



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:12 PM UTC

PDB ID : 8W8E / pdb_00008w8e
EMDB ID : EMD-37352
Title : human co-transcriptional RNA capping enzyme RNGTT
Authors : Li, Y.; Wang, Q.; Xu, Y.; Li, Z.
Deposited on : 2023-09-02
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

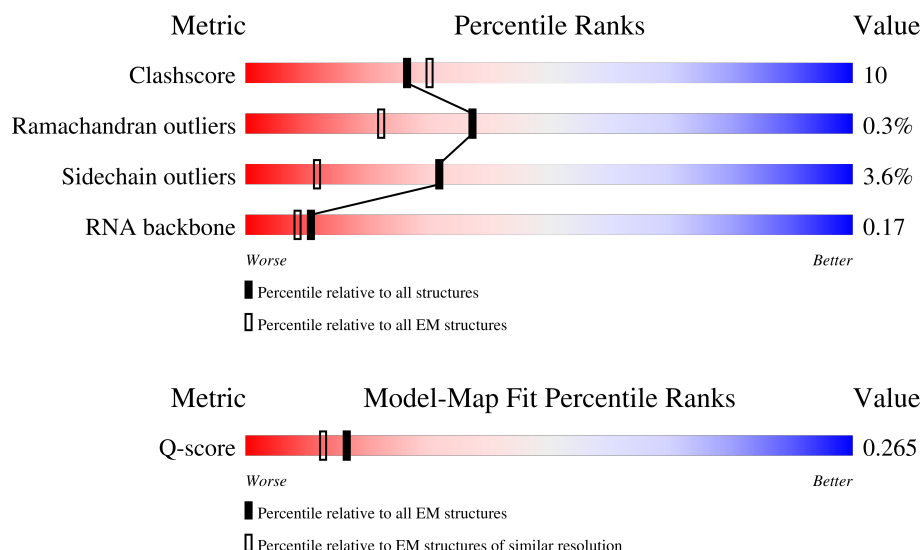
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.90 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.



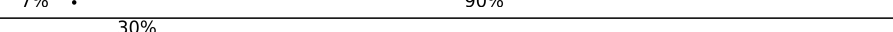
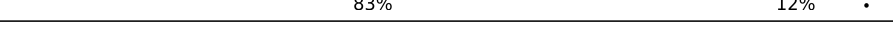
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	271	

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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	N	48	
14	P	16	
15	T	48	
16	U	528	
17	V	580	
18	W	584	
19	X	380	
20	Y	121	
21	Z	1087	
22	a	597	

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 50912 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	1426	Total	C	N	O	S	0	0
			11299	7111	2020	2099	69		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1133	Total	C	N	O	S	0	0
			9046	5723	1594	1665	64		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	258	Total	C	N	O	S	0	0
			2072	1301	353	412	6		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	128	Total	C	N	O	S	0	0
			997	629	169	195	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	82	Total	C	N	O	S	0	0
			658	418	113	122	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
			1305	852	205	240	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
			950	587	169	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 DNA-directed RNA polymerase II subunit RPB11-a.

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 RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			389	241	75	67	6		

- Molecule 13 is a DNA chain called DNA (36-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	34	Total	C	N	O	P	0	0
			714	333	147	200	34		

- Molecule 14 is a RNA chain called RNA (5'-D(*(GTP))-R(P*AP*GP*AP*GP*AP*GP*G

P*GP*AP*AP*CP*CP*CP*AP*CP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	16	Total	C	N	O	P	0	0
			347	155	69	107	16		

- Molecule 15 is a DNA chain called DNA (45-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	45	Total	C	N	O	P	0	0
			910	432	156	277	45		

- Molecule 16 is a protein called Negative elongation factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	183	Total	C	N	O	S	0	0
			1410	895	239	269	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	550	Total	C	N	O	S	0	0
			4411	2825	752	810	24		

- Molecule 18 is a protein called Negative elongation factor C/D.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	532	Total	C	N	O	S	0	0
			3823	2419	664	720	20		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	7	SER	-	expression tag	UNP Q8IXH7
W	8	ASN	-	expression tag	UNP Q8IXH7
W	9	ALA	-	expression tag	UNP Q8IXH7

- Molecule 19 is a protein called Negative elongation factor E.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	37	Total	C	N	O	S	0	0
			293	191	50	51	1		

- Molecule 20 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	116	Total	C	N	O	S	0	0
			911	570	159	173	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-3	GLY	-	expression tag	UNP P63272
Y	-2	PRO	-	expression tag	UNP P63272
Y	-1	GLY	-	expression tag	UNP P63272
Y	0	SER	-	expression tag	UNP P63272

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	360	Total	C	N	O	S	0	0
			2880	1835	495	537	13		

- Molecule 22 is a protein called mRNA-capping enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	a	506	Total	C	N	O	S	5	0
			4096	2614	710	740	32		

- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 24 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

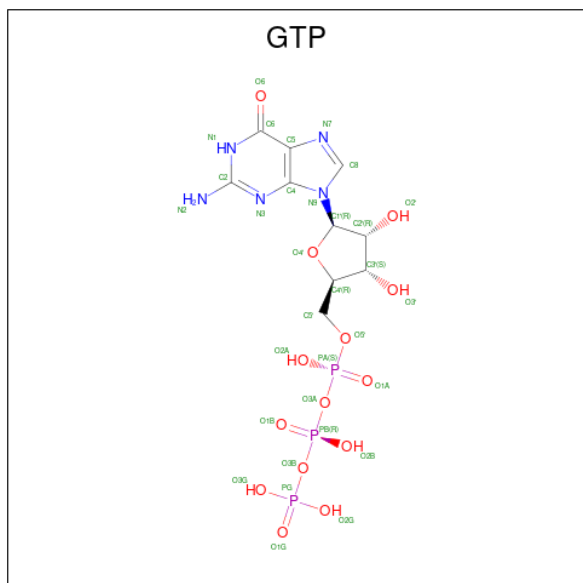
Mol	Chain	Residues	Atoms		AltConf
24	A	2	Total	Zn	0
			2	2	
24	B	1	Total	Zn	0
			1	1	
24	C	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
24	I	2	Total	Zn	0
			2	2	
24	L	1	Total	Zn	0
			1	1	
24	Y	1	Total	Zn	0
			1	1	

- Molecule 25 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).

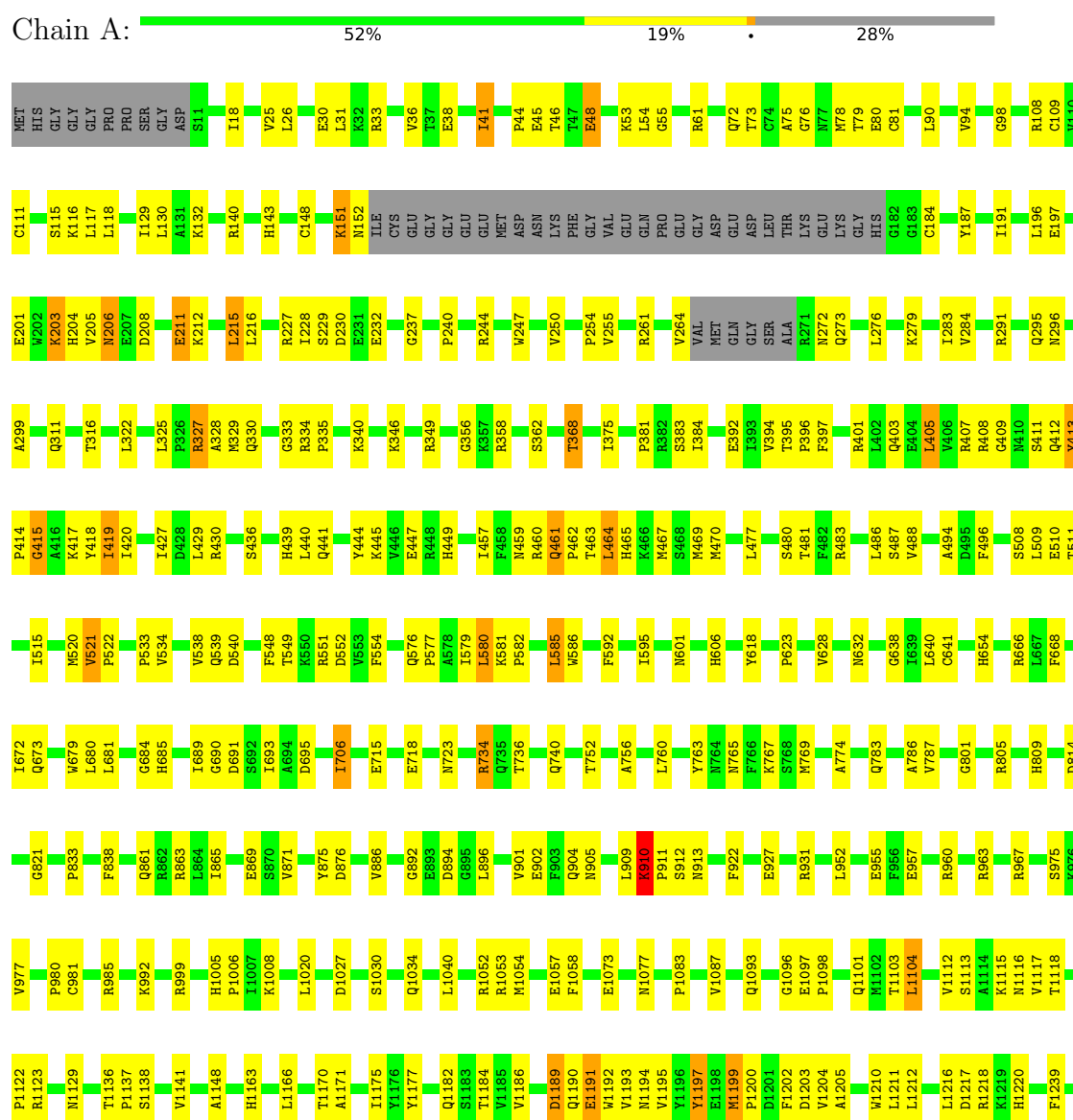


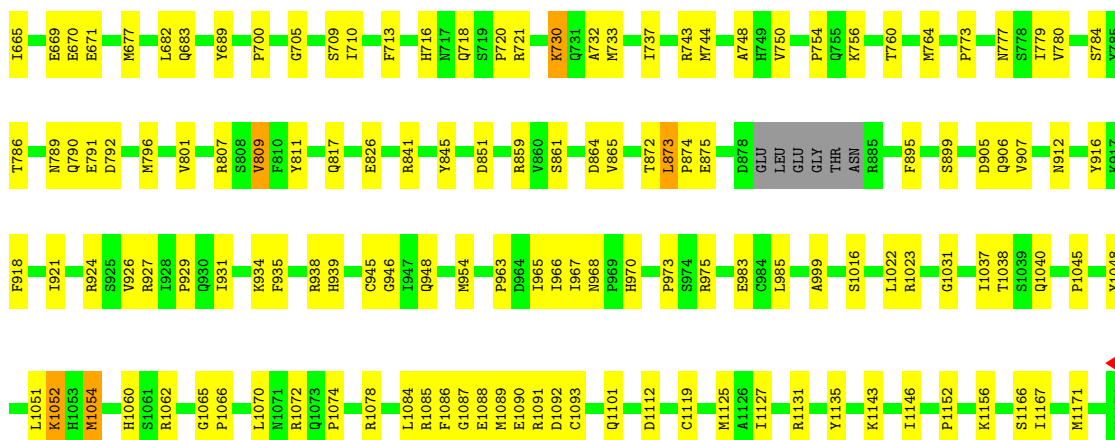
Mol	Chain	Residues	Atoms					AltConf
25	P	1	Total	C	N	O	P	0
			32	10	5	14	3	

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.

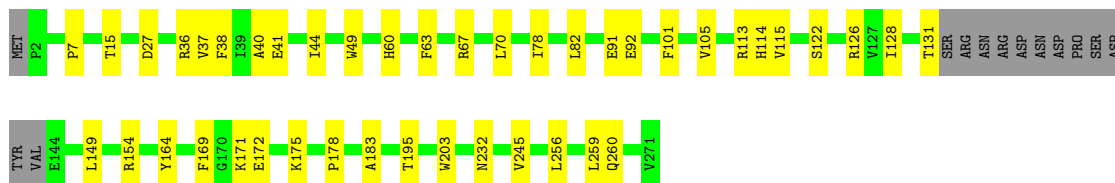
- Molecule 1: DNA-directed RNA polymerase subunit





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

Chain C: 79% 16% 5%



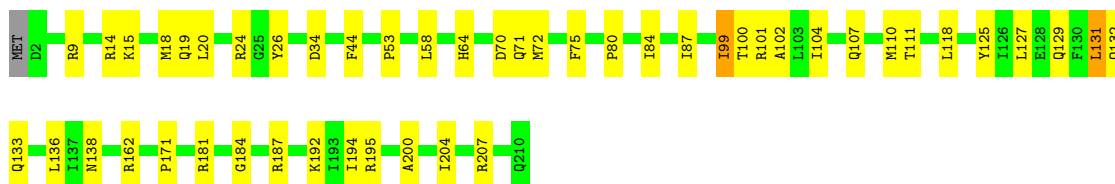
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D: 79% 11% 10%



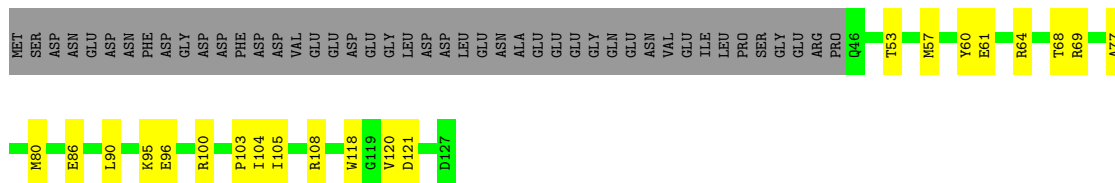
• Molecule 5: DNA-directed RNA polymerase II subunit E

Chain E: 77% 22%



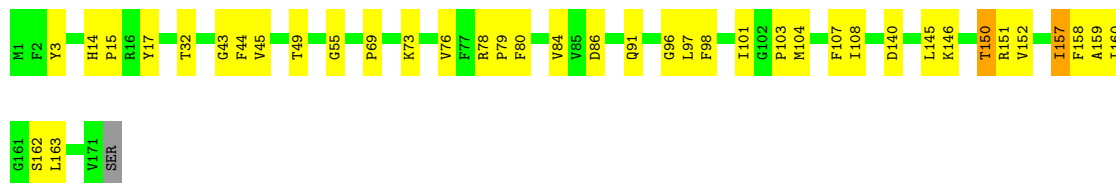
• Molecule 6: DNA-directed RNA polymerase II subunit F

Chain F: 48% 17% 35%



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

Chain G:  77% 22% ..



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

Chain H:  65% 32% ..



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

Chain I:  74% 18% 6%



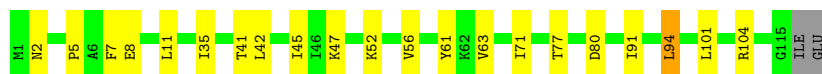
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:  79% 21%



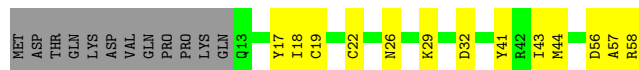
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

Chain K:  80% 17% ..

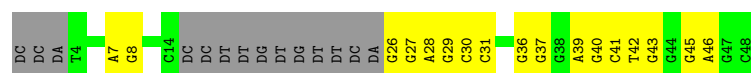


- Molecule 12: RPB12

Chain L:  57% 22% 21%



- Molecule 13: DNA (36-MER)



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|-----|
| A31 |
| G32 |
| A33 |
| G34 |
| A35 |
| G36 |
| G37 |
| G38 |
| A39 |
| A40 |
| C41 |
| C42 |
| C43 |
| A44 |
| C45 |
| U46 |

- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|----|----|----|----|----|----|----|--|-----|-----|--|-----|-----|-----|-----|--|-----|-----|-----|-----|-----|--|-----|-----|-----|-----|----|----|----|
| G1 | C2 | T3 | C4 | C5 | C6 | A7 | | C13 | T14 | | C20 | T21 | C22 | C23 | | G26 | T27 | G28 | G29 | G30 | | T42 | C43 | A44 | A45 | DT | DG | DG |
|----|----|----|----|----|----|----|--|-----|-----|--|-----|-----|-----|-----|--|-----|-----|-----|-----|-----|--|-----|-----|-----|-----|----|----|----|

- | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|----|----|------|------|------|------|------|------|------|
| MET | ALA | SER | MET | ARG | E6 | T9 | L17 | D21 | E22 | L23 | W24 | S28 | L29 | L38 | S39 | N40 | L41 | L48 | V52 | K53 | L54 | K55 | L56 | L57 | L58 | G59 | T60 | L61 | L78 | L79 | M92 | V93 | I96 | L97 | K98 | S99 | P100 | F101 | L106 | L110 | N116 | I120 | L121 |
|-----|-----|-----|-----|-----|----|----|------|------|------|------|------|------|------|

E126	K127	L137	L138	L139	E140	C141	Q142	Y143	L144	A148	T151	H162	F163	Q164	L165	K166	A172	R175	A186	Q187	Q188	LEU	LYS	ARG	SER	ALA	GLY	VAL	PRO	PHE	HIS	ALA	LYS	GLY	ARG	GLY	LEU	LEU	ARG	LYS	MET	ASP	THR	THR	THR	PRO	LEU	LYS	GLY	ILE	PRO	LYS
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GLN	ALA	PRO	PHE	ARG	SER	PRO	THR	THR	ALA	ALA	SER	SER	VAL	PHE	SER	SER	THR	THR	GLY	ASN	ARG	THR	THR	PRO	PRO	ILE	PRO	PRO	SER	SER	ARG	ARG	LEU	LEU	LEU	ARG	LYS	GLU	GLY	GLY	VAL	LYS	LEU	LEU	LEU	ASP	ASP	MET	VAL	GLY	LYS	ARG	ARG	ARG	LYS	THR	LEU	ASP
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ALA	GLU	VAL	GLU	VAL	GLU	LYS	PRO	ALA	ALA	LYS	GLU	GLU	THR	VAL	VAL	GLU	GLU	ASN	ALA	ALA	THR	PRO	ASP	TYR	ALA	ALA	GLY	GLY	LEU	VAL	SER	THR	GLN	LYS	LEU	GLY	SER	ASN	ASN	GLU	PRO	ALA	ALA	LEU	PRO	SER	THR	THR	SER	TYR	LEU	PRO	SER	SER	THR	PRO	SER	VAL	VAL	ALA	ALA	PRO	SER	SER	TYR	ILE	PRO
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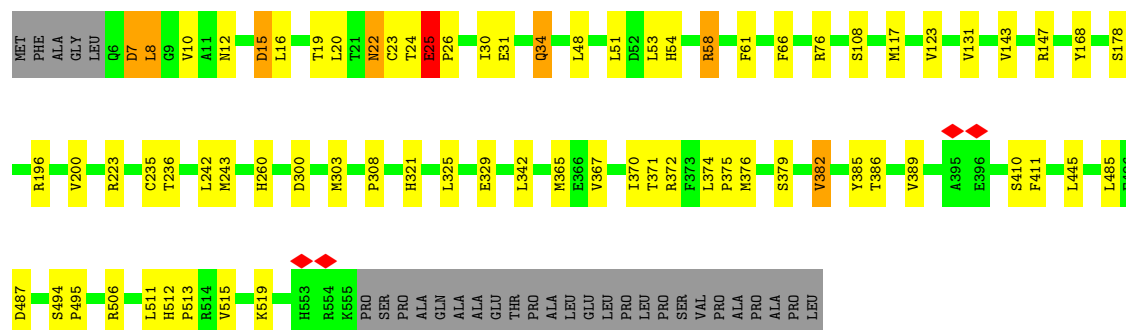
[illegible]

PRO	PRO	VAL	VAL	PRO	THR	THR	GLN	THR	PRO	PRO	VAL	VAL	ALA	ALA	GLN	THR	GLN	GLN	GLN	PRO	PRO	ALA	ALA	GLN	GLN	GLN	LYS	LYS	ASN	LEU	SR	LEU	THR	ARG	GLU	GLN	MET	ALA	ALA	ALA	ALA	GLN	GLU	MET	LYS	THR	LYS	ALA	ASN	LYS	VAL	THR	THR	ARG	PRO	PRO	GLU	LYS	ALA	ALA	LEU	LEU	ILE
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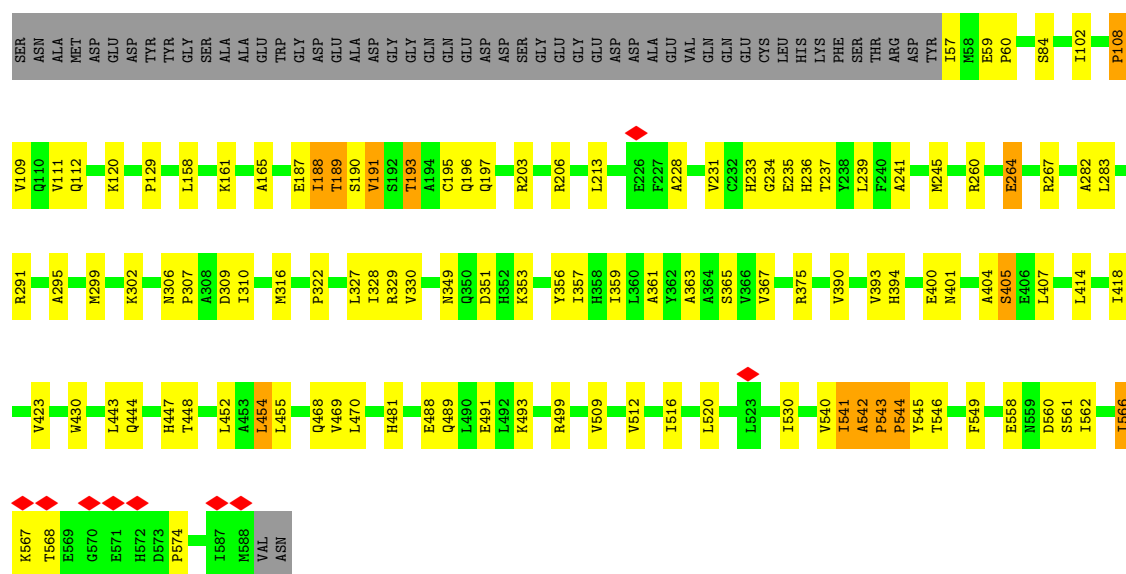
LEU GLY PHE MET ALA GLY SER ARG GLU ASN PRO PRO CYS GLN GLN GLY VAL TLE GLN TLE LYS LEU SER GLU HIS THR GLU ASP LEU PRO LYS ASP GLY GLY SER THR THR MET LEU VAL ASP THR VAL PHE GLU MET ASN TTR ALA THR GLN TTP THR ARG PHE LYS

LYS
TYR
LYS
PRO
MET
THR
ASN
VAL
SER

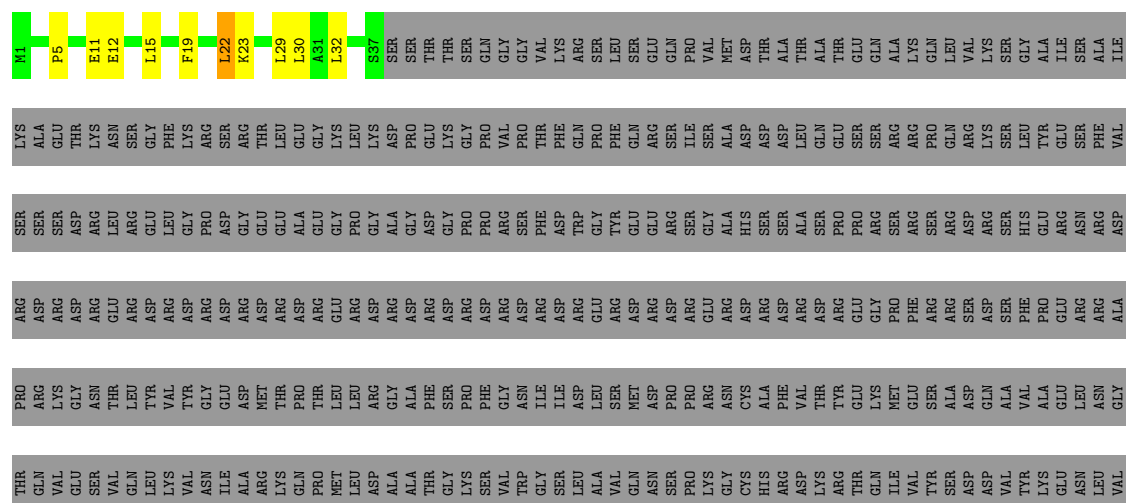
- Chain V:  82% 11% 5%



• Molecule 18: Negative elongation factor C/D



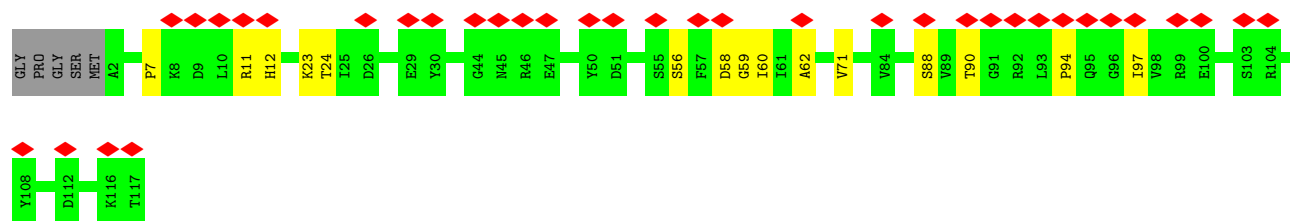
• Molecule 19: Negative elongation factor E



ASP
GLY
PHE

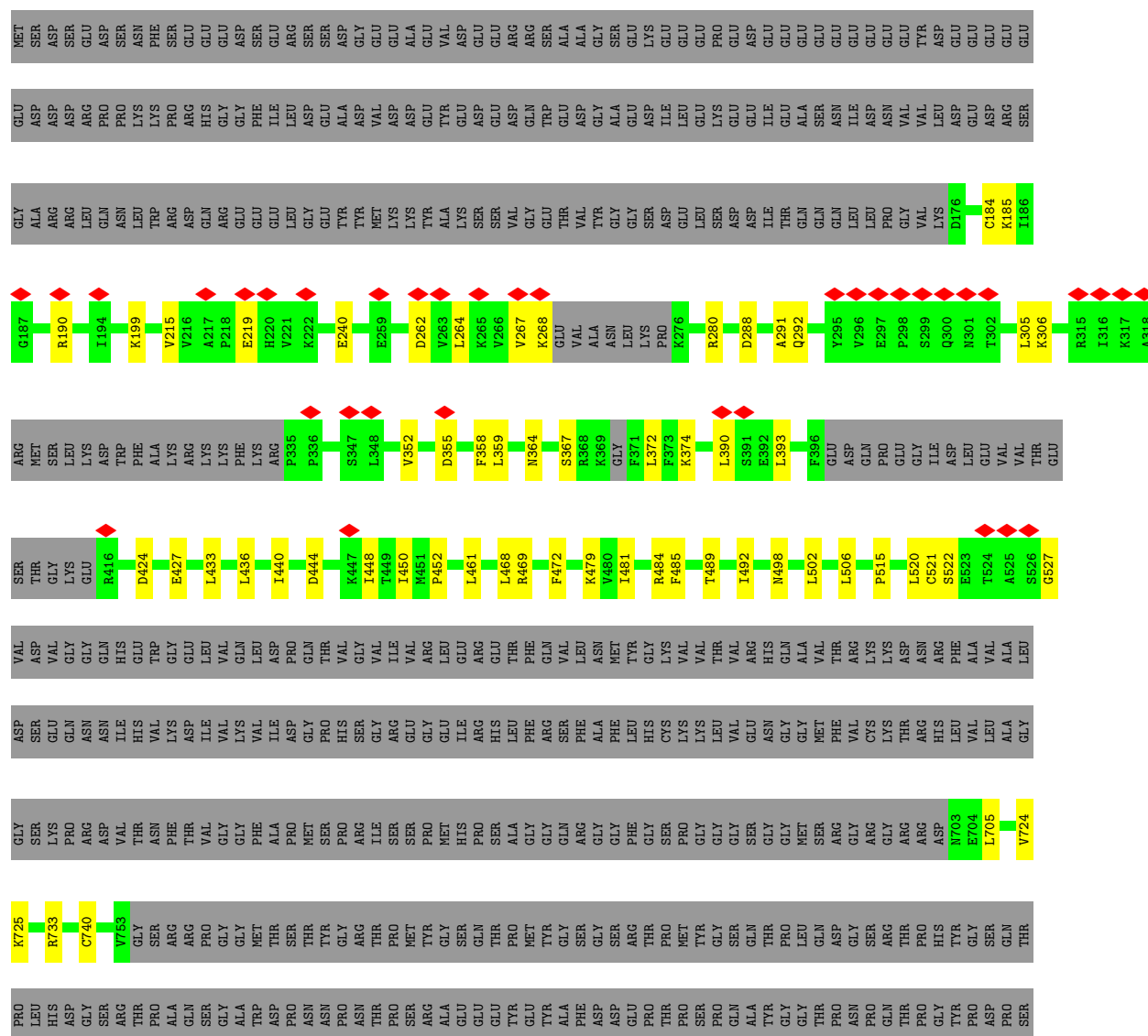
• Molecule 20: Transcription elongation factor SPT4

Chain Y: 30% 83% 12%

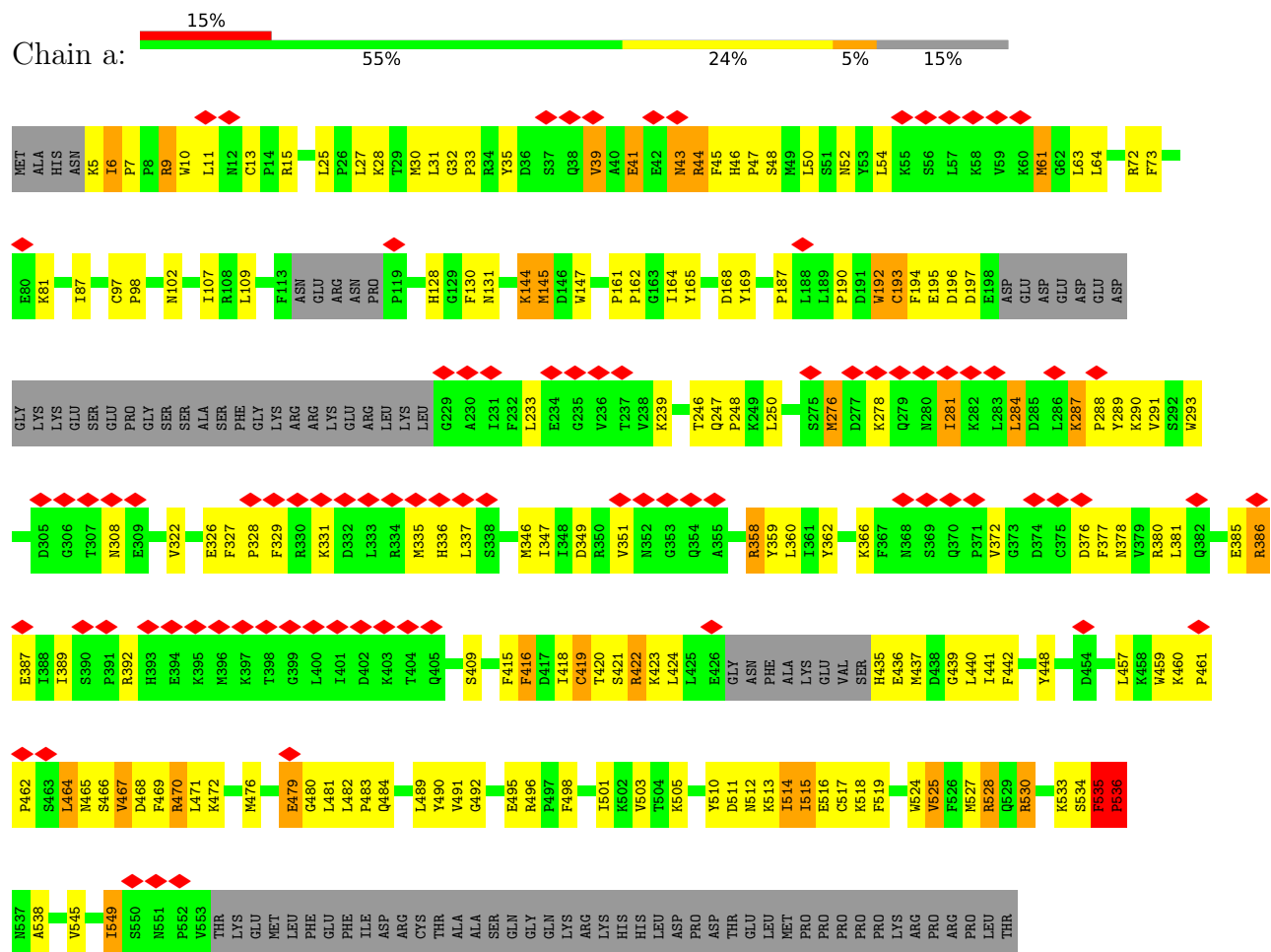


• Molecule 21: Transcription elongation factor SPT5

Chain Z: 28% 5% 67%



- Molecule 22: mRNA-capping enzyme



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.963	Depositor
Minimum map value	-1.420	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.22	Depositor
Map size (Å)	426.88, 426.88, 426.88	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.334, 1.334, 1.334	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.16	1/11509 (0.0%)	0.36	2/15542 (0.0%)
2	B	0.12	0/9226	0.36	3/12451 (0.0%)
3	C	0.10	0/2115	0.29	0/2873
4	D	0.08	0/1011	0.22	0/1364
5	E	0.10	0/1752	0.30	0/2366
6	F	0.08	0/668	0.24	0/901
7	G	0.10	0/1336	0.30	0/1820
8	H	0.09	0/1207	0.27	0/1628
9	I	0.08	0/973	0.26	0/1316
10	J	0.08	0/542	0.26	0/730
11	K	0.11	0/939	0.26	0/1271
12	L	0.10	0/395	0.28	0/524
13	N	0.21	0/804	0.42	0/1240
14	P	0.13	0/389	0.37	0/605
15	T	0.24	0/1015	0.52	0/1562
16	U	0.10	0/1434	0.28	0/1948
17	V	0.14	0/4496	0.31	0/6074
18	W	0.18	0/3891	0.43	1/5307 (0.0%)
19	X	0.14	0/295	0.36	0/388
20	Y	0.07	0/927	0.20	0/1250
21	Z	0.07	0/2928	0.25	0/3940
22	a	0.19	0/4213	0.49	4/5687 (0.1%)
All	All	0.14	1/52065 (0.0%)	0.35	10/70787 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	734	ARG	CA-C	-5.72	1.45	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	631	GLN	CA-C-N	-11.26	106.61	122.93
2	B	631	GLN	C-N-CA	-11.26	106.61	122.93
22	a	535	PHE	CA-CB-CG	10.91	124.71	113.80
1	A	415	GLY	CA-C-N	8.47	137.04	122.81
1	A	415	GLY	C-N-CA	8.47	137.04	122.81
22	a	535	PHE	CB-CA-C	8.08	126.08	110.17
22	a	536	PRO	CB-CA-C	-7.53	99.14	111.56
22	a	536	PRO	N-CA-C	6.48	125.81	112.47
2	B	631	GLN	N-CA-C	-5.48	99.14	110.80
18	W	405	SER	N-CA-C	-5.14	105.79	111.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11299	0	11416	278	0
2	B	9046	0	9078	218	0
3	C	2072	0	2016	35	0
4	D	997	0	953	13	0
5	E	1721	0	1737	32	0
6	F	658	0	684	14	0
7	G	1305	0	1267	26	0
8	H	1186	0	1147	41	0
9	I	950	0	880	18	0
10	J	533	0	557	9	0
11	K	920	0	942	15	0
12	L	389	0	395	11	0
13	N	714	0	379	22	0
14	P	347	0	175	10	0
15	T	910	0	507	21	0
16	U	1410	0	1455	37	0
17	V	4411	0	4503	72	0
18	W	3823	0	3520	93	0
19	X	293	0	340	17	0
20	Y	911	0	905	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	Z	2880	0	2925	38	0
22	a	4096	0	4076	162	0
23	A	1	0	0	0	0
24	A	2	0	0	0	0
24	B	1	0	0	0	0
24	C	1	0	0	0	0
24	I	2	0	0	0	0
24	L	1	0	0	0	0
24	Y	1	0	0	0	0
25	P	32	0	11	1	0
All	All	50912	0	49868	1009	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 10.

All (1009) 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)
18:W:404:ALA:HB1	18:W:407:LEU:HB3	1.30	1.06
2:B:630:LYS:C	2:B:632:LYS:H	1.64	1.04
17:V:54:HIS:HA	18:W:129:PRO:HG2	1.40	1.02
13:N:43:DG:N2	15:T:6:DC:N3	2.11	0.96
1:A:1115:LYS:HE3	1:A:1339:ASP:HA	1.47	0.96
18:W:404:ALA:CB	18:W:407:LEU:HB3	1.99	0.93
13:N:43:DG:H1	15:T:6:DC:H42	1.14	0.92
2:B:630:LYS:C	2:B:632:LYS:N	2.24	0.89
22:a:439:GLY:HA2	22:a:461:PRO:HD2	1.56	0.88
22:a:52:ASN:ND2	22:a:511:ASP:O	2.09	0.85
17:V:51:LEU:HA	17:V:54:HIS:HD2	1.42	0.85
22:a:470:ARG:HB2	22:a:536:PRO:HD3	1.61	0.82
3:C:37:VAL:HG13	3:C:41:GLU:HB2	1.63	0.79
22:a:44:ARG:HD2	22:a:46:HIS:CE1	2.18	0.78
16:U:164:GLN:HB3	18:W:543:PRO:HD2	1.64	0.77
22:a:46:HIS:HB2	22:a:534:SER:HB3	1.66	0.76
17:V:20:LEU:HD22	18:W:84:SER:HA	1.67	0.75
22:a:32:GLY:N	22:a:73:PHE:O	2.20	0.75
2:B:83:ARG:HH22	2:B:139:GLN:HB3	1.52	0.74
22:a:492:GLY:HA3	22:a:538:ALA:HA	1.69	0.74
1:A:206:ASN:HB3	1:A:211:GLU:HB3	1.68	0.74
1:A:327:ARG:NH2	1:A:329:MET:SD	2.60	0.74
2:B:750:VAL:HG23	2:B:809:VAL:HG13	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1141:VAL:HB	1:A:1336:LEU:HB2	1.69	0.73
13:N:42:DT:H2"	13:N:43:DG:C8	2.24	0.73
1:A:408:ARG:NH2	1:A:414:PRO:HD2	2.03	0.73
2:B:459:ALA:HB3	2:B:461:GLN:HE22	1.54	0.73
22:a:470:ARG:HB2	22:a:535:PHE:HB2	1.70	0.73
17:V:12:ASN:HB2	17:V:16:LEU:N	2.04	0.72
22:a:439:GLY:HA3	22:a:460:LYS:HA	1.71	0.72
21:Z:355:ASP:HB3	21:Z:358:PHE:HB3	1.72	0.72
22:a:535:PHE:CD1	22:a:536:PRO:HD2	2.23	0.72
1:A:409:GLY:O	1:A:415:GLY:HA3	1.88	0.72
17:V:61:PHE:CE1	18:W:120:LYS:HA	2.25	0.72
1:A:411:SER:OG	21:Z:733:ARG:NH1	2.23	0.71
22:a:46:HIS:HB3	22:a:535:PHE:CD2	2.24	0.71
1:A:94:VAL:HG13	1:A:311:GLN:HG2	1.72	0.71
2:B:473:LEU:HD21	2:B:1052:LYS:HD2	1.71	0.71
17:V:54:HIS:HA	18:W:129:PRO:CG	2.19	0.71
1:A:1287:CYS:SG	2:B:249:LYS:NZ	2.63	0.71
13:N:29:DG:H2"	13:N:30:DC:C5	2.25	0.71
2:B:754:PRO:HB2	2:B:773:PRO:HG2	1.73	0.71
16:U:139:LEU:HD13	18:W:267:ARG:HH21	1.56	0.71
2:B:859:ARG:HH22	21:Z:740:CYS:HA	1.55	0.70
22:a:161:PRO:HB2	22:a:162:PRO:HD3	1.72	0.70
21:Z:450:ILE:HG23	21:Z:452:PRO:HD3	1.74	0.70
2:B:1085:ARG:NH1	15:T:26:DG:OP1	2.25	0.70
22:a:468:ASP:HA	22:a:530:ARG:CZ	2.22	0.70
18:W:447:HIS:NE2	18:W:491:GLU:OE1	2.25	0.70
22:a:130:PHE:HE1	22:a:162:PRO:HD2	1.57	0.69
15:T:27:DT:H2'	15:T:28:DG:C8	2.28	0.69
22:a:48:SER:O	22:a:52:ASN:HB2	1.92	0.69
18:W:353:LYS:HE3	18:W:394:HIS:HD2	1.56	0.69
1:A:132:LYS:HG2	5:E:187:ARG:HH12	1.58	0.69
1:A:412:GLN:O	1:A:413:TYR:C	2.35	0.69
1:A:894:ASP:HB3	5:E:200:ALA:HB2	1.74	0.69
22:a:516:GLU:HA	22:a:530:ARG:NH1	2.08	0.69
21:Z:444:ASP:HB3	21:Z:448:ILE:HA	1.74	0.68
1:A:869:GLU:OE1	2:B:1091:ARG:NH1	2.24	0.68
22:a:9:ARG:HH11	22:a:9:ARG:HB3	1.57	0.68
4:D:60:VAL:HG13	7:G:103:PRO:HG3	1.75	0.68
2:B:458:LYS:NZ	2:B:459:ALA:O	2.20	0.68
25:P:101:GTP:O1G	22:a:72:ARG:NH1	2.27	0.68
18:W:452:LEU:HB3	18:W:499:ARG:HD2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Z:199:LYS:NZ	21:Z:240:GLU:O	2.27	0.67
1:A:486:LEU:HB3	1:A:538:VAL:HG21	1.73	0.67
22:a:514:ILE:HG13	22:a:530:ARG:HE	1.60	0.67
1:A:481:THR:OG1	1:A:483:ARG:NH1	2.28	0.67
5:E:20:LEU:HD21	5:E:24:ARG:HH21	1.60	0.67
2:B:748:ALA:HB3	2:B:811:TYR:HB2	1.75	0.67
22:a:9:ARG:O	22:a:128:HIS:NE2	2.28	0.67
17:V:24:THR:HG22	17:V:25:GLU:HB3	1.77	0.67
1:A:1468:THR:HG23	6:F:64:ARG:HB2	1.77	0.67
22:a:515:ILE:O	22:a:530:ARG:NH2	2.28	0.67
1:A:111:CYS:HB3	1:A:116:LYS:H	1.61	0.66
2:B:65:ILE:HD11	2:B:86:LEU:HD12	1.76	0.66
2:B:630:LYS:O	2:B:632:LYS:N	2.27	0.66
22:a:468:ASP:OD1	22:a:530:ARG:NH1	2.29	0.66
17:V:382:VAL:HG13	19:X:22:LEU:HD22	1.76	0.66
1:A:419:ILE:HG23	1:A:427:ILE:HB	1.78	0.66
18:W:188:ILE:HD13	18:W:188:ILE:H	1.60	0.66
2:B:274:ARG:NH2	2:B:281:ASP:OD1	2.28	0.65
8:H:14:ASP:HB2	8:H:29:HIS:HB2	1.78	0.65
22:a:471:LEU:O	22:a:512:ASN:N	2.27	0.65
18:W:444:GLN:NE2	18:W:488:GLU:OE2	2.29	0.65
1:A:420:ILE:HB	1:A:445:LYS:HB2	1.77	0.65
1:A:375:ILE:HG12	1:A:666:ARG:HG3	1.78	0.65
1:A:408:ARG:CD	1:A:414:PRO:HB2	2.26	0.65
1:A:520:MET:HB3	1:A:522:PRO:HD2	1.79	0.65
17:V:22:ASN:ND2	17:V:23:CYS:H	1.94	0.65
18:W:291:ARG:HB3	18:W:316:MET:HE1	1.79	0.65
22:a:514:ILE:HG13	22:a:530:ARG:NE	2.12	0.65
2:B:864:ASP:OD1	21:Z:725:LYS:NZ	2.30	0.64
1:A:886:VAL:HG23	5:E:171:PRO:HD3	1.78	0.64
3:C:7:PRO:O	11:K:104:ARG:NH1	2.30	0.64
1:A:1093:GLN:HE22	2:B:1093:CYS:HA	1.62	0.64
2:B:677:MET:HE2	2:B:700:PRO:HB3	1.79	0.64
9:I:80:ARG:HG3	9:I:95:VAL:HG12	1.80	0.64
16:U:120:ILE:HD12	18:W:206:ARG:HB2	1.79	0.64
2:B:501:LEU:HD12	2:B:505:LEU:HD13	1.78	0.63
1:A:623:PRO:HA	8:H:27:ARG:HH21	1.64	0.63
2:B:873:LEU:HD13	2:B:875:GLU:H	1.63	0.63
3:C:78:ILE:HD11	3:C:126:ARG:HD2	1.80	0.63
22:a:31:LEU:O	22:a:46:HIS:HD2	1.80	0.63
2:B:636:LYS:H	2:B:639:HIS:HD2	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:135:GLN:HE22	4:D:138:ARG:HH11	1.45	0.63
21:Z:427:GLU:OE2	21:Z:469:ARG:NH2	2.31	0.63
22:a:470:ARG:HB2	22:a:536:PRO:CD	2.28	0.63
2:B:483:ARG:HH12	2:B:528:LEU:HA	1.63	0.63
13:N:42:DT:H3	15:T:7:DA:H61	1.47	0.63
2:B:851:ASP:OD2	12:L:17:TYR:OH	2.17	0.63
22:a:291:VAL:HG11	22:a:421:SER:HB3	1.79	0.63
18:W:455:LEU:HD12	18:W:469:VAL:HG13	1.80	0.63
18:W:322:PRO:O	18:W:375:ARG:NH2	2.30	0.62
1:A:228:ILE:O	1:A:244:ARG:NH2	2.32	0.62
13:N:27:DG:H2'	13:N:28:DA:C4	2.34	0.62
1:A:408:ARG:HH21	1:A:414:PRO:HD2	1.62	0.62
2:B:780:VAL:HG12	2:B:965:ILE:HB	1.81	0.62
8:H:128:ASP:OD2	16:U:28:SER:OG	2.17	0.62
5:E:129:GLN:O	5:E:181:ARG:NH2	2.32	0.62
1:A:477:LEU:HB2	1:A:483:ARG:HH21	1.63	0.62
1:A:413:TYR:HB3	1:A:414:PRO:HD3	1.81	0.62
2:B:873:LEU:HD22	2:B:874:PRO:HD2	1.80	0.62
1:A:1115:LYS:NZ	1:A:1138:SER:OG	2.30	0.62
1:A:1239:PHE:HB3	1:A:1243:LEU:HD23	1.80	0.62
2:B:760:THR:OG1	2:B:764:MET:SD	2.56	0.62
9:I:68:ILE:O	9:I:122:ARG:NH1	2.32	0.62
22:a:35:TYR:HB2	22:a:44:ARG:HH22	1.64	0.62
22:a:52:ASN:CG	22:a:512:ASN:HB2	2.25	0.62
1:A:78:MET:O	2:B:1072:ARG:NH2	2.32	0.62
1:A:408:ARG:NE	1:A:414:PRO:HB2	2.14	0.61
17:V:48:LEU:O	17:V:58:ARG:NH2	2.31	0.61
22:a:195:GLU:OE1	22:a:247:GLN:NE2	2.28	0.61
2:B:1062:ARG:NH2	2:B:1066:PRO:O	2.29	0.61
1:A:48:GLU:HG2	1:A:53:LYS:HD3	1.82	0.61
22:a:33:PRO:HG2	22:a:492:GLY:HA2	1.82	0.61
21:Z:367:SER:HB2	21:Z:372:LEU:HD23	1.81	0.61
1:A:44:PRO:HB3	1:A:284:VAL:HG23	1.81	0.61
1:A:922:PHE:HA	1:A:1052:ARG:HD3	1.83	0.61
18:W:481:HIS:O	18:W:489:GLN:NE2	2.32	0.61
1:A:383:SER:H	11:K:2:ASN:HD21	1.49	0.61
1:A:680:LEU:HD21	2:B:784:SER:HB3	1.82	0.61
6:F:100:ARG:NH2	6:F:121:ASP:O	2.32	0.60
1:A:415:GLY:O	1:A:449:HIS:HD2	1.83	0.60
1:A:461:GLN:HG2	15:T:26:DG:H1'	1.83	0.60
1:A:905:ASN:ND2	1:A:975:SER:OG	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:51:LEU:HA	17:V:54:HIS:CD2	2.30	0.60
22:a:470:ARG:HD3	22:a:472:LYS:HG3	1.82	0.60
1:A:539:GLN:NE2	2:B:790:GLN:O	2.35	0.60
18:W:443:LEU:O	18:W:448:THR:OG1	2.19	0.60
21:Z:440:ILE:HG23	21:Z:450:ILE:HD11	1.84	0.60
1:A:1163:HIS:HE1	1:A:1297:THR:HG22	1.66	0.60
18:W:393:VAL:HG21	18:W:423:VAL:HG13	1.83	0.60
1:A:581:LYS:HB2	8:H:91:VAL:HG23	1.83	0.60
5:E:14:ARG:HE	5:E:18:MET:HE2	1.67	0.60
7:G:45:VAL:HA	7:G:76:VAL:HG12	1.81	0.60
2:B:631:GLN:O	2:B:683:GLN:HG2	2.01	0.60
3:C:260:GLN:HB2	11:K:91:ILE:HG21	1.84	0.60
18:W:540:VAL:HG23	18:W:541:ILE:HG23	1.84	0.60
13:N:27:DG:H2'	13:N:28:DA:C5	2.37	0.60
2:B:403:LEU:HD23	2:B:444:LEU:HD13	1.84	0.60
5:E:24:ARG:HH12	5:E:184:GLY:HA3	1.67	0.60
22:a:46:HIS:HB2	22:a:534:SER:CB	2.31	0.60
1:A:412:GLN:O	1:A:415:GLY:N	2.27	0.59
22:a:15:ARG:HA	22:a:28:LYS:HE2	1.83	0.59
2:B:718:GLN:HG2	2:B:720:PRO:HD2	1.83	0.59
2:B:796:MET:HB2	2:B:948:GLN:HG2	1.85	0.59
1:A:801:GLY:HA3	2:B:503:ASN:HB2	1.83	0.59
3:C:175:LYS:HZ2	12:L:57:ALA:HB3	1.65	0.59
17:V:8:LEU:HD13	17:V:8:LEU:H	1.67	0.59
22:a:439:GLY:CA	22:a:461:PRO:HD2	2.31	0.59
2:B:86:LEU:HD23	2:B:130:LYS:HB3	1.85	0.59
20:Y:94:PRO:HD2	20:Y:97:ILE:HD12	1.85	0.59
1:A:1005:HIS:HD2	1:A:1006:PRO:HD2	1.66	0.59
22:a:39:VAL:HG12	22:a:43:ASN:HD22	1.68	0.59
2:B:1135:TYR:HB3	2:B:1146:ILE:HD13	1.85	0.59
13:N:39:DA:H2''	13:N:40:DG:C8	2.38	0.59
22:a:372:VAL:HG12	22:a:380:ARG:HG2	1.83	0.59
22:a:284:LEU:O	22:a:284:LEU:HD22	2.03	0.59
1:A:115:SER:HB3	1:A:227:ARG:HD3	1.84	0.59
1:A:628:VAL:HA	1:A:638:GLY:HA3	1.84	0.59
22:a:470:ARG:CB	22:a:536:PRO:HD3	2.32	0.59
17:V:168:TYR:HB2	17:V:200:VAL:HG11	1.84	0.58
17:V:375:PRO:HB2	19:X:15:LEU:HD13	1.84	0.58
4:D:67:TYR:OH	7:G:86:ASP:O	2.20	0.58
16:U:24:TRP:HA	18:W:235:GLU:HB3	1.84	0.58
22:a:287:LYS:O	22:a:289:TYR:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:7:PRO:HG3	20:Y:23:LYS:HA	1.85	0.58
22:a:130:PHE:CE1	22:a:162:PRO:HD2	2.38	0.58
1:A:977:VAL:HG21	1:A:1040:LEU:HD21	1.85	0.58
17:V:16:LEU:O	17:V:20:LEU:HG	2.04	0.58
1:A:334:ARG:HH11	1:A:335:PRO:HD2	1.68	0.58
1:A:539:GLN:HA	1:A:774:ALA:HB1	1.85	0.58
2:B:334:LYS:HZ3	2:B:337:LYS:HD2	1.69	0.58
1:A:496:PHE:HD2	2:B:791:GLU:HB3	1.69	0.58
1:A:894:ASP:OD2	1:A:1396:ARG:NH2	2.37	0.58
2:B:59:VAL:HG21	2:B:91:ILE:HD12	1.85	0.58
22:a:420:THR:HG23	22:a:423:LYS:HD2	1.84	0.58
1:A:1309:MET:HB3	1:A:1336:LEU:HD23	1.86	0.58
2:B:380:ARG:HH21	2:B:609:GLU:HG2	1.68	0.58
2:B:631:GLN:HB3	2:B:683:GLN:HG3	1.86	0.58
7:G:108:ILE:HD11	7:G:145:LEU:HD22	1.84	0.58
1:A:395:THR:HG23	1:A:397:PHE:H	1.67	0.57
14:P:37:G:H3'	14:P:38:G:H8	1.69	0.57
16:U:138:PRO:HB2	16:U:140:GLU:HG2	1.87	0.57
17:V:61:PHE:HE1	18:W:120:LYS:HA	1.68	0.57
5:E:80:PRO:HA	5:E:107:GLN:HB2	1.86	0.57
17:V:48:LEU:HB3	17:V:58:ARG:HH22	1.69	0.57
1:A:467:MET:HG2	1:A:534:VAL:HG21	1.86	0.57
2:B:790:GLN:O	2:B:968:ASN:ND2	2.37	0.57
18:W:191:VAL:HG22	18:W:193:THR:HG23	1.86	0.57
4:D:114:LEU:HD22	7:G:84:VAL:HG11	1.86	0.57
1:A:480:SER:HB3	11:K:2:ASN:HB2	1.86	0.57
18:W:189:THR:C	18:W:191:VAL:H	2.12	0.57
18:W:195:CYS:HB2	18:W:237:THR:HG21	1.87	0.57
22:a:468:ASP:HA	22:a:530:ARG:NH1	2.20	0.57
1:A:508:SER:HB3	1:A:511:THR:HG22	1.87	0.57
2:B:387:HIS:NE2	2:B:671:GLU:OE2	2.38	0.57
22:a:281:ILE:HG13	22:a:284:LEU:HD12	1.85	0.57
22:a:530:ARG:HD2	22:a:533:LYS:HD3	1.87	0.57
1:A:521:VAL:HG22	1:A:522:PRO:HD3	1.87	0.57
6:F:53:THR:OG1	6:F:118:TRP:NE1	2.36	0.57
1:A:322:LEU:HG	1:A:325:LEU:HD12	1.86	0.57
2:B:1119:CYS:HA	2:B:1146:ILE:HA	1.86	0.56
1:A:394:VAL:HG21	1:A:440:LEU:HD22	1.86	0.56
6:F:86:GLU:OE2	6:F:95:LYS:NZ	2.39	0.56
6:F:53:THR:HG1	6:F:118:TRP:HE1	1.52	0.56
9:I:119:CYS:SG	9:I:120:GLY:N	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:U:137:LEU:O	18:W:260:ARG:NH1	2.35	0.56
18:W:102:ILE:CB	18:W:108:PRO:HB3	2.36	0.56
22:a:284:LEU:O	22:a:289:TYR:HB2	2.06	0.56
1:A:415:GLY:O	1:A:449:HIS:CD2	2.58	0.56
1:A:1194:ASN:HA	1:A:1197:TYR:HB2	1.87	0.56
2:B:483:ARG:NH2	2:B:527:ALA:O	2.38	0.56
1:A:552:ASP:HB2	8:H:24:ARG:HB2	1.86	0.56
2:B:1143:LYS:NZ	21:Z:522:SER:O	2.38	0.56
22:a:33:PRO:HB2	22:a:492:GLY:HA2	1.86	0.56
22:a:81[A]:LYS:HZ3	22:a:472:LYS:HD2	1.69	0.56
13:N:36:DG:H2''	13:N:37:DG:C8	2.39	0.56
18:W:543:PRO:HD2	18:W:544:PRO:HD3	1.87	0.56
2:B:153:PRO:HG2	2:B:448:LEU:HD12	1.87	0.56
2:B:721:ARG:HD2	2:B:975:ARG:HB3	1.88	0.56
7:G:17:TYR:HE2	22:a:480:GLY:HA3	1.71	0.56
5:E:9:ARG:HG3	5:E:136:LEU:HD21	1.86	0.56
2:B:1016:SER:HB2	2:B:1022:LEU:HD23	1.88	0.55
1:A:76:GLY:HA3	1:A:81:CYS:HB2	1.88	0.55
18:W:353:LYS:HE3	18:W:394:HIS:CD2	2.38	0.55
21:Z:479:LYS:HG3	21:Z:489:THR:HG22	1.88	0.55
17:V:22:ASN:HD22	17:V:22:ASN:N	2.05	0.55
17:V:34:GLN:NE2	18:W:59:GLU:O	2.37	0.55
20:Y:7:PRO:HB3	20:Y:24:THR:HG23	1.88	0.55
21:Z:280:ARG:HB3	21:Z:288:ASP:HA	1.87	0.55
2:B:94:SER:HB3	2:B:123:PRO:HG2	1.88	0.55
1:A:896:LEU:HB2	1:A:1396:ARG:HH21	1.70	0.55
2:B:1031:GLY:O	3:C:36:ARG:NH1	2.40	0.55
16:U:58:LEU:HD11	18:W:239:LEU:HD22	1.88	0.55
1:A:1193:VAL:O	1:A:1197:TYR:N	2.39	0.55
13:N:26:DG:H1	15:T:23:DC:N4	2.04	0.55
22:a:468:ASP:HA	22:a:530:ARG:NH2	2.22	0.55
22:a:514:ILE:HD11	22:a:536:PRO:HA	1.89	0.55
1:A:1170:THR:HA	1:A:1216:LEU:HD13	1.89	0.55
2:B:1038:THR:HA	3:C:195:THR:HA	1.88	0.55
18:W:196:GLN:HG3	18:W:197:GLN:HG3	1.88	0.55
1:A:957:GLU:OE2	1:A:960:ARG:NH2	2.40	0.55
1:A:1305:SER:OG	1:A:1339:ASP:HB3	2.07	0.55
2:B:378:GLY:HA3	9:I:102:ALA:HB3	1.89	0.55
1:A:554:PHE:HB3	1:A:585:LEU:HG	1.88	0.55
2:B:817:GLN:HB3	2:B:918:PHE:HD1	1.71	0.55
1:A:723:ASN:OD1	9:I:109:ARG:NE	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:913:ASN:OD1	1:A:963:ARG:NH1	2.40	0.54
2:B:205:VAL:O	2:B:371:ARG:NH1	2.39	0.54
2:B:223:SER:OG	2:B:350:HIS:ND1	2.27	0.54
2:B:229:SER:HA	2:B:405:ARG:HD3	1.88	0.54
6:F:77:ALA:HB2	7:G:15:PRO:HB3	1.88	0.54
21:Z:306:LYS:HA	21:Z:372:LEU:O	2.08	0.54
21:Z:352:VAL:HG23	21:Z:359:LEU:HD21	1.89	0.54
22:a:291:VAL:HG13	22:a:416:PHE:HD2	1.71	0.54
5:E:192:LYS:HE2	5:E:194:ILE:HD11	1.89	0.54
22:a:54:LEU:HD13	22:a:61:MET:HB2	1.89	0.54
8:H:7:GLU:HG3	8:H:59:VAL:HG22	1.89	0.54
22:a:284:LEU:HD23	22:a:442:PHE:HB3	1.89	0.54
1:A:1427:LEU:HB2	1:A:1456:GLU:HG3	1.90	0.54
2:B:192:LYS:HE3	2:B:449:ALA:HA	1.89	0.54
4:D:17:ALA:HB2	7:G:80:PHE:HB3	1.89	0.54
11:K:63:VAL:HG12	11:K:71:ILE:HG22	1.89	0.54
13:N:29:DG:N2	15:T:20:DC:N3	2.56	0.54
15:T:42:DT:H4'	15:T:43:DC:H5'	1.88	0.54
1:A:1175:ILE:HG12	9:I:54:TYR:HB3	1.89	0.54
22:a:9:ARG:NH1	22:a:197:ASP:OD1	2.40	0.54
1:A:327:ARG:HH21	1:A:329:MET:HB3	1.73	0.54
2:B:1062:ARG:HE	2:B:1065:GLY:H	1.56	0.54
1:A:1473:LEU:HD22	6:F:68:THR:HG21	1.89	0.54
2:B:934:LYS:HG2	2:B:1051:LEU:HD12	1.90	0.54
1:A:30:GLU:HA	1:A:33:ARG:HG2	1.88	0.54
1:A:457:ILE:HD11	1:A:515:ILE:HD12	1.90	0.54
1:A:833:PRO:HB2	2:B:506:TRP:HH2	1.73	0.54
2:B:454:GLY:HA3	2:B:458:LYS:HD3	1.90	0.54
17:V:367:VAL:HG22	19:X:5:PRO:HD3	1.89	0.54
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.90	0.54
18:W:414:LEU:O	18:W:418:ILE:HG13	2.07	0.54
17:V:379:SER:HB3	19:X:15:LEU:HD22	1.89	0.53
22:a:10:TRP:HE3	22:a:11:LEU:HD23	1.74	0.53
1:A:296:ASN:HB2	21:Z:267:VAL:HG21	1.90	0.53
1:A:1138:SER:H	1:A:1360:ASN:HB3	1.73	0.53
2:B:737:ILE:HG21	2:B:743:ARG:HD3	1.90	0.53
21:Z:184:CYS:SG	21:Z:185:LYS:N	2.82	0.53
2:B:230:ARG:NH1	2:B:231:PRO:O	2.42	0.53
16:U:61:LEU:HD21	18:W:282:ALA:HB2	1.90	0.53
22:a:515:ILE:HD12	22:a:517:CYS:SG	2.47	0.53
1:A:805:ARG:NH2	2:B:670:GLU:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:601:VAL:HG22	2:B:616:THR:HG23	1.91	0.53
2:B:779:ILE:HD13	2:B:1045:PRO:HB3	1.90	0.53
11:K:56:VAL:HG22	11:K:77:THR:HG22	1.90	0.53
16:U:23:LEU:HB2	18:W:234:GLY:HA2	1.91	0.53
21:Z:450:ILE:HG21	21:Z:468:LEU:HD11	1.91	0.53
21:Z:479:LYS:HD3	21:Z:521:CYS:HB2	1.89	0.53
8:H:60:ILE:HG21	8:H:135:PHE:HE1	1.73	0.53
22:a:545:VAL:O	22:a:549:ILE:HG23	2.08	0.53
1:A:1372:GLU:OE2	5:E:195:ARG:NH1	2.42	0.53
1:A:1473:LEU:HD23	6:F:104:ILE:HG21	1.91	0.53
5:E:44:PHE:HB3	5:E:53:PRO:HB3	1.91	0.53
22:a:377:PHE:HD1	22:a:380:ARG:HH21	1.56	0.53
2:B:826:GLU:H	2:B:872:THR:HG22	1.73	0.53
22:a:358:ARG:HG3	22:a:409:SER:HB3	1.91	0.53
1:A:734:ARG:NE	9:I:105:GLU:O	2.28	0.53
2:B:610:ARG:NH1	9:I:71:ASP:OD2	2.42	0.53
1:A:690:GLY:HA2	2:B:1023:ARG:HG2	1.91	0.53
18:W:234:GLY:O	18:W:237:THR:OG1	2.22	0.53
1:A:549:THR:HG21	1:A:640:LEU:H	1.74	0.52
16:U:24:TRP:CD1	18:W:235:GLU:HB2	2.44	0.52
16:U:127:LYS:HG3	18:W:213:LEU:HD23	1.90	0.52
17:V:375:PRO:C	19:X:15:LEU:HD13	2.34	0.52
2:B:665:ILE:HG23	2:B:669:GLU:HB3	1.90	0.52
2:B:954:MET:HG3	2:B:963:PRO:HD2	1.91	0.52
22:a:327:PHE:HB3	22:a:337:LEU:HD12	1.91	0.52
1:A:98:GLY:HA3	1:A:1440:MET:HE2	1.90	0.52
1:A:691:ASP:OD2	1:A:765:ASN:ND2	2.42	0.52
2:B:628:VAL:HG12	2:B:630:LYS:O	2.09	0.52
18:W:191:VAL:HG13	18:W:193:THR:H	1.75	0.52
1:A:760:LEU:HG	1:A:767:LYS:HB2	1.91	0.52
22:a:27:LEU:HD11	22:a:61:MET:HE1	1.90	0.52
17:V:16:LEU:HD13	18:W:57:ILE:N	2.24	0.52
22:a:335:MET:HE3	22:a:336:HIS:H	1.75	0.52
1:A:408:ARG:HD3	1:A:414:PRO:HB2	1.90	0.52
2:B:585:ASN:OD1	2:B:588:ARG:NH2	2.43	0.52
15:T:3:DT:H2"	15:T:4:DC:C5	2.45	0.52
17:V:445:LEU:HD21	17:V:485:LEU:HA	1.92	0.52
3:C:105:VAL:HG11	3:C:115:VAL:HG22	1.91	0.52
3:C:44:ILE:HG21	3:C:178:PRO:HB3	1.93	0.51
14:P:38:G:H2'	14:P:39:A:C8	2.45	0.51
18:W:191:VAL:HG13	18:W:193:THR:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:50:LEU:HD11	22:a:61:MET:HE3	1.92	0.51
22:a:419:CYS:O	22:a:422:ARG:NE	2.43	0.51
1:A:405:LEU:HD12	1:A:414:PRO:C	2.35	0.51
2:B:237:VAL:HG13	2:B:269:ILE:HD11	1.90	0.51
2:B:1125:MET:HE1	2:B:1156:LYS:HG2	1.92	0.51
4:D:56:GLU:HB3	22:a:505:LYS:HZ3	1.75	0.51
2:B:939:HIS:NE2	2:B:983:GLU:OE1	2.39	0.51
5:E:107:GLN:HA	5:E:132:GLN:HG3	1.91	0.51
18:W:260:ARG:NE	18:W:264:GLU:OE2	2.34	0.51
3:C:49:TRP:HB3	3:C:164:TYR:HB2	1.92	0.51
22:a:276:MET:HG3	22:a:457:LEU:HB3	1.91	0.51
22:a:535:PHE:HD1	22:a:536:PRO:HD2	1.73	0.51
1:A:1212:LEU:HB3	1:A:1259:ILE:HB	1.92	0.51
8:H:32:SER:OG	8:H:36:LYS:N	2.44	0.51
8:H:39:LEU:HD12	8:H:125:LEU:HD13	1.92	0.51
9:I:97:PHE:HB2	9:I:100:HIS:HE2	1.75	0.51
22:a:491:VAL:HG22	22:a:498:PHE:HB2	1.93	0.51
1:A:1104:LEU:O	1:A:1122:PRO:HD2	2.10	0.51
2:B:626:LEU:HD23	2:B:662:VAL:HG12	1.93	0.51
2:B:927:ARG:HG3	2:B:1054:MET:HE3	1.93	0.51
22:a:464:LEU:HG	22:a:518:LYS:HD3	1.92	0.51
1:A:756:ALA:HB2	1:A:786:ALA:HB2	1.93	0.51
1:A:1005:HIS:CD2	1:A:1006:PRO:HD2	2.45	0.51
22:a:287:LYS:HG2	22:a:289:TYR:CE1	2.46	0.51
1:A:61:ARG:HA	1:A:72:GLN:HB3	1.93	0.51
1:A:1461:GLY:HA3	2:B:1152:PRO:HD3	1.91	0.51
16:U:17:LEU:HB2	16:U:52:VAL:HG13	1.92	0.51
18:W:109:VAL:O	18:W:112:GLN:N	2.26	0.51
18:W:558:GLU:HA	18:W:562:ILE:HD11	1.91	0.51
1:A:999:ARG:NH1	8:H:103:GLU:OE1	2.44	0.51
1:A:1366:PHE:HB2	1:A:1374:VAL:HG21	1.92	0.51
2:B:26:CYS:O	2:B:29:VAL:HG12	2.10	0.51
4:D:42:GLU:HG2	4:D:65:LEU:HD11	1.93	0.51
18:W:516:ILE:HG23	18:W:530:ILE:HD12	1.91	0.51
22:a:459:TRP:CZ3	22:a:461:PRO:HD3	2.46	0.51
5:E:26:TYR:HD1	5:E:64:HIS:HA	1.74	0.51
8:H:49:PRO:O	8:H:147:LYS:NZ	2.43	0.51
1:A:76:GLY:HA2	1:A:80:GLU:HG3	1.93	0.50
1:A:459:ASN:HB3	1:A:469:MET:HG3	1.93	0.50
1:A:1118:THR:HG22	1:A:1136:THR:HB	1.92	0.50
1:A:1286:ARG:HD2	2:B:252:ILE:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:LEU:HD12	10:J:6:ARG:HD2	1.93	0.50
4:D:31:THR:HG22	7:G:3:TYR:HE1	1.76	0.50
4:D:70:ARG:NH1	7:G:140:ASP:OD1	2.43	0.50
8:H:15:ILE:HG13	8:H:52:LEU:HD12	1.93	0.50
11:K:7:PHE:HB2	11:K:11:LEU:HD12	1.93	0.50
18:W:541:ILE:HD12	18:W:545:TYR:HE1	1.77	0.50
22:a:30:MET:HB3	22:a:47:PRO:HD3	1.93	0.50
22:a:44:ARG:HH11	22:a:46:HIS:HE2	1.58	0.50
1:A:1005:HIS:HB3	1:A:1008:LYS:HG2	1.93	0.50
5:E:131:LEU:HD23	5:E:133:GLN:H	1.75	0.50
8:H:31:GLU:CD	18:W:302:LYS:HG3	2.36	0.50
22:a:293:TRP:HA	22:a:440:LEU:HD23	1.93	0.50
2:B:354:SER:OG	2:B:357:CYS:SG	2.58	0.50
2:B:525:ASN:HD22	2:B:526:LEU:N	2.09	0.50
18:W:187:GLU:HG3	18:W:188:ILE:HG23	1.93	0.50
1:A:901:VAL:HA	1:A:980:PRO:HA	1.92	0.50
2:B:330:VAL:HG12	2:B:331:THR:HG23	1.93	0.50
2:B:497:LYS:HG3	2:B:498:PRO:HD3	1.93	0.50
13:N:40:DG:H2"	13:N:41:DC:C5	2.47	0.50
16:U:9:THR:HG21	16:U:40:ASN:HB3	1.94	0.50
2:B:603:MET:HG3	2:B:614:ILE:HG12	1.94	0.50
4:D:16:ASP:OD2	4:D:18:SER:OG	2.22	0.50
5:E:110:MET:HE1	5:E:118:LEU:HD11	1.93	0.50
1:A:902:GLU:OE2	1:A:985:ARG:NH1	2.40	0.50
2:B:236:TRP:HB2	2:B:259:THR:HB	1.93	0.50
13:N:26:DG:C2	13:N:27:DG:C6	3.00	0.50
18:W:520:LEU:HD12	18:W:530:ILE:HG13	1.93	0.50
22:a:9:ARG:HD3	22:a:196:ASP:OD1	2.12	0.50
22:a:25:LEU:HD23	22:a:61:MET:HE2	1.94	0.50
22:a:495:GLU:CD	22:a:495:GLU:H	2.20	0.50
1:A:892:GLY:HA3	1:A:1396:ARG:HG3	1.93	0.50
1:A:911:PRO:HD2	1:A:967:ARG:HH21	1.76	0.50
2:B:116:ARG:NH1	2:B:118:LEU:HD11	2.27	0.50
2:B:677:MET:H	2:B:682:LEU:HD12	1.77	0.50
14:P:43:C:N4	15:T:29:DG:O6	2.45	0.50
22:a:47:PRO:HD2	22:a:535:PHE:CZ	2.47	0.50
22:a:276:MET:HG2	22:a:457:LEU:HD13	1.93	0.50
11:K:5:PRO:HG2	11:K:8:GLU:HG2	1.93	0.50
21:Z:472:PHE:HE1	21:Z:520:LEU:HB2	1.76	0.50
22:a:470:ARG:CZ	22:a:472:LYS:HZ1	2.25	0.50
1:A:18:ILE:HD12	2:B:1171:MET:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLU:H	1:A:61:ARG:HH12	1.60	0.49
16:U:116:ASN:O	16:U:120:ILE:HG12	2.12	0.49
2:B:480:SER:OG	2:B:525:ASN:OD1	2.18	0.49
2:B:764:MET:HE1	2:B:938:ARG:NH1	2.28	0.49
13:N:45:DG:H2''	13:N:46:DA:C8	2.47	0.49
17:V:54:HIS:ND1	18:W:129:PRO:HD3	2.26	0.49
17:V:512:HIS:CG	17:V:513:PRO:HD3	2.47	0.49
20:Y:60:ILE:HD13	21:Z:190:ARG:HG3	1.93	0.49
15:T:13:DC:H2'	15:T:14:DT:C6	2.47	0.49
16:U:54:LEU:HD11	16:U:93:VAL:HG21	1.93	0.49
16:U:166:LYS:N	18:W:540:VAL:O	2.37	0.49
17:V:26:PRO:O	17:V:30:ILE:HG13	2.12	0.49
17:V:375:PRO:HB2	19:X:15:LEU:CD1	2.42	0.49
1:A:689:ILE:HG21	2:B:985:LEU:HD22	1.95	0.49
2:B:56:GLN:NE2	2:B:89:GLU:O	2.38	0.49
20:Y:71:VAL:HG13	21:Z:264:LEU:HD11	1.95	0.49
22:a:527:MET:HG3	22:a:528:ARG:HG3	1.95	0.49
1:A:510:GLU:OE2	2:B:1101:GLN:NE2	2.46	0.49
22:a:192:TRP:CD1	22:a:192:TRP:H	2.25	0.49
22:a:327:PHE:CD1	22:a:392:ARG:HD2	2.47	0.49
2:B:931:ILE:HA	2:B:945:CYS:HB3	1.95	0.49
3:C:91:GLU:O	3:C:92:GLU:HG3	2.13	0.49
6:F:80:MET:HG3	6:F:103:PRO:HD3	1.94	0.49
8:H:96:VAL:HA	8:H:116:VAL:HA	1.94	0.49
12:L:17:TYR:HB3	12:L:44:MET:HB3	1.94	0.49
22:a:190:PRO:HB3	22:a:192:TRP:CZ3	2.48	0.49
22:a:329:PHE:HD1	22:a:331:LYS:H	1.59	0.49
22:a:476:MET:HG2	22:a:484:GLN:O	2.13	0.49
1:A:1097:GLU:O	1:A:1101:GLN:NE2	2.46	0.49
8:H:97:TYR:CZ	8:H:115:TYR:HB3	2.48	0.49
8:H:100:GLU:HG2	8:H:115:TYR:HE1	1.78	0.49
20:Y:59:GLY:H	21:Z:219:GLU:HB2	1.77	0.49
21:Z:292:GLN:HB3	21:Z:306:LYS:HB3	1.95	0.49
1:A:863:ARG:HH12	1:A:1129:ASN:ND2	2.10	0.49
1:A:1073:GLU:OE2	1:A:1077:ASN:ND2	2.45	0.49
17:V:372:ARG:HB3	19:X:11:GLU:CD	2.38	0.49
2:B:54:SER:O	2:B:58:ILE:HG12	2.12	0.48
2:B:99:TRP:HE1	2:B:105:PRO:HG3	1.78	0.48
2:B:565:THR:HG22	2:B:610:ARG:HB3	1.95	0.48
2:B:826:GLU:N	2:B:872:THR:HG22	2.27	0.48
13:N:30:DC:H2''	13:N:31:DC:H5'	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:28:DG:H2''	15:T:29:DG:H5'	1.94	0.48
16:U:23:LEU:HB3	18:W:236:HIS:CD2	2.48	0.48
16:U:172:ALA:O	16:U:175:ARG:HG3	2.12	0.48
2:B:26:CYS:O	2:B:30:ILE:HG12	2.12	0.48
2:B:561:ILE:HD11	2:B:566:LYS:HG2	1.94	0.48
2:B:584:MET:HG3	2:B:605:ARG:HB2	1.94	0.48
4:D:56:GLU:HB3	22:a:505:LYS:NZ	2.27	0.48
5:E:24:ARG:NH1	5:E:184:GLY:HA3	2.28	0.48
7:G:150:THR:HA	7:G:159:ALA:HA	1.94	0.48
17:V:236:THR:OG1	17:V:308:PRO:HD2	2.13	0.48
2:B:899:SER:OG	2:B:1078:ARG:NH2	2.46	0.48
11:K:47:LYS:HD3	11:K:61:TYR:HD1	1.78	0.48
14:P:31:A:N3	14:P:31:A:H2'	2.28	0.48
1:A:392:GLU:OE2	1:A:401:ARG:NH2	2.40	0.48
2:B:760:THR:O	2:B:999:ALA:N	2.46	0.48
3:C:38:PHE:HE1	3:C:245:VAL:HA	1.77	0.48
8:H:40:ILE:O	8:H:123:MET:HA	2.13	0.48
8:H:52:LEU:HD21	18:W:307:PRO:HB2	1.96	0.48
17:V:382:VAL:HG13	19:X:22:LEU:HD13	1.96	0.48
22:a:482:LEU:HB3	22:a:484:GLN:HB2	1.96	0.48
22:a:514:ILE:HG21	22:a:533:LYS:HB3	1.94	0.48
1:A:601:ASN:OD1	1:A:632:ASN:N	2.35	0.48
2:B:87:LYS:HB3	2:B:129:THR:HG23	1.96	0.48
9:I:11:PHE:HA	9:I:55:VAL:HG11	1.94	0.48
16:U:100:PHE:HB3	16:U:101:PRO:HD3	1.95	0.48
18:W:295:ALA:HB1	18:W:309:ASP:OD1	2.12	0.48
22:a:131:ASN:HB3	22:a:169:TYR:CE2	2.48	0.48
1:A:1053:ARG:NE	1:A:1057:GLU:OE2	2.32	0.48
22:a:47:PRO:HD2	22:a:535:PHE:CE2	2.49	0.48
1:A:90:LEU:HD23	1:A:90:LEU:H	1.79	0.48
1:A:397:PHE:HZ	1:A:1486:ILE:HG12	1.78	0.48
17:V:329:GLU:CD	19:X:23:LYS:HD3	2.39	0.48
18:W:357:ILE:HD12	18:W:390:VAL:HG12	1.95	0.48
1:A:356:GLY:HA3	2:B:1087:GLY:HA2	1.96	0.48
2:B:65:ILE:HB	2:B:416:ARG:HH11	1.79	0.48
3:C:259:LEU:HG	11:K:42:LEU:HD21	1.96	0.48
18:W:109:VAL:C	18:W:111:VAL:N	2.69	0.48
22:a:44:ARG:HD2	22:a:46:HIS:NE2	2.27	0.48
2:B:744:MET:HE1	2:B:906:GLN:HG3	1.96	0.48
1:A:1138:SER:HB2	1:A:1360:ASN:HB2	1.96	0.48
8:H:20:LYS:HE2	8:H:23:ASP:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:TYR:O	1:A:414:PRO:C	2.57	0.47
2:B:280:SER:OG	9:I:21:ASN:O	2.31	0.47
5:E:15:LYS:HE2	5:E:34:ASP:HA	1.96	0.47
12:L:56:ASP:CG	12:L:58:ARG:HH11	2.22	0.47
13:N:28:DA:C5	13:N:29:DG:C6	3.02	0.47
17:V:19:THR:O	17:V:22:ASN:ND2	2.47	0.47
18:W:241:ALA:O	18:W:245:MET:HG2	2.14	0.47
1:A:340:LYS:HG2	1:A:1436:VAL:HG21	1.95	0.47
1:A:875:TYR:HA	1:A:1083:PRO:HB3	1.95	0.47
7:G:44:PHE:CE2	7:G:104:MET:HB2	2.49	0.47
17:V:371:THR:O	19:X:12:GLU:HB2	2.14	0.47
22:a:39:VAL:HG21	22:a:44:ARG:NH2	2.29	0.47
1:A:460:ARG:HD2	1:A:494:ALA:HB2	1.95	0.47
1:A:1177:TYR:H	9:I:51:SER:HB3	1.80	0.47
2:B:130:LYS:O	2:B:141:GLN:HA	2.13	0.47
17:V:367:VAL:HG13	19:X:5:PRO:HG3	1.94	0.47
18:W:329:ARG:NE	18:W:363:ALA:O	2.43	0.47
22:a:33:PRO:CB	22:a:492:GLY:HA2	2.43	0.47
1:A:606:HIS:CE1	1:A:641:CYS:HB3	2.49	0.47
3:C:259:LEU:HD21	11:K:35:ILE:HD12	1.95	0.47
17:V:235:CYS:HB3	17:V:303:MET:O	2.15	0.47
1:A:264:VAL:HG21	14:P:37:G:O2'	2.13	0.47
2:B:1040:GLN:NE2	3:C:195:THR:OG1	2.48	0.47
7:G:151:ARG:HA	7:G:151:ARG:HD3	1.64	0.47
16:U:48:LEU:HD23	16:U:48:LEU:H	1.80	0.47
1:A:1343:LEU:C	1:A:1345:ARG:H	2.22	0.47
2:B:274:ARG:NH1	2:B:312:GLN:HA	2.30	0.47
2:B:1088:GLU:CD	2:B:1088:GLU:H	2.22	0.47
16:U:79:ILE:HD13	16:U:98:LYS:HA	1.95	0.47
1:A:809:HIS:HE1	2:B:506:TRP:CE2	2.33	0.47
1:A:1027:ASP:OD1	1:A:1027:ASP:N	2.45	0.47
1:A:1115:LYS:HZ3	1:A:1136:THR:HG22	1.80	0.47
1:A:1211:LEU:HD22	1:A:1258:ARG:HH21	1.79	0.47
12:L:26:ASN:HD21	12:L:44:MET:HE1	1.79	0.47
17:V:12:ASN:HB3	17:V:15:ASP:HB2	1.96	0.47
21:Z:484:ARG:HH11	21:Z:485:PHE:HE1	1.62	0.47
1:A:31:LEU:HD11	1:A:254:PRO:HB3	1.97	0.47
1:A:417:LYS:HD3	1:A:430:ARG:HH21	1.80	0.47
2:B:270:ILE:HG13	2:B:305:LEU:HA	1.97	0.47
13:N:29:DG:H1	15:T:20:DC:H42	1.63	0.47
21:Z:433:LEU:HB3	21:Z:436:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Z:705:LEU:HG	21:Z:724:VAL:HG21	1.96	0.47
1:A:577:PRO:HG3	1:A:586:TRP:CZ2	2.50	0.47
1:A:695:ASP:N	1:A:695:ASP:OD1	2.48	0.47
2:B:967:ILE:HG21	2:B:1048:TYR:OH	2.15	0.47
3:C:256:LEU:HD13	11:K:94:LEU:HB3	1.97	0.47
17:V:53:LEU:O	18:W:129:PRO:HG2	2.15	0.47
18:W:193:THR:HB	18:W:233:HIS:NE2	2.30	0.47
22:a:165:TYR:HA	22:a:187:PRO:HD2	1.96	0.47
22:a:246:THR:HG22	22:a:248:PRO:HD2	1.97	0.47
1:A:140:ARG:HH11	1:A:237:GLY:HA2	1.80	0.47
1:A:909:LEU:C	1:A:911:PRO:HD3	2.40	0.47
22:a:32:GLY:O	22:a:44:ARG:NH1	2.48	0.47
1:A:693:ILE:HG21	2:B:1023:ARG:HH21	1.79	0.46
1:A:912:SER:O	1:A:913:ASN:C	2.58	0.46
1:A:1218:ARG:NH2	1:A:1252:ALA:O	2.49	0.46
7:G:91:GLN:HB3	7:G:98:PHE:HB2	1.98	0.46
15:T:27:DT:H2'	15:T:28:DG:H8	1.75	0.46
1:A:362:SER:HB2	2:B:1084:LEU:HD12	1.98	0.46
1:A:496:PHE:HB2	2:B:791:GLU:O	2.15	0.46
1:A:693:ILE:HD12	2:B:1023:ARG:HE	1.80	0.46
1:A:1210:TRP:HZ3	9:I:28:GLU:HB3	1.79	0.46
1:A:1321:ILE:HG12	1:A:1331:LEU:HD13	1.96	0.46
2:B:401:ALA:O	2:B:405:ARG:HG3	2.15	0.46
17:V:117:MET:HE3	17:V:123:VAL:HG11	1.97	0.46
21:Z:291:ALA:HB1	21:Z:305:LEU:HB3	1.98	0.46
21:Z:506:LEU:HD21	21:Z:527:GLY:HA2	1.97	0.46
1:A:592:PHE:HA	1:A:595:ILE:HD12	1.97	0.46
1:A:821:GLY:HA2	1:A:838:PHE:CD2	2.50	0.46
22:a:349:ASP:OD2	22:a:358:ARG:NH1	2.46	0.46
1:A:299:ALA:HA	21:Z:262:ASP:HB3	1.97	0.46
1:A:1113:SER:C	1:A:1115:LYS:H	2.24	0.46
2:B:801:VAL:HG13	2:B:929:PRO:HD2	1.98	0.46
2:B:924:ARG:NH1	3:C:60:HIS:HB2	2.31	0.46
3:C:101:PHE:CE1	3:C:122:SER:HB2	2.51	0.46
7:G:97:LEU:HD23	7:G:108:ILE:HD12	1.97	0.46
21:Z:492:ILE:HG22	21:Z:502:LEU:HB3	1.97	0.46
2:B:438:ARG:O	2:B:442:ASP:HB2	2.16	0.46
2:B:573:TRP:NE1	2:B:575:GLY:O	2.48	0.46
2:B:807:ARG:HA	2:B:929:PRO:HD3	1.98	0.46
10:J:10:CYS:SG	10:J:42:ARG:NE	2.88	0.46
21:Z:424:ASP:HB2	21:Z:440:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1344:MET:H	1:A:1347:LEU:HD12	1.81	0.46
2:B:84:TYR:HB3	2:B:132:VAL:HG23	1.98	0.46
3:C:154:ARG:HD3	10:J:64:PRO:HD3	1.97	0.46
20:Y:58:ASP:HB2	20:Y:88:SER:HB3	1.97	0.46
2:B:733:MET:HE3	2:B:1051:LEU:O	2.15	0.46
3:C:60:HIS:CE1	3:C:63:PHE:HB2	2.51	0.46
5:E:72:MET:HA	5:E:101:ARG:O	2.15	0.46
5:E:75:PHE:HB2	5:E:104:ILE:HG22	1.97	0.46
10:J:35:LEU:HD13	10:J:46:ARG:HB3	1.97	0.46
17:V:143:VAL:O	17:V:147:ARG:HG3	2.15	0.46
18:W:566:ILE:HD13	18:W:574:PRO:HG3	1.96	0.46
1:A:129:ILE:HD13	1:A:143:HIS:HB3	1.97	0.46
1:A:1123:ARG:NH2	1:A:1360:ASN:OD1	2.49	0.46
2:B:442:ASP:C	2:B:456:GLN:HE22	2.24	0.46
2:B:502:HIS:N	2:B:505:LEU:HD12	2.30	0.46
2:B:1062:ARG:NH1	2:B:1074:PRO:HB3	2.31	0.46
3:C:131:THR:HG21	10:J:16:ASN:HD22	1.80	0.46
5:E:100:THR:HB	5:E:125:TYR:HA	1.97	0.46
17:V:34:GLN:HB3	18:W:60:PRO:HA	1.97	0.46
1:A:327:ARG:NH2	1:A:329:MET:HB3	2.31	0.46
1:A:1248:ASN:HD22	1:A:1249:ASP:H	1.64	0.46
2:B:777:ASN:O	10:J:47:ARG:NH1	2.49	0.46
3:C:40:ALA:HB1	3:C:171:LYS:HG3	1.98	0.46
5:E:171:PRO:O	5:E:207:ARG:HA	2.16	0.46
11:K:35:ILE:HB	11:K:71:ILE:HG12	1.97	0.46
14:P:42:C:H2'	14:P:43:C:C6	2.50	0.46
17:V:7:ASP:OD1	17:V:7:ASP:N	2.29	0.46
1:A:769:MET:SD	2:B:973:PRO:HG3	2.56	0.46
1:A:1182:GLN:H	1:A:1182:GLN:CD	2.23	0.46
2:B:254:GLN:H	2:B:254:GLN:HG2	1.51	0.46
7:G:14:HIS:NE2	22:a:479:GLU:OE2	2.49	0.46
18:W:542:ALA:HB3	18:W:543:PRO:HD3	1.98	0.46
22:a:98:PRO:HA	22:a:102:ASN:HD22	1.81	0.46
1:A:151:LYS:HA	1:A:151:LYS:HD3	1.50	0.45
1:A:910:LYS:N	1:A:911:PRO:HD3	2.31	0.45
2:B:242:ARG:HD2	2:B:242:ARG:HA	1.55	0.45
13:N:29:DG:H2''	13:N:30:DC:H5	1.78	0.45
22:a:466:SER:HA	22:a:518:LYS:HA	1.98	0.45
22:a:489:LEU:HD11	22:a:501:ILE:HB	1.98	0.45
1:A:439:HIS:CG	22:a:496:ARG:HH11	2.34	0.45
8:H:98:ARG:HB3	8:H:115:TYR:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:29:DG:H4'	15:T:30:DG:OP1	2.15	0.45
21:Z:390:LEU:HD23	21:Z:393:LEU:HD12	1.99	0.45
22:a:469:PHE:CD2	22:a:489:LEU:HD13	2.51	0.45
1:A:1097:GLU:HB3	1:A:1098:PRO:HD3	1.97	0.45
1:A:1457:ASN:HD22	1:A:1462:GLN:HE21	1.65	0.45
2:B:710:ILE:HA	2:B:764:MET:HE2	1.98	0.45
3:C:40:ALA:O	3:C:169:PHE:HB2	2.17	0.45
22:a:470:ARG:CB	22:a:535:PHE:HB2	2.44	0.45
1:A:117:LEU:HD21	1:A:232:GLU:HB3	1.97	0.45
1:A:533:PRO:HD3	1:A:654:HIS:CD2	2.50	0.45
2:B:705:GLY:O	2:B:709:SER:OG	2.26	0.45
5:E:71:GLN:HB2	5:E:99:ILE:HD12	1.99	0.45
5:E:111:THR:HG21	13:N:39:DA:OP1	2.16	0.45
8:H:41:LEU:HG	8:H:43:VAL:HG13	1.99	0.45
12:L:29:LYS:HB3	12:L:32:ASP:HB2	1.99	0.45
13:N:7:DA:H2''	13:N:8:DG:C8	2.50	0.45
21:Z:364:ASN:O	21:Z:374:LYS:NZ	2.31	0.45
22:a:6:ILE:HG22	22:a:7[B]:PRO:HD3	1.98	0.45
1:A:75:ALA:HB1	2:B:1131:ARG:HH11	1.80	0.45
1:A:203:LYS:HD2	1:A:203:LYS:HA	1.47	0.45
17:V:376:MET:SD	17:V:411:PHE:HB2	2.56	0.45
22:a:190:PRO:HB2	22:a:193:CYS:HB3	1.99	0.45
22:a:435:HIS:CG	22:a:436:GLU:N	2.84	0.45
1:A:291:ARG:O	1:A:295:GLN:HB2	2.17	0.45
1:A:540:ASP:HB3	2:B:790:GLN:HE22	1.81	0.45
1:A:668:PHE:CZ	1:A:672:ILE:HD11	2.52	0.45
3:C:38:PHE:CE1	3:C:245:VAL:HA	2.51	0.45
3:C:78:ILE:HG22	3:C:82:LEU:HG	1.98	0.45
9:I:24:LEU:HB3	9:I:37:TYR:HB3	1.99	0.45
16:U:162:HIS:HB3	18:W:549:PHE:HB2	1.99	0.45
22:a:33:PRO:CG	22:a:492:GLY:HA2	2.46	0.45
22:a:87:ILE:HG21	22:a:109:LEU:HD22	1.99	0.45
1:A:1244:ASN:HD22	1:A:1245:CYS:N	2.15	0.45
1:A:1343:LEU:O	1:A:1344:MET:HG2	2.17	0.45
8:H:13:LYS:HG3	8:H:31:GLU:CD	2.41	0.45
8:H:59:VAL:O	8:H:144:LEU:HB2	2.16	0.45
1:A:465:HIS:CD2	1:A:467:MET:HB2	2.51	0.45
1:A:618:TYR:HB3	1:A:623:PRO:HD3	1.98	0.45
6:F:61:GLU:OE2	6:F:108:ARG:NE	2.50	0.45
7:G:101:ILE:HB	7:G:104:MET:HE2	1.99	0.45
17:V:54:HIS:CE1	18:W:129:PRO:HD3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:58:ASP:OD2	21:Z:268:LYS:NZ	2.31	0.45
22:a:469:PHE:H	22:a:530:ARG:NH2	2.15	0.45
1:A:418:TYR:HB2	1:A:447:GLU:HB2	1.97	0.45
1:A:1248:ASN:HD22	1:A:1249:ASP:N	2.14	0.45
2:B:442:ASP:HB3	2:B:456:GLN:NE2	2.32	0.45
2:B:484:ARG:NH2	2:B:730:LYS:HE3	2.32	0.45
7:G:84:VAL:HG22	7:G:146:LYS:HB2	1.99	0.45
17:V:511:LEU:O	17:V:515:VAL:HG23	2.17	0.45
21:Z:433:LEU:HD13	21:Z:461:LEU:HD13	1.98	0.45
22:a:35:TYR:HB2	22:a:44:ARG:NH2	2.30	0.45
1:A:272:ASN:HD22	1:A:273:GLN:N	2.15	0.45
1:A:1353:ASP:O	1:A:1357:THR:OG1	2.31	0.45
7:G:49:THR:N	7:G:73:LYS:O	2.50	0.45
13:N:41:DC:H2"	13:N:42:DT:C6	2.52	0.45
16:U:38:ILE:HD13	16:U:41:ILE:HD12	1.99	0.45
16:U:96:ILE:HA	16:U:110:LEU:HD21	1.99	0.45
22:a:13[A]:CYS:SG	22:a:28:LYS:HD3	2.57	0.45
22:a:467:VAL:HG23	22:a:545:VAL:HG11	1.98	0.45
1:A:25:VAL:HG23	1:A:247:TRP:HE3	1.82	0.44
1:A:551:ARG:HG2	8:H:25:VAL:HG11	1.99	0.44
1:A:1440:MET:SD	2:B:1167:ILE:HD11	2.57	0.44
2:B:411:LEU:HD21	2:B:435:ILE:HG23	1.99	0.44
7:G:150:THR:OG1	7:G:157:ILE:HG22	2.16	0.44
13:N:26:DG:H2"	13:N:27:DG:C8	2.52	0.44
17:V:76:ARG:HD2	17:V:76:ARG:HA	1.55	0.44
22:a:13[B]:CYS:SG	22:a:28:LYS:HD3	2.57	0.44
22:a:346:MET:SD	22:a:359:TYR:HB2	2.58	0.44
1:A:349:ARG:HH22	2:B:1070:LEU:HD21	1.82	0.44
1:A:911:PRO:HD2	1:A:967:ARG:NH2	2.31	0.44
1:A:952:LEU:O	1:A:955:GLU:HG3	2.18	0.44
19:X:19:PHE:CE2	19:X:23:LYS:HE2	2.52	0.44
22:a:347:ILE:HD13	22:a:360:LEU:HD11	1.99	0.44
1:A:581:LYS:HA	1:A:581:LYS:HD2	1.76	0.44
2:B:483:ARG:O	2:B:525:ASN:ND2	2.50	0.44
8:H:64:LEU:HB3	8:H:83:SER:HB2	2.00	0.44
22:a:293:TRP:HB2	22:a:437:MET:HB3	1.98	0.44
1:A:871:VAL:HG11	1:A:1400:LEU:HD11	1.99	0.44
5:E:84:ILE:HA	5:E:87:ILE:HG12	2.00	0.44
18:W:228:ALA:HA	18:W:231:VAL:HG22	2.00	0.44
1:A:109:CYS:HA	1:A:148:CYS:SG	2.57	0.44
1:A:215:LEU:H	1:A:215:LEU:HG	1.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:GLN:HE21	1:A:334:ARG:HB3	1.83	0.44
2:B:628:VAL:HG22	2:B:633:LEU:HD23	1.98	0.44
2:B:905:ASP:HB2	2:B:924:ARG:HB2	1.99	0.44
2:B:907:VAL:HG13	2:B:921:ILE:HG12	2.00	0.44
2:B:1040:GLN:HG2	3:C:203:TRP:CZ2	2.53	0.44
17:V:242:LEU:HD21	17:V:260:HIS:HA	1.99	0.44
18:W:470:LEU:HD13	18:W:512:VAL:HG22	1.99	0.44
22:a:6:ILE:HG22	22:a:7[A]:PRO:HD3	1.98	0.44
1:A:417:LYS:HA	1:A:429:LEU:HB2	2.00	0.44
1:A:579:ILE:HD13	8:H:92:MET:HG2	2.00	0.44
1:A:922:PHE:HB2	1:A:1052:ARG:HB2	2.00	0.44
2:B:733:MET:HE1	2:B:1054:MET:SD	2.58	0.44
1:A:927:GLU:O	1:A:931:ARG:HG2	2.18	0.44
1:A:992:LYS:HA	1:A:992:LYS:HD3	1.81	0.44
1:A:1020:LEU:O	1:A:1034:GLN:NE2	2.50	0.44
1:A:1365:ILE:O	1:A:1369:LEU:N	2.46	0.44
2:B:92:TYR:HB2	2:B:125:TYR:HB2	1.99	0.44
5:E:24:ARG:HD2	5:E:26:TYR:CE2	2.52	0.44
17:V:66:PHE:CE1	17:V:108:SER:HB2	2.53	0.44
1:A:261:ARG:O	1:A:261:ARG:HG2	2.18	0.44
1:A:736:THR:O	1:A:740:GLN:HG2	2.17	0.44
1:A:1212:LEU:HB2	1:A:1285:LEU:HD21	1.98	0.44
2:B:861:SER:N	2:B:864:ASP:OD2	2.48	0.44
12:L:19:CYS:HB2	12:L:22:CYS:HB2	1.99	0.44
18:W:489:GLN:O	18:W:493:LYS:HG2	2.18	0.44
22:a:380:ARG:HH12	22:a:448:TYR:N	2.15	0.44
2:B:125:TYR:HD1	2:B:148:PHE:HA	1.83	0.44
2:B:629:GLU:CD	2:B:634:LEU:HD11	2.42	0.44
2:B:792:ASP:OD2	2:B:975:ARG:NH2	2.32	0.44
3:C:67:ARG:NH2	3:C:149:LEU:O	2.37	0.44
8:H:35:PHE:HB3	8:H:37:MET:HE3	2.00	0.44
17:V:8:LEU:O	17:V:10:VAL:HG23	2.17	0.44
17:V:51:LEU:O	17:V:54:HIS:HB2	2.18	0.44
22:a:41:GLU:HA	22:a:533:LYS:HB2	1.99	0.44
2:B:113:ALA:HA	2:B:118:LEU:HB2	1.99	0.43
2:B:201:ALA:HB3	2:B:206:TYR:OH	2.18	0.43
17:V:66:PHE:HE1	17:V:108:SER:HB2	1.83	0.43
22:a:516:GLU:N	22:a:528:ARG:O	2.43	0.43
1:A:36:VAL:HG21	1:A:73:THR:OG1	2.18	0.43
1:A:623:PRO:HA	8:H:27:ARG:NH2	2.32	0.43
2:B:929:PRO:HB3	2:B:935:PHE:HZ	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:385:TYR:O	17:V:389:VAL:HG23	2.18	0.43
18:W:407:LEU:HD11	18:W:430:TRP:HH2	1.83	0.43
22:a:145:MET:HB3	22:a:147:TRP:CD1	2.53	0.43
1:A:1191:GLU:HG2	1:A:1195:VAL:HG23	2.00	0.43
2:B:42:GLN:HE22	2:B:483:ARG:HA	1.83	0.43
4:D:87:LEU:HB3	4:D:97:LEU:HG	2.00	0.43
8:H:89:GLU:OE2	8:H:147:LYS:HG2	2.18	0.43
1:A:462:PRO:O	1:A:464:LEU:HG	2.19	0.43
1:A:470:MET:HB3	1:A:521:VAL:HG12	2.00	0.43
1:A:783:GLN:HA	1:A:787:VAL:O	2.19	0.43
1:A:1030:SER:OG	5:E:162:ARG:NE	2.51	0.43
1:A:1307:VAL:HG13	1:A:1338:THR:HA	2.00	0.43
2:B:84:TYR:HA	2:B:131:THR:O	2.18	0.43
2:B:258:ALA:HB2	2:B:269:ILE:HD13	2.00	0.43
2:B:387:HIS:CD2	2:B:504:THR:HG21	2.53	0.43
2:B:506:TRP:HZ2	2:B:677:MET:HE1	1.84	0.43
9:I:65:LEU:HD22	9:I:122:ARG:HG2	2.01	0.43
17:V:22:ASN:ND2	17:V:22:ASN:N	2.65	0.43
17:V:31:GLU:O	17:V:34:GLN:HG3	2.19	0.43
17:V:223:ARG:HH21	17:V:300:ASP:CG	2.25	0.43
17:V:365:MET:HE3	17:V:370:ILE:HD11	2.01	0.43
1:A:552:ASP:HB3	8:H:22:PHE:HB3	1.99	0.43
1:A:685:HIS:HB3	2:B:784:SER:HB2	1.99	0.43
2:B:591:ARG:HD3	2:B:603:MET:HE1	1.99	0.43
2:B:927:ARG:HG3	2:B:1054:MET:CE	2.48	0.43
16:U:92:MET:O	16:U:96:ILE:HG13	2.19	0.43
2:B:22:TRP:CZ3	2:B:635:LEU:HD23	2.54	0.43
2:B:502:HIS:H	2:B:505:LEU:HD12	1.84	0.43
5:E:70:ASP:OD1	5:E:70:ASP:N	2.51	0.43
5:E:194:ILE:HG13	5:E:204:ILE:HG12	2.00	0.43
16:U:121:LEU:HB3	16:U:125:ARG:NH1	2.34	0.43
17:V:30:ILE:CG2	18:W:59:GLU:HA	2.49	0.43
1:A:684:GLY:HA3	2:B:1037:ILE:HG23	2.00	0.43
1:A:1423:ASP:OD1	1:A:1423:ASP:N	2.47	0.43
2:B:629:GLU:O	2:B:630:LYS:HB2	2.18	0.43
22:a:44:ARG:NH1	22:a:46:HIS:HE2	2.16	0.43
22:a:290:LYS:HB3	22:a:415:PHE:HB3	2.01	0.43
1:A:487:SER:OG	1:A:673:GLN:NE2	2.51	0.43
1:A:876:ASP:OD1	1:A:876:ASP:N	2.45	0.43
2:B:93:LEU:HD23	2:B:124:LEU:HD13	1.99	0.43
2:B:463:ARG:HD2	2:B:466:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:587:LEU:HD13	2:B:603:MET:HG2	2.01	0.43
8:H:13:LYS:HB3	18:W:306:ASN:CG	2.43	0.43
16:U:24:TRP:HA	18:W:235:GLU:CB	2.48	0.43
17:V:487:ASP:OD2	17:V:519:LYS:NZ	2.50	0.43
1:A:61:ARG:O	1:A:73:THR:OG1	2.37	0.43
1:A:681:LEU:HD11	2:B:786:THR:HA	2.01	0.43
1:A:763:TYR:OH	8:H:23:ASP:OD2	2.37	0.43
2:B:841:ARG:CZ	14:P:34:G:H21	2.31	0.43
8:H:116:VAL:HG13	8:H:123:MET:HB3	2.01	0.43
18:W:361:ALA:O	18:W:365:SER:CB	2.67	0.43
22:a:284:LEU:HD13	22:a:418:ILE:HD13	1.99	0.43
22:a:328:PRO:HD2	22:a:392:ARG:HG2	2.01	0.43
1:A:469:MET:HE1	2:B:1086:PHE:CE1	2.53	0.43
1:A:1301:ILE:HD12	1:A:1342:SER:HB3	2.01	0.43
2:B:968:ASN:ND2	2:B:970:HIS:HB2	2.34	0.43
6:F:57:MET:HE1	6:F:120:VAL:HG13	2.00	0.43
16:U:162:HIS:HA	18:W:546:THR:HB	2.01	0.43
18:W:161:LYS:O	18:W:165:ALA:HB2	2.18	0.43
18:W:560:ASP:O	18:W:561:SER:OG	2.33	0.43
22:a:514:ILE:HD13	22:a:535:PHE:HA	2.01	0.43
1:A:395:THR:OG1	1:A:396:PRO:HD2	2.19	0.42
1:A:1474:LEU:HB2	6:F:105:ILE:HB	2.01	0.42
7:G:43:GLY:HA2	7:G:157:ILE:HD11	2.01	0.42
1:A:358:ARG:HH12	15:T:27:DT:P	2.42	0.42
1:A:486:LEU:HD21	2:B:790:GLN:HG3	2.01	0.42
2:B:841:ARG:HH12	14:P:35:A:H1'	1.84	0.42
3:C:172:GLU:OE2	12:L:58:ARG:NH2	2.52	0.42
8:H:94:GLY:HA3	8:H:118:TYR:HA	2.01	0.42
8:H:103:GLU:HB3	8:H:109:ALA:HB2	2.00	0.42
16:U:144:LEU:HD12	16:U:148:ALA:HB1	2.01	0.42
22:a:519:PHE:CD2	22:a:549:ILE:HD12	2.53	0.42
1:A:381:PRO:HB3	1:A:480:SER:HA	2.01	0.42
1:A:548:PHE:HD1	1:A:679:TRP:CD2	2.37	0.42
1:A:1199:MET:O	1:A:1200:PRO:C	2.62	0.42
2:B:507:GLY:HA3	2:B:623:ARG:NH1	2.34	0.42
18:W:189:THR:O	18:W:191:VAL:N	2.49	0.42
22:a:46:HIS:HB3	22:a:535:PHE:CG	2.55	0.42
22:a:424:LEU:HD13	22:a:440:LEU:HD21	2.00	0.42
1:A:79:THR:HA	2:B:1072:ARG:HH22	1.84	0.42
1:A:316:THR:HG21	1:A:328:ALA:HB3	2.00	0.42
1:A:368:THR:OG1	2:B:946:GLY:HA2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:LYS:HB3	1:A:582:PRO:HD3	2.01	0.42
2:B:317:ALA:O	2:B:321:ILE:HG12	2.20	0.42
2:B:713:PHE:HB3	2:B:716:HIS:ND1	2.34	0.42
18:W:158:LEU:HA	18:W:190:SER:CB	2.49	0.42
18:W:361:ALA:O	18:W:365:SER:OG	2.34	0.42
22:a:516:GLU:HA	22:a:530:ARG:CZ	2.48	0.42
1:A:184:CYS:HB2	1:A:187:TYR:HB3	2.02	0.42
1:A:329:MET:SD	1:A:333:GLY:HA2	2.59	0.42
1:A:381:PRO:HD2	1:A:384:ILE:HD12	2.02	0.42
1:A:1115:LYS:NZ	1:A:1137:PRO:O	2.46	0.42
2:B:348:LEU:HB3	2:B:351:VAL:HG22	2.01	0.42
16:U:148:ALA:HA	18:W:367:VAL:HG12	2.01	0.42
21:Z:498:ASN:O	21:Z:515:PRO:HD3	2.20	0.42
1:A:229:SER:OG	1:A:230:ASP:N	2.52	0.42
1:A:441:GLN:HG2	1:A:444:TYR:CE2	2.55	0.42
1:A:1468:THR:H	6:F:60:TYR:HB3	1.84	0.42
3:C:172:GLU:CG	12:L:58:ARG:HH21	2.33	0.42
17:V:329:GLU:HA	19:X:19:PHE:CE2	2.54	0.42
22:a:276:MET:CG	22:a:457:LEU:HB3	2.50	0.42
22:a:287:LYS:HG2	22:a:289:TYR:HE1	1.84	0.42
22:a:386:ARG:HG2	22:a:387:GLU:HG2	2.01	0.42
1:A:75:ALA:HB1	2:B:1131:ARG:NH1	2.35	0.42
2:B:180:ASP:OD1	2:B:472:ARG:NH2	2.52	0.42
2:B:285:LEU:HD23	9:I:16:PHE:HZ	1.84	0.42
6:F:69:ARG:NE	6:F:96:GLU:OE1	2.42	0.42
19:X:11:GLU:HG2	19:X:15:LEU:HD11	2.01	0.42
1:A:1217:ASP:OD2	1:A:1220:HIS:ND1	2.34	0.42
15:T:22:DC:O3'	15:T:23:DC:H3'	2.19	0.42
16:U:92:MET:HE2	16:U:92:MET:HB2	1.84	0.42
17:V:512:HIS:ND1	17:V:513:PRO:HD3	2.35	0.42
22:a:15:ARG:HG2	22:a:45:PHE:HB2	2.01	0.42
22:a:469:PHE:HE2	22:a:524:TRP:CD2	2.38	0.42
1:A:415:GLY:C	1:A:449:HIS:HD2	2.28	0.42
1:A:861:GLN:NE2	1:A:1096:GLY:O	2.52	0.42
5:E:75:PHE:HD2	5:E:104:ILE:HG22	1.85	0.42
18:W:349:ASN:O	18:W:351:ASP:N	2.53	0.42
1:A:1244:ASN:O	1:A:1259:ILE:HA	2.20	0.42
3:C:67:ARG:NH1	10:J:3:ILE:O	2.48	0.42
10:J:66:GLU:HA	12:L:18:ILE:HD13	2.01	0.42
12:L:41:TYR:CE2	12:L:43:ILE:HB	2.55	0.42
14:P:37:G:H3'	14:P:38:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:12:ASN:HB2	17:V:15:ASP:C	2.45	0.42
17:V:22:ASN:ND2	17:V:23:CYS:N	2.65	0.42
20:Y:11:ARG:HG2	20:Y:12:HIS:CD2	2.54	0.42
20:Y:56:SER:HB2	20:Y:90:THR:HB	2.01	0.42
1:A:41:ILE:HG13	1:A:55:GLY:O	2.20	0.41
1:A:417:LYS:HD3	1:A:430:ARG:NH2	2.35	0.41
1:A:1171:ALA:O	9:I:59:THR:N	2.45	0.41
8:H:91:VAL:HG22	8:H:144:LEU:HD13	2.02	0.41
18:W:454:LEU:HD13	18:W:454:LEU:HA	1.85	0.41
1:A:197:GLU:OE2	1:A:311:GLN:NE2	2.53	0.41
2:B:290:TYR:HB3	2:B:561:ILE:HG23	2.02	0.41
2:B:809:VAL:HA	2:B:926:VAL:HA	2.01	0.41
8:H:27:ARG:HH11	8:H:40:ILE:HG22	1.85	0.41
17:V:196:ARG:HD3	17:V:243:MET:HB2	2.02	0.41
20:Y:62:ALA:HB3	21:Z:215:VAL:HB	2.02	0.41
22:a:530:ARG:H	22:a:530:ARG:HG3	1.74	0.41
1:A:1432:PHE:CD2	1:A:1433:GLU:HG2	2.56	0.41
2:B:417:ILE:HG22	2:B:421:LYS:NZ	2.35	0.41
2:B:845:TYR:CE1	2:B:865:VAL:HG11	2.54	0.41
2:B:1054:MET:H	2:B:1054:MET:HG2	1.64	0.41
5:E:19:GLN:OE1	5:E:138:ASN:ND2	2.48	0.41
7:G:78:ARG:HD2	7:G:79:PRO:HD2	2.02	0.41
17:V:372:ARG:HB3	19:X:11:GLU:OE1	2.20	0.41
22:a:107:ILE:HG23	22:a:144:LYS:HD3	2.02	0.41
22:a:168:ASP:OD1	22:a:168:ASP:N	2.52	0.41
22:a:471:LEU:HB2	22:a:515:ILE:HD11	2.02	0.41
1:A:327:ARG:H	1:A:327:ARG:HG3	1.30	0.41
1:A:910:LYS:HB2	1:A:910:LYS:HE3	1.82	0.41
2:B:756:LYS:O	2:B:777:ASN:ND2	2.50	0.41
8:H:8:ASP:OD1	8:H:9:ILE:N	2.51	0.41
17:V:494:SER:OG	17:V:495:PRO:HD3	2.20	0.41
18:W:353:LYS:O	18:W:357:ILE:HG12	2.20	0.41
22:a:190:PRO:HB3	22:a:192:TRP:CE3	2.55	0.41
1:A:461:GLN:HG2	15:T:26:DG:C1'	2.50	0.41
17:V:342:LEU:HD11	17:V:374:LEU:HD11	2.03	0.41
22:a:470:ARG:HB3	22:a:490:TYR:HB2	2.03	0.41
15:T:27:DT:C2	15:T:28:DG:N7	2.88	0.41
22:a:44:ARG:O	22:a:534:SER:OG	2.38	0.41
1:A:715:GLU:HA	1:A:718:GLU:HG2	2.03	0.41
1:A:1359:SER:HB3	1:A:1365:ILE:HD11	2.03	0.41
2:B:274:ARG:NH1	2:B:311:ILE:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:463:ARG:HE	2:B:463:ARG:HB3	1.66	0.41
2:B:789:ASN:ND2	2:B:966:ILE:HG22	2.35	0.41
16:U:41:ILE:HG21	16:U:56:LEU:HD21	2.02	0.41
18:W:310:ILE:HG21	18:W:356:TYR:CD1	2.55	0.41
18:W:567:LYS:HG2	18:W:568:THR:HG23	2.03	0.41
22:a:276:MET:HE3	22:a:442:PHE:CD2	2.54	0.41
22:a:441:ILE:HG13	22:a:442:PHE:H	1.86	0.41
1:A:1148:ALA:HB1	1:A:1333:GLU:HB2	2.02	0.41
2:B:1112:ASP:OD1	2:B:1112:ASP:N	2.54	0.41
3:C:7:PRO:HB2	11:K:101:LEU:HD13	2.03	0.41
5:E:102:ALA:HB3	5:E:127:LEU:HD23	2.02	0.41
14:P:41:C:H2'	14:P:42:C:C6	2.56	0.41
17:V:372:ARG:HE	19:X:11:GLU:HB2	1.86	0.41
18:W:299:MET:HB2	18:W:309:ASP:OD2	2.21	0.41
22:a:459:TRP:HZ3	22:a:461:PRO:HD3	1.85	0.41
1:A:585:LEU:HD12	1:A:585:LEU:HA	1.92	0.41
1:A:706:ILE:HD12	1:A:752:THR:HG21	2.03	0.41
1:A:904:GLN:NE2	1:A:981:CYS:O	2.54	0.41
2:B:474:THR:OG1	2:B:732:ALA:O	2.39	0.41
2:B:565:THR:HG21	2:B:580:PRO:HB3	2.01	0.41
2:B:912:ASN:OD1	2:B:916:TYR:N	2.52	0.41
7:G:17:TYR:CG	22:a:482:LEU:HD11	2.56	0.41
7:G:55:GLY:HA3	7:G:69:PRO:HG2	2.03	0.41
7:G:96:GLY:HA3	7:G:107:PHE:CE1	2.56	0.41
16:U:151:THR:HG21	18:W:367:VAL:HB	2.03	0.41
17:V:321:HIS:O	17:V:325:LEU:HG	2.21	0.41
18:W:328:ILE:HD11	18:W:359:ILE:HG23	2.03	0.41
22:a:39:VAL:HG21	22:a:44:ARG:CZ	2.50	0.41
22:a:470:ARG:NH2	22:a:472:LYS:HZ1	2.19	0.41
1:A:26:LEU:HD12	2:B:1166:SER:HA	2.03	0.41
1:A:279:LYS:O	1:A:283:ILE:HG12	2.21	0.41
8:H:41:LEU:HD13	8:H:123:MET:HG3	2.02	0.41
16:U:29:ILE:HG12	16:U:59:GLY:HA3	2.03	0.41
16:U:100:PHE:HB2	16:U:106:LEU:HD23	2.03	0.41
18:W:542:ALA:O	18:W:545:TYR:CZ	2.74	0.41
22:a:284:LEU:HD21	22:a:442:PHE:CD1	2.55	0.41
22:a:366:LYS:HE2	22:a:366:LYS:HB2	1.94	0.41
1:A:108:ARG:HE	1:A:191:ILE:HB	1.86	0.40
1:A:403:GLN:O	1:A:407:ARG:HG2	2.21	0.40
1:A:436:SER:O	22:a:496:ARG:CZ	2.69	0.40
1:A:1216:LEU:HB2	1:A:1255:LEU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1382:LEU:HD21	1:A:1401:LEU:HD23	2.03	0.40
3:C:27:ASP:OD2	11:K:52:LYS:HD2	2.21	0.40
10:J:17:LYS:HB3	10:J:38:LEU:HD13	2.03	0.40
17:V:22:ASN:ND2	17:V:22:ASN:H	2.19	0.40
1:A:552:ASP:HB3	8:H:25:VAL:HG12	2.02	0.40
2:B:249:LYS:HA	2:B:249:LYS:HD2	1.90	0.40
2:B:603:MET:HE2	2:B:603:MET:HB2	1.95	0.40
9:I:64:GLU:O	9:I:68:ILE:HG12	2.22	0.40
17:V:117:MET:HE1	17:V:131:VAL:HG21	2.03	0.40
18:W:203:ARG:HG3	18:W:206:ARG:HH21	1.85	0.40
22:a:52:ASN:ND2	22:a:513:LYS:HG2	2.35	0.40
1:A:196:LEU:HD22	1:A:311:GLN:HE22	1.87	0.40
1:A:368:THR:HG21	2:B:931:ILE:HD12	2.03	0.40
1:A:865:ILE:HG21	2:B:1092:ASP:CG	2.46	0.40
1:A:1054:MET:HA	1:A:1058:PHE:HB2	2.03	0.40
1:A:1189:ASP:HB2	1:A:1192:TRP:CZ2	2.57	0.40
1:A:1436:VAL:O	1:A:1440:MET:HG2	2.21	0.40
2:B:473:LEU:CD2	2:B:1052:LYS:HD2	2.46	0.40
2:B:524:LYS:HE2	2:B:524:LYS:HB2	1.82	0.40
2:B:1087:GLY:N	2:B:1090:GLU:OE1	2.55	0.40
3:C:113:ARG:NH1	3:C:114:HIS:O	2.55	0.40
16:U:142:GLN:HE22	18:W:468:GLN:HE22	1.68	0.40
17:V:376:MET:N	19:X:15:LEU:HD13	2.37	0.40
22:a:41:GLU:HG2	22:a:533:LYS:H	1.86	0.40
22:a:517:CYS:HA	22:a:525:VAL:O	2.22	0.40
1:A:230:ASP:HA	1:A:240:PRO:HG2	2.03	0.40
1:A:814:ASP:OD2	2:B:689:TYR:OH	2.32	0.40
4:D:26:PHE:HE2	7:G:78:ARG:HG2	1.85	0.40
17:V:178:SER:O	17:V:506:ARG:NH2	2.54	0.40
22:a:30:MET:HE1	22:a:64:LEU:HD21	2.04	0.40
22:a:439:GLY:CA	22:a:460:LYS:HA	2.45	0.40
1:A:356:GLY:HA2	2:B:1086:PHE:O	2.21	0.40
1:A:576:GLN:HE21	1:A:580:LEU:HD21	1.85	0.40
1:A:1312:PRO:HG2	1:A:1318:LYS:HG2	2.03	0.40
2:B:393:LEU:HD22	2:B:485:LEU:HD22	2.02	0.40
2:B:865:VAL:HG12	2:B:895:PHE:CE1	2.56	0.40
2:B:1060:HIS:HB3	2:B:1078:ARG:HE	1.86	0.40
8:H:28:LEU:O	8:H:40:ILE:HA	2.21	0.40
15:T:1:DG:H2"	15:T:2:DC:C6	2.56	0.40
18:W:189:THR:C	18:W:191:VAL:N	2.79	0.40
22:a:11:LEU:HD22	22:a:43:ASN:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:192:TRP:CD1	22:a:192:TRP:N	2.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1418/1970 (72%)	1308 (92%)	106 (8%)	4 (0%)	36	69
2	B	1123/1174 (96%)	1054 (94%)	68 (6%)	1 (0%)	48	80
3	C	254/271 (94%)	248 (98%)	6 (2%)	0	100	100
4	D	126/142 (89%)	121 (96%)	5 (4%)	0	100	100
5	E	207/210 (99%)	199 (96%)	8 (4%)	0	100	100
6	F	80/127 (63%)	79 (99%)	1 (1%)	0	100	100
7	G	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
8	H	146/150 (97%)	138 (94%)	8 (6%)	0	100	100
9	I	115/125 (92%)	108 (94%)	7 (6%)	0	100	100
10	J	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
11	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
12	L	44/58 (76%)	42 (96%)	2 (4%)	0	100	100
16	U	181/528 (34%)	178 (98%)	3 (2%)	0	100	100
17	V	548/580 (94%)	529 (96%)	18 (3%)	1 (0%)	43	74
18	W	530/584 (91%)	462 (87%)	62 (12%)	6 (1%)	11	43
19	X	35/380 (9%)	35 (100%)	0	0	100	100
20	Y	114/121 (94%)	113 (99%)	1 (1%)	0	100	100
21	Z	348/1087 (32%)	335 (96%)	13 (4%)	0	100	100
22	a	503/597 (84%)	457 (91%)	42 (8%)	4 (1%)	16	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	6119/8460 (72%)	5743 (94%)	360 (6%)	16 (0%)	37 69

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	910	LYS
1	A	1205	ALA
17	V	25	GLU
18	W	400	GLU
18	W	401	ASN
22	a	288	PRO
22	a	462	PRO
18	W	542	ALA
18	W	543	PRO
22	a	536	PRO
1	A	1203	ASP
1	A	413	TYR
2	B	631	GLN
18	W	108	PRO
18	W	544	PRO
22	a	483	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1255/1749 (72%)	1198 (96%)	57 (4%)	24 49
2	B	989/1027 (96%)	962 (97%)	27 (3%)	39 60
3	C	235/248 (95%)	233 (99%)	2 (1%)	70 75
4	D	104/126 (82%)	104 (100%)	0	100 100
5	E	191/192 (100%)	188 (98%)	3 (2%)	55 69
6	F	71/111 (64%)	70 (99%)	1 (1%)	59 71
7	G	138/153 (90%)	130 (94%)	8 (6%)	18 44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	129/131 (98%)	125 (97%)	4 (3%)	35	57
9	I	105/112 (94%)	104 (99%)	1 (1%)	68	75
10	J	56/56 (100%)	54 (96%)	2 (4%)	31	54
11	K	104/106 (98%)	100 (96%)	4 (4%)	29	52
12	L	43/55 (78%)	43 (100%)	0	100	100
16	U	158/451 (35%)	155 (98%)	3 (2%)	50	66
17	V	493/515 (96%)	483 (98%)	10 (2%)	48	65
18	W	359/511 (70%)	346 (96%)	13 (4%)	31	54
19	X	33/331 (10%)	29 (88%)	4 (12%)	5	21
20	Y	102/105 (97%)	102 (100%)	0	100	100
21	Z	319/940 (34%)	318 (100%)	1 (0%)	86	85
22	a	456/534 (85%)	401 (88%)	55 (12%)	5	21
All	All	5340/7453 (72%)	5145 (96%)	195 (4%)	32	53

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ILE
1	A	45	GLU
1	A	46	THR
1	A	48	GLU
1	A	54	LEU
1	A	118	LEU
1	A	130	LEU
1	A	151	LYS
1	A	152	ASN
1	A	201	GLU
1	A	203	LYS
1	A	204	HIS
1	A	205	VAL
1	A	206	ASN
1	A	208	ASP
1	A	211	GLU
1	A	212	LYS
1	A	215	LEU
1	A	216	LEU
1	A	250	VAL
1	A	255	VAL

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Mol	Chain	Res	Type
1	A	276	LEU
1	A	327	ARG
1	A	346	LYS
1	A	368	THR
1	A	405	LEU
1	A	419	ILE
1	A	461	GLN
1	A	463	THR
1	A	464	LEU
1	A	488	VAL
1	A	509	LEU
1	A	521	VAL
1	A	580	LEU
1	A	585	LEU
1	A	706	ILE
1	A	910	LYS
1	A	1087	VAL
1	A	1103	THR
1	A	1104	LEU
1	A	1112	VAL
1	A	1116	ASN
1	A	1117	VAL
1	A	1166	LEU
1	A	1184	THR
1	A	1186	VAL
1	A	1189	ASP
1	A	1190	GLN
1	A	1191	GLU
1	A	1197	TYR
1	A	1199	MET
1	A	1202	PHE
1	A	1204	VAL
1	A	1323	THR
1	A	1374	VAL
1	A	1378	LEU
1	A	1463	LEU
2	B	29	VAL
2	B	163	LEU
2	B	230	ARG
2	B	238	SER
2	B	240	LEU
2	B	242	ARG

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Mol	Chain	Res	Type
2	B	248	LYS
2	B	249	LYS
2	B	254	GLN
2	B	257	VAL
2	B	336	ILE
2	B	361	LYS
2	B	377	LEU
2	B	455	ASP
2	B	457	LYS
2	B	463	ARG
2	B	576	ILE
2	B	616	THR
2	B	629	GLU
2	B	630	LYS
2	B	730	LYS
2	B	809	VAL
2	B	873	LEU
2	B	1052	LYS
2	B	1054	MET
2	B	1089	MET
2	B	1127	ILE
3	C	15	THR
3	C	128	ILE
5	E	58	LEU
5	E	99	ILE
5	E	131	LEU
6	F	90	LEU
7	G	32	THR
7	G	150	THR
7	G	152	VAL
7	G	157	ILE
7	G	158	PHE
7	G	160	ILE
7	G	162	SER
7	G	163	LEU
8	H	60	ILE
8	H	96	VAL
8	H	143	LEU
8	H	148	LEU
9	I	119	CYS
10	J	7	CYS
10	J	53	VAL

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Mol	Chain	Res	Type
11	K	41	THR
11	K	45	ILE
11	K	80	ASP
11	K	94	LEU
16	U	53	LYS
16	U	78	ILE
16	U	97	LEU
17	V	7	ASP
17	V	8	LEU
17	V	15	ASP
17	V	22	ASN
17	V	25	GLU
17	V	34	GLN
17	V	58	ARG
17	V	382	VAL
17	V	386	THR
17	V	410	SER
18	W	188	ILE
18	W	189	THR
18	W	191	VAL
18	W	193	THR
18	W	264	GLU
18	W	283	LEU
18	W	327	LEU
18	W	330	VAL
18	W	405	SER
18	W	454	LEU
18	W	509	VAL
18	W	541	ILE
18	W	566	ILE
19	X	22	LEU
19	X	29	LEU
19	X	30	LEU
19	X	32	LEU
21	Z	481	ILE
22	a	5	LYS
22	a	6	ILE
22	a	9	ARG
22	a	39	VAL
22	a	41	GLU
22	a	43	ASN
22	a	44	ARG

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Mol	Chain	Res	Type
22	a	61	MET
22	a	63	LEU
22	a	97[A]	CYS
22	a	97[B]	CYS
22	a	144	LYS
22	a	145	MET
22	a	164	ILE
22	a	192	TRP
22	a	193	CYS
22	a	194	PHE
22	a	233	LEU
22	a	239	LYS
22	a	250	LEU
22	a	276	MET
22	a	278	LYS
22	a	281	ILE
22	a	284	LEU
22	a	287	LYS
22	a	308	ASN
22	a	322	VAL
22	a	326	GLU
22	a	351	VAL
22	a	358	ARG
22	a	362	TYR
22	a	376	ASP
22	a	378	ASN
22	a	381	LEU
22	a	385	GLU
22	a	386	ARG
22	a	389	ILE
22	a	416	PHE
22	a	419	CYS
22	a	422	ARG
22	a	464	LEU
22	a	465	ASN
22	a	467	VAL
22	a	470	ARG
22	a	479	GLU
22	a	481	LEU
22	a	503	VAL
22	a	510	TYR
22	a	514	ILE

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Mol	Chain	Res	Type
22	a	515	ILE
22	a	525	VAL
22	a	528	ARG
22	a	530	ARG
22	a	535	PHE
22	a	549	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	136	GLN
1	A	188	GLN
1	A	206	ASN
1	A	210	GLN
1	A	272	ASN
1	A	273	GLN
1	A	278	HIS
1	A	311	GLN
1	A	372	ASN
1	A	472	HIS
1	A	529	GLN
1	A	576	GLN
1	A	654	HIS
1	A	662	HIS
1	A	711	GLN
1	A	809	HIS
1	A	905	ASN
1	A	989	ASN
1	A	1005	HIS
1	A	1032	GLN
1	A	1093	GLN
1	A	1105	ASN
1	A	1129	ASN
1	A	1163	HIS
1	A	1194	ASN
1	A	1244	ASN
1	A	1248	ASN
1	A	1299	GLN
1	A	1332	GLN
1	A	1384	HIS
1	A	1457	ASN

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Mol	Chain	Res	Type
2	B	111	ASN
2	B	164	ASN
2	B	245	GLN
2	B	420	GLN
2	B	456	GLN
2	B	461	GLN
2	B	486	ASN
2	B	518	HIS
2	B	577	HIS
2	B	639	HIS
2	B	650	ASN
2	B	699	HIS
2	B	731	GLN
2	B	749	HIS
2	B	1003	ASN
2	B	1021	HIS
2	B	1025	ASN
2	B	1053	HIS
2	B	1094	GLN
2	B	1145	GLN
3	C	55	ASN
3	C	66	HIS
4	D	66	ASN
4	D	129	GLN
4	D	135	GLN
5	E	22	HIS
5	E	92	GLN
5	E	95	GLN
5	E	132	GLN
5	E	169	GLN
8	H	44	ASN
8	H	76	ASN
9	I	22	ASN
9	I	41	ASN
9	I	45	GLN
11	K	49	GLN
16	U	142	GLN
17	V	22	ASN
17	V	119	HIS
17	V	323	GLN
17	V	358	GLN
17	V	418	GLN

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Mol	Chain	Res	Type
17	V	435	GLN
18	W	223	ASN
18	W	250	GLN
18	W	352	HIS
18	W	354	HIS
18	W	394	HIS
18	W	444	GLN
18	W	481	HIS
18	W	502	HIS
20	Y	12	HIS
20	Y	45	ASN
22	a	43	ASN
22	a	102	ASN
22	a	243	GLN
22	a	258	HIS
22	a	272	GLN
22	a	279	GLN
22	a	405	GLN
22	a	465	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	15/16 (93%)	10 (66%)	0

All (10) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	33	A
14	P	34	G
14	P	35	A
14	P	36	G
14	P	37	G
14	P	38	G
14	P	42	C
14	P	44	A
14	P	45	C
14	P	46	U

There are no RNA pucker outliers to report.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
25	GTP	P	101	14	33,34,34	0.96	2 (6%)	50,54,54	1.56	8 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	GTP	P	101	14	-	5/22/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	P	101	GTP	C2-N3	2.15	1.38	1.33
25	P	101	GTP	PA-O3A	2.11	1.61	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	101	GTP	C5-C4-N3	-4.84	120.69	128.39
25	P	101	GTP	C2-N3-C4	4.56	120.16	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	101	GTP	N9-C4-N3	3.02	131.99	125.95
25	P	101	GTP	C2-N1-C6	-2.84	119.97	125.11
25	P	101	GTP	N9-C8-N7	-2.77	108.27	113.40
25	P	101	GTP	C8-N7-C5	2.54	108.78	104.26
25	P	101	GTP	C5-C6-N1	2.47	119.53	113.25
25	P	101	GTP	O6-C6-C5	-2.37	120.27	126.53

There are no chirality outliers.

All (5) torsion outliers are listed below:

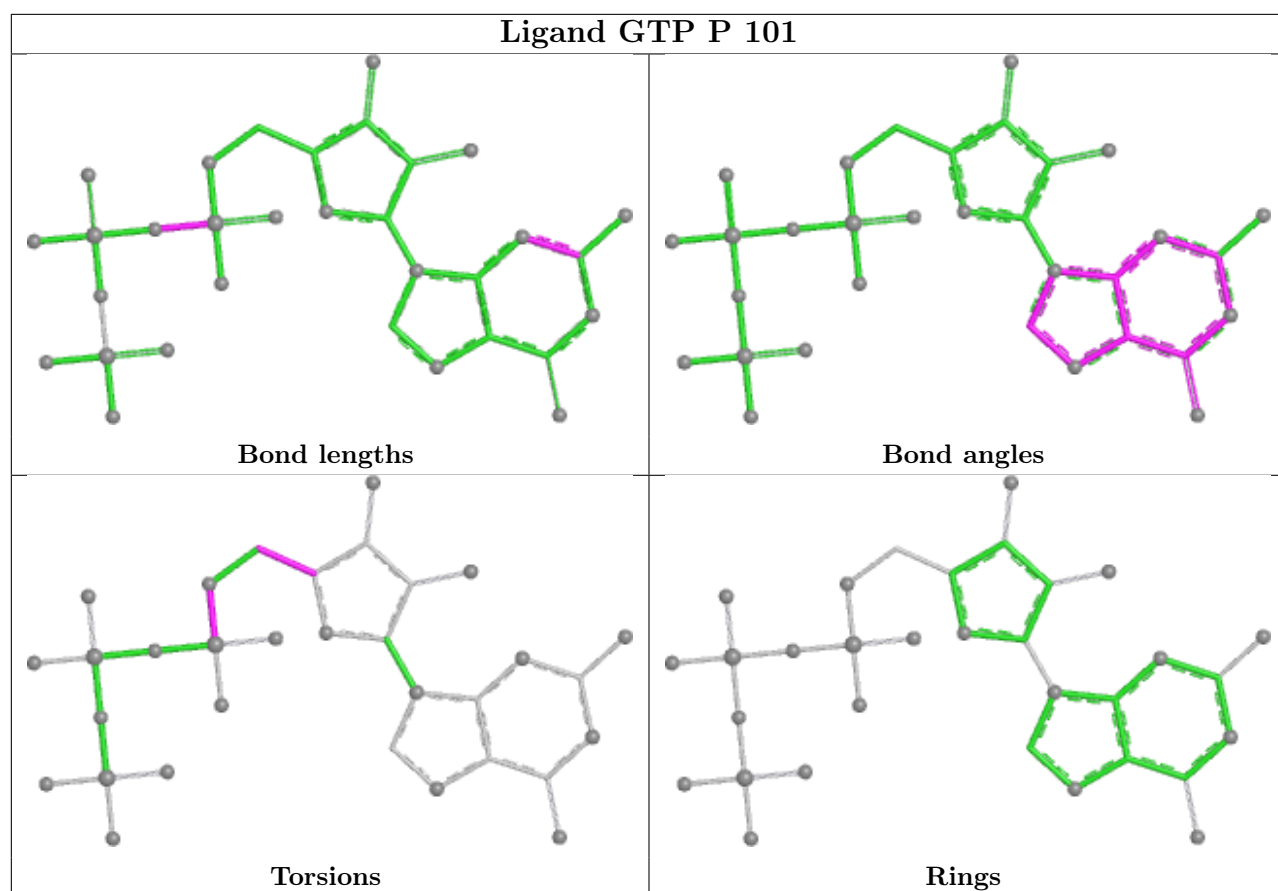
Mol	Chain	Res	Type	Atoms
25	P	101	GTP	C5'-O5'-PA-O3A
25	P	101	GTP	C5'-O5'-PA-O1A
25	P	101	GTP	C5'-O5'-PA-O2A
25	P	101	GTP	O4'-C4'-C5'-O5'
25	P	101	GTP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	P	101	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

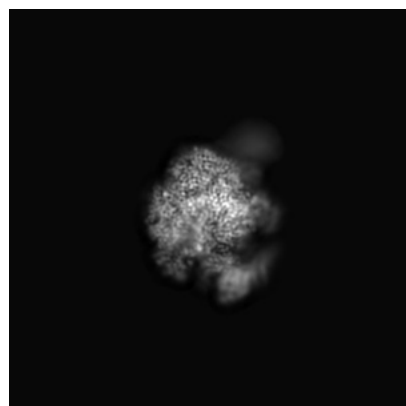
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37352. These allow visual inspection of the internal detail of the map and identification of artifacts.

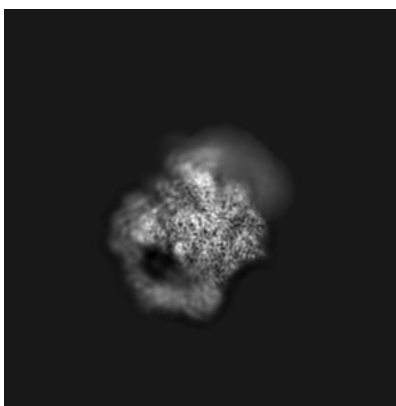
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

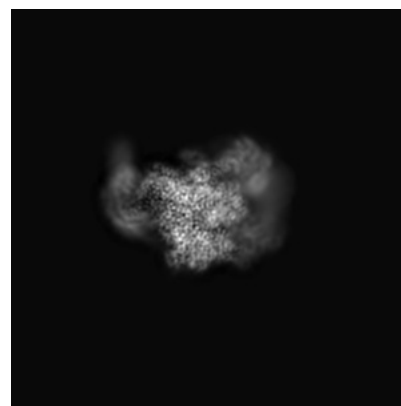
6.1.1 Primary map



X

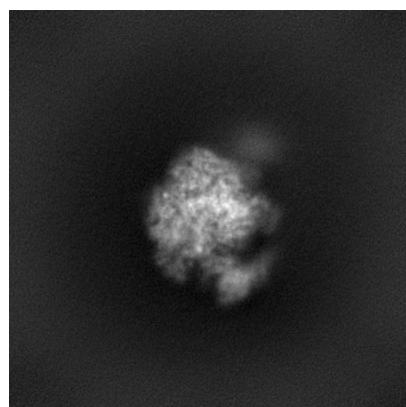


Y

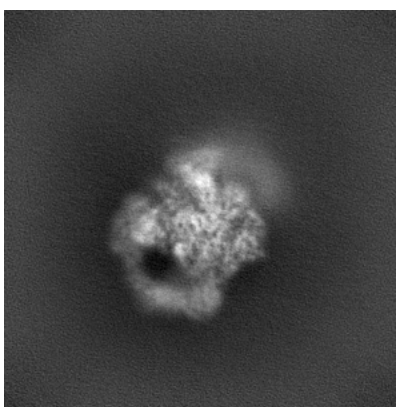


Z

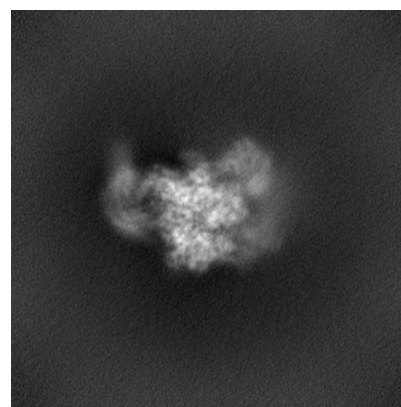
6.1.2 Raw map



X



Y

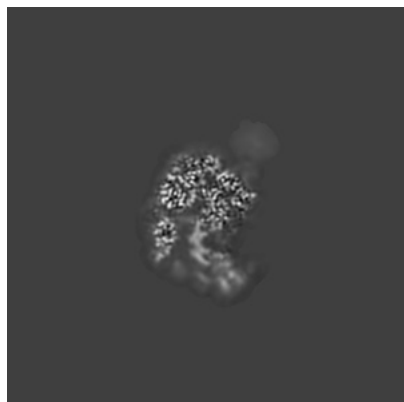


Z

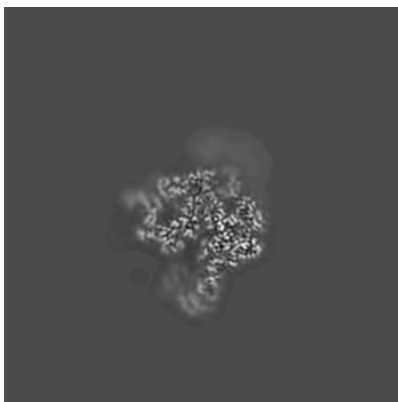
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

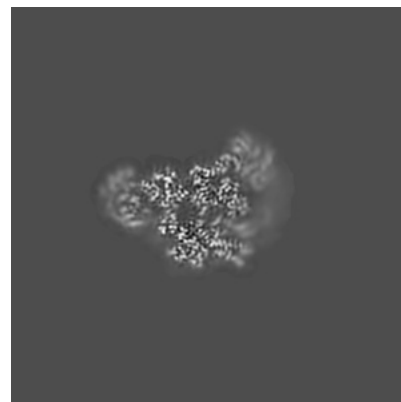
6.2.1 Primary map



X Index: 160

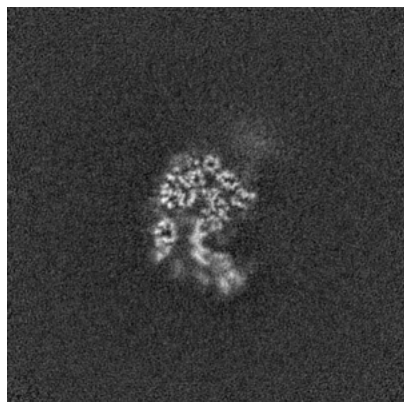


Y Index: 160

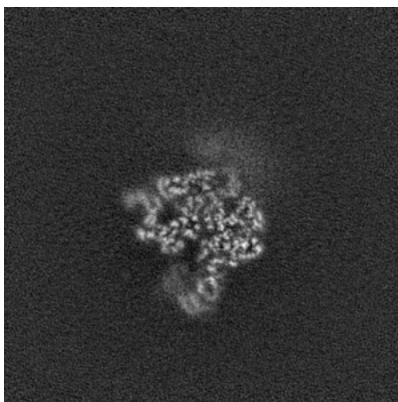


Z Index: 160

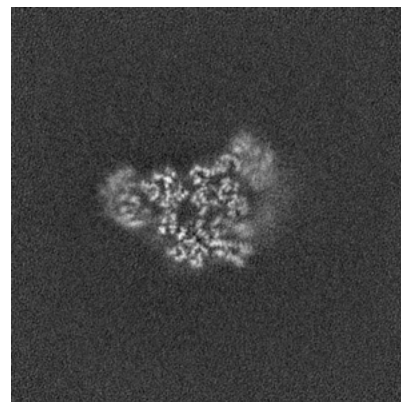
6.2.2 Raw map



X Index: 160



Y Index: 160

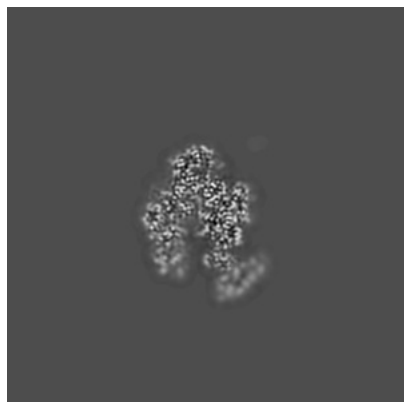


Z Index: 160

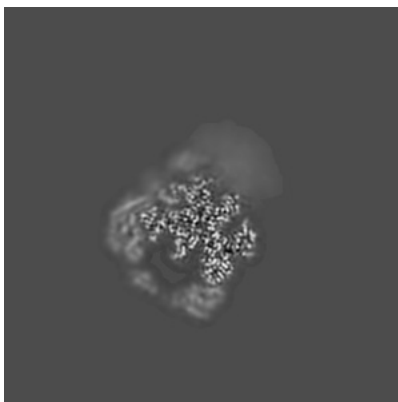
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

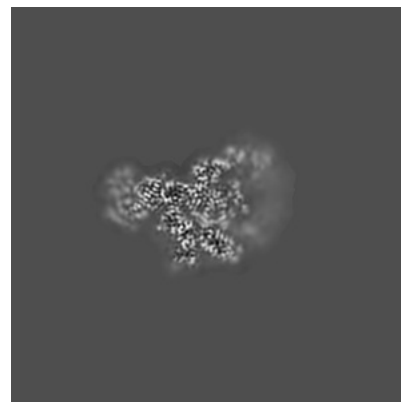
6.3.1 Primary map



X Index: 150

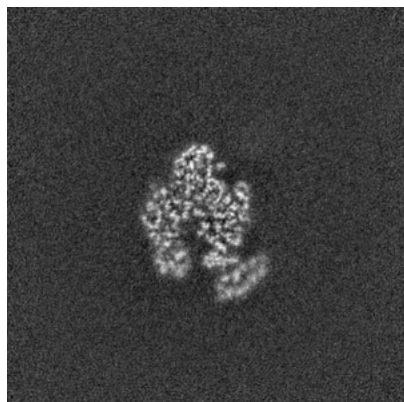


Y Index: 173

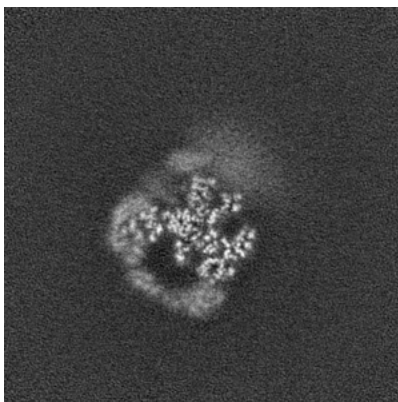


Z Index: 166

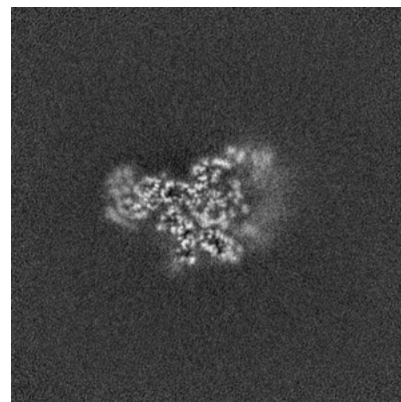
6.3.2 Raw map



X Index: 148



Y Index: 176

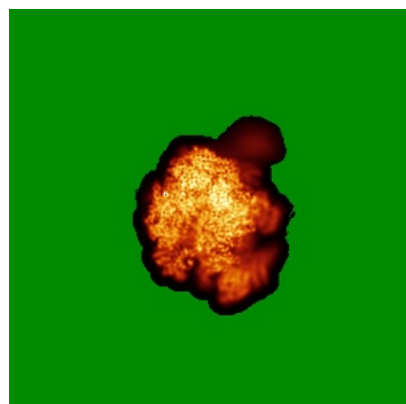


Z Index: 166

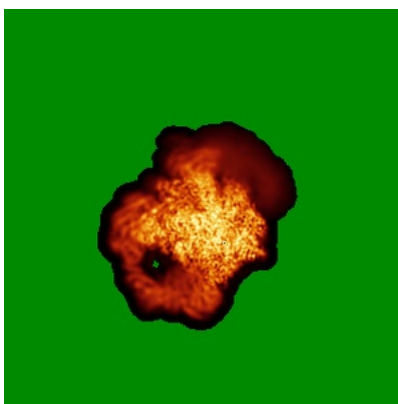
The images above show the largest variance slices of the map in three orthogonal directions.

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

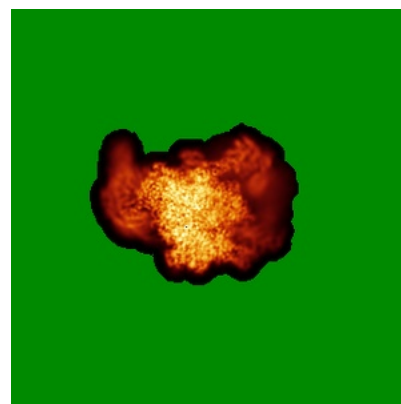
6.4.1 Primary map



X

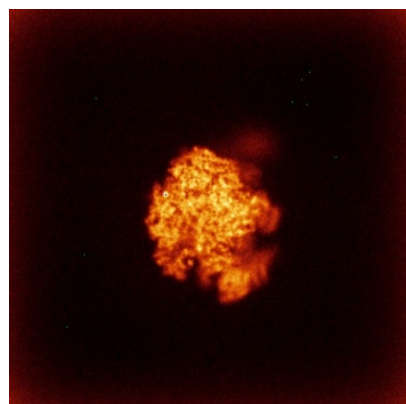


Y

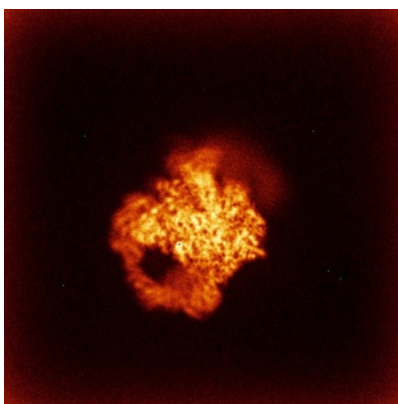


Z

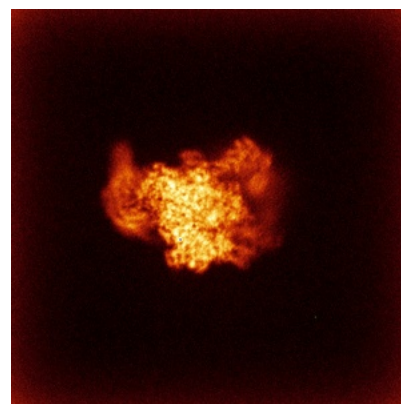
6.4.2 Raw map



X



Y



Z

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

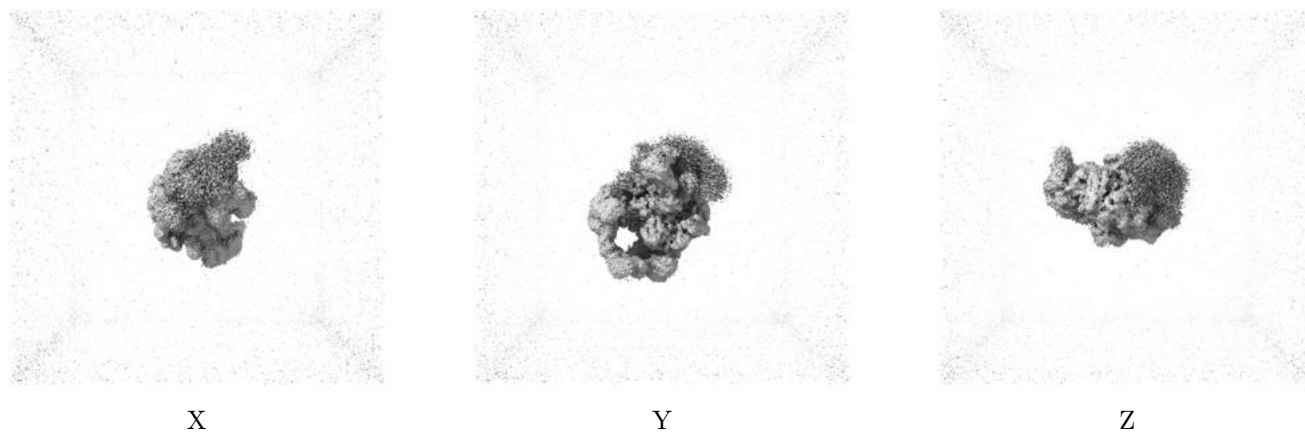
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.22. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

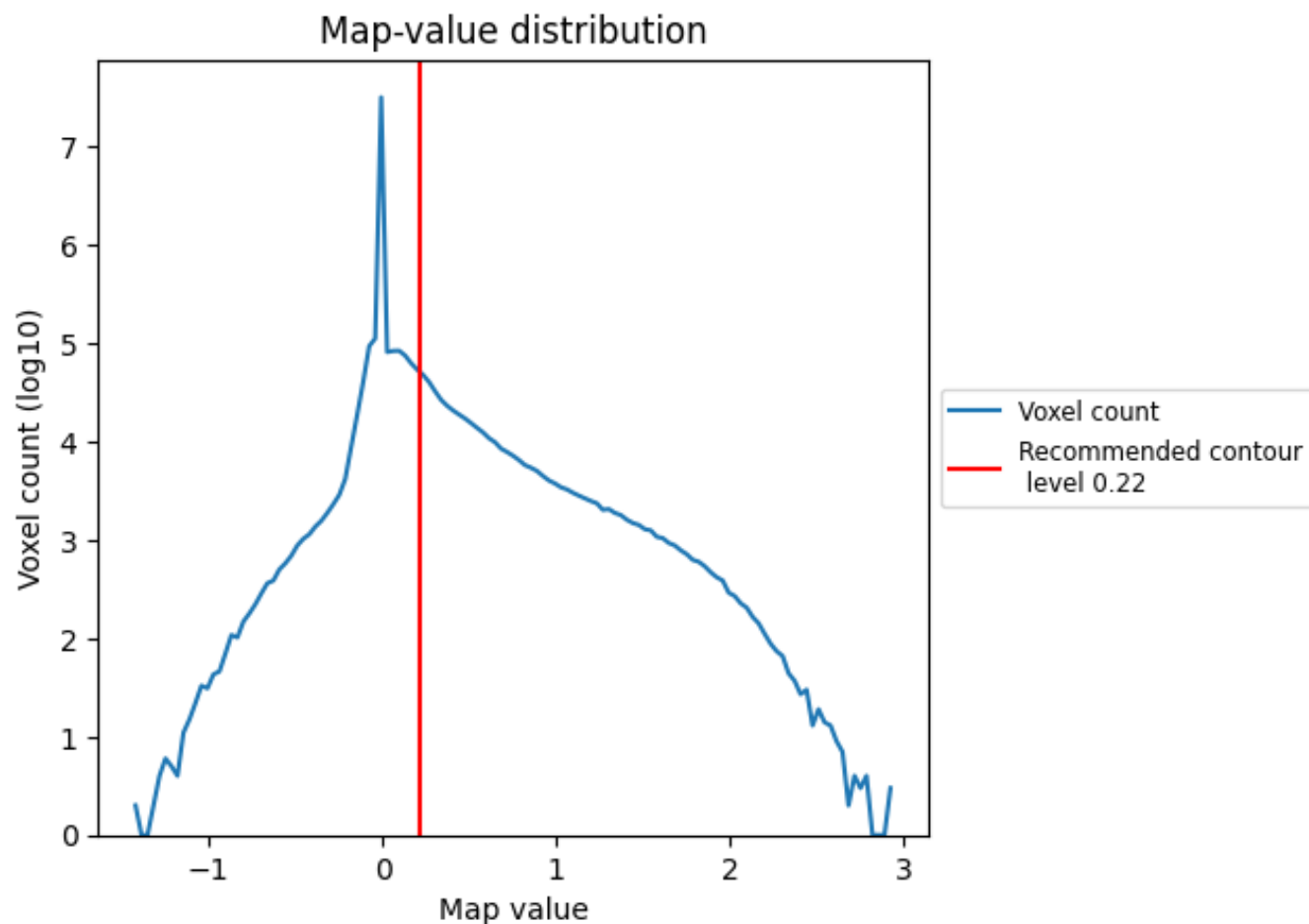
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

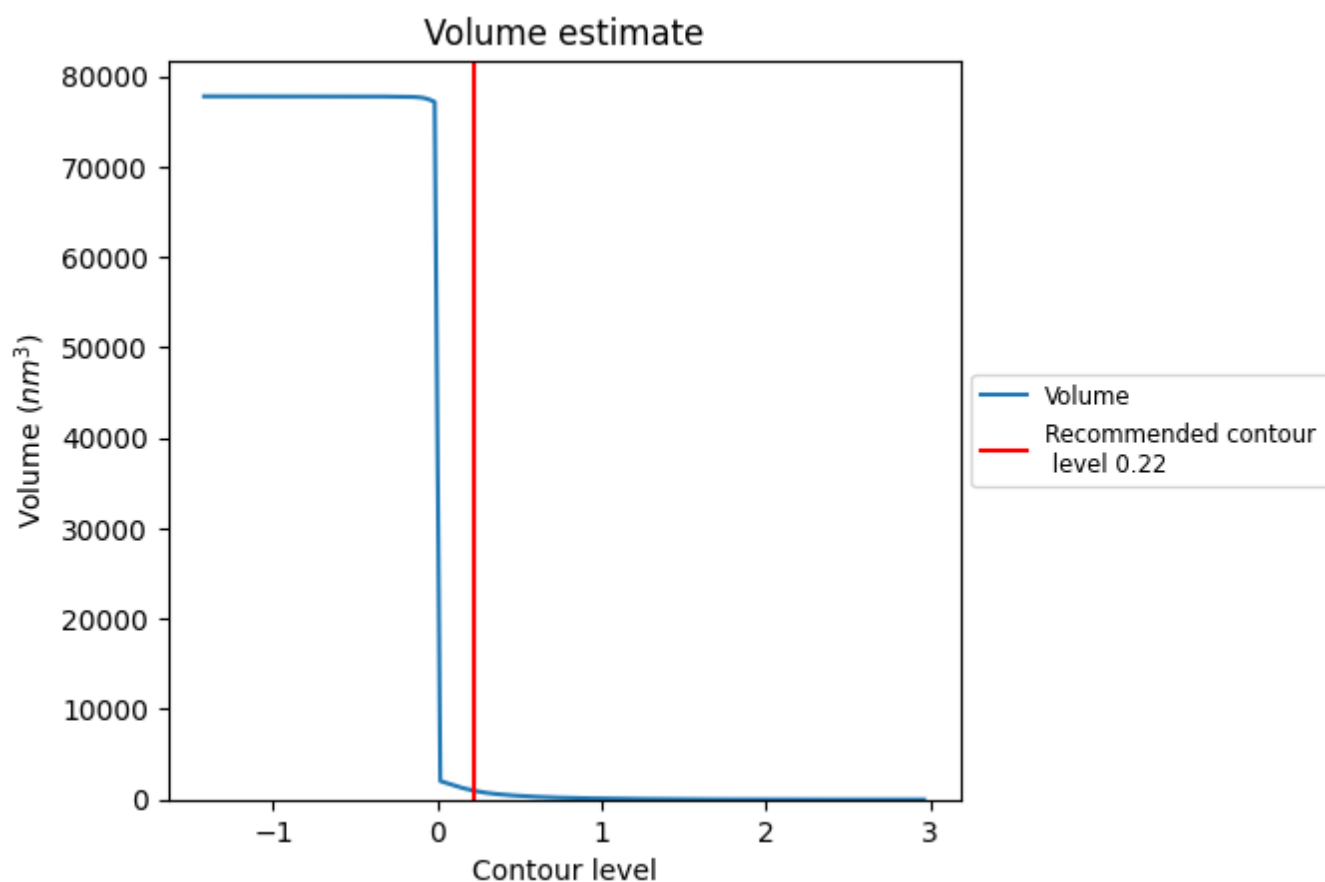
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

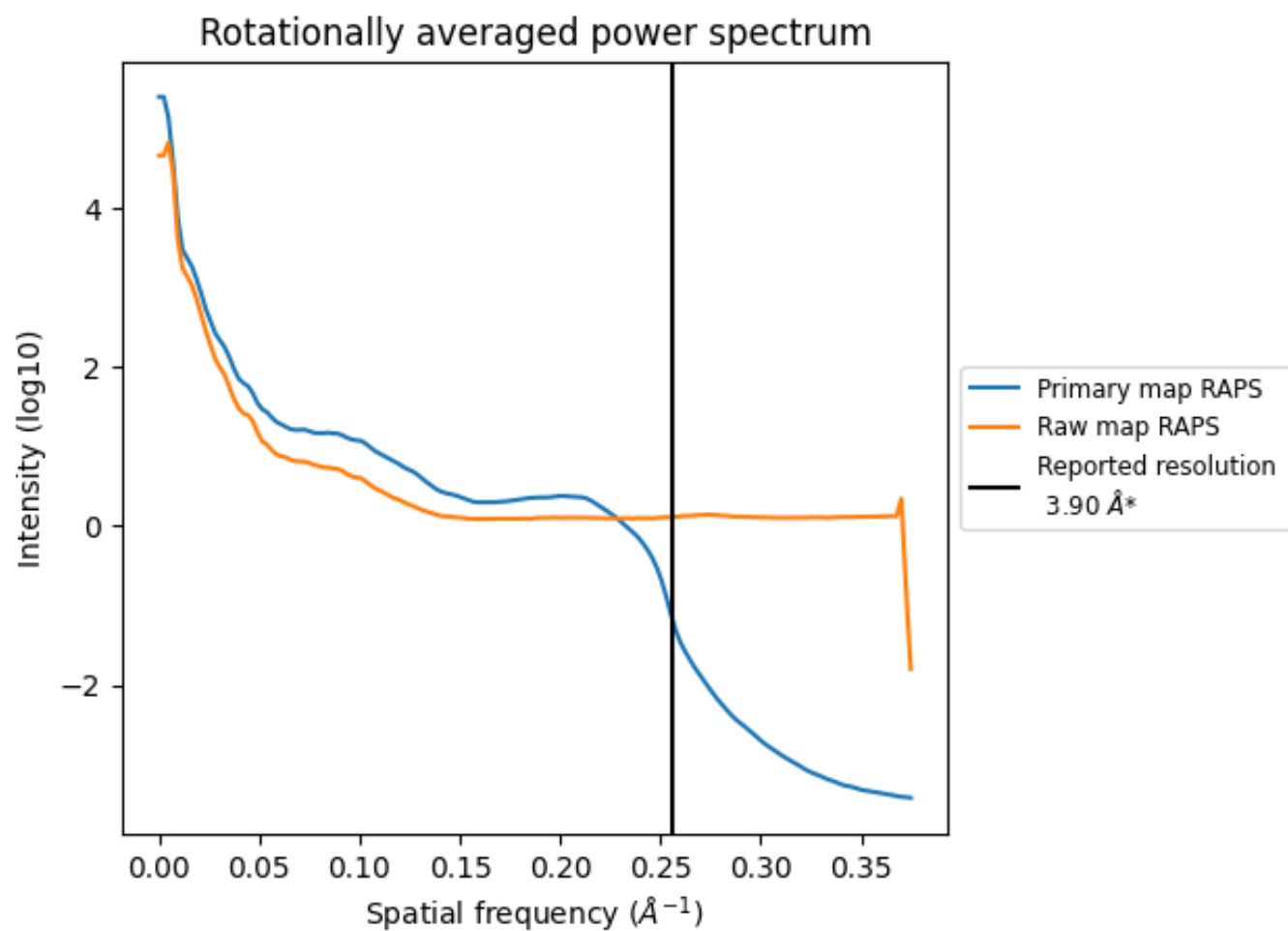
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 991 nm^3 ; this corresponds to an approximate mass of 896 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 ⓘ

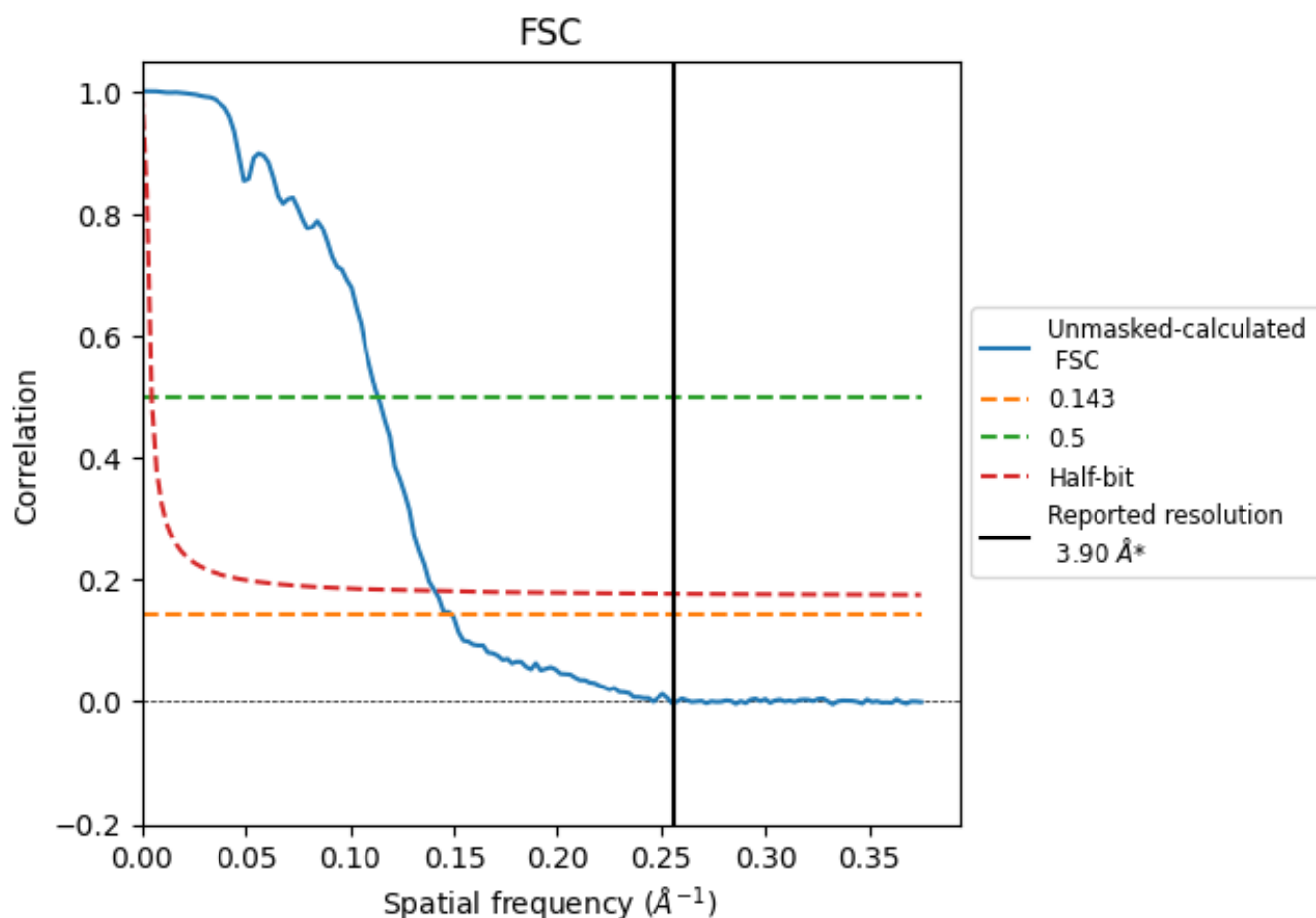


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

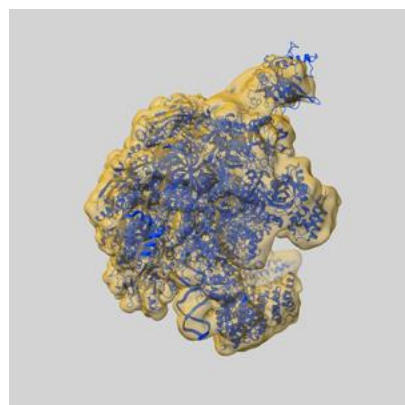
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.72	8.80	7.10

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.72 differs from the reported value 3.9 by more than 10 %

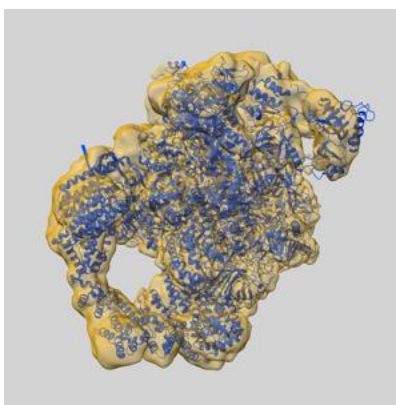
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37352 and PDB model 8W8E. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

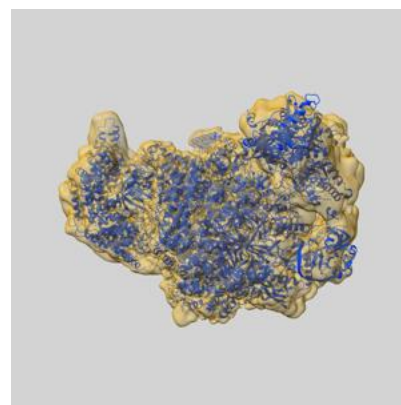
9.1 Map-model overlay [i](#)



X



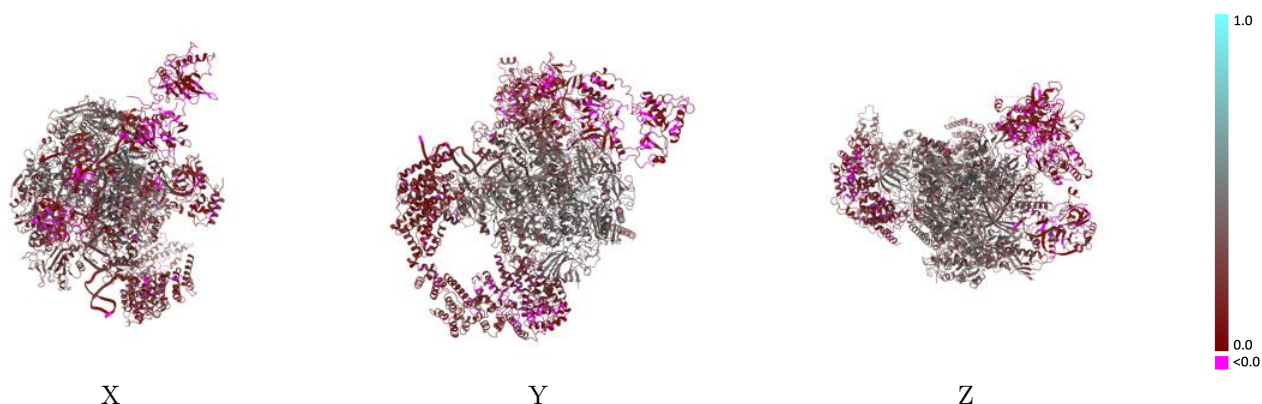
Y



Z

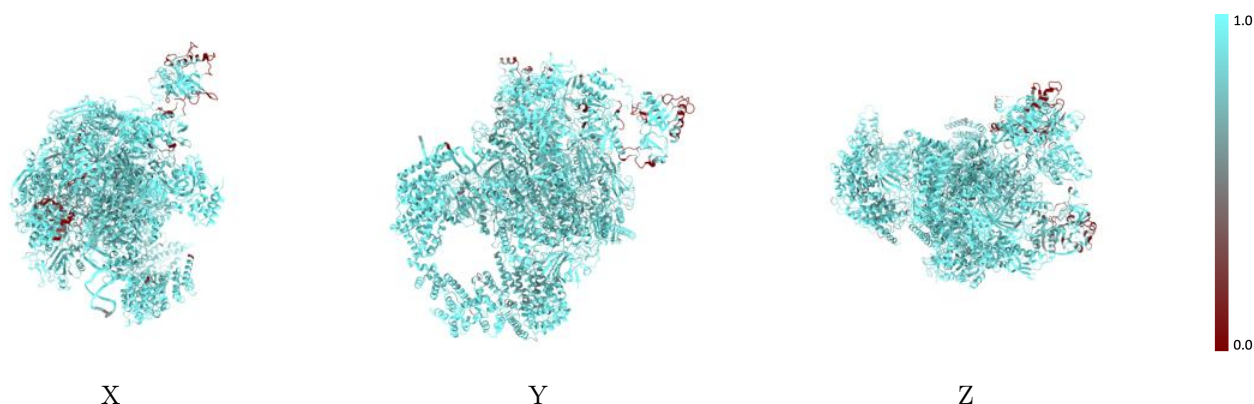
The images above show the 3D surface view of the map at the recommended contour level 0.22 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



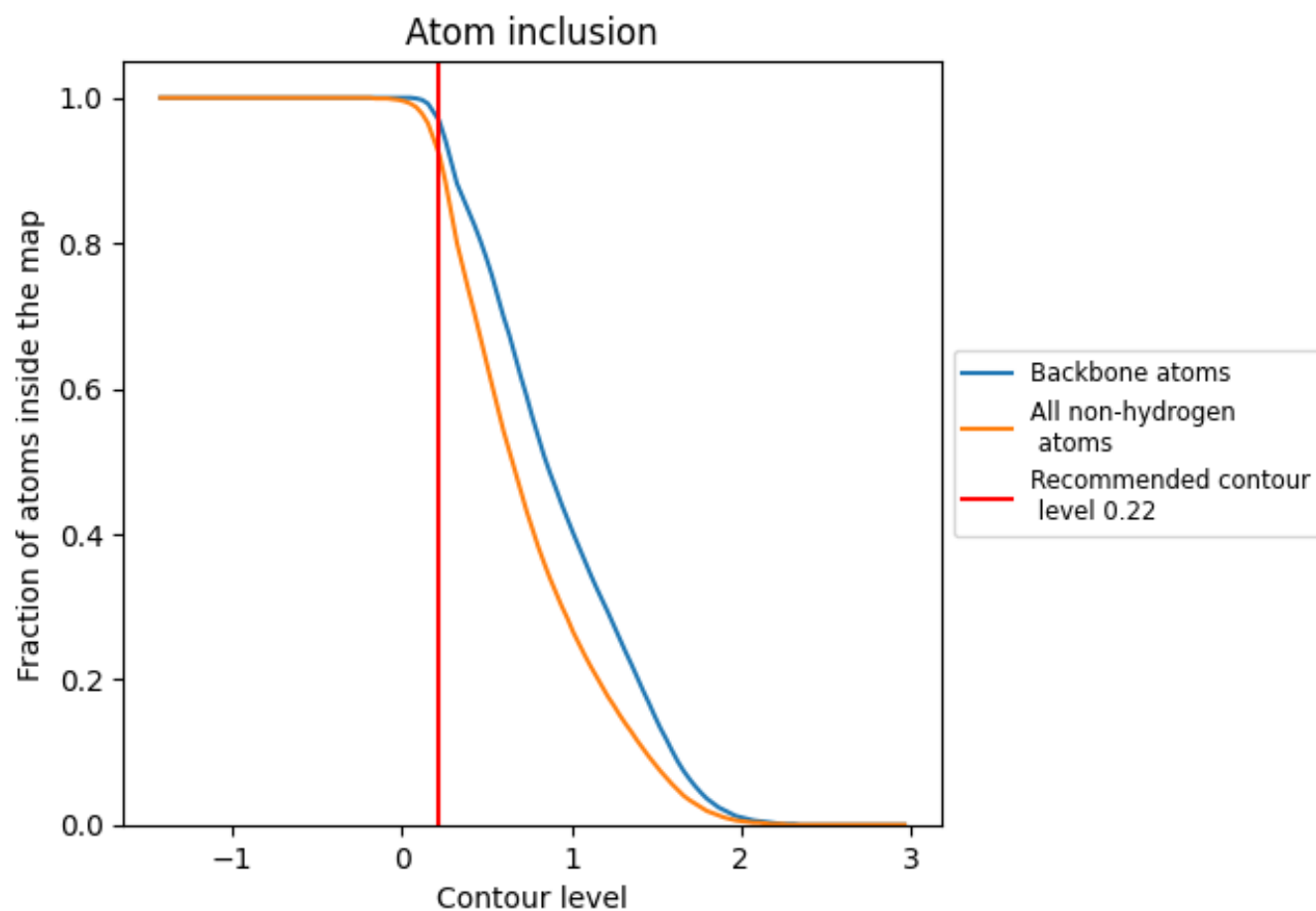
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.22).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 92% 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 (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9240	 0.2650
A	 0.9410	 0.3600
B	 0.9550	 0.3700
C	 0.9640	 0.3770
D	 0.9690	 0.1650
E	 0.9530	 0.3450
F	 0.9300	 0.3680
G	 0.9640	 0.2120
H	 0.9580	 0.3910
I	 0.9650	 0.3180
J	 0.9460	 0.3840
K	 0.9560	 0.3890
L	 0.9810	 0.3530
N	 0.9230	 0.2000
P	 0.9840	 0.2490
T	 0.9570	 0.2330
U	 0.9420	 0.1020
V	 0.9480	 0.1600
W	 0.9310	 0.1380
X	 0.9730	 0.1600
Y	 0.6420	 0.0910
Z	 0.8380	 0.1200
a	 0.7870	 0.0560

