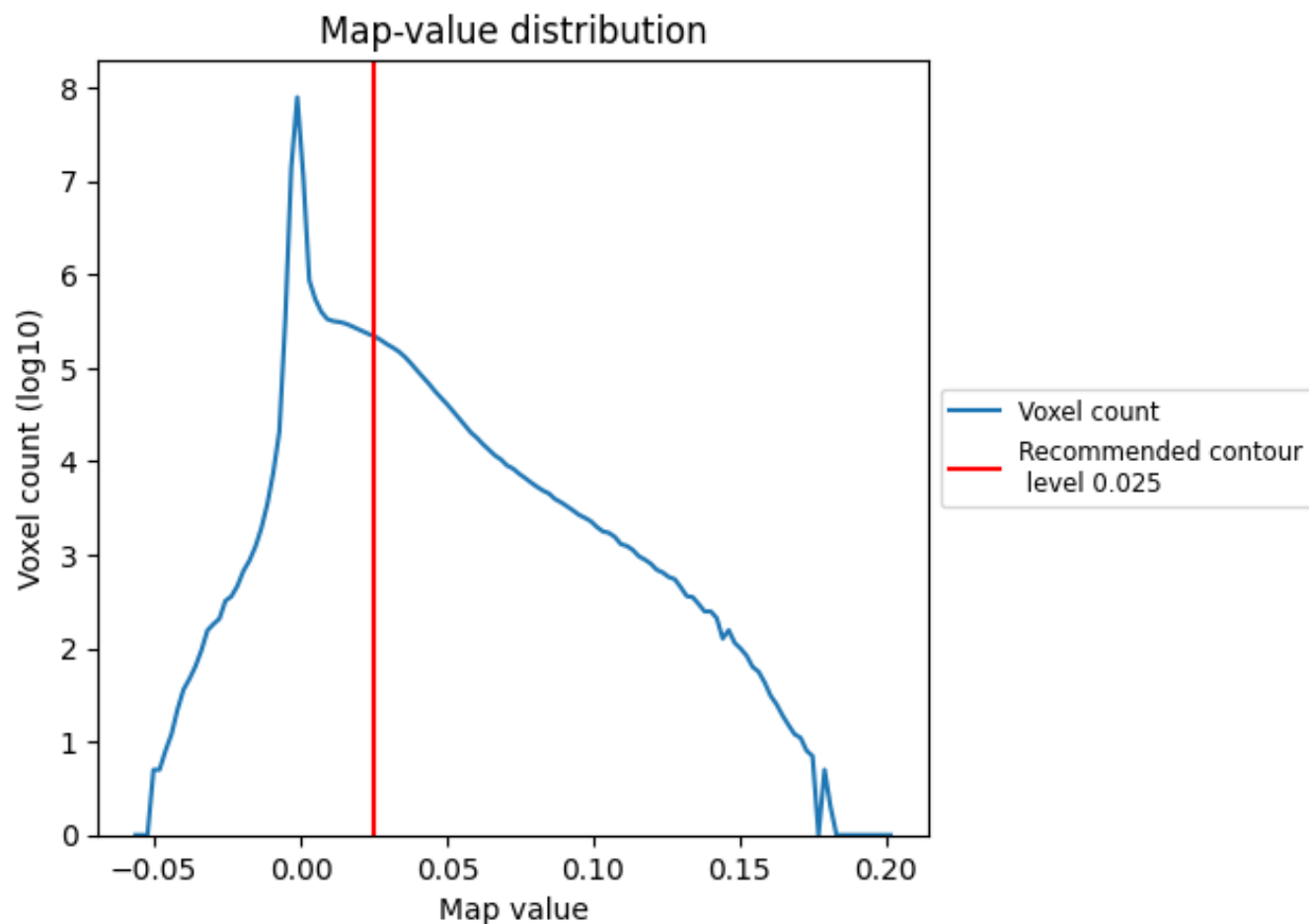


Z

7 Map analysis [i](#)

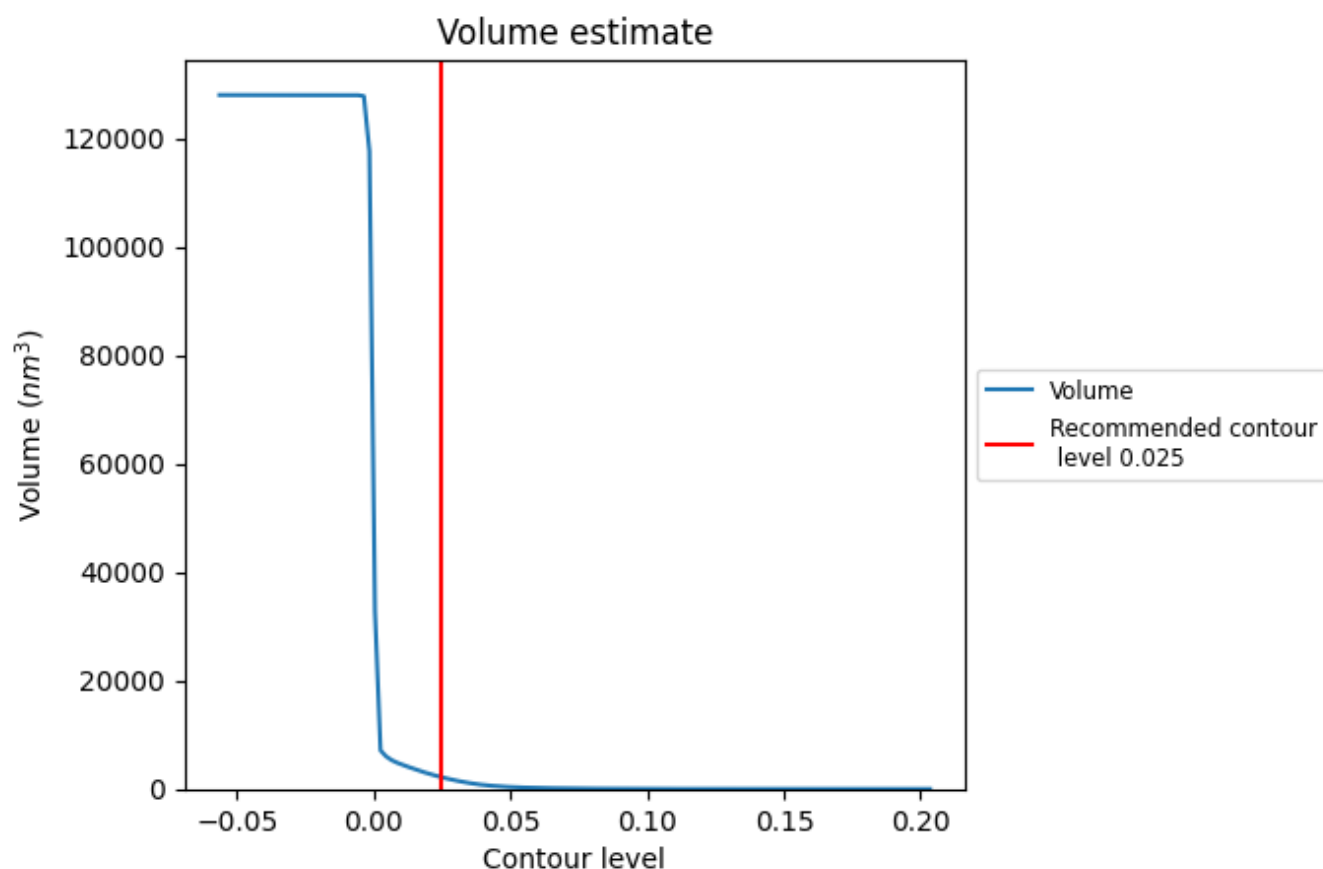
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

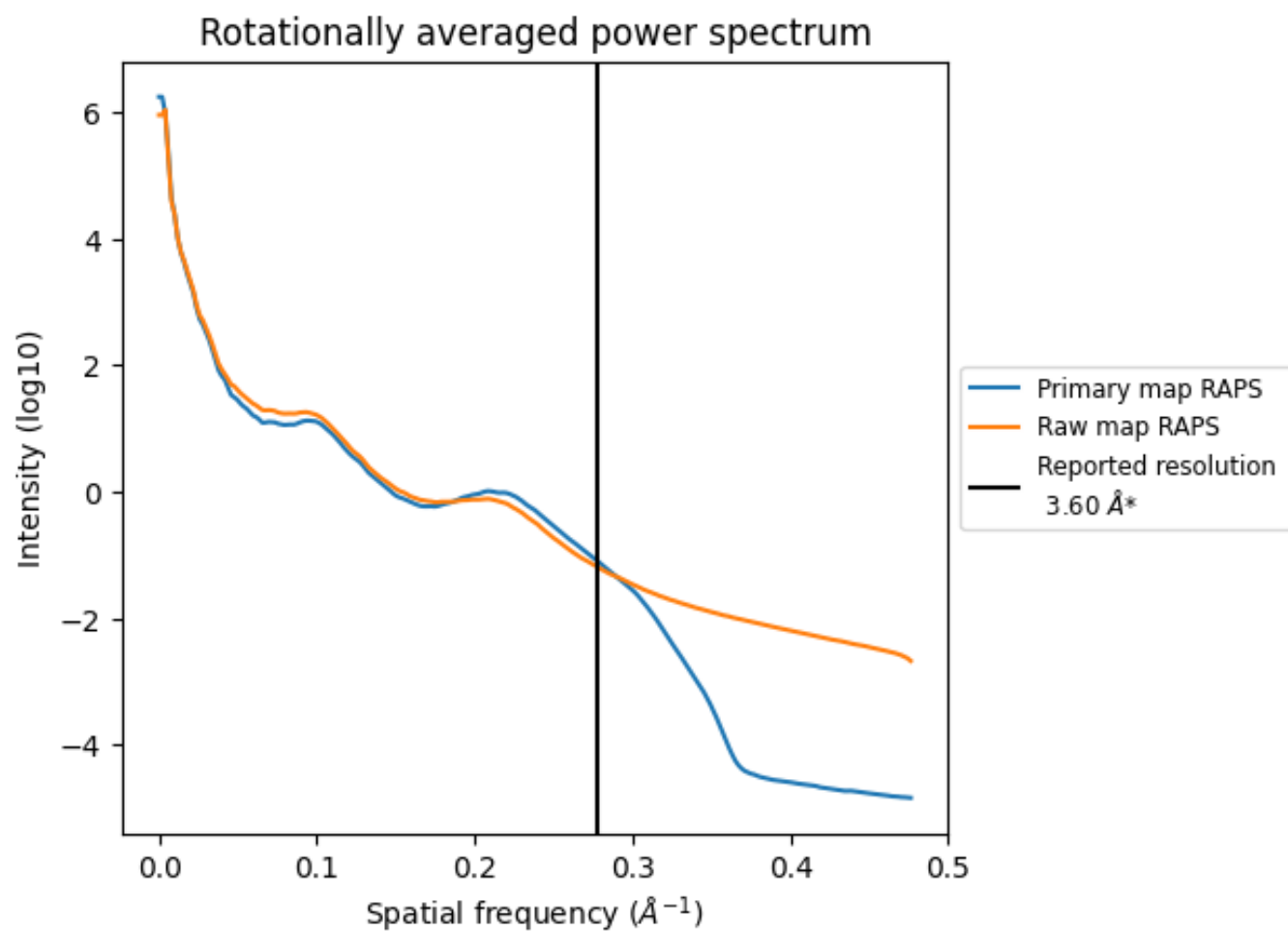
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2154 nm^3 ; this corresponds to an approximate mass of 1946 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 ⓘ

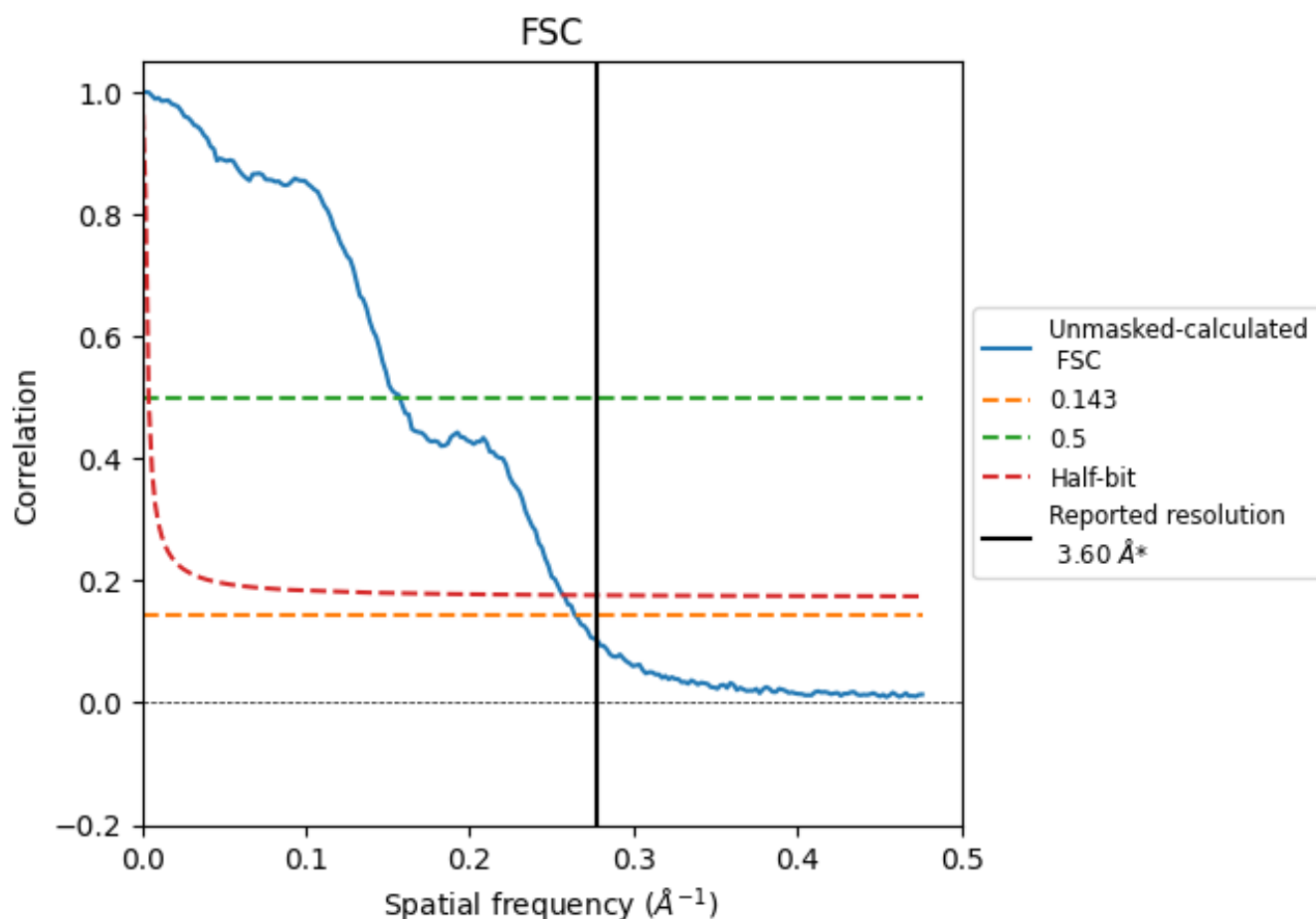


*Reported resolution corresponds to spatial frequency of $0.278 \text{ \AA}^{-1}$

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 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

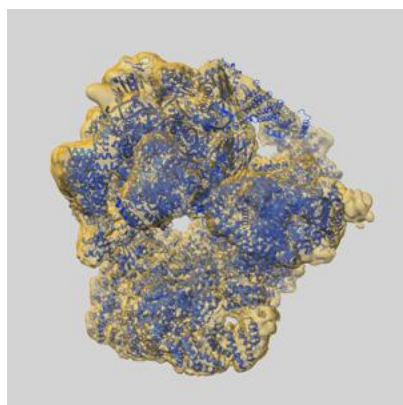
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.78	6.36	3.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

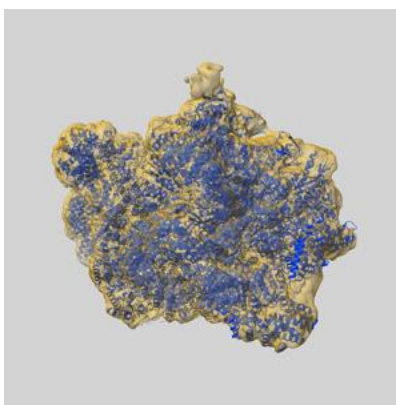
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13479 and PDB model 7PKS. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

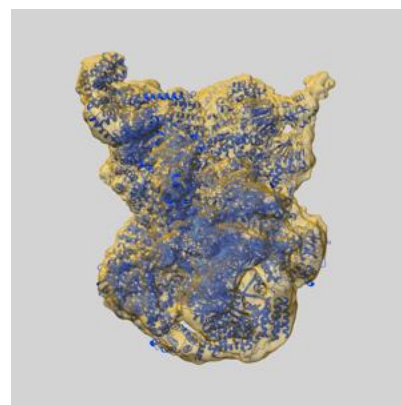
9.1 Map-model overlay [i](#)



X



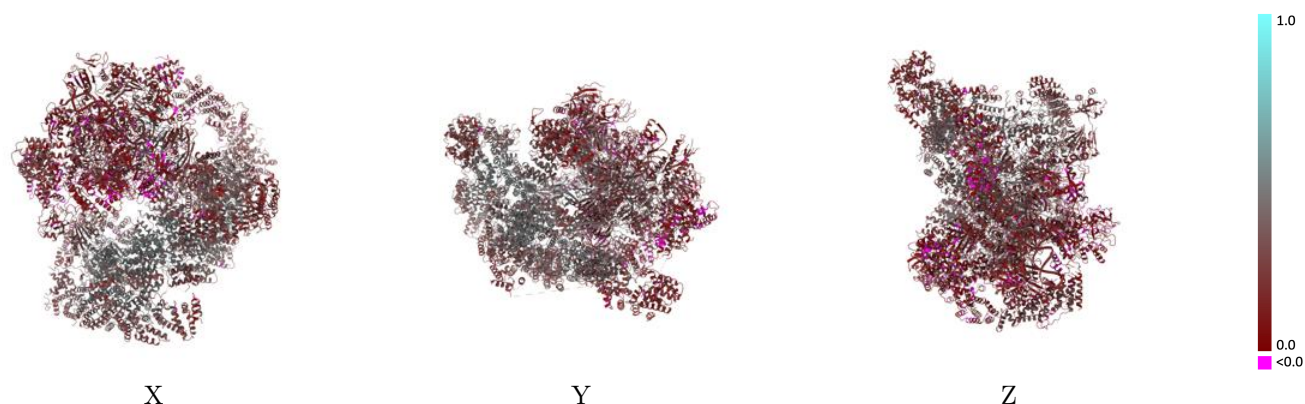
Y



Z

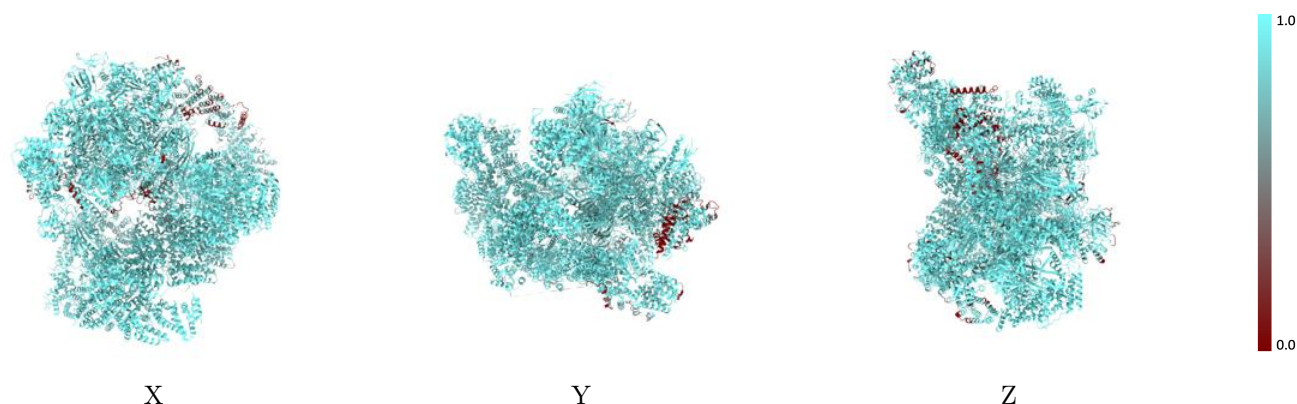
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



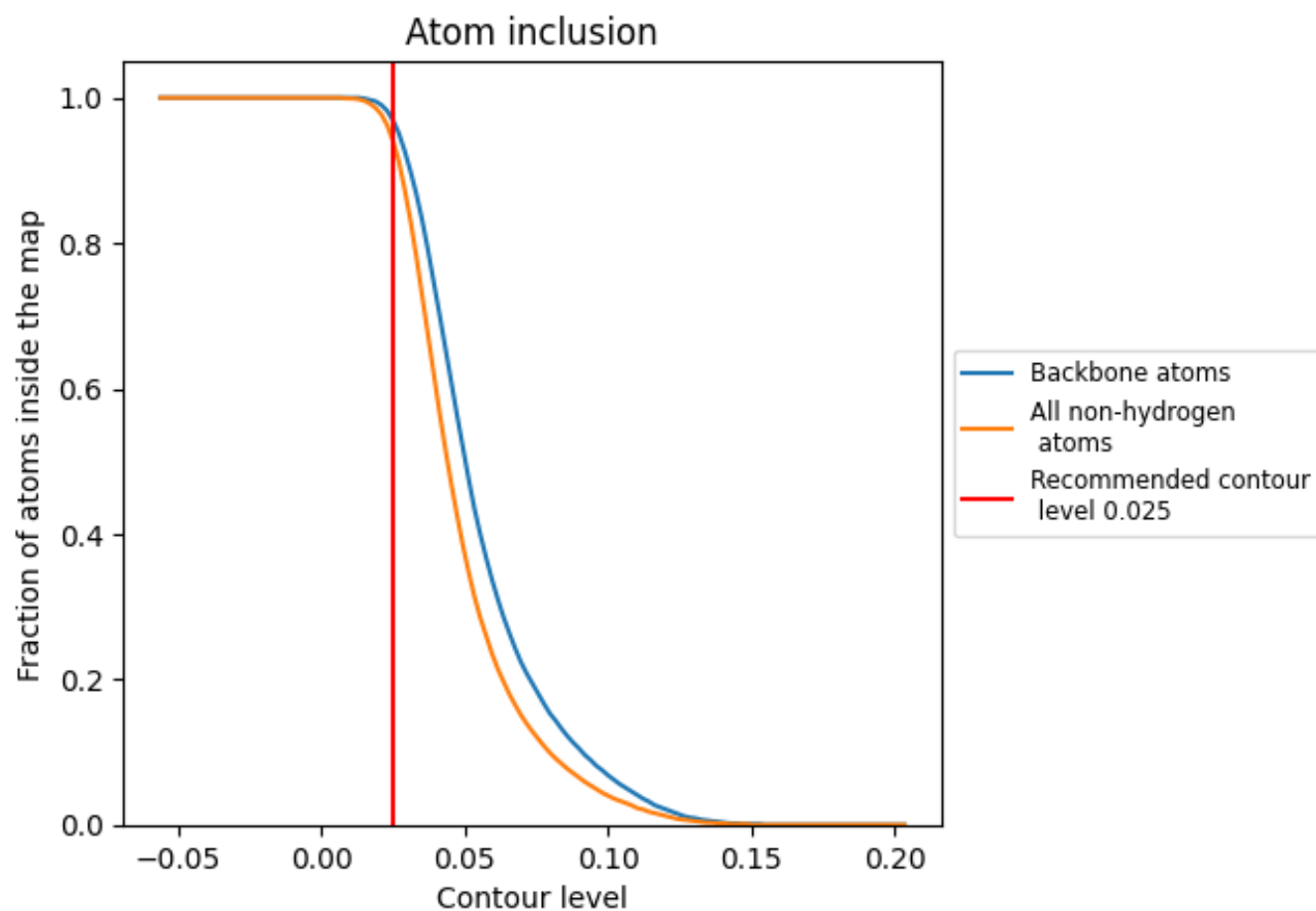
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 94% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9390	 0.2780
A	 0.9690	 0.2060
B	 0.9800	 0.2510
C	 0.8940	 0.2310
D	 0.8210	 0.1010
E	 0.9740	 0.1810
F	 0.9060	 0.1770
G	 0.9190	 0.1100
H	 0.9020	 0.1600
I	 0.9800	 0.1810
J	 0.9370	 0.2740
K	 0.8320	 0.1460
L	 0.9760	 0.2390
M	 0.8600	 0.5230
N	 0.9410	 0.1600
P	 0.9610	 0.1820
T	 0.9780	 0.2170
U	 0.8220	 0.1280
V	 0.9350	 0.1880
W	 0.9120	 0.1280
X	 0.9910	 0.1730
Z	 0.8300	 0.0840
a	 0.7910	 0.2410
b	 0.9620	 0.3980
d	 0.9650	 0.3400
e	 0.9780	 0.4090
f	 0.9590	 0.2910
g	 0.9690	 0.4280
h	 0.9700	 0.3550
i	 0.9700	 0.3500
k	 0.9640	 0.2540
p	 0.9410	 0.2370
q	 0.9700	 0.4230
u	 0.9930	 0.4520

