



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 04:35 AM UTC

PDB ID : 9FD2 / pdb_00009fd2
EMDB ID : EMD-50325
Title : Structure of Pol II-TC-NER-STK19 complex
Authors : Lee, S.-H.; Sixma, T.K.
Deposited on : 2024-05-16
Resolution : 3.40 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

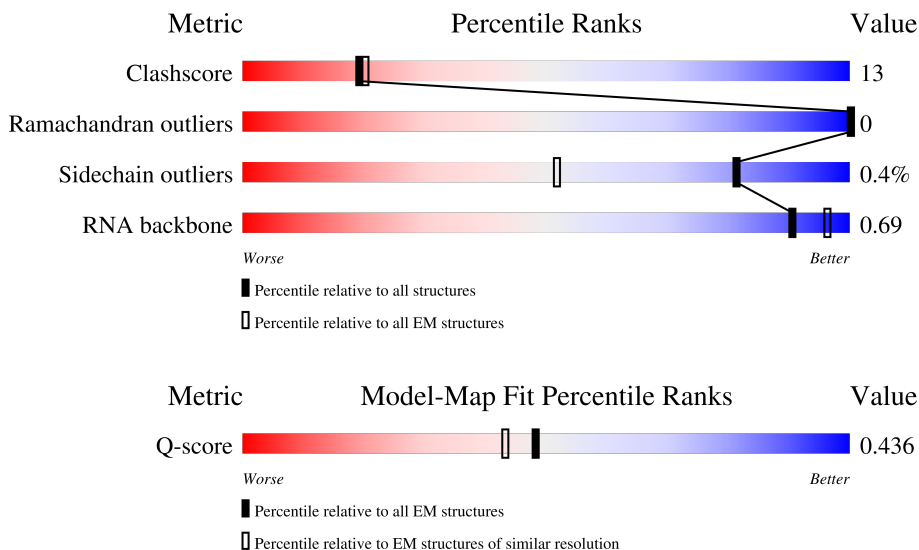
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 51%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 28%; height: 10px; background-color: grey;"></div> </div>
2	B	1300	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 63%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div>
3	C	275	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 67%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 27%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div>

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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	f	85	
14	N	60	
15	M	25	
16	T	60	
17	a	408	
18	b	1160	
19	c	152	
20	g	257	
21	e	1493	
22	d	729	

2 Entry composition [i](#)

There are 24 unique types of molecules in this entry. The entry contains 51949 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
			Total	C	N	O	S		
1	A	1409	11161	7022	1998	2070	71	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1130	9048	5725	1591	1668	64	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	260	2089	1309	359	415	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	128	1050	656	178	212	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	209	1720	1089	300	323	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	82	657	418	113	121	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	148	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
			Total	C	N	O	S		
9	I	117	Total	C	N	O	S	0	0
			949	587	169	182	11		

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

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

- Molecule 12 is a protein called RNA polymerase II, I and III subunit K.

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

- Molecule 13 is a protein called Transcription elongation factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	f	64	Total	C	N	O	S	0	0
			505	312	81	105	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	-1	GLY	-	expression tag	UNP P60002
f	0	ALA	-	expression tag	UNP P60002

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
14	N	40	831	393	162	236	40	0	0

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
15	M	10	220	98	45	67	10	0	0

- Molecule 16 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
16	T	54	1091	521	187	329	54	0	0

- Molecule 17 is a protein called DNA excision repair protein ERCC-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	a	377	2951	1842	520	570	19	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	397	GLY	-	expression tag	UNP Q13216
a	398	THR	-	expression tag	UNP Q13216
a	399	SER	-	expression tag	UNP Q13216
a	400	ALA	-	expression tag	UNP Q13216
a	401	TRP	-	expression tag	UNP Q13216
a	402	SER	-	expression tag	UNP Q13216
a	403	HIS	-	expression tag	UNP Q13216
a	404	PRO	-	expression tag	UNP Q13216
a	405	GLN	-	expression tag	UNP Q13216
a	406	PHE	-	expression tag	UNP Q13216
a	407	GLU	-	expression tag	UNP Q13216
a	408	LYS	-	expression tag	UNP Q13216

- Molecule 18 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	b	814	6405	4059	1079	1231	36	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	-19	MET	-	initiating methionine	UNP Q16531
b	-18	ALA	-	expression tag	UNP Q16531
b	-17	HIS	-	expression tag	UNP Q16531
b	-16	HIS	-	expression tag	UNP Q16531
b	-15	HIS	-	expression tag	UNP Q16531
b	-14	HIS	-	expression tag	UNP Q16531
b	-13	HIS	-	expression tag	UNP Q16531
b	-12	HIS	-	expression tag	UNP Q16531
b	-11	SER	-	expression tag	UNP Q16531
b	-10	ALA	-	expression tag	UNP Q16531
b	-9	ALA	-	expression tag	UNP Q16531
b	-8	LEU	-	expression tag	UNP Q16531
b	-7	GLU	-	expression tag	UNP Q16531
b	-6	VAL	-	expression tag	UNP Q16531
b	-5	LEU	-	expression tag	UNP Q16531
b	-4	PHE	-	expression tag	UNP Q16531
b	-3	GLN	-	expression tag	UNP Q16531
b	-2	GLY	-	expression tag	UNP Q16531
b	-1	PRO	-	expression tag	UNP Q16531
b	0	GLY	-	expression tag	UNP Q16531

- Molecule 19 is a protein called DET1- and DDB1-associated protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	c	36	302	199	49	54	0	0

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	103	ASP	-	expression tag	UNP Q9BW61
c	104	VAL	-	expression tag	UNP Q9BW61
c	105	LEU	-	expression tag	UNP Q9BW61
c	106	PHE	-	expression tag	UNP Q9BW61
c	107	GLN	-	expression tag	UNP Q9BW61

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Chain	Residue	Modelled	Actual	Comment	Reference
c	108	GLY	-	expression tag	UNP Q9BW61
c	109	PRO	-	expression tag	UNP Q9BW61
c	110	GLY	-	expression tag	UNP Q9BW61
c	111	ALA	-	expression tag	UNP Q9BW61
c	112	TRP	-	expression tag	UNP Q9BW61
c	113	SER	-	expression tag	UNP Q9BW61
c	114	HIS	-	expression tag	UNP Q9BW61
c	115	PRO	-	expression tag	UNP Q9BW61
c	116	GLN	-	expression tag	UNP Q9BW61
c	117	PHE	-	expression tag	UNP Q9BW61
c	118	GLU	-	expression tag	UNP Q9BW61
c	119	LYS	-	expression tag	UNP Q9BW61
c	120	GLY	-	expression tag	UNP Q9BW61
c	121	GLY	-	expression tag	UNP Q9BW61
c	122	GLY	-	expression tag	UNP Q9BW61
c	123	SER	-	expression tag	UNP Q9BW61
c	124	GLY	-	expression tag	UNP Q9BW61
c	125	GLY	-	expression tag	UNP Q9BW61
c	126	GLY	-	expression tag	UNP Q9BW61
c	127	SER	-	expression tag	UNP Q9BW61
c	128	GLY	-	expression tag	UNP Q9BW61
c	129	GLY	-	expression tag	UNP Q9BW61
c	130	GLY	-	expression tag	UNP Q9BW61
c	131	SER	-	expression tag	UNP Q9BW61
c	132	TRP	-	expression tag	UNP Q9BW61
c	133	SER	-	expression tag	UNP Q9BW61
c	134	HIS	-	expression tag	UNP Q9BW61
c	135	PRO	-	expression tag	UNP Q9BW61
c	136	GLN	-	expression tag	UNP Q9BW61
c	137	PHE	-	expression tag	UNP Q9BW61
c	138	GLU	-	expression tag	UNP Q9BW61
c	139	LYS	-	expression tag	UNP Q9BW61
c	140	GLY	-	expression tag	UNP Q9BW61
c	141	ALA	-	expression tag	UNP Q9BW61
c	142	SER	-	expression tag	UNP Q9BW61
c	143	GLY	-	expression tag	UNP Q9BW61
c	144	GLU	-	expression tag	UNP Q9BW61
c	145	ASP	-	expression tag	UNP Q9BW61
c	146	TYR	-	expression tag	UNP Q9BW61
c	147	LYS	-	expression tag	UNP Q9BW61
c	148	ASP	-	expression tag	UNP Q9BW61
c	149	ASP	-	expression tag	UNP Q9BW61

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Chain	Residue	Modelled	Actual	Comment	Reference
c	150	ASP	-	expression tag	UNP Q9BW61
c	151	ASP	-	expression tag	UNP Q9BW61
c	152	LYS	-	expression tag	UNP Q9BW61

- Molecule 20 is a protein called Inactive serine/threonine-protein kinase 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	g	220	1721	1098	308	309	6	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	-2	GLY	-	expression tag	UNP P49842
g	-1	PRO	-	expression tag	UNP P49842
g	0	GLY	-	expression tag	UNP P49842

- Molecule 21 is a protein called DNA excision repair protein ERCC-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	e	590	4820	3091	847	859	23	0	0

- Molecule 22 is a protein called UV-stimulated scaffold protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	d	249	2040	1274	397	361	8	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	-19	MET	-	initiating methionine	UNP Q2YD98
d	-18	ALA	-	expression tag	UNP Q2YD98
d	-17	HIS	-	expression tag	UNP Q2YD98
d	-16	HIS	-	expression tag	UNP Q2YD98
d	-15	HIS	-	expression tag	UNP Q2YD98
d	-14	HIS	-	expression tag	UNP Q2YD98
d	-13	HIS	-	expression tag	UNP Q2YD98
d	-12	HIS	-	expression tag	UNP Q2YD98
d	-11	SER	-	expression tag	UNP Q2YD98

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Chain	Residue	Modelled	Actual	Comment	Reference
d	-10	ALA	-	expression tag	UNP Q2YD98
d	-9	ALA	-	expression tag	UNP Q2YD98
d	-8	LEU	-	expression tag	UNP Q2YD98
d	-7	GLU	-	expression tag	UNP Q2YD98
d	-6	VAL	-	expression tag	UNP Q2YD98
d	-5	LEU	-	expression tag	UNP Q2YD98
d	-4	PHE	-	expression tag	UNP Q2YD98
d	-3	GLN	-	expression tag	UNP Q2YD98
d	-2	GLY	-	expression tag	UNP Q2YD98
d	-1	PRO	-	expression tag	UNP Q2YD98
d	0	GLY	-	expression tag	UNP Q2YD98

- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
23	A	2	Total Zn 2 2	0
23	B	1	Total Zn 1 1	0
23	C	1	Total Zn 1 1	0
23	I	2	Total Zn 2 2	0
23	J	1	Total Zn 1 1	0
23	L	1	Total Zn 1 1	0
23	f	1	Total Zn 1 1	0
23	d	1	Total Zn 1 1	0

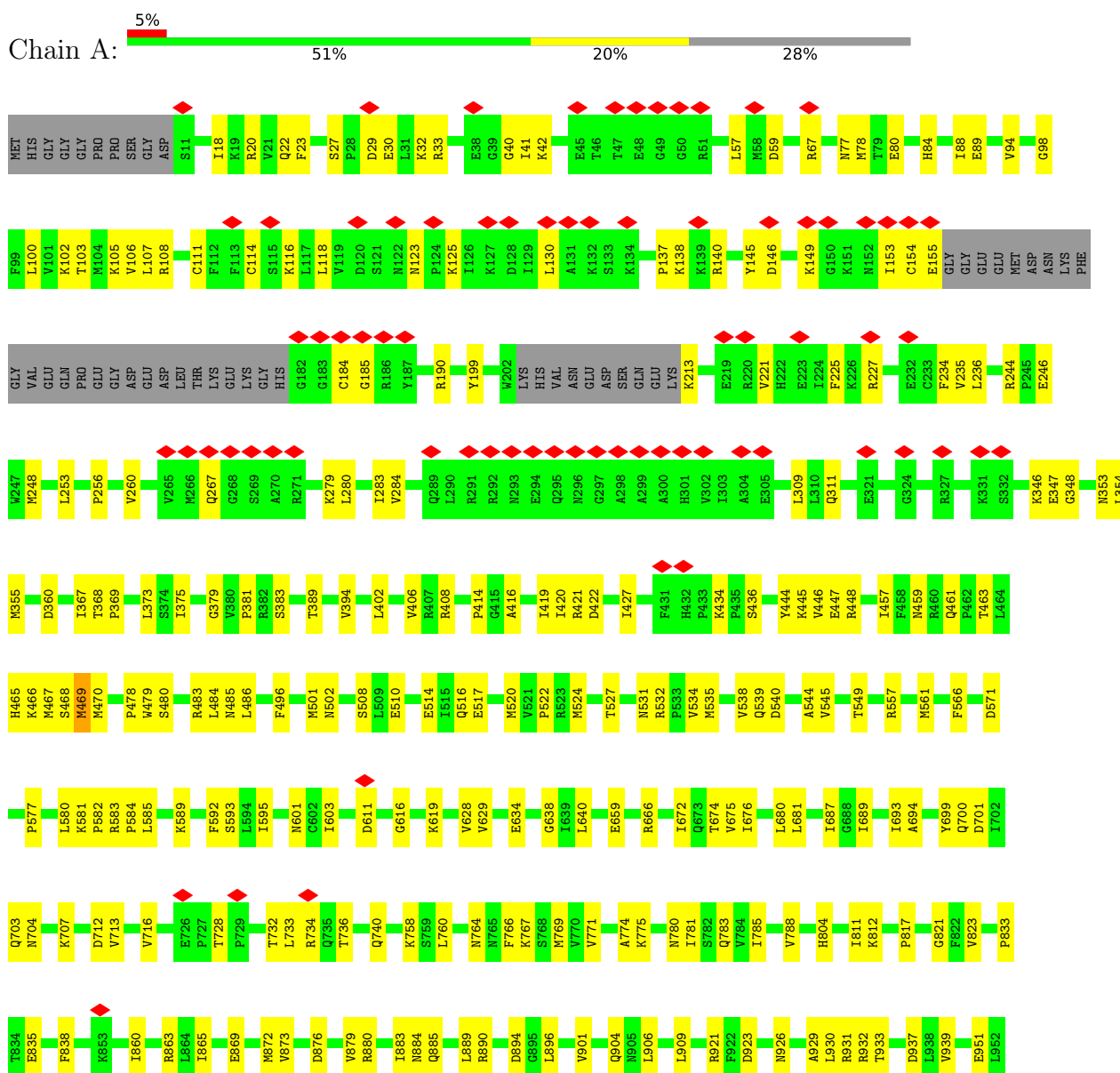
- Molecule 24 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

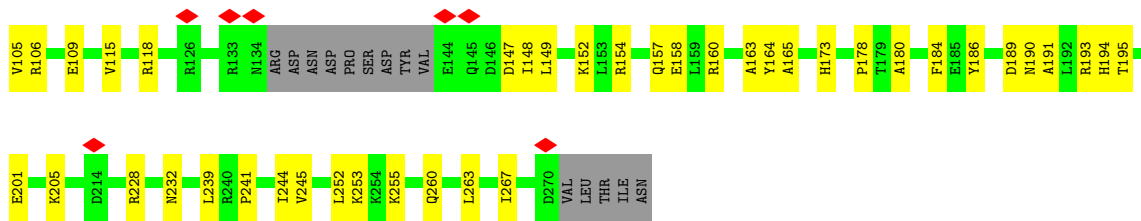
Mol	Chain	Residues	Atoms	AltConf
24	A	1	Total Mg 1 1	0

3 Residue-property plots i

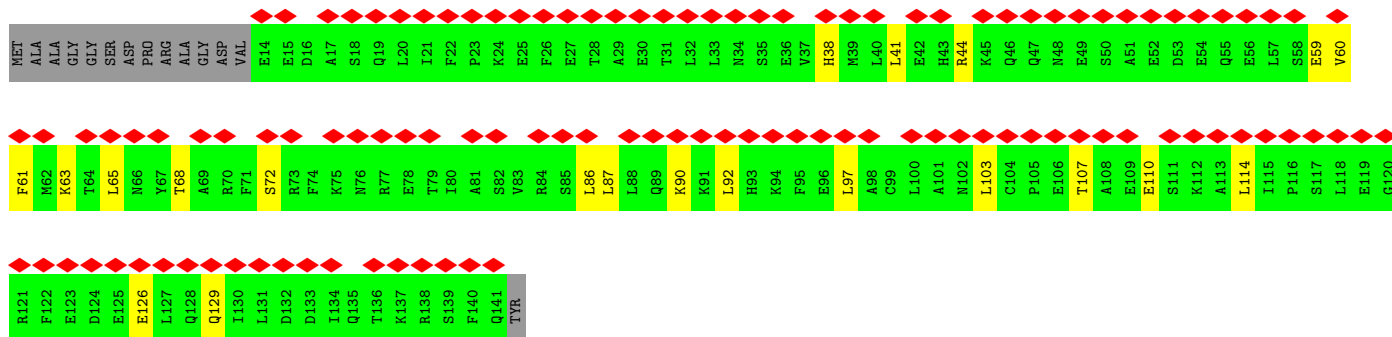
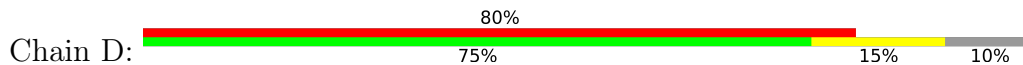
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

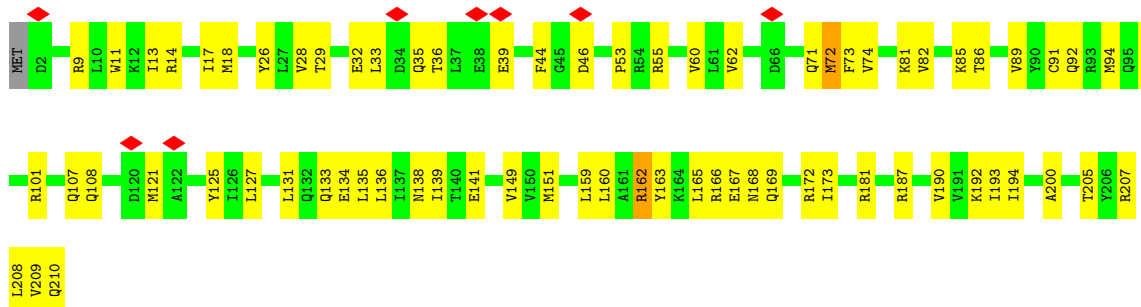




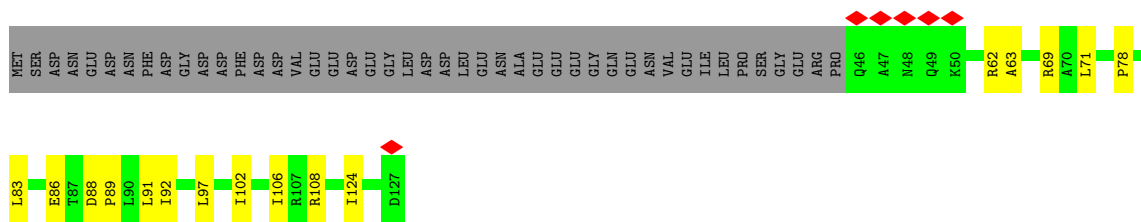
• Molecule 4: RNA polymerase II subunit D



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

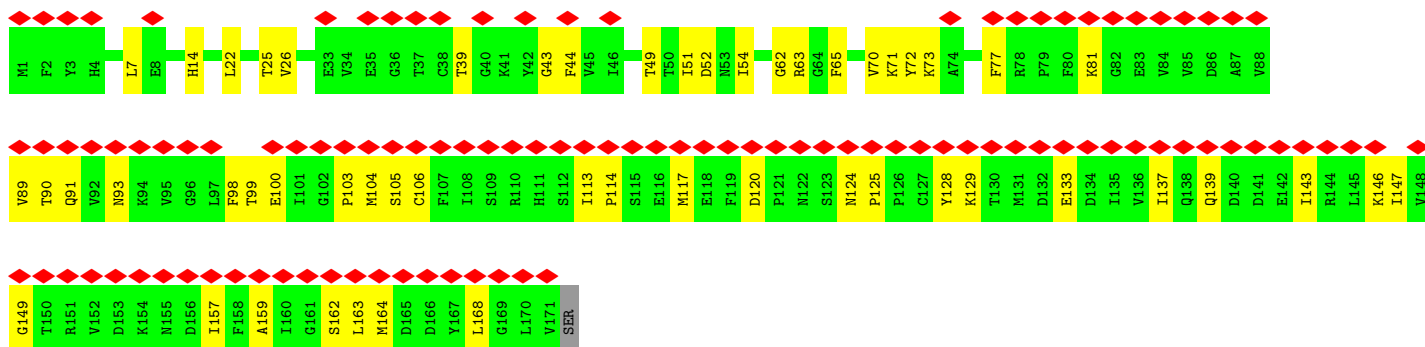


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



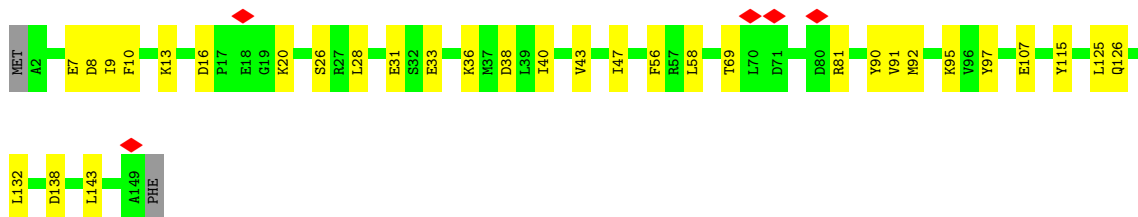
• Molecule 7: DNA-directed RNA polymerase subunit





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

Chain H: 77% 21%



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

Chain I: 16% 70% 22% 6%



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

Chain J: 75% 25%

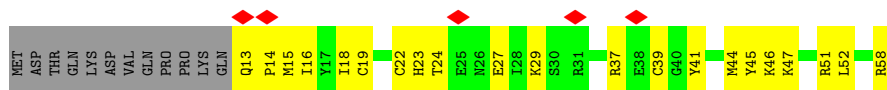
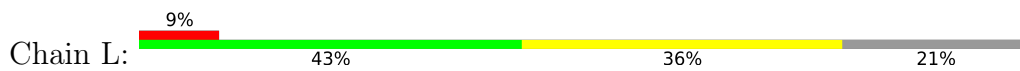


- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

Chain K: 74% 25%



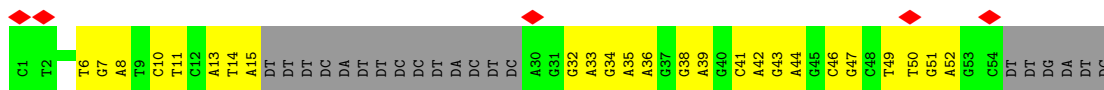
- Molecule 12: RNA polymerase II, I and III subunit K



• Molecule 13: Transcription elongation factor 1 homolog



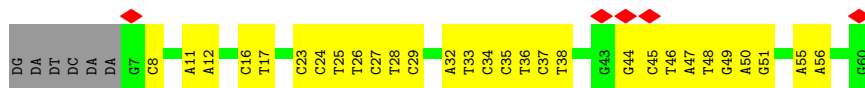
• Molecule 14: Non-template DNA



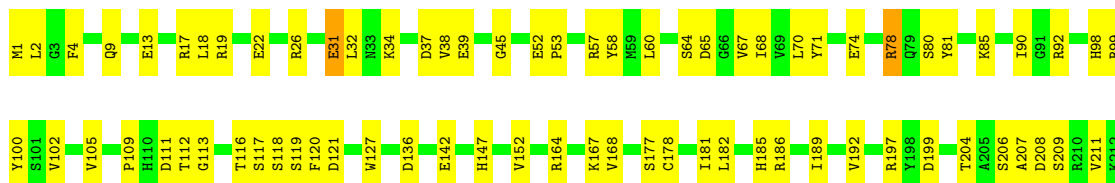
• Molecule 15: RNA

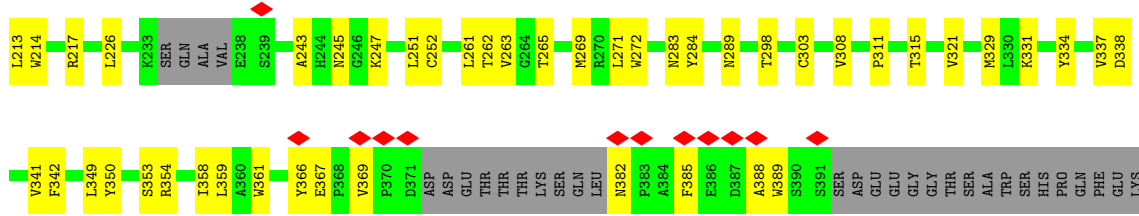


• Molecule 16: Template DNA

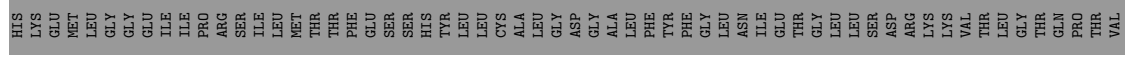
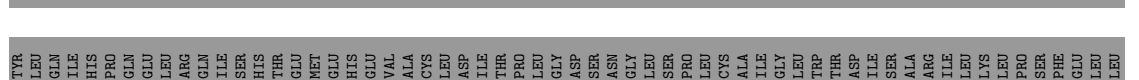
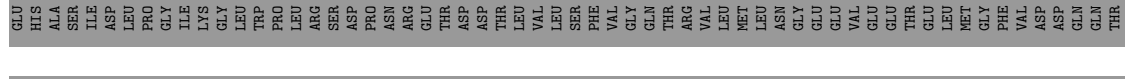
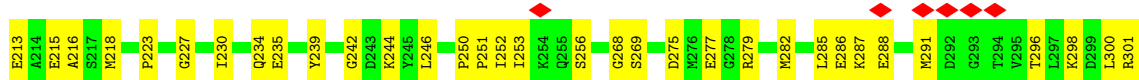


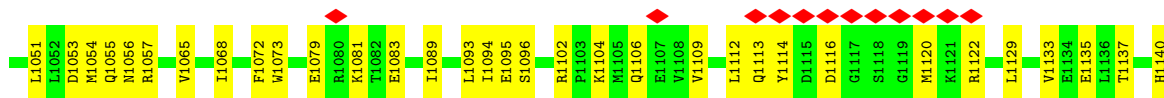
• Molecule 17: DNA excision repair protein ERCC-8



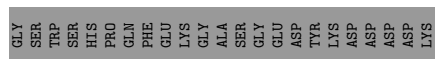
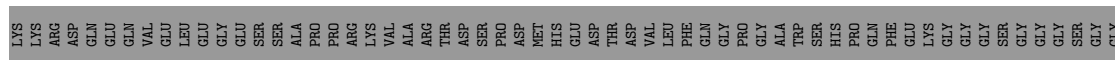


• Molecule 18: DNA damage-binding protein 1

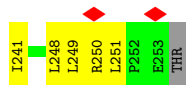
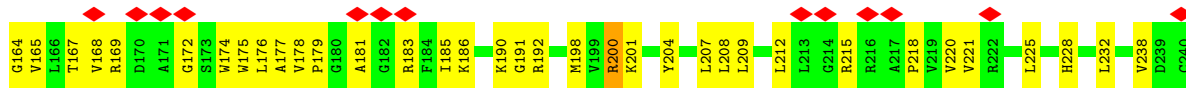
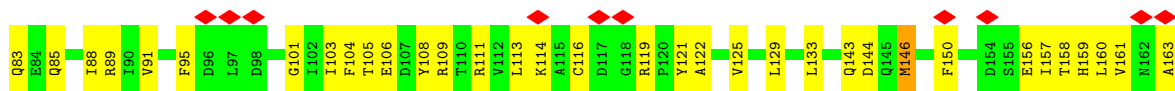
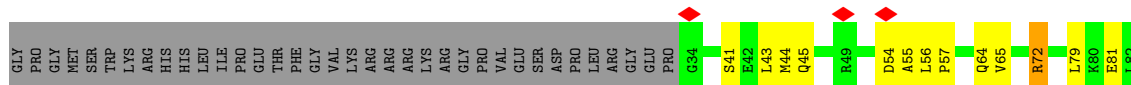




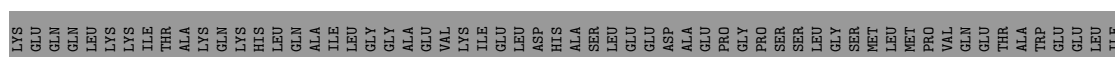
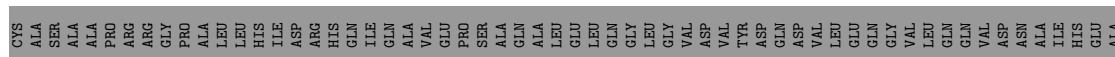
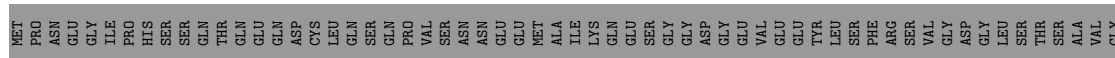
• Molecule 19: DET1- and DDB1-associated protein 1

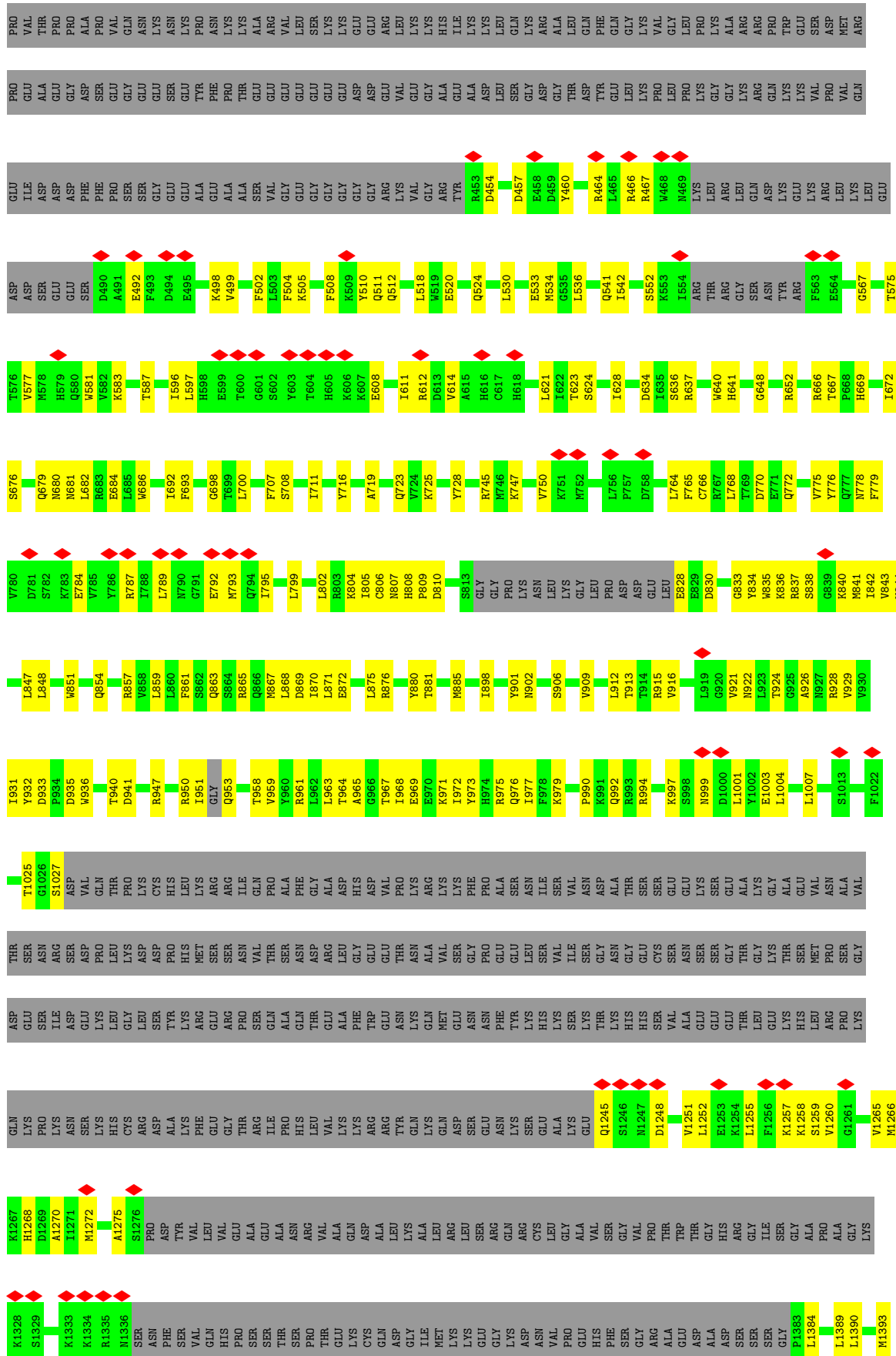


• Molecule 20: Inactive serine/threonine-protein kinase 19



• Molecule 21: DNA excision repair protein ERCC-6





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	257539	Depositor
Resolution determination method	OTHER	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)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	114.502	Depositor
Minimum map value	-1.609	Depositor
Average map value	0.029	Depositor
Map value standard deviation	1.373	Depositor
Recommended contour level	4.4	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	0.17	0/11364	0.35	0/15342
2	B	0.17	0/9229	0.33	0/12458
3	C	0.15	0/2132	0.29	0/2896
4	D	0.08	0/1064	0.22	0/1428
5	E	0.17	0/1751	0.35	0/2366
6	F	0.12	0/667	0.25	0/901
7	G	0.09	0/1382	0.27	0/1874
8	H	0.13	0/1207	0.28	0/1628
9	I	0.19	0/972	0.41	0/1316
10	J	0.13	0/542	0.27	0/730
11	K	0.14	0/939	0.28	0/1271
12	L	0.19	0/394	0.42	0/524
13	f	0.14	0/515	0.31	0/700
14	N	0.19	0/934	0.36	0/1439
15	M	0.13	0/247	0.21	0/384
16	T	0.23	0/1218	0.57	0/1874
17	a	0.19	0/3015	0.39	0/4086
18	b	0.17	0/6518	0.34	0/8810
19	c	0.10	0/311	0.31	0/420
20	g	0.25	0/1753	0.52	0/2374
21	e	0.21	0/4929	0.42	0/6642
22	d	0.20	0/2077	0.38	0/2783
All	All	0.18	0/53160	0.36	0/72246

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
1	A	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
5	E	0	2
9	I	0	1
12	L	0	1
13	f	0	1
17	a	0	1
18	b	0	3
20	g	0	3
21	e	0	4
22	d	0	1
All	All	0	21

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1160	ARG	Sidechain
1	A	20	ARG	Sidechain
1	A	532	ARG	Sidechain
2	B	975	ARG	Sidechain
5	E	162	ARG	Sidechain
5	E	166	ARG	Sidechain
9	I	33	ARG	Sidechain
12	L	51	ARG	Sidechain
17	a	78	ARG	Sidechain
18	b	753	ARG	Sidechain
18	b	847	ARG	Sidechain
18	b	889	ARG	Sidechain
22	d	44	ARG	Sidechain
21	e	464	ARG	Sidechain
21	e	466	ARG	Sidechain
21	e	467	ARG	Sidechain
21	e	612	ARG	Sidechain
13	f	43	ARG	Sidechain
20	g	192	ARG	Sidechain
20	g	200	ARG	Sidechain
20	g	72	ARG	Sidechain

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	11161	0	11297	305	0
2	B	9048	0	9084	215	0
3	C	2089	0	2031	62	0
4	D	1050	0	1033	16	0
5	E	1720	0	1737	59	0
6	F	657	0	684	12	0
7	G	1351	0	1358	37	0
8	H	1186	0	1147	23	0
9	I	949	0	879	24	0
10	J	533	0	553	17	0
11	K	920	0	942	29	0
12	L	388	0	393	16	0
13	f	505	0	463	18	0
14	N	831	0	450	23	0
15	M	220	0	109	5	0
16	T	1091	0	610	28	0
17	a	2951	0	2853	97	0
18	b	6405	0	6384	169	0
19	c	302	0	297	13	0
20	g	1721	0	1760	72	0
21	e	4820	0	4836	151	0
22	d	2040	0	2079	68	0
23	A	2	0	0	0	0
23	B	1	0	0	0	0
23	C	1	0	0	0	0
23	I	2	0	0	0	0
23	J	1	0	0	0	0
23	L	1	0	0	0	0
23	d	1	0	0	0	0
23	f	1	0	0	0	0
24	A	1	0	0	0	0
All	All	51949	0	50979	1308	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 13.

All (1308) 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)
5:E:187:ARG:NH2	5:E:210:GLN:HE22	1.54	1.05
5:E:187:ARG:CZ	5:E:210:GLN:OE1	2.18	0.91
5:E:187:ARG:HH21	5:E:210:GLN:HE22	0.93	0.88
3:C:90:CYS:SG	3:C:94:CYS:HB3	2.14	0.87
5:E:187:ARG:NH2	5:E:210:GLN:NE2	2.21	0.87
17:a:167:LYS:HE2	17:a:181:ILE:HD11	1.59	0.85
21:e:1027:SER:HB3	21:e:1266:MET:HA	1.57	0.84
2:B:532:ILE:HG22	2:B:621:ILE:HG13	1.60	0.81
2:B:1122:CYS:HB3	2:B:1140:CYS:SG	2.20	0.81
17:a:13:GLU:HG2	17:a:17:ARG:HD3	1.62	0.80
18:b:830:ILE:HD13	18:b:850:VAL:HG22	1.62	0.80
1:A:508:SER:OG	1:A:510:GLU:OE1	1.99	0.80
2:B:228:SER:O	2:B:405:ARG:NH2	2.16	0.77
17:a:111:ASP:OD1	17:a:112:THR:N	2.18	0.77
18:b:282:MET:HE2	18:b:305:LEU:HD21	1.66	0.76
1:A:549:THR:HG21	1:A:640:LEU:HD12	1.67	0.75
18:b:5:TYR:HE1	18:b:1094:ILE:HD11	1.51	0.75
2:B:18:THR:OG1	2:B:20:ASP:OD1	2.05	0.74
5:E:187:ARG:HH21	5:E:210:GLN:NE2	1.76	0.74
18:b:215:GLU:HG3	18:b:234:GLN:HB3	1.68	0.74
5:E:72:MET:HB2	5:E:101:ARG:HB2	1.69	0.74
2:B:934:LYS:HG2	2:B:1051:LEU:HD12	1.69	0.74
18:b:127:GLU:HB2	18:b:129:ARG:HH12	1.53	0.74
18:b:830:ILE:HG13	18:b:873:MET:HE1	1.67	0.74
3:C:72:PRO:HG3	10:J:13:ILE:HD11	1.70	0.73
20:g:167:THR:HG23	20:g:177:ALA:HB2	1.71	0.73
21:e:648:GLY:HA3	21:e:672:ILE:HG23	1.70	0.73
2:B:395:LEU:HD11	2:B:532:ILE:HD11	1.71	0.72
21:e:834:TYR:HD1	21:e:836:LYS:H	1.36	0.72
12:L:22:CYS:SG	12:L:24:THR:OG1	2.47	0.72
20:g:56:LEU:HD12	20:g:57:PRO:HD2	1.70	0.72
21:e:567:GLY:H	21:e:641:HIS:HD2	1.36	0.71
1:A:461:GLN:OE1	1:A:502:ASN:ND2	2.22	0.71
2:B:388:TYR:H	2:B:504:THR:HG21	1.55	0.71
21:e:836:LYS:HA	21:e:842:ILE:HD11	1.73	0.71
1:A:463:THR:HG23	1:A:468:SER:HB2	1.72	0.70
3:C:118:ARG:NH1	3:C:147:ASP:OD2	2.23	0.70
3:C:106:ARG:HG2	3:C:158:GLU:HG3	1.74	0.70
2:B:737:ILE:HG21	2:B:743:ARG:HD3	1.74	0.70
20:g:129:LEU:HA	20:g:133:LEU:HD23	1.73	0.70
18:b:1081:LYS:NZ	18:b:1083:GLU:OE1	2.21	0.70
5:E:13:ILE:HD11	5:E:136:LEU:HD22	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:7:DG:H2''	14:N:8:DA:H5''	1.74	0.70
18:b:291:MET:SD	18:b:291:MET:N	2.64	0.69
21:e:857:ARG:NH1	21:e:901:TYR:O	2.26	0.69
21:e:973:TYR:OH	21:e:1268:HIS:ND1	2.26	0.69
13:f:54:LEU:HB2	17:a:354:ARG:HH12	1.57	0.69
16:T:47:DA:H2''	16:T:48:DT:H5'	1.75	0.69
21:e:499:VAL:HG11	21:e:504:PHE:HD1	1.57	0.69
18:b:207:TRP:HB3	18:b:242:GLY:HA2	1.72	0.69
20:g:54:ASP:OD1	20:g:111:ARG:NH2	2.25	0.69
2:B:1105:GLU:HA	2:B:1109:GLU:HB2	1.74	0.69
18:b:256:SER:HB3	18:b:277:GLU:HG2	1.73	0.69
2:B:23:GLN:HE22	2:B:699:HIS:HE1	1.39	0.68
13:f:24:PHE:HB2	13:f:35:CYS:HB2	1.74	0.68
20:g:43:LEU:HD13	20:g:64:GLN:HG3	1.75	0.68
20:g:119:ARG:HD2	20:g:121:TYR:HE2	1.56	0.68
2:B:634:LEU:HB3	2:B:661:VAL:HG12	1.75	0.68
13:f:53:CYS:O	17:a:354:ARG:NH1	2.27	0.68
18:b:1109:VAL:HG12	18:b:1112:LEU:HD12	1.76	0.68
2:B:866:ILE:HG13	2:B:867:ILE:HG13	1.75	0.68
5:E:165:LEU:HB2	5:E:169:GLN:HG3	1.76	0.68
18:b:102:THR:OG1	18:b:1065:VAL:O	2.11	0.68
18:b:329:GLY:O	18:b:355:ASN:ND2	2.27	0.67
21:e:454:ASP:HB3	21:e:596:ILE:HD12	1.75	0.67
3:C:27:ASP:OD2	11:K:52:LYS:NZ	2.26	0.67
1:A:1368:VAL:HG13	1:A:1369:LEU:HG	1.76	0.67
5:E:138:ASN:HB3	5:E:141:GLU:HG3	1.74	0.67
5:E:167:GLU:HB3	5:E:208:LEU:HD13	1.74	0.67
8:H:8:ASP:OD2	8:H:9:ILE:N	2.27	0.67
1:A:1371:ILE:HG13	1:A:1406:THR:HG23	1.76	0.67
3:C:190:ASN:ND2	3:C:195:THR:O	2.28	0.67
21:e:768:LEU:HD23	21:e:772:GLN:HG2	1.75	0.67
21:e:776:TYR:CE1	21:e:802:LEU:HD11	2.30	0.67
17:a:369:VAL:HG12	18:b:887:THR:HG21	1.77	0.67
2:B:385:ARG:O	2:B:391:LYS:NZ	2.29	0.66
1:A:1216:LEU:HD12	1:A:1228:MET:HE1	1.76	0.66
2:B:93:LEU:HG	2:B:124:LEU:HD13	1.77	0.66
2:B:508:MET:HB3	2:B:621:ILE:HD13	1.76	0.66
18:b:210:GLU:N	18:b:210:GLU:OE1	2.29	0.66
21:e:1384:LEU:HD23	21:e:1389:LEU:HB2	1.78	0.66
17:a:52:GLU:OE2	17:a:58:TYR:N	2.22	0.66
21:e:967:THR:HG23	21:e:969:GLU:H	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1325:ASP:OD1	1:A:1326:GLY:N	2.29	0.66
22:d:691:ARG:NH1	22:d:692:MET:SD	2.69	0.66
18:b:1095:GLU:HG2	18:b:1137:THR:HG22	1.78	0.65
20:g:178:VAL:HG13	20:g:181:ALA:HB2	1.78	0.65
17:a:269:MET:HE1	17:a:308:VAL:HG21	1.78	0.65
1:A:1211:LEU:HD12	1:A:1260:ARG:HE	1.60	0.65
2:B:223:SER:OG	2:B:350:HIS:ND1	2.26	0.65
21:e:533:GLU:OE2	21:e:747:LYS:NZ	2.30	0.65
2:B:242:ARG:HD3	22:d:689:MET:HE1	1.78	0.65
1:A:478:PRO:HD2	11:K:67:LEU:HD23	1.78	0.65
1:A:1430:CYS:HB2	1:A:1435:THR:HG23	1.78	0.65
20:g:209:LEU:HA	20:g:212:LEU:HD23	1.79	0.65
21:e:861:PHE:HE1	21:e:912:LEU:HD13	1.60	0.65
21:e:881:THR:OG1	21:e:906:SER:O	2.13	0.65
3:C:201:GLU:OE1	3:C:201:GLU:N	2.20	0.64
18:b:720:SER:OG	18:b:738:SER:O	2.15	0.64
1:A:811:ILE:HD12	9:I:79:PRO:HB3	1.79	0.64
2:B:1119:CYS:HB3	2:B:1122:CYS:SG	2.36	0.64
16:T:25:DT:H2'	16:T:26:DT:H71	1.80	0.64
18:b:118:THR:HB	18:b:134:ARG:HH22	1.62	0.64
1:A:98:GLY:HA3	1:A:1440:MET:HE3	1.78	0.64
5:E:11:TRP:NE1	5:E:35:GLN:O	2.29	0.64
18:b:824:ASP:OD2	18:b:828:TYR:OH	2.15	0.64
2:B:565:THR:OG1	2:B:610:ARG:O	2.11	0.64
3:C:37:VAL:HG13	3:C:41:GLU:HB2	1.79	0.64
21:e:614:VAL:HG11	21:e:621:LEU:HB2	1.80	0.64
1:A:957:GLU:OE1	1:A:960:ARG:NH2	2.27	0.64
13:f:30:ASN:HB2	17:a:100:TYR:HD2	1.63	0.64
16:T:49:DG:H5''	21:e:865:ARG:H	1.62	0.64
21:e:775:VAL:HA	21:e:778:ASN:HD22	1.62	0.64
21:e:913:THR:HG22	21:e:915:ARG:H	1.62	0.64
1:A:280:LEU:O	1:A:284:VAL:HG23	1.98	0.63
18:b:795:ASP:HB2	18:b:802:LEU:HD11	1.79	0.63
1:A:486:LEU:HB3	1:A:538:VAL:HG21	1.80	0.63
14:N:49:DT:H2''	14:N:50:DT:H5''	1.81	0.63
1:A:1458:ILE:HD13	2:B:1091:ARG:HD2	1.81	0.63
4:D:87:LEU:HD13	4:D:97:LEU:HG	1.81	0.63
1:A:1009:VAL:O	1:A:1013:VAL:HG23	1.99	0.62
2:B:847:LYS:NZ	2:B:864:ASP:OD2	2.29	0.62
18:b:234:GLN:O	18:b:234:GLN:NE2	2.31	0.62
18:b:879:LYS:HE3	18:b:890:LEU:HD21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:b:1093:LEU:O	18:b:1096:SER:OG	2.14	0.62
22:d:69:PHE:HE1	22:d:76:ARG:HG3	1.64	0.62
2:B:754:PRO:HB2	2:B:773:PRO:HG2	1.81	0.62
17:a:53:PRO:HG3	17:a:109:PRO:HA	1.82	0.62
1:A:137:PRO:HB2	1:A:1445:HIS:HD1	1.65	0.62
18:b:3:TYR:HB3	18:b:1048:TYR:HB2	1.82	0.62
18:b:1120:MET:SD	18:b:1120:MET:N	2.73	0.62
21:e:510:TYR:O	21:e:745:ARG:NH1	2.33	0.62
21:e:840:LYS:HG2	21:e:932:TYR:CZ	2.33	0.62
22:d:88:GLU:HB3	22:d:94:ASP:HB2	1.81	0.62
2:B:550:MET:HE3	2:B:575:GLY:HA3	1.80	0.62
20:g:156:GLU:HA	20:g:159:HIS:HD2	1.65	0.62
21:e:1245:GLN:HB3	21:e:1248:ASP:HB2	1.82	0.62
20:g:169:ARG:H	20:g:174:TRP:HA	1.65	0.62
22:d:55:ALA:HA	22:d:58:ARG:HB2	1.81	0.62
22:d:87:LEU:HD21	22:d:138:LEU:HD11	1.82	0.62
21:e:833:GLY:HA3	21:e:870:ILE:HD11	1.82	0.62
1:A:1210:TRP:HZ3	9:I:53:ILE:HG13	1.65	0.61
2:B:281:ASP:HB3	9:I:22:ASN:HA	1.83	0.61
2:B:699:HIS:HD2	2:B:701:SER:H	1.48	0.61
20:g:54:ASP:HA	20:g:111:ARG:HH21	1.65	0.61
22:d:76:ARG:HD2	22:d:128:TYR:CE2	2.36	0.61
21:e:997:LYS:NZ	21:e:999:ASN:HB2	2.15	0.61
1:A:1190:GLN:O	1:A:1194:ASN:ND2	2.34	0.61
11:K:81:TYR:OH	11:K:89:ASN:OD1	2.19	0.61
2:B:602:SER:OG	2:B:620:ARG:NH1	2.33	0.61
21:e:968:ILE:HD12	21:e:971:LYS:HB2	1.82	0.61
1:A:904:GLN:NE2	1:A:981:CYS:O	2.34	0.61
4:D:60:VAL:HG13	7:G:103:PRO:HB3	1.83	0.61
8:H:92:MET:HE2	8:H:143:LEU:HD22	1.83	0.61
3:C:180:ALA:O	10:J:42:ARG:NH2	2.33	0.60
22:d:117:VAL:HA	22:d:120:TRP:HB2	1.83	0.60
5:E:167:GLU:HB3	5:E:208:LEU:CD1	2.31	0.60
2:B:387:HIS:NE2	2:B:671:GLU:OE2	2.31	0.60
9:I:24:LEU:HD23	9:I:37:TYR:HB3	1.83	0.60
18:b:285:LEU:HD22	18:b:300:LEU:HD22	1.82	0.60
3:C:190:ASN:O	3:C:193:ARG:NH1	2.33	0.60
18:b:69:PRO:HA	18:b:128:CYS:SG	2.42	0.60
21:e:492:GLU:HG2	21:e:498:LYS:HG2	1.83	0.60
1:A:860:ILE:HD11	1:A:1125:LYS:HB2	1.82	0.60
3:C:86:ARG:HD2	11:K:11:LEU:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:9:ARG:O	5:E:13:ILE:HG12	2.02	0.60
2:B:726:SER:O	2:B:730:LYS:NZ	2.34	0.60
2:B:1060:HIS:NE2	2:B:1082:GLY:O	2.31	0.60
17:a:58:TYR:HB3	17:a:70:LEU:HD11	1.82	0.60
18:b:83:LYS:NZ	18:b:1072:PHE:O	2.35	0.60
20:g:109:ARG:HG3	20:g:129:LEU:HD11	1.84	0.60
17:a:199:ASP:OD1	17:a:199:ASP:N	2.34	0.59
1:A:733:LEU:HD13	9:I:107:ALA:H	1.66	0.59
7:G:113:ILE:HG13	7:G:114:PRO:HD2	1.84	0.59
17:a:209:SER:O	17:a:243:ALA:N	2.33	0.59
21:e:636:SER:O	21:e:666:ARG:NH1	2.32	0.59
2:B:223:SER:HG	2:B:350:HIS:HD1	1.50	0.59
17:a:243:ALA:HB1	17:a:272:TRP:CH2	2.36	0.59
18:b:380:GLY:HA3	18:b:385:GLY:HA2	1.84	0.59
1:A:107:LEU:HD13	1:A:221:VAL:HG12	1.85	0.59
2:B:242:ARG:HD2	2:B:254:GLN:HG2	1.85	0.59
18:b:925:ASP:OD1	18:b:926:LEU:N	2.35	0.59
1:A:517:GLU:OE1	6:F:62:ARG:NH1	2.35	0.59
18:b:301:ARG:NH2	18:b:303:GLU:OE2	2.36	0.59
2:B:288:ILE:HD13	2:B:366:GLY:HA2	1.85	0.59
6:F:97:LEU:HD12	6:F:102:ILE:HG13	1.85	0.59
9:I:37:TYR:HD1	9:I:48:ALA:HB2	1.67	0.59
1:A:566:PHE:HB3	1:A:674:THR:HG22	1.85	0.59
18:b:319:ASN:ND2	19:c:15:ASN:O	2.36	0.58
2:B:627:ILE:HB	2:B:634:LEU:HD12	1.85	0.58
17:a:4:PHE:HB3	17:a:18:LEU:HD13	1.83	0.58
20:g:200:ARG:HG2	20:g:251:LEU:HD21	1.84	0.58
21:e:641:HIS:O	21:e:641:HIS:ND1	2.36	0.58
2:B:1085:ARG:NE	16:T:34:DC:OP1	2.27	0.58
17:a:116:THR:OG1	17:a:147:HIS:NE2	2.37	0.58
18:b:738:SER:OG	18:b:787:GLU:OE2	2.21	0.58
20:g:121:TYR:HB2	20:g:159:HIS:HB3	1.84	0.58
21:e:725:LYS:HB3	21:e:1399:LEU:HB3	1.85	0.58
2:B:117:ASN:HA	2:B:189:GLY:HA3	1.85	0.58
2:B:859:ARG:HH21	2:B:903:ILE:HD11	1.69	0.58
3:C:49:TRP:HB3	3:C:164:TYR:HB2	1.84	0.58
3:C:260:GLN:HB2	11:K:91:ILE:HG21	1.86	0.58
14:N:10:DC:H2'	14:N:11:DT:H71	1.84	0.58
21:e:787:ARG:HB3	21:e:792:GLU:HB2	1.84	0.58
1:A:1311:LEU:HD12	1:A:1332:GLN:HG3	1.85	0.58
2:B:602:SER:HB2	2:B:615:TYR:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:13:ILE:O	5:E:17:ILE:HG12	2.04	0.58
18:b:963:ASP:OD1	18:b:963:ASP:N	2.36	0.58
1:A:1279:MET:SD	1:A:1280:ASP:N	2.76	0.58
18:b:126:PRO:HD3	18:b:169:PHE:HB3	1.85	0.58
21:e:766:CYS:O	21:e:964:THR:HA	2.04	0.58
21:e:863:GLN:O	21:e:915:ARG:NH2	2.36	0.58
1:A:767:LYS:O	1:A:771:VAL:HG22	2.04	0.58
2:B:99:TRP:HZ3	2:B:151:LYS:HD3	1.69	0.58
18:b:338:VAL:HG13	19:c:6:LYS:HG3	1.85	0.58
22:d:82:ASN:ND2	22:d:85:GLU:OE1	2.36	0.58
22:d:107:GLN:OE1	22:d:110:ARG:NH1	2.33	0.58
17:a:204:THR:OG1	17:a:214:TRP:NE1	2.29	0.58
1:A:373:LEU:O	1:A:485:ASN:ND2	2.36	0.57
3:C:99:VAL:HB	3:C:165:ALA:HB3	1.86	0.57
1:A:467:MET:HE3	1:A:527:THR:HG22	1.86	0.57
5:E:187:ARG:NH2	5:E:210:GLN:CD	2.61	0.57
1:A:659:GLU:OE2	1:A:985:ARG:NH1	2.37	0.57
18:b:370:GLN:N	18:b:370:GLN:OE1	2.37	0.57
16:T:11:DA:H2 ^{''}	16:T:12:DA:H8	1.69	0.57
22:d:69:PHE:O	22:d:76:ARG:NH1	2.37	0.57
1:A:687:ILE:HD12	1:A:769:MET:HE1	1.86	0.57
1:A:18:ILE:HD11	2:B:1149:VAL:HG21	1.86	0.57
1:A:712:ASP:O	1:A:716:VAL:HG23	2.05	0.57
2:B:195:ILE:O	2:B:197:GLN:NE2	2.35	0.57
13:f:30:ASN:HB2	17:a:100:TYR:CD2	2.39	0.57
13:f:50:CYS:SG	13:f:51:THR:N	2.77	0.57
17:a:136:ASP:OD2	21:e:1396:ARG:NH1	2.37	0.57
18:b:756:ALA:HB1	18:b:801:VAL:HG21	1.87	0.57
21:e:935:ASP:HB3	21:e:940:THR:HG21	1.87	0.57
1:A:381:PRO:HB3	1:A:480:SER:HA	1.87	0.57
7:G:162:SER:HB2	7:G:164:MET:HE3	1.85	0.57
18:b:1014:MET:HE2	18:b:1014:MET:HA	1.87	0.57
21:e:810:ASP:HB2	21:e:837:ARG:HH21	1.69	0.57
2:B:849:ASP:HB3	12:L:15:MET:HE1	1.87	0.57
3:C:48:ASP:OD2	12:L:58:ARG:NH2	2.36	0.57
17:a:208:ASP:OD2	17:a:208:ASP:N	2.35	0.57
20:g:105:THR:HB	20:g:109:ARG:HH22	1.70	0.57
21:e:498:LYS:O	21:e:552:SER:OG	2.23	0.57
21:e:499:VAL:HG11	21:e:504:PHE:CD1	2.38	0.57
21:e:682:LEU:HD11	21:e:711:ILE:HG21	1.87	0.57
5:E:187:ARG:NH2	5:E:210:GLN:OE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:26:TYR:HB3	5:E:62:VAL:HG22	1.87	0.56
1:A:860:ILE:HG12	1:A:1128:ILE:HD11	1.86	0.56
1:A:1157:ILE:HA	1:A:1160:ARG:HD3	1.87	0.56
2:B:288:ILE:HG22	2:B:289:ILE:HG13	1.87	0.56
2:B:330:VAL:O	2:B:335:ARG:NH1	2.39	0.56
2:B:598:VAL:HG22	2:B:601:VAL:HG23	1.87	0.56
18:b:359:ILE:HG21	18:b:362:MET:HE3	1.87	0.56
21:e:975:ARG:HD3	21:e:1001:LEU:HD21	1.87	0.56
1:A:1166:LEU:HD23	1:A:1292:MET:HB3	1.86	0.56
2:B:808:SER:OG	2:B:1050:ARG:NH1	2.39	0.56
5:E:44:PHE:HB3	5:E:53:PRO:HB3	1.86	0.56
3:C:148:ILE:HG21	10:J:5:VAL:HG13	1.86	0.56
3:C:180:ALA:HB1	10:J:12:LYS:HB2	1.87	0.56
7:G:100:GLU:HA	7:G:105:SER:HA	1.88	0.56
14:N:15:DA:N1	16:T:46:DT:H72	2.20	0.56
18:b:328:LEU:HB3	18:b:381:ALA:HB3	1.88	0.56
9:I:17:CYS:N	9:I:22:ASN:O	2.37	0.56
17:a:111:ASP:OD1	17:a:113:GLY:N	2.39	0.56
1:A:465:HIS:CD2	1:A:467:MET:HB2	2.40	0.56
1:A:681:LEU:HG	2:B:1030:ASN:HD21	1.70	0.56
18:b:817:VAL:HG23	18:b:830:ILE:HG23	1.87	0.56
1:A:539:GLN:HB3	2:B:970:HIS:CD2	2.40	0.56
13:f:39:MET:SD	13:f:41:ARG:HG2	2.45	0.56
18:b:286:GLU:N	18:b:286:GLU:OE1	2.39	0.56
18:b:909:ILE:HD12	18:b:927:MET:HB2	1.87	0.56
20:g:146:MET:HA	20:g:150:PHE:HD2	1.69	0.56
22:d:22:PRO:HB2	22:d:26:LYS:HE3	1.88	0.56
18:b:735:VAL:HG12	18:b:792:LEU:HB2	1.88	0.56
21:e:765:PHE:HB3	21:e:965:ALA:HB2	1.87	0.56
1:A:1250:ASP:HA	1:A:1255:LEU:HD21	1.87	0.56
2:B:268:PRO:HG2	2:B:271:ILE:HG12	1.89	0.56
7:G:81:LYS:HE3	7:G:149:GLY:HA2	1.87	0.56
1:A:728:THR:H	1:A:736:THR:HG21	1.71	0.55
2:B:506:TRP:CZ2	2:B:677:MET:HE1	2.41	0.55
17:a:243:ALA:HB1	17:a:272:TRP:HH2	1.70	0.55
1:A:123:ASN:HD21	1:A:125:LYS:HB2	1.70	0.55
13:f:54:LEU:HB2	17:a:354:ARG:NH1	2.21	0.55
16:T:46:DT:H71	16:T:47:DA:C6	2.41	0.55
17:a:334:TYR:OH	22:d:130:LYS:O	2.21	0.55
22:d:55:ALA:H	22:d:100:PRO:HG2	1.72	0.55
1:A:1305:SER:HB3	1:A:1339:ASP:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:LEU:HD11	2:B:485:LEU:HD13	1.88	0.55
18:b:333:LEU:HB2	18:b:351:GLU:HG3	1.87	0.55
2:B:212:ASP:N	2:B:212:ASP:OD1	2.40	0.55
5:E:149:VAL:HG13	5:E:192:LYS:HB3	1.87	0.55
7:G:52:ASP:N	7:G:71:LYS:O	2.40	0.55
18:b:55:VAL:HG21	18:b:1065:VAL:HG21	1.88	0.55
1:A:694:ALA:HB3	1:A:699:TYR:CE1	2.41	0.55
22:d:59:LEU:HB2	22:d:109:LEU:HB2	1.88	0.55
1:A:40:GLY:O	1:A:42:LYS:NZ	2.39	0.55
1:A:1218:ARG:O	1:A:1221:MET:HB2	2.07	0.55
17:a:338:ASP:OD1	17:a:338:ASP:N	2.36	0.55
18:b:1024:THR:HB	18:b:1041:THR:HG21	1.89	0.55
21:e:844:VAL:HB	21:e:932:TYR:HE1	1.71	0.55
18:b:244:LYS:NZ	18:b:246:LEU:HB2	2.22	0.55
1:A:408:ARG:HH21	1:A:414:PRO:HB2	1.71	0.55
1:A:833:PRO:HB2	2:B:677:MET:HE2	1.89	0.55
1:A:865:ILE:O	1:A:869:GLU:HB3	2.07	0.55
2:B:258:ALA:HB2	2:B:269:ILE:HG22	1.89	0.55
2:B:581:GLU:O	2:B:585:ASN:ND2	2.30	0.55
4:D:41:LEU:HB3	4:D:65:LEU:HD12	1.88	0.55
22:d:73:HIS:HA	22:d:76:ARG:HB3	1.88	0.55
4:D:41:LEU:HD13	4:D:65:LEU:HA	1.89	0.55
1:A:153:ILE:HG21	20:g:186:LYS:HD3	1.89	0.55
1:A:865:ILE:HG12	2:B:1092:ASP:CG	2.31	0.55
5:E:18:MET:HE2	5:E:32:GLU:HB3	1.89	0.55
21:e:776:TYR:HH	21:e:967:THR:HG1	1.50	0.55
22:d:12:LEU:HB3	22:d:20:LEU:HD13	1.89	0.55
1:A:111:CYS:HB3	1:A:116:LYS:H	1.71	0.54
1:A:1294:THR:HG21	22:d:685:VAL:HG13	1.89	0.54
12:L:27:GLU:OE2	12:L:37:ARG:NH1	2.40	0.54
21:e:851:TRP:NE1	21:e:928:ARG:HG3	2.22	0.54
7:G:99:THR:OG1	7:G:106:CYS:SG	2.65	0.54
1:A:32:LYS:NZ	1:A:89:GLU:OE2	2.40	0.54
1:A:1416:ARG:NH2	16:T:29:DC:O2	2.41	0.54
2:B:556:ILE:HG21	2:B:576:ILE:HG12	1.89	0.54
7:G:117:MET:HE2	7:G:128:TYR:HB3	1.89	0.54
18:b:165:ILE:HB	18:b:181:VAL:HG13	1.88	0.54
1:A:360:ASP:OD1	2:B:1062:ARG:NE	2.39	0.54
1:A:582:PRO:HD2	8:H:47:ILE:HD12	1.89	0.54
11:K:73:ILE:HD12	11:K:87:PHE:HZ	1.72	0.54
20:g:55:ALA:HB3	20:g:183:ARG:HH22	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:g:83:GLN:HA	20:g:88:ILE:HG22	1.90	0.54
21:e:634:ASP:OD1	21:e:637:ARG:NH1	2.39	0.54
1:A:1228:MET:HE3	1:A:1255:LEU:HB3	1.90	0.54
1:A:1301:ILE:HG23	1:A:1345:ARG:HE	1.73	0.54
7:G:52:ASP:HB2	7:G:71:LYS:HB3	1.89	0.54
18:b:127:GLU:HB2	18:b:129:ARG:NH1	2.19	0.54
22:d:53:GLU:HG2	22:d:54:HIS:N	2.22	0.54
1:A:593:SER:HB3	1:A:634:GLU:HA	1.90	0.54
1:A:896:LEU:HD13	1:A:980:PRO:HG3	1.89	0.54
2:B:344:GLN:O	2:B:361:LYS:NZ	2.39	0.54
2:B:812:ARG:NE	2:B:897:ARG:HG3	2.23	0.54
6:F:83:LEU:HD22	6:F:86:GLU:HB2	1.89	0.54
16:T:11:DA:H2"	16:T:12:DA:C8	2.42	0.54
21:e:921:VAL:O	21:e:950:ARG:NH2	2.41	0.54
2:B:538:PRO:HG3	2:B:570:ASN:HD22	1.73	0.54
5:E:60:VAL:HB	5:E:74:VAL:HB	1.89	0.54
1:A:77:ASN:H	1:A:80:GLU:HG2	1.73	0.54
1:A:863:ARG:HB3	1:A:1414:ILE:HG22	1.90	0.54
2:B:448:LEU:O	2:B:467:SER:OG	2.23	0.54
2:B:541:ILE:HG12	2:B:597:ILE:HG12	1.90	0.54
1:A:1004:LEU:HD13	1:A:1062:GLY:HA2	1.90	0.54
1:A:1030:SER:OG	5:E:162:ARG:HD2	2.07	0.54
2:B:309:PHE:CZ	9:I:40:ARG:HG3	2.43	0.54
21:e:922:ASN:HA	21:e:950:ARG:HH22	1.73	0.54
21:e:931:ILE:HG13	21:e:961:ARG:HD3	1.90	0.54
1:A:1011:GLU:OE1	1:A:1011:GLU:N	2.40	0.53
19:c:44:GLU:HG2	19:c:45:GLN:HG2	1.89	0.53
1:A:544:ALA:HB2	1:A:680:LEU:HD22	1.90	0.53
1:A:592:PHE:HE1	1:A:672:ILE:HG12	1.72	0.53
17:a:152:VAL:O	18:b:111:ARG:NH2	2.41	0.53
21:e:865:ARG:HA	21:e:868:LEU:HG	1.89	0.53
1:A:516:GLN:HA	1:A:520:MET:HE3	1.90	0.53
17:a:119:SER:OG	17:a:120:PHE:N	2.40	0.53
21:e:992:GLN:HG3	21:e:1275:ALA:HA	1.90	0.53
21:e:997:LYS:HZ2	21:e:999:ASN:HB2	1.73	0.53
1:A:930:LEU:HB3	1:A:939:VAL:HG23	1.89	0.53
13:f:24:PHE:O	13:f:34:SER:N	2.38	0.53
21:e:835:TRP:H	21:e:835:TRP:CD1	2.26	0.53
1:A:1477:ALA:HA	7:G:22:LEU:HD21	1.90	0.53
2:B:276:LEU:HG	2:B:343:LEU:HD11	1.90	0.53
2:B:373:LEU:O	2:B:377:LEU:HD12	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:187:ARG:CZ	5:E:210:GLN:CD	2.82	0.53
2:B:297:MET:O	2:B:301:VAL:HG23	2.08	0.53
5:E:46:ASP:OD1	5:E:46:ASP:N	2.42	0.53
17:a:168:VAL:HG22	17:a:189:ILE:HD13	1.91	0.53
18:b:253:ILE:HD11	18:b:302:VAL:HG11	1.91	0.53
22:d:565:HIS:NE2	22:d:581:ASP:O	2.41	0.53
1:A:227:ARG:CZ	20:g:168:VAL:HG21	2.38	0.53
1:A:369:PRO:HD3	1:A:496:PHE:CG	2.44	0.53
1:A:467:MET:SD	1:A:524:MET:HE3	2.47	0.53
2:B:796:MET:HE1	2:B:929:PRO:HB2	1.90	0.53
14:N:51:DG:H2''	14:N:52:DA:C8	2.44	0.53
17:a:80:SER:O	17:a:81:TYR:C	2.51	0.53
18:b:1095:GLU:OE2	18:b:1140:HIS:NE2	2.37	0.53
1:A:1141:VAL:HA	1:A:1357:THR:HG23	1.91	0.53
1:A:1429:LYS:HB2	1:A:1438:VAL:HG21	1.90	0.53
16:T:37:DC:H2'	16:T:38:DT:C6	2.44	0.53
17:a:57:ARG:NE	17:a:74:GLU:OE2	2.42	0.53
21:e:667:THR:HG22	21:e:669:HIS:H	1.73	0.53
1:A:227:ARG:NH1	20:g:168:VAL:HG21	2.24	0.52
2:B:998:ASP:OD1	2:B:1000:THR:OG1	2.27	0.52
18:b:14:ALA:HB1	18:b:327:ARG:HD2	1.90	0.52
21:e:922:ASN:HA	21:e:950:ARG:HH12	1.74	0.52
1:A:595:ILE:HD11	1:A:675:VAL:HG11	1.91	0.52
1:A:1461:GLY:HA3	2:B:1152:PRO:HD3	1.91	0.52
2:B:86:LEU:HD23	2:B:130:LYS:HB2	1.91	0.52
2:B:474:THR:HG23	2:B:477:SER:H	1.74	0.52
1:A:904:GLN:OE1	1:A:1044:HIS:NE2	2.39	0.52
20:g:167:THR:O	20:g:174:TRP:HB3	2.09	0.52
1:A:1184:THR:OG1	1:A:1190:GLN:OE1	2.21	0.52
12:L:13:GLN:O	12:L:29:LYS:NZ	2.42	0.52
17:a:177:SER:OG	17:a:178:CYS:N	2.34	0.52
17:a:329:MET:HB2	17:a:331:LYS:HZ2	1.74	0.52
20:g:143:GLN:N	20:g:172:GLY:O	2.43	0.52
18:b:1113:GLN:NE2	18:b:1114:TYR:O	2.43	0.52
1:A:592:PHE:CE1	1:A:672:ILE:HG12	2.43	0.52
1:A:804:HIS:NE2	9:I:100:HIS:HB2	2.25	0.52
2:B:50:PHE:HB2	2:B:397:GLY:HA2	1.91	0.52
2:B:794:VAL:HG12	2:B:967:ILE:HG22	1.90	0.52
5:E:91:CYS:HA	5:E:94:MET:HE3	1.91	0.52
14:N:7:DG:H2''	14:N:8:DA:H8	1.75	0.52
1:A:459:ASN:HB2	1:A:469:MET:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:863:ARG:NH2	1:A:1129:ASN:OD1	2.42	0.52
7:G:22:LEU:HA	7:G:25:THR:HG22	1.90	0.52
7:G:129:LYS:HD3	7:G:133:GLU:HG2	1.90	0.52
10:J:67:LYS:HD2	12:L:23:HIS:HB2	1.90	0.52
15:M:2:U:H2'	15:M:3:C:C6	2.45	0.52
16:T:55:DA:H4'	16:T:56:DA:OP1	2.09	0.52
17:a:353:SER:OG	17:a:354:ARG:N	2.42	0.52
21:e:502:PHE:HA	21:e:505:LYS:HE3	1.92	0.52
2:B:15:ASP:OD1	2:B:15:ASP:N	2.41	0.52
2:B:907:VAL:HG12	2:B:921:ILE:HG12	1.92	0.52
9:I:98:GLN:O	9:I:100:HIS:ND1	2.38	0.52
20:g:160:LEU:HD12	20:g:160:LEU:H	1.75	0.52
1:A:1027:ASP:OD1	1:A:1027:ASP:N	2.41	0.52
2:B:188:ASN:OD1	2:B:445:LYS:NZ	2.41	0.52
2:B:675:LEU:HD22	2:B:697:GLU:HG2	1.90	0.52
3:C:253:LYS:HG2	11:K:95:ILE:HD13	1.92	0.52
9:I:49:ASP:OD1	9:I:49:ASP:N	2.41	0.52
11:K:39:ASP:OD1	11:K:39:ASP:N	2.42	0.52
17:a:81:TYR:HE2	22:d:129:LYS:NZ	2.08	0.52
17:a:283:ASN:HB3	20:g:72:ARG:HH21	1.75	0.52
22:d:27:GLU:O	22:d:30:LYS:HG2	2.10	0.52
8:H:69:THR:HG21	8:H:81:ARG:HH22	1.75	0.52
20:g:91:VAL:O	20:g:101:GLY:N	2.41	0.52
20:g:104:PHE:CE1	20:g:106:GLU:HB2	2.45	0.52
21:e:871:LEU:O	21:e:875:LEU:N	2.39	0.52
1:A:549:THR:O	1:A:589:LYS:NZ	2.36	0.51
2:B:282:ARG:O	2:B:286:GLU:HG3	2.09	0.51
2:B:759:VAL:HG13	2:B:986:GLN:HG2	1.92	0.51
2:B:955:PRO:HB2	2:B:1028:LEU:HD13	1.91	0.51
2:B:1027:VAL:HG13	3:C:195:THR:HG21	1.93	0.51
17:a:142:GLU:HB3	17:a:164:ARG:HB3	1.92	0.51
20:g:248:LEU:HD12	20:g:249:LEU:H	1.75	0.51
1:A:514:GLU:HA	6:F:63:ALA:HB1	1.93	0.51
1:A:1129:ASN:HA	1:A:1413:ALA:HB1	1.90	0.51
17:a:19:ARG:NH1	18:b:1079:GLU:OE2	2.38	0.51
18:b:27:GLU:N	18:b:27:GLU:OE1	2.43	0.51
18:b:53:LYS:HD2	19:c:35:TYR:HB2	1.92	0.51
1:A:406:VAL:HG21	1:A:419:ILE:HD11	1.92	0.51
1:A:1218:ARG:O	1:A:1222:THR:HG23	2.10	0.51
3:C:20:LYS:HE2	3:C:232:ASN:ND2	2.25	0.51
7:G:52:ASP:OD2	7:G:73:LYS:NZ	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:99:THR:HG21	7:G:143:ILE:HD11	1.91	0.51
17:a:38:VAL:HG11	17:a:358:ILE:HB	1.92	0.51
17:a:217:ARG:HB3	21:e:524:GLN:HB3	1.92	0.51
18:b:149:ASN:O	19:c:45:GLN:NE2	2.43	0.51
1:A:267:GLN:O	2:B:890:ARG:NH2	2.44	0.51
1:A:580:LEU:HB3	8:H:91:VAL:HG13	1.93	0.51
1:A:1227:THR:HG23	1:A:1230:GLN:H	1.76	0.51
2:B:764:MET:HA	2:B:767:LEU:HB2	1.93	0.51
2:B:956:PHE:HE2	3:C:184:PHE:HB3	1.76	0.51
17:a:329:MET:HB2	17:a:331:LYS:NZ	2.25	0.51
18:b:1116:ASP:OD1	18:b:1116:ASP:N	2.40	0.51
21:e:728:TYR:CE1	21:e:990:PRO:HB2	2.46	0.51
1:A:1175:ILE:HG23	1:A:1285:LEU:HD23	1.92	0.51
2:B:196:ALA:HB2	2:B:395:LEU:HD23	1.92	0.51
13:f:82:ASN:HA	17:a:92:ARG:NH1	2.26	0.51
16:T:24:DC:H2'	16:T:25:DT:H71	1.93	0.51
18:b:223:PRO:HD2	18:b:268:GLY:HA3	1.93	0.51
1:A:713:VAL:HG11	1:A:817:PRO:HD3	1.93	0.51
3:C:109:GLU:OE1	3:C:109:GLU:N	2.44	0.51
21:e:681:ASN:N	21:e:681:ASN:OD1	2.43	0.51
22:d:53:GLU:HG2	22:d:54:HIS:H	1.75	0.51
1:A:577:PRO:HG2	1:A:580:LEU:HD13	1.93	0.51
1:A:603:ILE:HG12	1:A:629:VAL:HG22	1.93	0.51
1:A:1167:ARG:HD3	22:d:692:MET:HE2	1.93	0.51
2:B:528:LEU:HB3	2:B:702:MET:HE3	1.92	0.51
2:B:1129:ASN:OD1	2:B:1131:ARG:N	2.44	0.51
14:N:34:DG:H2''	14:N:35:DA:H8	1.74	0.51
14:N:43:DG:H2''	14:N:44:DA:C8	2.44	0.51
20:g:212:LEU:HD12	20:g:225:LEU:HD11	1.91	0.51
1:A:354:LEU:HD13	1:A:1459:MET:HG2	1.93	0.51
1:A:1029:LEU:HD23	5:E:162:ARG:NE	2.25	0.51
11:K:10:PHE:HA	11:K:37:LYS:HB3	1.91	0.51
1:A:420:ILE:HB	1:A:445:LYS:HG3	1.93	0.51
2:B:225:LEU:HB3	2:B:227:ASN:O	2.10	0.51
17:a:262:THR:HG21	17:a:272:TRP:CZ3	2.45	0.51
1:A:1324:GLU:HG2	1:A:1325:ASP:N	2.26	0.51
2:B:565:THR:HG21	2:B:580:PRO:HB3	1.92	0.51
22:d:594:ARG:NH2	22:d:609:GLU:OE2	2.43	0.51
1:A:102:LYS:NZ	1:A:1441:GLU:OE1	2.43	0.50
2:B:942:LYS:NZ	15:M:10:A:OP1	2.30	0.50
4:D:107:THR:HG23	4:D:110:GLU:H	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:55:ARG:NH1	5:E:107:GLN:OE1	2.42	0.50
14:N:34:DG:H2'	14:N:35:DA:C8	2.46	0.50
21:e:912:LEU:HB3	21:e:916:VAL:HG11	1.93	0.50
1:A:921:ARG:NH2	1:A:953:GLU:OE2	2.38	0.50
5:E:14:ARG:O	5:E:18:MET:HG2	2.11	0.50
18:b:32:LEU:HD13	18:b:66:LEU:HD11	1.93	0.50
18:b:381:ALA:O	18:b:720:SER:HB3	2.11	0.50
20:g:204:TYR:HE1	22:d:49:GLN:HE21	1.59	0.50
2:B:69:ALA:HB3	2:B:81:PRO:HB3	1.92	0.50
7:G:90:THR:O	7:G:139:GLN:NE2	2.38	0.50
21:e:652:ARG:HB2	21:e:684:GLU:HG3	1.92	0.50
22:d:54:HIS:O	22:d:57:ILE:N	2.43	0.50
2:B:506:TRP:HZ2	2:B:677:MET:HE1	1.76	0.50
2:B:759:VAL:HG12	2:B:999:ALA:HB2	1.94	0.50
3:C:9:VAL:HG21	11:K:105:PHE:HA	1.94	0.50
16:T:23:DC:H5'	22:d:683:ARG:CZ	2.42	0.50
21:e:869:ASP:OD2	21:e:869:ASP:N	2.44	0.50
2:B:761:THR:HG23	2:B:1000:THR:HA	1.94	0.50
6:F:69:ARG:NH2	6:F:78:PRO:O	2.43	0.50
9:I:35:LEU:HD22	9:I:51:SER:HA	1.94	0.50
10:J:1:MET:HA	10:J:55:LEU:HB2	1.94	0.50
1:A:583:ARG:HG2	1:A:584:PRO:HD2	1.92	0.50
2:B:96:PRO:HG2	2:B:162:LEU:HD12	1.93	0.50
2:B:236:TRP:HB2	2:B:259:THR:HB	1.93	0.50
7:G:62:GLY:O	7:G:63:ARG:HG2	2.12	0.50
8:H:13:LYS:HG3	8:H:31:GLU:HG3	1.93	0.50
12:L:13:GLN:N	12:L:14:PRO:HD2	2.27	0.50
1:A:687:ILE:HD11	1:A:766:PHE:CE1	2.47	0.50
3:C:19:VAL:HB	3:C:241:PRO:HB2	1.93	0.50
4:D:87:LEU:HD21	4:D:92:LEU:HD23	1.93	0.50
18:b:34:ALA:HB2	18:b:64:MET:SD	2.51	0.50
18:b:269:SER:OG	18:b:287:LYS:NZ	2.43	0.50
21:e:457:ASP:HB3	21:e:460:TYR:HB3	1.93	0.50
21:e:680:ASN:N	21:e:684:GLU:OE1	2.38	0.50
1:A:375:ILE:HD12	1:A:535:MET:HE1	1.93	0.50
1:A:926:ASN:HB3	1:A:929:ALA:HB3	1.94	0.50
1:A:1123:ARG:HH21	1:A:1381:GLU:HG3	1.77	0.50
16:T:33:DT:H2'	16:T:34:DC:C6	2.46	0.50
18:b:133:LEU:HB3	18:b:135:LEU:HD13	1.93	0.50
18:b:740:ILE:HG23	18:b:785:GLU:CD	2.36	0.50
21:e:676:SER:OG	21:e:679:GLN:NE2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:823:VAL:HG22	1:A:835:GLU:HB3	1.93	0.50
2:B:827:GLU:HG3	2:B:871:VAL:HB	1.93	0.50
3:C:7:PRO:HB2	11:K:101:LEU:HD13	1.94	0.50
16:T:47:DA:H2''	16:T:48:DT:C5'	2.40	0.50
21:e:924:THR:O	21:e:953:GLN:NE2	2.44	0.50
22:d:13:THR:HB	22:d:57:ILE:HG23	1.94	0.50
21:e:776:TYR:OH	21:e:806:CYS:SG	2.70	0.49
21:e:847:LEU:HB3	21:e:851:TRP:CZ3	2.46	0.49
21:e:848:LEU:HB3	21:e:880:TYR:HE2	1.76	0.49
22:d:23:GLU:HA	22:d:26:LYS:HD2	1.94	0.49
1:A:190:ARG:HH22	14:N:38:DG:H3'	1.77	0.49
2:B:52:GLN:HB3	2:B:53:MET:SD	2.51	0.49
2:B:110:PRO:HG2	2:B:163:LEU:HD11	1.95	0.49
2:B:795:ILE:HG12	2:B:947:ILE:HG22	1.94	0.49
2:B:1116:VAL:HG21	2:B:1125:MET:SD	2.51	0.49
17:a:60:LEU:HD23	17:a:70:LEU:HD13	1.94	0.49
18:b:883:SER:HB3	18:b:914:LEU:HD11	1.94	0.49
21:e:928:ARG:HD2	21:e:958:THR:HG23	1.94	0.49
1:A:421:ARG:HE	1:A:427:ILE:HD11	1.76	0.49
3:C:24:GLU:HG2	3:C:228:ARG:HG3	1.93	0.49
18:b:310:ILE:HG21	18:b:328:LEU:HD12	1.94	0.49
21:e:534:MET:O	21:e:747:LYS:NZ	2.45	0.49
21:e:716:TYR:O	21:e:994:ARG:NH1	2.46	0.49
22:d:59:LEU:HA	22:d:109:LEU:HD13	1.94	0.49
1:A:375:ILE:HG12	1:A:666:ARG:HG3	1.94	0.49
1:A:1128:ILE:HB	1:A:1414:ILE:HB	1.94	0.49
7:G:147:ILE:HD13	7:G:159:ALA:HB1	1.93	0.49
18:b:188:ARG:NH1	18:b:216:ALA:O	2.45	0.49
1:A:138:LYS:HA	1:A:1445:HIS:HE1	1.77	0.49
2:B:320:PHE:CE2	13:f:64:LEU:HD21	2.47	0.49
21:e:583:LYS:O	21:e:587:THR:HG23	2.12	0.49
22:d:76:ARG:HD2	22:d:128:TYR:CZ	2.48	0.49
1:A:383:SER:HB2	11:K:2:ASN:OD1	2.13	0.49
1:A:1375:ARG:HD2	1:A:1402:CYS:HB3	1.94	0.49
2:B:274:ARG:NH1	2:B:311:ILE:O	2.46	0.49
17:a:105:VAL:HG12	17:a:117:SER:HB2	1.95	0.49
18:b:288:GLU:OE1	18:b:296:THR:OG1	2.30	0.49
21:e:841:MET:HE2	21:e:932:TYR:OH	2.12	0.49
1:A:520:MET:HB3	1:A:522:PRO:HD2	1.93	0.49
2:B:295:PRO:O	2:B:299:GLU:HG3	2.12	0.49
3:C:18:ASN:ND2	3:C:232:ASN:OD1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:263:LEU:HD13	11:K:19:ILE:HD13	1.94	0.49
10:J:66:GLU:HG2	12:L:18:ILE:HD12	1.95	0.49
17:a:349:LEU:HB3	17:a:361:TRP:HB2	1.95	0.49
18:b:368:GLU:O	18:b:369:ARG:HG2	2.13	0.49
21:e:686:TRP:NE1	21:e:698:GLY:O	2.34	0.49
1:A:527:THR:HG23	1:A:534:VAL:HB	1.93	0.49
1:A:821:GLY:HA2	1:A:838:PHE:CD2	2.47	0.49
1:A:1199:MET:HE3	1:A:1200:PRO:HD2	1.95	0.49
3:C:45:ILE:HG22	3:C:73:LEU:HD12	1.94	0.49
7:G:89:VAL:HG22	7:G:99:THR:HG22	1.94	0.49
17:a:247:LYS:O	17:a:265:THR:HG23	2.11	0.49
18:b:275:ASP:OD2	18:b:279:ARG:HB2	2.13	0.49
18:b:303:GLU:HG3	19:c:5:LEU:HD21	1.93	0.49
18:b:363:CYS:HB2	18:b:724:ILE:HG23	1.95	0.49
20:g:157:ILE:O	20:g:161:VAL:HG23	2.12	0.49
1:A:1138:SER:N	1:A:1360:ASN:OD1	2.46	0.49
2:B:228:SER:OG	2:B:405:ARG:NH2	2.44	0.49
7:G:117:MET:HE1	7:G:137:ILE:HD12	1.95	0.49
17:a:31:GLU:OE1	17:a:32:LEU:N	2.46	0.49
1:A:108:ARG:HD2	1:A:145:TYR:HE1	1.77	0.49
2:B:289:ILE:HD11	2:B:301:VAL:HG21	1.94	0.49
6:F:83:LEU:HD21	6:F:92:ILE:HG23	1.94	0.49
18:b:129:ARG:HE	18:b:176:PRO:HG3	1.77	0.49
18:b:966:LEU:HD22	18:b:1040:VAL:HG11	1.93	0.49
18:b:1002:GLU:OE2	18:b:1034:ASN:HB2	2.12	0.49
20:g:168:VAL:HA	20:g:174:TRP:HD1	1.76	0.49
21:e:931:ILE:HB	21:e:961:ARG:HA	1.95	0.49
1:A:419:ILE:HB	1:A:427:ILE:HB	1.93	0.48
2:B:589:LYS:HB2	2:B:589:LYS:HE3	1.57	0.48
12:L:39:CYS:SG	12:L:41:TYR:HB2	2.53	0.48
18:b:59:GLY:HA2	18:b:1073:TRP:CZ3	2.48	0.48
18:b:770:LEU:HD13	18:b:865:GLU:HG3	1.95	0.48
1:A:923:ASP:O	1:A:930:LEU:HD21	2.13	0.48
2:B:1128:ALA:HB1	2:B:1135:TYR:HD1	1.78	0.48
4:D:126:GLU:O	4:D:129:GLN:HG3	2.13	0.48
17:a:388:ALA:HB3	22:d:71:ARG:HA	1.95	0.48
7:G:39:THR:O	7:G:43:GLY:N	2.47	0.48
18:b:1051:LEU:O	18:b:1055:GLN:N	2.38	0.48
20:g:116:CYS:O	20:g:122:ALA:HB2	2.13	0.48
21:e:921:VAL:HG13	21:e:947:ARG:HG3	1.95	0.48
1:A:479:TRP:H	1:A:483:ARG:HH22	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:ARG:O	1:A:561:MET:HG3	2.13	0.48
4:D:87:LEU:HD22	4:D:97:LEU:HD12	1.95	0.48
4:D:87:LEU:HA	4:D:90:LYS:HZ3	1.78	0.48
5:E:187:ARG:HG2	5:E:187:ARG:HH11	1.78	0.48
18:b:39:LEU:HB3	18:b:55:VAL:HG13	1.95	0.48
1:A:27:SER:OG	1:A:29:ASP:OD1	2.18	0.48
1:A:244:ARG:NH2	1:A:246:GLU:OE2	2.44	0.48
1:A:833:PRO:HG3	2:B:1002:PHE:CG	2.48	0.48
1:A:865:ILE:HG12	2:B:1092:ASP:OD2	2.13	0.48
2:B:385:ARG:HH11	2:B:385:ARG:HG2	1.78	0.48
16:T:28:DT:H1'	16:T:29:DC:H5'	1.95	0.48
18:b:1010:GLY:O	18:b:1027:SER:OG	2.28	0.48
2:B:783:ALA:O	2:B:789:ASN:ND2	2.47	0.48
10:J:2:ILE:HD12	10:J:56:ILE:HD13	1.96	0.48
17:a:81:TYR:HE2	22:d:129:LYS:HZ2	1.61	0.48
17:a:303:CYS:O	18:b:114:ARG:NH2	2.46	0.48
17:a:341:VAL:HG12	17:a:350:TYR:HB2	1.94	0.48
18:b:63:VAL:HG22	18:b:80:LEU:HB3	1.96	0.48
18:b:112:ILE:HD12	18:b:113:GLY:H	1.77	0.48
21:e:764:LEU:HD22	21:e:1265:VAL:HG22	1.96	0.48
5:E:71:GLN:OE1	5:E:71:GLN:N	2.47	0.48
18:b:213:GLU:HG3	18:b:215:GLU:H	1.78	0.48
18:b:953:TRP:HB2	18:b:970:ASN:HB2	1.96	0.48
22:d:566:TRP:HE1	22:d:580:GLN:HE21	1.62	0.48
18:b:129:ARG:NE	18:b:176:PRO:HG3	2.29	0.48
18:b:1016:ASN:OD1	18:b:1020:THR:N	2.47	0.48
20:g:89:ARG:HG2	20:g:105:THR:HG22	1.96	0.48
20:g:113:LEU:HA	20:g:116:CYS:SG	2.54	0.48
2:B:17:ILE:HG21	2:B:22:TRP:HE3	1.79	0.48
2:B:924:ARG:NH1	3:C:62:GLU:OE2	2.47	0.48
2:B:1028:LEU:HD12	2:B:1041:ILE:HD12	1.95	0.48
21:e:772:GLN:NE2	21:e:805:ILE:O	2.46	0.48
21:e:872:GLU:O	21:e:876:ARG:HG2	2.13	0.48
2:B:115:LEU:HD22	2:B:908:MET:HE2	1.95	0.48
8:H:10:PHE:HB2	8:H:56:PHE:CE1	2.48	0.48
18:b:288:GLU:HB2	18:b:298:LYS:HG3	1.96	0.48
21:e:772:GLN:HE21	21:e:805:ILE:HG22	1.79	0.48
1:A:114:CYS:HB3	1:A:184:CYS:SG	2.54	0.47
1:A:379:GLY:HA3	1:A:483:ARG:HB2	1.96	0.47
2:B:407:MET:HA	2:B:410:ASN:HD22	1.78	0.47
5:E:17:ILE:HG21	5:E:74:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:43:ARG:HG3	22:d:103:ARG:HH22	1.79	0.47
1:A:355:MET:HE2	1:A:1431:SER:OG	2.14	0.47
2:B:289:ILE:HG12	2:B:297:MET:HB3	1.97	0.47
2:B:709:SER:HB3	2:B:763:SER:HB2	1.96	0.47
3:C:105:VAL:HG11	3:C:115:VAL:HG22	1.94	0.47
4:D:38:HIS:HB2	4:D:68:THR:HB	1.97	0.47
4:D:59:GLU:HG3	4:D:63:LYS:HD2	1.95	0.47
5:E:134:GLU:OE2	5:E:181:ARG:NH2	2.47	0.47
17:a:32:LEU:O	17:a:34:LYS:N	2.48	0.47
18:b:1053:ASP:HA	18:b:1056:ASN:HB2	1.96	0.47
21:e:1259:SER:OG	21:e:1260:VAL:N	2.47	0.47
1:A:466:LYS:HE2	1:A:524:MET:HE1	1.95	0.47
1:A:1228:MET:HB3	1:A:1247:PHE:CD2	2.49	0.47
1:A:1343:LEU:HD23	1:A:1368:VAL:HG11	1.95	0.47
1:A:1389:ASP:OD2	1:A:1391:SER:OG	2.27	0.47
2:B:819:SER:OG	2:B:827:GLU:OE1	2.26	0.47
3:C:7:PRO:HD2	11:K:100:LEU:HD23	1.96	0.47
8:H:38:ASP:HB3	8:H:126:GLN:HG2	1.96	0.47
14:N:6:DT:H2''	14:N:7:DG:H5''	1.96	0.47
17:a:185:HIS:CE1	17:a:206:SER:HB3	2.49	0.47
18:b:165:ILE:HG13	18:b:188:ARG:NH1	2.29	0.47
18:b:1051:LEU:HB2	18:b:1089:ILE:HD13	1.94	0.47
1:A:540:ASP:HB2	2:B:790:GLN:CD	2.39	0.47
18:b:1051:LEU:HA	18:b:1054:MET:HB3	1.95	0.47
21:e:941:ASP:OD2	21:e:976:GLN:NE2	2.48	0.47
22:d:110:ARG:O	22:d:114:THR:HG23	2.14	0.47
2:B:150:GLY:HA2	2:B:437:THR:HB	1.96	0.47
3:C:47:ILE:HA	3:C:165:ALA:HA	1.95	0.47
8:H:20:LYS:NZ	8:H:26:SER:OG	2.43	0.47
1:A:571:ASP:N	1:A:571:ASP:OD1	2.42	0.47
11:K:26:LYS:HE2	11:K:26:LYS:HB2	1.70	0.47
17:a:31:GLU:OE2	17:a:34:LYS:HB3	2.15	0.47
17:a:192:VAL:HG12	17:a:204:THR:HG22	1.96	0.47
1:A:466:LYS:HG3	1:A:524:MET:HE1	1.96	0.47
1:A:812:LYS:HE3	9:I:77:THR:HG21	1.96	0.47
1:A:1151:ALA:O	1:A:1155:LYS:HG3	2.15	0.47
3:C:101:PHE:HB2	3:C:163:ALA:HB3	1.97	0.47
11:K:1:MET:HG2	11:K:2:ASN:OD1	2.15	0.47
11:K:19:ILE:HG13	11:K:35:ILE:HG12	1.96	0.47
18:b:252:ILE:HD11	18:b:302:VAL:HG13	1.97	0.47
20:g:121:TYR:CZ	20:g:163:ALA:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:e:901:TYR:HE2	21:e:926:ALA:HB2	1.79	0.47
21:e:963:LEU:HD21	21:e:973:TYR:HB2	1.97	0.47
21:e:1251:VAL:O	21:e:1255:LEU:N	2.47	0.47
1:A:539:GLN:HA	1:A:774:ALA:HB1	1.95	0.47
2:B:735:VAL:HG21	10:J:55:LEU:HD13	1.97	0.47
21:e:1258:LYS:HE2	21:e:1258:LYS:HA	1.97	0.47
1:A:932:ARG:NH1	8:H:107:GLU:O	2.48	0.47
2:B:848:LEU:HD21	2:B:865:VAL:HG12	1.97	0.47
5:E:28:VAL:HG11	5:E:33:LEU:HD13	1.97	0.47
17:a:1:MET:HE3	17:a:1:MET:O	2.15	0.47
17:a:32:LEU:HD12	17:a:32:LEU:HA	1.81	0.47
17:a:197:ARG:NH2	18:b:112:ILE:O	2.48	0.47
18:b:147:ARG:HH22	19:c:44:GLU:HG3	1.80	0.47
18:b:1102:ARG:HH12	18:b:1106:GLN:HG2	1.79	0.47
1:A:1118:THR:HG23	1:A:1123:ARG:HD3	1.96	0.47
1:A:1160:ARG:O	1:A:1300:GLY:HA2	2.16	0.47
2:B:897:ARG:HB2	2:B:900:GLU:HG3	1.96	0.47
4:D:68:THR:O	4:D:72:SER:HB3	2.15	0.47
16:T:36:DT:H2'	16:T:37:DC:C6	2.51	0.47
16:T:44:DG:H4'	16:T:45:DC:H5'	1.97	0.47
17:a:263:VAL:HG12	17:a:289:ASN:HD22	1.79	0.47
1:A:457:ILE:HG12	1:A:469:MET:HG2	1.97	0.46
1:A:539:GLN:HE21	1:A:775:LYS:NZ	2.13	0.46
8:H:16:ASP:OD2	8:H:26:SER:HB3	2.16	0.46
18:b:905:HIS:CG	18:b:933:LEU:HD11	2.50	0.46
1:A:628:VAL:HA	1:A:638:GLY:HA3	1.98	0.46
1:A:1125:LYS:HA	1:A:1128:ILE:HG12	1.97	0.46
2:B:674:MET:H	2:B:694:THR:HG22	1.80	0.46
18:b:147:ARG:HH12	19:c:45:GLN:HG3	1.80	0.46
18:b:877:ASN:ND2	18:b:919:ASP:OD1	2.49	0.46
2:B:1152:PRO:HG2	2:B:1155:CYS:HB2	1.97	0.46
3:C:239:LEU:HB2	3:C:244:ILE:HG13	1.97	0.46
8:H:95:LYS:HE2	8:H:138:ASP:HA	1.98	0.46
14:N:38:DG:H1'	14:N:39:DA:H5'	1.97	0.46
14:N:46:DC:H2''	14:N:47:DG:N7	2.30	0.46
17:a:45:GLY:O	17:a:64:SER:N	2.45	0.46
18:b:244:LYS:HE2	18:b:246:LEU:HD12	1.96	0.46
18:b:922:LEU:HD11	18:b:965:PHE:HB3	1.96	0.46
21:e:623:THR:HG21	21:e:628:ILE:HD11	1.96	0.46
21:e:971:LYS:NZ	21:e:1003:GLU:O	2.48	0.46
1:A:367:ILE:HG21	1:A:501:MET:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1194:ASN:O	1:A:1198:GLU:HG2	2.16	0.46
19:c:13:LYS:O	19:c:17:SER:OG	2.24	0.46
21:e:766:CYS:SG	21:e:843:VAL:HG21	2.56	0.46
21:e:898:ILE:O	21:e:902:ASN:ND2	2.48	0.46
1:A:1192:TRP:HZ3	1:A:1246:ILE:HG22	1.80	0.46
2:B:86:LEU:HD11	2:B:429:PHE:HZ	1.80	0.46
3:C:72:PRO:CG	10:J:13:ILE:HD11	2.44	0.46
15:M:3:C:H2'	15:M:4:G:C8	2.49	0.46
17:a:359:LEU:HD21	22:d:133:LEU:HD21	1.98	0.46
18:b:900:ARG:HB3	18:b:900:ARG:NH1	2.30	0.46
21:e:508:PHE:O	21:e:512:GLN:HG3	2.15	0.46
1:A:185:GLY:HA3	20:g:185:ILE:HG23	1.97	0.46
1:A:421:ARG:NH1	1:A:444:TYR:OH	2.45	0.46
2:B:458:LYS:HB3	2:B:461:GLN:HB2	1.96	0.46
17:a:263:VAL:HG22	17:a:269:MET:HG3	1.98	0.46
1:A:872:MET:HE2	1:A:1084:GLY:HA2	1.96	0.46
1:A:1134:PRO:HG2	1:A:1361:ASP:HB2	1.97	0.46
3:C:20:LYS:HE2	3:C:232:ASN:HD21	1.80	0.46
5:E:173:ILE:HG22	5:E:207:ARG:HB3	1.98	0.46
18:b:44:VAL:HG13	19:c:16:PHE:CE1	2.51	0.46
21:e:977:ILE:HD12	21:e:1272:MET:HE1	1.96	0.46
1:A:88:ILE:HB	1:A:253:LEU:HB3	1.97	0.46
1:A:1137:PRO:HB2	1:A:1341:VAL:HG13	1.98	0.46
1:A:1211:LEU:HD12	1:A:1260:ARG:NE	2.28	0.46
1:A:1301:ILE:HB	1:A:1304:ILE:HD12	1.96	0.46
2:B:710:ILE:HG23	2:B:764:MET:HE3	1.97	0.46
2:B:1116:VAL:HG11	2:B:1151:MET:HE2	1.96	0.46
21:e:682:LEU:HD12	21:e:708:SER:HA	1.97	0.46
1:A:760:LEU:HD11	1:A:781:ILE:HG21	1.97	0.46
1:A:783:GLN:HG2	1:A:788:VAL:HA	1.98	0.46
1:A:1130:ILE:HG12	1:A:1411:LEU:HB3	1.98	0.46
1:A:1217:ASP:OD1	1:A:1219:LYS:HG2	2.15	0.46
2:B:82:PRO:HA	2:B:134:LYS:HA	1.97	0.46
4:D:41:LEU:HD23	4:D:61:PHE:CZ	2.51	0.46
9:I:37:TYR:CD1	9:I:48:ALA:HB2	2.49	0.46
18:b:287:LYS:O	18:b:298:LYS:NZ	2.43	0.46
21:e:768:LEU:HB3	21:e:772:GLN:HG2	1.98	0.46
22:d:70:VAL:HG23	22:d:71:ARG:HG3	1.97	0.46
1:A:256:PRO:HD2	1:A:280:LEU:HD11	1.97	0.46
2:B:378:GLY:HA3	9:I:102:ALA:HB3	1.97	0.46
2:B:827:GLU:HG2	2:B:869:LYS:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:b:741:GLU:HG3	18:b:788:VAL:HG12	1.98	0.46
20:g:212:LEU:HD13	20:g:215:ARG:NH2	2.31	0.46
21:e:775:VAL:HG11	21:e:809:PRO:HB3	1.97	0.46
21:e:799:LEU:HD21	21:e:1004:LEU:HG	1.98	0.46
1:A:510:GLU:OE2	7:G:62:GLY:HA2	2.16	0.45
1:A:1173:THR:HG21	1:A:1293:LEU:HD11	1.98	0.45
7:G:120:ASP:HB2	7:G:129:LYS:HG2	1.97	0.45
18:b:1055:GLN:HG3	18:b:1093:LEU:HD23	1.98	0.45
11:K:80:ASP:OD1	11:K:80:ASP:N	2.40	0.45
22:d:94:ASP:OD2	22:d:97:GLN:HG3	2.16	0.45
1:A:909:LEU:HD13	1:A:966:LEU:HB3	1.98	0.45
18:b:321:VAL:HG21	19:c:16:PHE:HD2	1.82	0.45
21:e:977:ILE:HD11	21:e:1268:HIS:HE1	1.82	0.45
22:d:33:LYS:O	22:d:34:SER:C	2.59	0.45
22:d:124:PHE:HB3	22:d:128:TYR:CD2	2.50	0.45
1:A:470:MET:HG2	1:A:524:MET:HG3	1.98	0.45
1:A:951:GLU:HB3	1:A:1007:ILE:HD11	1.98	0.45
7:G:91:GLN:NE2	7:G:93:ASN:OD1	2.47	0.45
11:K:57:LEU:N	11:K:76:GLN:O	2.49	0.45
13:f:37:VAL:HG22	13:f:48:ILE:HD12	1.99	0.45
15:M:5:A:H2'	15:M:6:G:C8	2.51	0.45
20:g:157:ILE:HA	20:g:160:LEU:HD13	1.97	0.45
1:A:1362:ILE:HG21	1:A:1378:LEU:HD13	1.98	0.45
1:A:1375:ARG:NE	1:A:1403:ASP:OD1	2.44	0.45
2:B:691:SER:O	2:B:691:SER:OG	2.31	0.45
3:C:4:ALA:HB2	11:K:93:ASP:HB3	1.98	0.45
17:a:102:VAL:HA	17:a:119:SER:HA	1.98	0.45
18:b:362:MET:HB2	18:b:375:LEU:HD11	1.99	0.45
1:A:402:LEU:O	1:A:406:VAL:HG12	2.16	0.45
1:A:883:ILE:O	1:A:884:ASN:HB2	2.16	0.45
2:B:611:GLU:OE1	2:B:613:ARG:NH2	2.49	0.45
2:B:993:LYS:HG3	2:B:1018:TYR:OH	2.16	0.45
7:G:22:LEU:O	7:G:26:VAL:HG12	2.15	0.45
13:f:41:ARG:HD2	13:f:63:TYR:HA	1.99	0.45
20:g:81:GLU:OE1	20:g:85:GLN:NE2	2.49	0.45
1:A:154:CYS:O	1:A:155:GLU:HG3	2.17	0.45
1:A:1054:MET:HE3	1:A:1065:PHE:HE1	1.82	0.45
2:B:148:PHE:CD2	2:B:437:THR:HG21	2.51	0.45
2:B:934:LYS:HE3	2:B:1051:LEU:HD12	1.98	0.45
16:T:16:DC:H2'	16:T:17:DT:H71	1.99	0.45
17:a:367:GLU:N	17:a:367:GLU:OE1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LYS:HB3	1:A:248:MET:HE1	1.99	0.45
1:A:700:GLN:HG3	1:A:704:ASN:HD21	1.82	0.45
17:a:39:GLU:O	17:a:71:TYR:OH	2.32	0.45
1:A:138:LYS:HA	1:A:1445:HIS:CE1	2.52	0.45
2:B:785:TYR:CE2	2:B:955:PRO:HD3	2.52	0.45
14:N:32:DG:H2''	14:N:33:DA:H8	1.82	0.45
20:g:144:ASP:OD1	20:g:144:ASP:N	2.49	0.45
1:A:29:ASP:OD1	1:A:30:GLU:N	2.49	0.45
1:A:346:LYS:O	1:A:347:GLU:HB3	2.16	0.45
2:B:58:ILE:HD13	2:B:58:ILE:HA	1.80	0.45
2:B:159:THR:HA	2:B:164:ASN:ND2	2.32	0.45
2:B:331:THR:HG23	2:B:334:LYS:H	1.82	0.45
18:b:230:ILE:HD11	18:b:285:LEU:HD11	1.99	0.45
18:b:743:GLN:HE22	18:b:782:PHE:HD1	1.64	0.45
20:g:119:ARG:HD2	20:g:121:TYR:CE2	2.46	0.45
21:e:510:TYR:CE1	21:e:511:GLN:HG2	2.52	0.45
21:e:795:ILE:HG12	21:e:799:LEU:HD12	1.98	0.45
1:A:146:ASP:HA	1:A:149:LYS:HE3	1.99	0.44
1:A:368:THR:HG23	2:B:946:GLY:HA2	1.99	0.44
1:A:539:GLN:HB3	2:B:970:HIS:CG	2.52	0.44
1:A:1155:LYS:HE3	1:A:1155:LYS:HB3	1.83	0.44
16:T:46:DT:C7	16:T:47:DA:C6	3.01	0.44
21:e:510:TYR:CD2	21:e:750:VAL:HG11	2.53	0.44
2:B:802:ASP:HB3	3:C:173:HIS:NE2	2.33	0.44
3:C:51:GLN:OE1	12:L:52:LEU:HB3	2.17	0.44
20:g:238:VAL:HB	20:g:249:LEU:HB3	1.99	0.44
1:A:1097:GLU:OE2	1:A:1101:GLN:NE2	2.51	0.44
2:B:748:ALA:HB3	2:B:811:TYR:HB2	1.99	0.44
2:B:1068:GLN:NE2	2:B:1076:GLU:OE2	2.50	0.44
8:H:36:LYS:HA	8:H:36:LYS:HD3	1.73	0.44
9:I:59:THR:O	9:I:60:HIS:C	2.60	0.44
18:b:1104:LYS:H	18:b:1104:LYS:HG2	1.68	0.44
22:d:5:LEU:HD21	22:d:42:ALA:HB2	1.99	0.44
22:d:46:LEU:HD11	22:d:68:LEU:HD12	1.99	0.44
1:A:33:ARG:HH11	2:B:1141:ARG:HH22	1.64	0.44
1:A:353:ASN:OD1	2:B:1071:ASN:ND2	2.50	0.44
1:A:484:LEU:HD12	1:A:485:ASN:O	2.17	0.44
2:B:340:LYS:HB2	2:B:340:LYS:HE2	1.82	0.44
2:B:781:ALA:HB2	2:B:1043:ILE:HG13	2.00	0.44
5:E:18:MET:HE3	5:E:28:VAL:HG22	1.99	0.44
17:a:389:TRP:HA	22:d:71:ARG:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:b:227:GLY:O	18:b:239:TYR:OH	2.33	0.44
22:d:693:ASP:O	22:d:697:HIS:ND1	2.51	0.44
1:A:510:GLU:OE2	6:F:71:LEU:HD22	2.17	0.44
2:B:570:ASN:HD21	2:B:616:THR:HB	1.82	0.44
5:E:151:MET:HE3	5:E:190:VAL:HB	2.00	0.44
20:g:208:LEU:HD23	20:g:208:LEU:HA	1.80	0.44
1:A:105:LYS:HE3	1:A:105:LYS:HB3	1.76	0.44
1:A:461:GLN:NE2	2:B:1090:GLU:OE2	2.50	0.44
1:A:1428:MET:HG2	1:A:1455:SER:OG	2.18	0.44
2:B:269:ILE:HD13	2:B:369:VAL:HG21	1.99	0.44
11:K:31:CYS:SG	11:K:32:LEU:N	2.91	0.44
14:N:49:DT:H4'	20:g:201:LYS:HD2	1.99	0.44
20:g:169:ARG:HA	20:g:175:TRP:CZ2	2.53	0.44
20:g:241:ILE:O	20:g:248:LEU:N	2.37	0.44
21:e:577:VAL:HG12	21:e:581:TRP:HD1	1.82	0.44
21:e:719:ALA:HB1	21:e:723:GLN:HB2	2.00	0.44
1:A:94:VAL:HG13	1:A:311:GLN:OE1	2.18	0.44
1:A:103:THR:HG22	1:A:225:PHE:HE2	1.83	0.44
1:A:804:HIS:HB2	1:A:812:LYS:HG2	2.00	0.44
1:A:982:ASN:O	1:A:986:MET:HG3	2.18	0.44
2:B:934:LYS:HE2	2:B:1053:HIS:CD2	2.53	0.44
5:E:13:ILE:HD12	5:E:135:LEU:HB3	2.00	0.44
18:b:111:ARG:H	18:b:111:ARG:HG3	1.48	0.44
18:b:308:THR:O	18:b:383:LYS:NZ	2.49	0.44
21:e:640:TRP:O	21:e:667:THR:OG1	2.31	0.44
1:A:734:ARG:NE	9:I:105:GLU:O	2.51	0.44
1:A:760:LEU:HD13	1:A:764:ASN:HD22	1.83	0.44
1:A:1361:ASP:OD2	1:A:1364:GLU:HB2	2.16	0.44
3:C:38:PHE:CE1	3:C:245:VAL:HA	2.53	0.44
15:M:4:G:H2'	15:M:5:A:C8	2.53	0.44
18:b:733:PHE:HB2	18:b:794:ILE:HB	2.00	0.44
18:b:915:LYS:HG2	18:b:957:VAL:HG23	1.99	0.44
21:e:692:ILE:HG13	21:e:693:PHE:N	2.33	0.44
1:A:1371:ILE:HD12	1:A:1371:ILE:HA	1.87	0.44
2:B:1003:ASN:HD21	2:B:1005:ALA:HB3	1.83	0.44
3:C:60:HIS:HD2	3:C:62:GLU:HB2	1.82	0.44
17:a:90:ILE:HD13	17:a:127:TRP:CZ3	2.53	0.44
18:b:31:LEU:HD13	18:b:317:LEU:HD21	1.99	0.44
18:b:834:ALA:HB2	18:b:869:ALA:HA	2.00	0.44
20:g:103:ILE:HG22	20:g:108:TYR:HB2	2.00	0.44
21:e:518:LEU:HD23	21:e:518:LEU:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:e:652:ARG:HB2	21:e:684:GLU:CG	2.48	0.44
1:A:102:LYS:O	1:A:106:VAL:HG12	2.17	0.43
1:A:1366:PHE:HB2	1:A:1374:VAL:HG21	2.00	0.43
1:A:1406:THR:HG22	5:E:207:ARG:HH22	1.83	0.43
2:B:623:ARG:CZ	2:B:625:LEU:HD21	2.47	0.43
5:E:159:LEU:HD12	5:E:163:TYR:HD1	1.83	0.43
7:G:164:MET:N	7:G:164:MET:HE2	2.33	0.43
17:a:85:LYS:NZ	17:a:85:LYS:HB2	2.32	0.43
17:a:217:ARG:HH11	21:e:524:GLN:HA	1.82	0.43
18:b:365:VAL:HG21	18:b:733:PHE:CE1	2.53	0.43
22:d:87:LEU:HD23	22:d:87:LEU:HA	1.73	0.43
1:A:309:LEU:HD12	1:A:309:LEU:HA	1.84	0.43
1:A:758:LYS:HE2	1:A:758:LYS:HB3	1.77	0.43
1:A:1369:LEU:O	5:E:139:ILE:HD11	2.17	0.43
5:E:85:LYS:O	5:E:89:VAL:HG12	2.18	0.43
8:H:33:GLU:OE1	8:H:33:GLU:N	2.50	0.43
10:J:48:MET:HE3	10:J:48:MET:HB3	1.77	0.43
11:K:21:ILE:HG23	11:K:31:CYS:SG	2.58	0.43
17:a:78:ARG:HD3	18:b:990:GLN:HE22	1.83	0.43
20:g:146:MET:HA	20:g:150:PHE:CD2	2.53	0.43
20:g:228:HIS:O	20:g:232:LEU:HD12	2.18	0.43
21:e:770:ASP:OD1	21:e:770:ASP:N	2.51	0.43
22:d:91:LEU:HD21	22:d:114:THR:HG22	1.99	0.43
1:A:434:LYS:HD3	1:A:436:SER:HB3	1.99	0.43
1:A:1177:TYR:CZ	9:I:28:GLU:HG2	2.53	0.43
2:B:44:LEU:HD13	2:B:155:MET:HE3	2.00	0.43
2:B:713:PHE:HB3	2:B:716:HIS:ND1	2.33	0.43
2:B:861:SER:HA	2:B:901:THR:HA	1.99	0.43
5:E:121:MET:HE2	5:E:125:TYR:HB2	1.99	0.43
5:E:160:LEU:HD11	5:E:167:GLU:HG2	1.99	0.43
14:N:43:DG:H2'	14:N:44:DA:H8	1.83	0.43
16:T:50:DA:H2'	16:T:51:DG:C8	2.53	0.43
17:a:65:ASP:OD2	17:a:67:VAL:HG22	2.18	0.43
18:b:11:LYS:HD2	18:b:38:ARG:CD	2.48	0.43
20:g:218:PRO:HB2	20:g:220:VAL:HG22	2.00	0.43
1:A:539:GLN:H	1:A:539:GLN:HG3	1.56	0.43
1:A:901:VAL:HB	1:A:978:VAL:HG12	1.99	0.43
1:A:1095:LEU:HD13	1:A:1401:LEU:HD22	2.00	0.43
1:A:1259:ILE:HG21	1:A:1292:MET:HE1	2.00	0.43
5:E:168:ASN:HA	5:E:172:ARG:HH12	1.83	0.43
7:G:77:PHE:HE2	7:G:104:MET:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:65:LEU:HD21	12:L:45:TYR:CG	2.54	0.43
13:f:41:ARG:HA	13:f:41:ARG:HD3	1.81	0.43
18:b:366:ASP:OD1	18:b:366:ASP:N	2.45	0.43
20:g:57:PRO:HG2	20:g:103:ILE:HD12	2.00	0.43
21:e:719:ALA:HB3	21:e:994:ARG:HH12	1.84	0.43
21:e:808:HIS:HE2	21:e:833:GLY:HA2	1.81	0.43
22:d:91:LEU:HB3	22:d:93:THR:HG23	2.00	0.43
2:B:91:ILE:HB	2:B:124:LEU:HD11	2.00	0.43
2:B:184:TYR:CE1	2:B:191:GLU:HG2	2.54	0.43
17:a:99:ARG:C	17:a:100:TYR:HD1	2.27	0.43
20:g:95:PHE:HB3	20:g:185:ILE:HD11	2.01	0.43
21:e:707:PHE:O	21:e:711:ILE:HG22	2.18	0.43
21:e:808:HIS:NE2	21:e:833:GLY:HA2	2.34	0.43
22:d:55:ALA:N	22:d:100:PRO:HG2	2.33	0.43
22:d:74:GLN:O	22:d:78:LEU:HG	2.18	0.43
1:A:1086:MET:HG3	2:B:1095:ILE:O	2.19	0.43
2:B:240:LEU:H	2:B:240:LEU:HD22	1.83	0.43
12:L:13:GLN:HG2	12:L:14:PRO:HD3	1.99	0.43
16:T:46:DT:H2"	16:T:47:DA:OP1	2.18	0.43
18:b:250:PRO:HA	18:b:251:PRO:HD3	1.91	0.43
18:b:1057:ARG:HD3	18:b:1112:LEU:HD11	2.01	0.43
1:A:84:HIS:CE1	2:B:1127:ILE:HG23	2.53	0.43
1:A:581:LYS:HB2	8:H:91:VAL:HG12	1.99	0.43
1:A:681:LEU:HD12	1:A:681:LEU:HA	1.85	0.43
1:A:937:ASP:OD1	1:A:937:ASP:N	2.51	0.43
1:A:1199:MET:HG2	22:d:571:ARG:HH21	1.84	0.43
2:B:402:PHE:HA	2:B:405:ARG:HH11	1.84	0.43
3:C:44:ILE:HG21	3:C:178:PRO:HB3	2.00	0.43
17:a:99:ARG:NH1	17:a:121:ASP:HB2	2.34	0.43
17:a:118:SER:HG	17:a:147:HIS:CE1	2.33	0.43
21:e:719:ALA:H	21:e:994:ARG:HH12	1.65	0.43
21:e:808:HIS:ND1	21:e:838:SER:HB3	2.34	0.43
21:e:929:VAL:HG13	21:e:959:VAL:HG22	2.00	0.43
21:e:1251:VAL:HG23	21:e:1252:LEU:H	1.84	0.43
22:d:4:LYS:HA	22:d:7:LYS:HD2	2.00	0.43
22:d:59:LEU:HD13	22:d:109:LEU:HA	2.00	0.43
1:A:140:ARG:NH1	1:A:234:PHE:O	2.49	0.43
1:A:402:LEU:HD13	1:A:446:VAL:HG12	2.01	0.43
1:A:883:ILE:HG22	1:A:885:GLN:HG3	1.99	0.43
2:B:395:LEU:HD21	2:B:532:ILE:HD11	2.00	0.43
3:C:205:LYS:HA	3:C:205:LYS:HD3	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:252:LEU:HA	3:C:255:LYS:HZ3	1.84	0.43
10:J:4:PRO:HB2	10:J:48:MET:HE1	2.01	0.43
12:L:47:LYS:HE3	12:L:47:LYS:HB3	1.81	0.43
13:f:27:PRO:HG2	13:f:28:PHE:CD2	2.54	0.43
18:b:1112:LEU:HD23	18:b:1112:LEU:HA	1.84	0.43
21:e:530:LEU:HD11	21:e:541:GLN:OE1	2.19	0.43
21:e:768:LEU:HD23	21:e:772:GLN:CG	2.47	0.43
1:A:416:ALA:HB2	1:A:448:ARG:HA	2.01	0.43
2:B:423:ILE:HD13	2:B:423:ILE:HA	1.87	0.43
2:B:665:ILE:HG23	2:B:669:GLU:HB3	2.00	0.43
2:B:1036:LYS:HB2	3:C:194:HIS:HB3	2.01	0.43
17:a:98:HIS:NE2	17:a:117:SER:OG	2.49	0.43
17:a:284:TYR:OH	17:a:321:VAL:O	2.29	0.43
20:g:91:VAL:N	20:g:101:GLY:O	2.50	0.43
21:e:510:TYR:OH	21:e:536:LEU:O	2.27	0.43
21:e:848:LEU:HB3	21:e:880:TYR:CE2	2.54	0.43
21:e:885:MET:HE2	21:e:912:LEU:HD23	2.00	0.43
22:d:609:GLU:HA	22:d:612:ARG:HD2	2.01	0.43
1:A:889:LEU:O	1:A:890:ARG:NH1	2.50	0.43
7:G:163:LEU:H	7:G:164:MET:HE2	1.84	0.43
8:H:92:MET:H	8:H:143:LEU:HB3	1.83	0.43
1:A:545:VAL:HG12	1:A:676:ILE:HG13	2.01	0.42
16:T:48:DT:OP1	21:e:804:LYS:NZ	2.50	0.42
17:a:2:LEU:HD13	18:b:814:LEU:HD21	2.01	0.42
17:a:9:GLN:OE1	18:b:360:VAL:HG13	2.18	0.42
18:b:213:GLU:OE1	18:b:235:GLU:HB2	2.19	0.42
18:b:1133:VAL:O	18:b:1137:THR:HG23	2.18	0.42
21:e:807:ASN:OD1	21:e:867:MET:HE2	2.19	0.42
21:e:851:TRP:HA	21:e:854:GLN:HE22	1.84	0.42
22:d:80:VAL:HG13	22:d:130:LYS:HB3	2.00	0.42
1:A:279:LYS:HA	1:A:279:LYS:HD3	1.76	0.42
1:A:929:ALA:O	1:A:933:THR:OG1	2.32	0.42
1:A:1405:MET:HE3	1:A:1414:ILE:HG12	2.01	0.42
2:B:225:LEU:HD12	2:B:225:LEU:HA	1.94	0.42
5:E:62:VAL:O	5:E:71:GLN:HB2	2.19	0.42
7:G:7:LEU:HB3	7:G:72:TYR:CZ	2.54	0.42
7:G:54:ILE:HD13	7:G:70:VAL:HG12	2.00	0.42
9:I:72:VAL:HG22	9:I:78:LEU:HD11	2.01	0.42
18:b:80:LEU:HD23	18:b:120:ILE:HG21	2.01	0.42
18:b:941:ASN:C	18:b:941:ASN:OD1	2.62	0.42
21:e:979:LYS:HE2	21:e:979:LYS:HB2	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:THR:HB	1:A:447:GLU:HB3	2.01	0.42
2:B:566:LYS:O	2:B:612:ILE:N	2.46	0.42
2:B:666:ASP:OD1	2:B:666:ASP:C	2.62	0.42
3:C:154:ARG:NE	10:J:64:PRO:HD3	2.34	0.42
6:F:124:ILE:HD12	6:F:124:ILE:H	1.84	0.42
11:K:51:LEU:HD23	11:K:51:LEU:HA	1.85	0.42
17:a:26:ARG:NE	18:b:927:MET:HE2	2.34	0.42
18:b:53:LYS:HE2	18:b:98:ILE:HD11	2.00	0.42
20:g:89:ARG:HH21	20:g:176:LEU:HD13	1.84	0.42
20:g:111:ARG:HA	20:g:114:LYS:HG2	2.02	0.42
21:e:542:ILE:HD13	21:e:542:ILE:HA	1.93	0.42
1:A:106:VAL:HG23	1:A:236:LEU:HD13	2.01	0.42
1:A:1371:ILE:O	1:A:1374:VAL:HG12	2.20	0.42
3:C:149:LEU:HD21	3:C:152:LYS:HE3	2.02	0.42
14:N:6:DT:H2"	14:N:7:DG:C8	2.54	0.42
17:a:382:ASN:HB3	17:a:385:PHE:HB2	2.00	0.42
20:g:157:ILE:HD12	20:g:158:THR:N	2.34	0.42
20:g:198:MET:H	20:g:198:MET:HG3	1.72	0.42
21:e:779:PHE:CD2	21:e:802:LEU:HD13	2.54	0.42
1:A:1162:GLU:O	1:A:1300:GLY:HA3	2.20	0.42
1:A:1423:ASP:OD1	1:A:1423:ASP:N	2.53	0.42
2:B:62:ALA:HB1	2:B:412:LEU:HD11	2.02	0.42
2:B:83:ARG:HG2	2:B:133:ILE:HB	2.02	0.42
2:B:128:ILE:O	2:B:144:HIS:N	2.45	0.42
2:B:623:ARG:NH2	2:B:697:GLU:OE2	2.40	0.42
6:F:91:LEU:HD12	6:F:91:LEU:H	1.83	0.42
7:G:14:HIS:HD2	7:G:65:PHE:HE1	1.67	0.42
7:G:44:PHE:HE1	7:G:157:ILE:HB	1.84	0.42
8:H:28:LEU:O	8:H:40:ILE:HA	2.20	0.42
8:H:97:TYR:CZ	8:H:115:TYR:HB3	2.54	0.42
17:a:311:PRO:HB3	17:a:337:VAL:HG13	2.02	0.42
18:b:6:VAL:HG22	18:b:1040:VAL:HG22	2.00	0.42
20:g:44:MET:HE3	20:g:44:MET:HB3	1.76	0.42
1:A:199:TYR:HD2	1:A:213:LYS:HG2	1.83	0.42
1:A:987:ILE:HD13	1:A:1058:PHE:CE2	2.55	0.42
2:B:44:LEU:HA	2:B:155:MET:HE1	2.02	0.42
2:B:288:ILE:HD13	2:B:288:ILE:HA	1.87	0.42
2:B:1108:PHE:CE1	2:B:1113:PRO:HA	2.55	0.42
6:F:88:ASP:HB3	6:F:91:LEU:HD12	2.01	0.42
9:I:91:HIS:CD2	9:I:116:ALA:HB2	2.55	0.42
18:b:85:ASN:HD22	18:b:1068:ILE:HG12	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:e:575:THR:HG22	21:e:624:SER:HB2	2.01	0.42
21:e:842:ILE:HG21	21:e:1260:VAL:HG21	2.02	0.42
1:A:1436:VAL:O	1:A:1440:MET:HG2	2.20	0.42
2:B:391:LYS:HB2	2:B:391:LYS:HE2	1.74	0.42
2:B:546:GLU:OE2	2:B:552:ASN:ND2	2.50	0.42
3:C:104:ASP:OD1	3:C:160:ARG:HD3	2.19	0.42
5:E:193:ILE:HB	5:E:205:THR:HG23	2.02	0.42
9:I:107:ALA:C	9:I:109:ARG:H	2.27	0.42
18:b:840:GLU:OE2	18:b:844:LYS:NZ	2.52	0.42
18:b:928:ARG:H	18:b:928:ARG:HG2	1.52	0.42
18:b:1113:GLN:HE22	18:b:1122:ARG:H	1.68	0.42
18:b:1129:LEU:HD13	18:b:1129:LEU:HA	1.89	0.42
20:g:65:VAL:HG11	20:g:79:LEU:HD11	2.01	0.42
20:g:105:THR:HB	20:g:109:ARG:NH2	2.34	0.42
20:g:250:ARG:HH11	22:d:44:ARG:HE	1.67	0.42
1:A:457:ILE:HG21	2:B:1102:PHE:CZ	2.54	0.42
1:A:527:THR:CG2	1:A:534:VAL:HB	2.49	0.42
1:A:601:ASN:HD22	1:A:988:TRP:CG	2.38	0.42
1:A:1288:ILE:HG22	1:A:1292:MET:HE3	2.02	0.42
1:A:1294:THR:OG1	22:d:685:VAL:HG22	2.20	0.42
2:B:131:THR:HG22	2:B:141:GLN:HB3	2.02	0.42
2:B:587:LEU:HB3	2:B:603:MET:SD	2.60	0.42
2:B:604:ILE:HG12	2:B:668:LEU:HB3	2.02	0.42
2:B:907:VAL:CG2	12:L:46:LYS:HB2	2.50	0.42
2:B:1051:LEU:C	2:B:1053:HIS:H	2.26	0.42
8:H:58:LEU:HD23	8:H:58:LEU:HA	1.81	0.42
20:g:164:GLY:HA3	20:g:179:PRO:HA	2.01	0.42
21:e:936:TRP:CZ3	21:e:972:ILE:HG12	2.55	0.42
22:d:111:GLN:O	22:d:115:ARG:HG3	2.20	0.42
1:A:108:ARG:HH11	1:A:145:TYR:HE1	1.68	0.42
1:A:422:ASP:OD1	1:A:422:ASP:N	2.52	0.42
1:A:561:MET:SD	11:K:51:LEU:HD21	2.59	0.42
1:A:876:ASP:OD2	1:A:880:ARG:NH2	2.51	0.42
1:A:953:GLU:O	1:A:957:GLU:HG2	2.20	0.42
1:A:959:MET:HE1	1:A:1050:CYS:SG	2.60	0.42
1:A:1065:PHE:O	1:A:1069:LEU:HG	2.19	0.42
1:A:1135:LYS:HB3	1:A:1135:LYS:HE3	1.88	0.42
3:C:189:ASP:O	3:C:191:ALA:N	2.52	0.42
11:K:11:LEU:HD23	11:K:11:LEU:HA	1.86	0.42
18:b:70:LYS:NZ	18:b:127:GLU:O	2.52	0.42
18:b:96:GLU:H	18:b:96:GLU:HG3	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:b:152:LEU:HD12	18:b:152:LEU:H	1.85	0.42
20:g:41:SER:O	20:g:45:GLN:HG2	2.20	0.42
20:g:207:LEU:HD22	20:g:212:LEU:HD22	2.02	0.42
21:e:1257:LYS:HG3	21:e:1258:LYS:HG2	2.01	0.42
22:d:21:ASN:HB3	22:d:24:LYS:HG2	2.02	0.42
1:A:469:MET:HE3	2:B:1093:CYS:SG	2.59	0.42
2:B:953:ASP:OD1	3:C:36:ARG:NH1	2.52	0.42
3:C:49:TRP:O	3:C:163:ALA:HA	2.20	0.42
3:C:263:LEU:HD21	11:K:87:PHE:HB3	2.02	0.42
7:G:91:GLN:HG3	7:G:98:PHE:HB2	2.02	0.42
17:a:206:SER:OG	17:a:207:ALA:N	2.52	0.42
18:b:128:CYS:SG	18:b:128:CYS:O	2.78	0.42
2:B:927:ARG:HH22	2:B:1057:ASP:CG	2.27	0.41
3:C:37:VAL:HG21	3:C:252:LEU:HD13	2.01	0.41
4:D:103:LEU:HD13	4:D:114:LEU:HD13	2.02	0.41
10:J:6:ARG:HD2	10:J:11:GLY:O	2.20	0.41
13:f:50:CYS:HB3	13:f:55:GLU:H	1.85	0.41
14:N:7:DG:H2''	14:N:8:DA:C8	2.55	0.41
16:T:34:DC:H2'	16:T:35:DC:H6	1.85	0.41
17:a:186:ARG:HA	17:a:186:ARG:HD3	1.78	0.41
18:b:1002:GLU:OE1	18:b:1036:MET:HE3	2.20	0.41
18:b:1135:GLU:H	18:b:1135:GLU:CD	2.28	0.41
21:e:872:GLU:HA	21:e:875:LEU:HB2	2.02	0.41
1:A:41:ILE:HG21	1:A:57:LEU:HD23	2.02	0.41
1:A:67:ARG:HG3	1:A:78:MET:HG2	2.02	0.41
1:A:118:LEU:HD22	1:A:154:CYS:HA	2.02	0.41
1:A:931:ARG:HD3	1:A:939:VAL:HG11	2.02	0.41
1:A:1375:ARG:HB2	1:A:1406:THR:HG21	2.02	0.41
2:B:323:SER:HB2	2:B:324:ARG:HH11	1.85	0.41
3:C:49:TRP:CD1	3:C:93:PHE:HZ	2.39	0.41
8:H:7:GLU:HA	8:H:58:LEU:O	2.21	0.41
18:b:218:MET:HB2	18:b:218:MET:HE3	1.78	0.41
20:g:121:TYR:CD1	20:g:125:VAL:HG11	2.54	0.41
21:e:597:LEU:HD11	21:e:611:ILE:HG12	2.02	0.41
22:d:116:ALA:HB1	22:d:120:TRP:CD1	2.55	0.41
1:A:22:GLN:NE2	1:A:23:PHE:O	2.40	0.41
1:A:1443:ALA:HB2	2:B:1167:ILE:HG23	2.01	0.41
2:B:1112:ASP:N	2:B:1112:ASP:OD1	2.51	0.41
3:C:58:VAL:HB	10:J:59:LEU:HD23	2.02	0.41
5:E:187:ARG:CZ	5:E:210:GLN:NE2	2.82	0.41
8:H:43:VAL:HG13	8:H:90:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:41:DC:H2''	14:N:42:DA:H8	1.85	0.41
18:b:378:CYS:SG	18:b:724:ILE:HB	2.61	0.41
18:b:945:ILE:HD13	18:b:945:ILE:HA	1.85	0.41
18:b:975:PHE:HA	18:b:996:GLY:O	2.21	0.41
21:e:686:TRP:CD2	21:e:700:LEU:HD13	2.55	0.41
1:A:256:PRO:HG3	2:B:1164:SER:OG	2.21	0.41
1:A:355:MET:HE1	1:A:1455:SER:HB2	2.03	0.41
1:A:781:ILE:HG23	1:A:785:ILE:HD12	2.02	0.41
1:A:804:HIS:CE1	9:I:100:HIS:HB2	2.55	0.41
1:A:1009:VAL:HA	1:A:1065:PHE:CE2	2.56	0.41
1:A:1161:LEU:HD21	1:A:1349:GLU:HG3	2.02	0.41
1:A:1234:LYS:HG3	1:A:1296:MET:HE2	2.02	0.41
2:B:360:LYS:NZ	2:B:554:GLU:OE2	2.53	0.41
2:B:632:LYS:HB3	2:B:632:LYS:HE3	1.72	0.41
3:C:56:SER:HB2	3:C:157:GLN:HA	2.03	0.41
5:E:81:LYS:HB2	5:E:81:LYS:HE2	1.73	0.41
5:E:81:LYS:NZ	5:E:108:GLN:OE1	2.41	0.41
17:a:251:LEU:HD12	17:a:262:THR:HG22	2.03	0.41
18:b:830:ILE:HD11	18:b:848:ILE:HG22	2.03	0.41
20:g:157:ILE:H	20:g:157:ILE:HG13	1.70	0.41
20:g:165:VAL:C	20:g:177:ALA:HB3	2.44	0.41
21:e:520:GLU:O	21:e:524:GLN:HG3	2.20	0.41
1:A:253:LEU:HD22	1:A:283:ILE:HG21	2.02	0.41
1:A:510:GLU:OE1	1:A:510:GLU:N	2.35	0.41
1:A:873:VAL:HG22	1:A:879:VAL:HG22	2.03	0.41
3:C:35:ARG:O	3:C:38:PHE:HB2	2.21	0.41
3:C:70:LEU:HD22	10:J:6:ARG:HG3	2.02	0.41
5:E:131:LEU:HB3	5:E:133:GLN:HG2	2.02	0.41
16:T:48:DT:P	21:e:804:LYS:NZ	2.94	0.41
17:a:252:CYS:O	17:a:261:LEU:HB2	2.21	0.41
17:a:261:LEU:HD21	17:a:271:LEU:HD12	2.03	0.41
17:a:298:THR:HG21	17:a:342:PHE:HB2	2.02	0.41
17:a:315:THR:HG22	17:a:331:LYS:HA	2.01	0.41
18:b:15:VAL:HG21	18:b:325:GLY:HA3	2.01	0.41
22:d:62:PHE:CZ	22:d:113:THR:HA	2.55	0.41
1:A:130:LEU:HD11	1:A:235:VAL:HG13	2.03	0.41
1:A:346:LYS:C	1:A:348:GLY:H	2.26	0.41
1:A:890:ARG:NH2	1:A:1023:VAL:HG22	2.36	0.41
1:A:1382:LEU:HB3	1:A:1398:LEU:HD21	2.03	0.41
3:C:267:ILE:HD11	11:K:84:GLN:HB3	2.02	0.41
9:I:14:ILE:HB	9:I:23:MET:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:a:37:ASP:OD2	17:a:38:VAL:N	2.53	0.41
18:b:338:VAL:HA	19:c:6:LYS:HG3	2.03	0.41
22:d:91:LEU:HD23	22:d:91:LEU:HA	1.93	0.41
1:A:479:TRP:N	1:A:483:ARG:HH22	2.16	0.41
1:A:894:ASP:HB3	5:E:200:ALA:HB2	2.02	0.41
1:A:1020:LEU:HD21	1:A:1073:GLU:HA	2.02	0.41
2:B:99:TRP:HE1	2:B:105:PRO:HB3	1.85	0.41
3:C:23:ILE:HD13	11:K:101:LEU:HD21	2.02	0.41
5:E:29:THR:OG1	5:E:32:GLU:OE1	2.38	0.41
5:E:131:LEU:HB2	5:E:134:GLU:OE1	2.20	0.41
6:F:88:ASP:HA	6:F:89:PRO:HD3	1.97	0.41
12:L:16:ILE:HA	12:L:27:GLU:HA	2.03	0.41
17:a:68:ILE:HG23	17:a:90:ILE:HB	2.02	0.41
17:a:168:VAL:HB	17:a:182:LEU:HB2	2.03	0.41
18:b:28:ASP:N	18:b:28:ASP:OD1	2.53	0.41
18:b:318:ASP:OD1	18:b:319:ASN:N	2.54	0.41
20:g:156:GLU:OE1	20:g:156:GLU:N	2.53	0.41
22:d:116:ALA:HB1	22:d:120:TRP:NE1	2.35	0.41
1:A:611:ASP:OD1	1:A:611:ASP:N	2.53	0.41
1:A:616:GLY:O	1:A:619:LYS:HG2	2.21	0.41
1:A:906:LEU:HD22	1:A:966:LEU:HD11	2.02	0.41
1:A:1364:GLU:O	1:A:1368:VAL:HG12	2.21	0.41
14:N:13:DA:H5''	21:e:652:ARG:NH1	2.35	0.41
14:N:13:DA:C2	14:N:14:DT:H71	2.56	0.41
14:N:35:DA:H2''	14:N:36:DA:H8	1.86	0.41
18:b:112:ILE:HD12	18:b:113:GLY:N	2.36	0.41
20:g:160:LEU:HB3	20:g:165:VAL:CG1	2.51	0.41
22:d:563:VAL:HG11	22:d:580:GLN:HB3	2.02	0.41
1:A:100:LEU:HD12	1:A:100:LEU:HA	1.91	0.41
1:A:154:CYS:HB3	1:A:185:GLY:H	1.86	0.41
1:A:394:VAL:HG22	1:A:402:LEU:HD12	2.02	0.41
1:A:732:THR:O	1:A:736:THR:HG23	2.21	0.41
1:A:992:LYS:HA	1:A:992:LYS:HD3	1.88	0.41
1:A:1426:PRO:HD2	1:A:1449:ASP:OD1	2.21	0.41
2:B:724:TYR:O	2:B:728:MET:HB2	2.21	0.41
2:B:1151:MET:SD	2:B:1171:MET:HE1	2.60	0.41
5:E:82:VAL:HG13	5:E:86:THR:OG1	2.21	0.41
8:H:125:LEU:HG	8:H:132:LEU:HD21	2.01	0.41
9:I:57:LYS:HE3	9:I:57:LYS:HB3	1.89	0.41
14:N:6:DT:H2''	14:N:7:DG:H8	1.84	0.41
16:T:32:DA:H2'	16:T:33:DT:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:a:22:GLU:HG2	18:b:926:LEU:HD21	2.02	0.41
17:a:211:VAL:O	17:a:226:LEU:HD12	2.21	0.41
18:b:131:ILE:HB	18:b:143:ILE:HB	2.02	0.41
21:e:533:GLU:OE1	21:e:747:LYS:HG3	2.21	0.41
21:e:608:GLU:CD	21:e:608:GLU:H	2.29	0.41
21:e:793:MET:HE3	21:e:793:MET:HB3	1.76	0.41
21:e:828:GLU:C	21:e:830:ASP:H	2.29	0.41
21:e:867:MET:O	21:e:870:ILE:HG22	2.21	0.41
21:e:1389:LEU:HD21	21:e:1393:MET:HE3	2.02	0.41
22:d:64:ILE:O	22:d:68:LEU:HG	2.21	0.41
1:A:689:ILE:O	1:A:693:ILE:HG12	2.21	0.41
1:A:769:MET:HE3	1:A:769:MET:HB2	1.86	0.41
1:A:1097:GLU:N	1:A:1098:PRO:HD2	2.36	0.41
1:A:1169:VAL:HG12	1:A:1220:HIS:HB3	2.03	0.41
20:g:186:LYS:HZ1	20:g:190:LYS:HE2	1.86	0.41
21:e:859:LEU:HB2	21:e:929:VAL:HG23	2.02	0.41
1:A:583:ARG:HH12	1:A:585:LEU:HD11	1.86	0.40
1:A:1234:LYS:HB2	1:A:1234:LYS:HE2	1.73	0.40
2:B:348:LEU:O	2:B:361:LYS:HE2	2.21	0.40
2:B:388:TYR:HB2	2:B:504:THR:CG2	2.52	0.40
2:B:1129:ASN:OD1	2:B:1129:ASN:C	2.63	0.40
4:D:86:LEU:O	4:D:90:LYS:NZ	2.54	0.40
5:E:92:GLN:O	5:E:96:GLU:HG2	2.21	0.40
5:E:94:MET:HE1	5:E:127:LEU:CD2	2.50	0.40
6:F:106:ILE:HG22	6:F:108:ARG:HG3	2.03	0.40
11:K:32:LEU:HD23	11:K:32:LEU:HA	1.83	0.40
16:T:27:DC:H2 ⁺	16:T:28:DT:H71	2.03	0.40
18:b:849:VAL:HG22	18:b:863:GLU:HG3	2.03	0.40
18:b:926:LEU:O	18:b:953:TRP:HA	2.21	0.40
21:e:1025:THR:HB	21:e:1270:ALA:HB1	2.03	0.40
22:d:86:PHE:O	22:d:90:THR:OG1	2.28	0.40
1:A:260:VAL:HA	2:B:1157:LEU:HD11	2.03	0.40
2:B:265:GLN:HB3	2:B:324:ARG:HE	1.85	0.40
2:B:625:LEU:HD13	2:B:675:LEU:HD21	2.02	0.40
2:B:829:PHE:HD2	2:B:917:LYS:HD2	1.86	0.40
2:B:931:ILE:HD11	2:B:947:ILE:HD12	2.03	0.40
7:G:51:ILE:HA	7:G:72:TYR:HA	2.02	0.40
12:L:19:CYS:HA	12:L:44:MET:HG2	2.03	0.40
18:b:40:GLU:HG3	18:b:54:GLU:OE1	2.22	0.40
20:g:191:GLY:HA2	20:g:221:VAL:HB	2.03	0.40
21:e:951:ILE:O	21:e:953:GLN:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:MET:HE3	1:A:469:MET:HB2	1.94	0.40
1:A:544:ALA:HB1	1:A:676:ILE:HG22	2.03	0.40
1:A:703:GLN:O	1:A:707:LYS:HG2	2.21	0.40
1:A:780:ASN:ND2	2:B:976:MET:HE2	2.36	0.40
1:A:980:PRO:HD2	1:A:1041:PHE:CD1	2.56	0.40
1:A:1224:ARG:HB3	1:A:1226:LEU:HG	2.03	0.40
1:A:1420:ASN:O	1:A:1429:LYS:HD3	2.21	0.40
2:B:153:PRO:HD2	2:B:444:LEU:HD13	2.02	0.40
5:E:36:THR:HG22	5:E:39:GLU:HG3	2.03	0.40
5:E:173:ILE:O	5:E:209:VAL:HA	2.20	0.40
7:G:124:ASN:HB2	7:G:125:PRO:HD3	2.02	0.40
17:a:121:ASP:OD1	17:a:121:ASP:C	2.64	0.40
18:b:36:ASN:OD1	18:b:60:LYS:NZ	2.49	0.40
18:b:321:VAL:HG11	19:c:16:PHE:HE2	1.86	0.40
18:b:723:LYS:HB3	18:b:723:LYS:HE3	1.90	0.40
21:e:875:LEU:HD11	21:e:909:VAL:HG11	2.03	0.40
22:d:51:THR:HG22	22:d:89:LEU:HD21	2.03	0.40
2:B:33:TYR:HD1	2:B:653:TRP:CE2	2.39	0.40
2:B:191:GLU:OE1	2:B:743:ARG:NH1	2.50	0.40
2:B:417:ILE:HD13	2:B:417:ILE:HA	1.94	0.40
2:B:532:ILE:HD13	2:B:532:ILE:HG21	1.82	0.40
7:G:163:LEU:HA	7:G:168:LEU:HD12	2.02	0.40
13:f:32:GLU:H	13:f:32:GLU:HG2	1.74	0.40
17:a:22:GLU:OE1	17:a:366:TYR:OH	2.39	0.40
17:a:78:ARG:NH1	18:b:944:GLU:O	2.54	0.40
3:C:186:TYR:OH	3:C:194:HIS:ND1	2.43	0.40
4:D:44:ARG:HH22	7:G:49:THR:HA	1.85	0.40
5:E:85:LYS:H	5:E:85:LYS:HG3	1.60	0.40
7:G:146:LYS:HG3	7:G:168:LEU:HD11	2.04	0.40
8:H:13:LYS:HE3	8:H:13:LYS:HB3	1.92	0.40
16:T:8:DC:H6	16:T:8:DC:H2'	1.73	0.40
17:a:213:LEU:HD23	17:a:226:LEU:HD11	2.02	0.40
18:b:909:ILE:HD11	18:b:928:ARG:HD3	2.03	0.40
21:e:834:TYR:CE1	21:e:836:LYS:HB2	2.57	0.40
21:e:936:TRP:HH2	21:e:968:ILE:HD11	1.86	0.40
21:e:1390:LEU:HD23	21:e:1390:LEU:HA	1.86	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	1399/1970 (71%)	1349 (96%)	50 (4%)	0	100	100
2	B	1122/1300 (86%)	1078 (96%)	44 (4%)	0	100	100
3	C	256/275 (93%)	250 (98%)	6 (2%)	0	100	100
4	D	126/142 (89%)	123 (98%)	3 (2%)	0	100	100
5	E	207/210 (99%)	203 (98%)	4 (2%)	0	100	100
6	F	80/127 (63%)	77 (96%)	3 (4%)	0	100	100
7	G	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
8	H	146/150 (97%)	144 (99%)	2 (1%)	0	100	100
9	I	115/125 (92%)	104 (90%)	11 (10%)	0	100	100
10	J	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
11	K	113/117 (97%)	112 (99%)	1 (1%)	0	100	100
12	L	44/58 (76%)	42 (96%)	2 (4%)	0	100	100
13	f	62/85 (73%)	60 (97%)	2 (3%)	0	100	100
17	a	371/408 (91%)	345 (93%)	26 (7%)	0	100	100
18	b	806/1160 (70%)	766 (95%)	40 (5%)	0	100	100
19	c	32/152 (21%)	32 (100%)	0	0	100	100
20	g	218/257 (85%)	210 (96%)	8 (4%)	0	100	100
21	e	574/1493 (38%)	546 (95%)	28 (5%)	0	100	100
22	d	243/729 (33%)	234 (96%)	9 (4%)	0	100	100
All	All	6148/8997 (68%)	5900 (96%)	248 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1241/1749 (71%)	1234 (99%)	7 (1%)	78	80
2	B	992/1127 (88%)	991 (100%)	1 (0%)	88	89
3	C	237/252 (94%)	237 (100%)	0	100	100
4	D	118/126 (94%)	118 (100%)	0	100	100
5	E	191/192 (100%)	188 (98%)	3 (2%)	55	68
6	F	71/111 (64%)	71 (100%)	0	100	100
7	G	152/153 (99%)	152 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	105/112 (94%)	104 (99%)	1 (1%)	68	75
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	43/55 (78%)	43 (100%)	0	100	100
13	f	59/76 (78%)	59 (100%)	0	100	100
17	a	331/358 (92%)	329 (99%)	2 (1%)	78	80
18	b	712/1014 (70%)	709 (100%)	3 (0%)	84	83
19	c	35/128 (27%)	35 (100%)	0	100	100
20	g	183/215 (85%)	182 (100%)	1 (0%)	81	81
21	e	527/1297 (41%)	523 (99%)	4 (1%)	73	77
22	d	216/623 (35%)	216 (100%)	0	100	100
All	All	5502/7881 (70%)	5480 (100%)	22 (0%)	81	83

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ASP
1	A	469	MET
1	A	531	ASN
1	A	701	ASP

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Mol	Chain	Res	Type
1	A	740	GLN
1	A	1341	VAL
1	A	1374	VAL
2	B	1008	VAL
5	E	72	MET
5	E	73	PHE
5	E	194	ILE
9	I	14	ILE
17	a	31	GLU
17	a	245	ASN
18	b	355	ASN
18	b	386	SER
18	b	809	GLN
20	g	146	MET
21	e	784	GLU
21	e	789	LEU
21	e	933	ASP
21	e	1007	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	278	HIS
1	A	441	GLN
1	A	459	ASN
1	A	461	GLN
1	A	493	ASN
1	A	502	ASN
1	A	539	GLN
1	A	590	GLN
1	A	673	GLN
1	A	704	ASN
1	A	735	GLN
1	A	739	ASN
1	A	742	ASN
1	A	791	GLN
1	A	825	ASN
1	A	1291	ASN
1	A	1299	GLN
1	A	1462	GLN
2	B	23	GLN
2	B	319	ASN

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Mol	Chain	Res	Type
2	B	370	HIS
2	B	410	ASN
2	B	471	ASN
2	B	500	GLN
2	B	570	ASN
2	B	631	GLN
2	B	642	GLN
2	B	968	ASN
2	B	986	GLN
2	B	1003	ASN
2	B	1049	GLN
2	B	1068	GLN
2	B	1073	GLN
2	B	1097	HIS
3	C	18	ASN
3	C	108	ASN
3	C	145	GLN
3	C	232	ASN
4	D	48	ASN
5	E	92	GLN
5	E	132	GLN
5	E	138	ASN
7	G	9	HIS
7	G	24	ASN
7	G	60	GLN
8	H	126	GLN
8	H	131	ASN
9	I	18	GLN
9	I	91	HIS
17	a	139	ASN
17	a	169	GLN
17	a	185	HIS
17	a	187	GLN
17	a	228	GLN
17	a	343	GLN
17	a	345	ASN
18	b	4	ASN
18	b	290	GLN
18	b	1009	HIS
20	g	159	HIS
20	g	193	GLN
20	g	228	HIS

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Mol	Chain	Res	Type
20	g	236	GLN
21	e	641	HIS
21	e	718	ASN
21	e	772	GLN
21	e	773	HIS
21	e	778	ASN
21	e	854	GLN
21	e	956	GLN
21	e	1398	HIS
22	d	49	GLN
22	d	580	GLN
22	d	664	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	M	9/25 (36%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	M	8	G

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 11 ligands modelled in this entry, 11 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

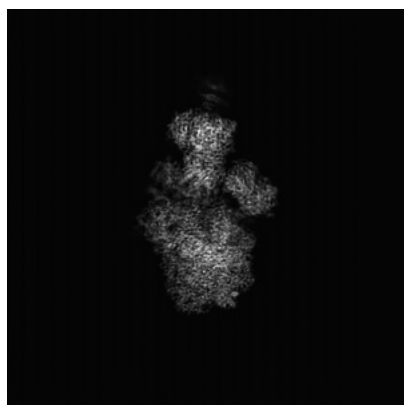
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50325. These allow visual inspection of the internal detail of the map and identification of artifacts.

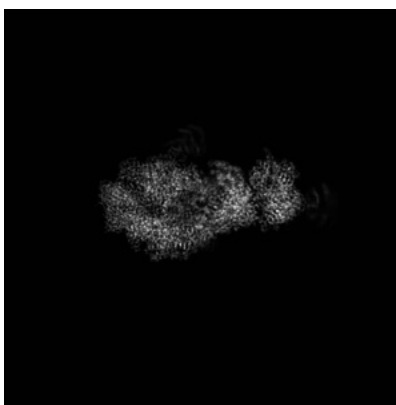
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

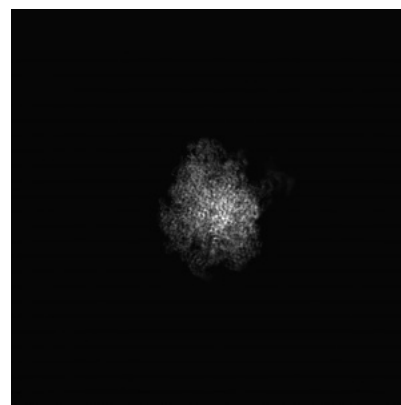
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

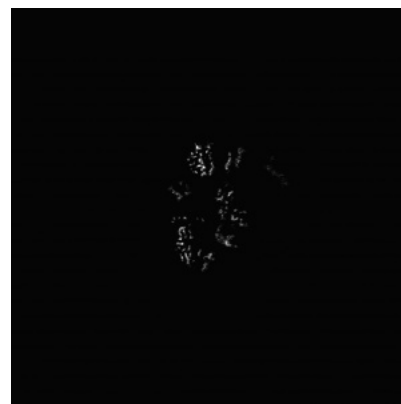
6.2.1 Primary map



X Index: 200



Y Index: 200



Z Index: 200

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: 214



Y Index: 191

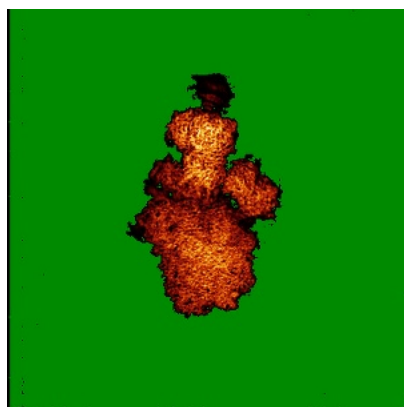


Z Index: 160

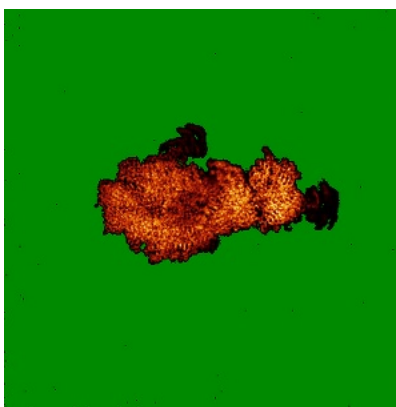
The images above show the largest variance slices of the map in three orthogonal directions.

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

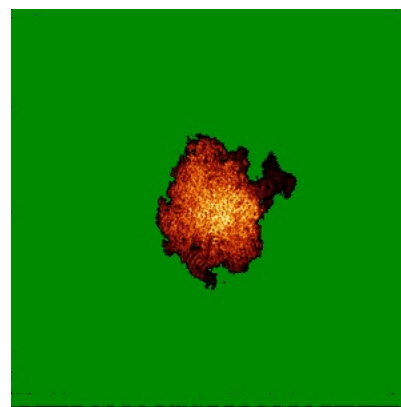
6.4.1 Primary map



X



Y

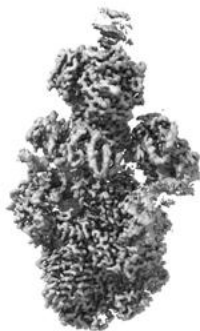


Z

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

6.5 Orthogonal surface views [i](#)

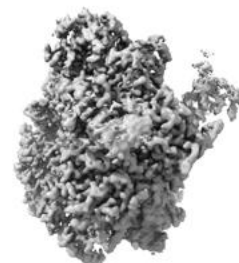
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

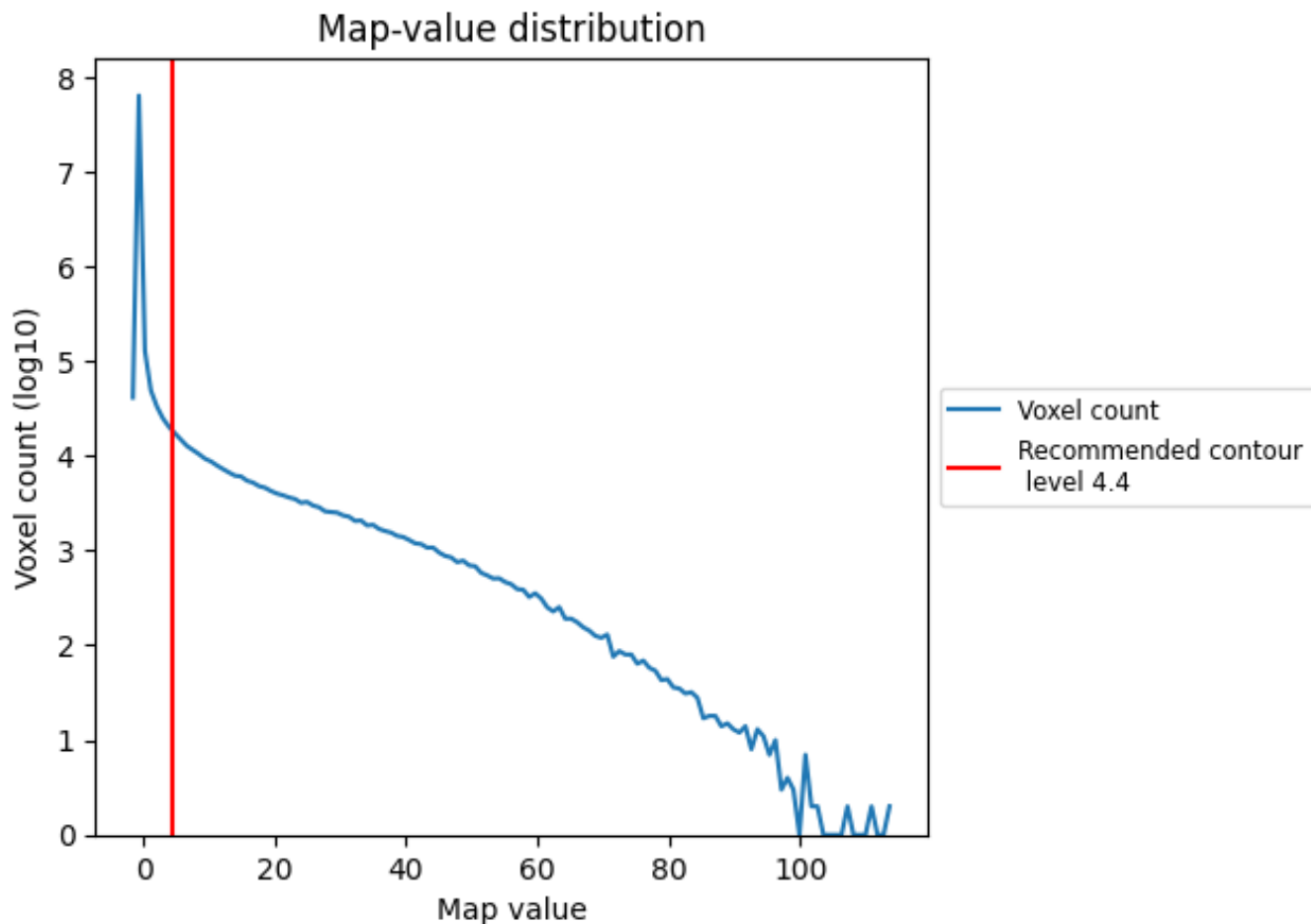
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

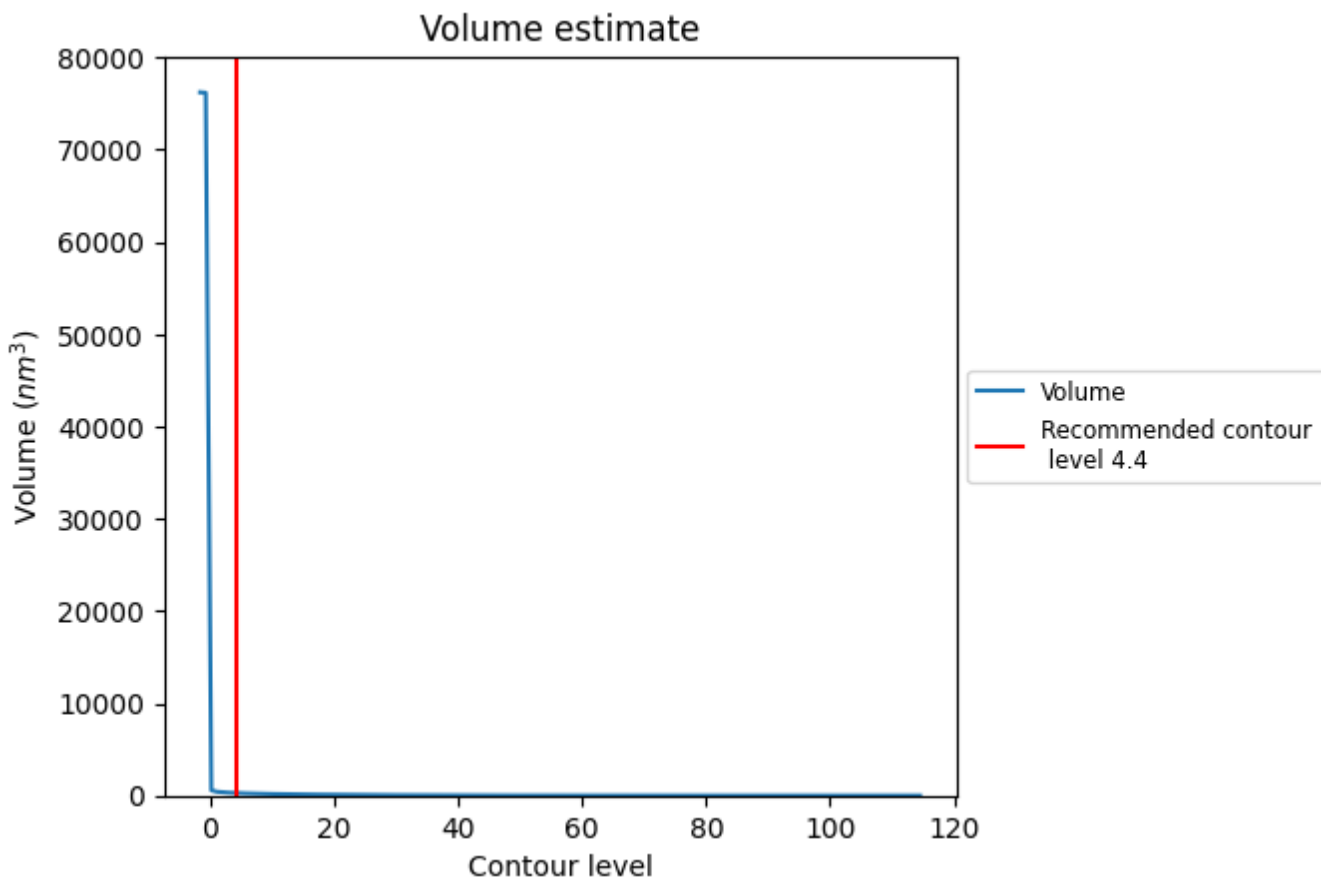
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

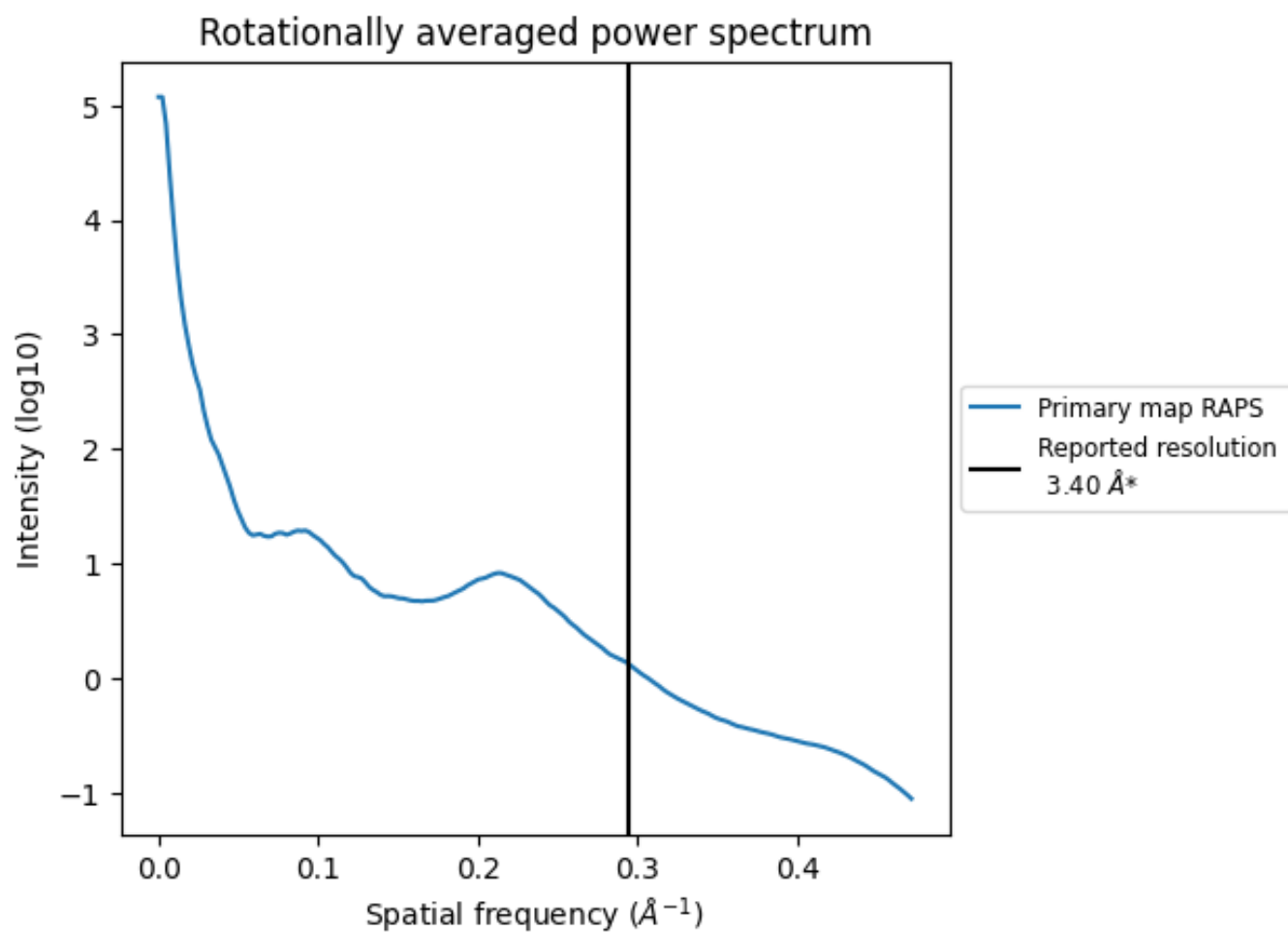
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 269 nm³; this corresponds to an approximate mass of 243 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

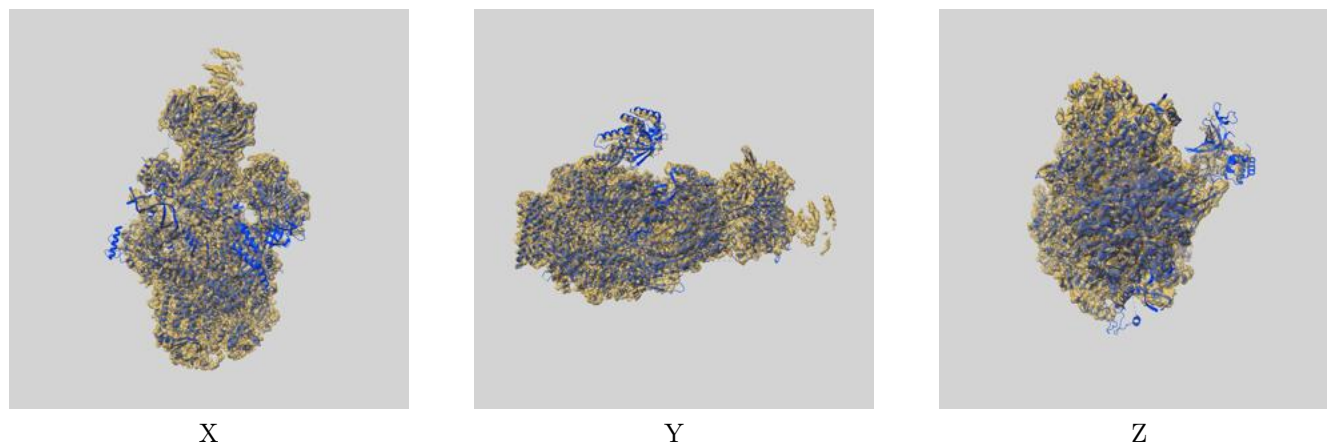
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

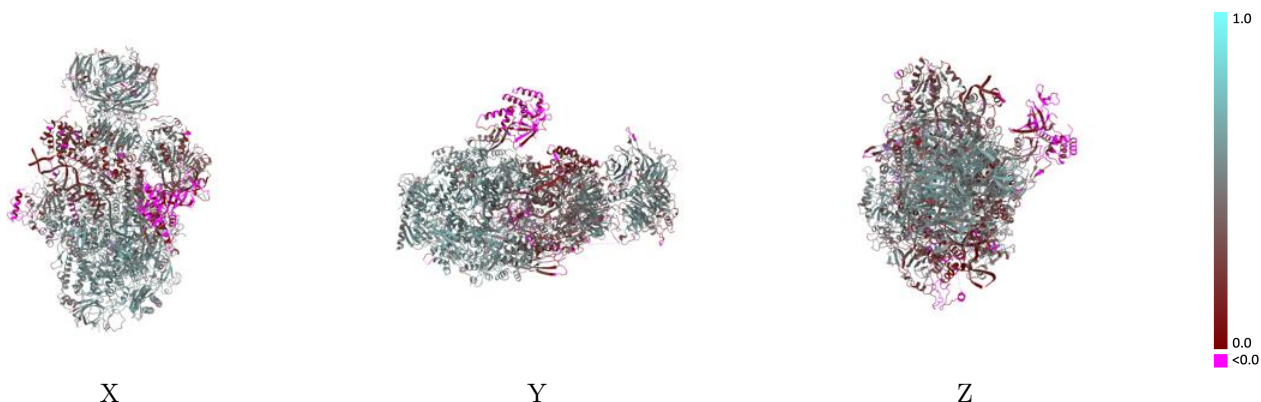
This section contains information regarding the fit between EMDB map EMD-50325 and PDB model 9FD2. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



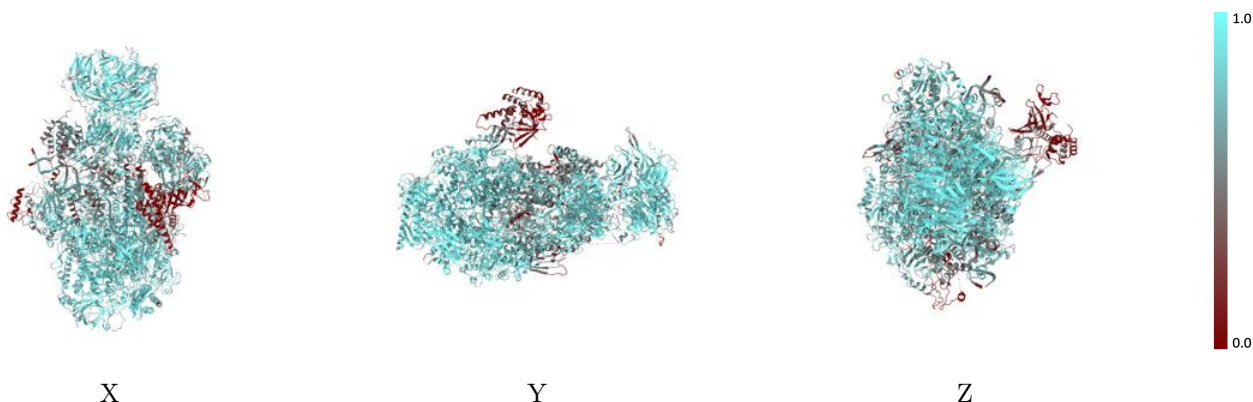
The images above show the 3D surface view of the map at the recommended contour level 4.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



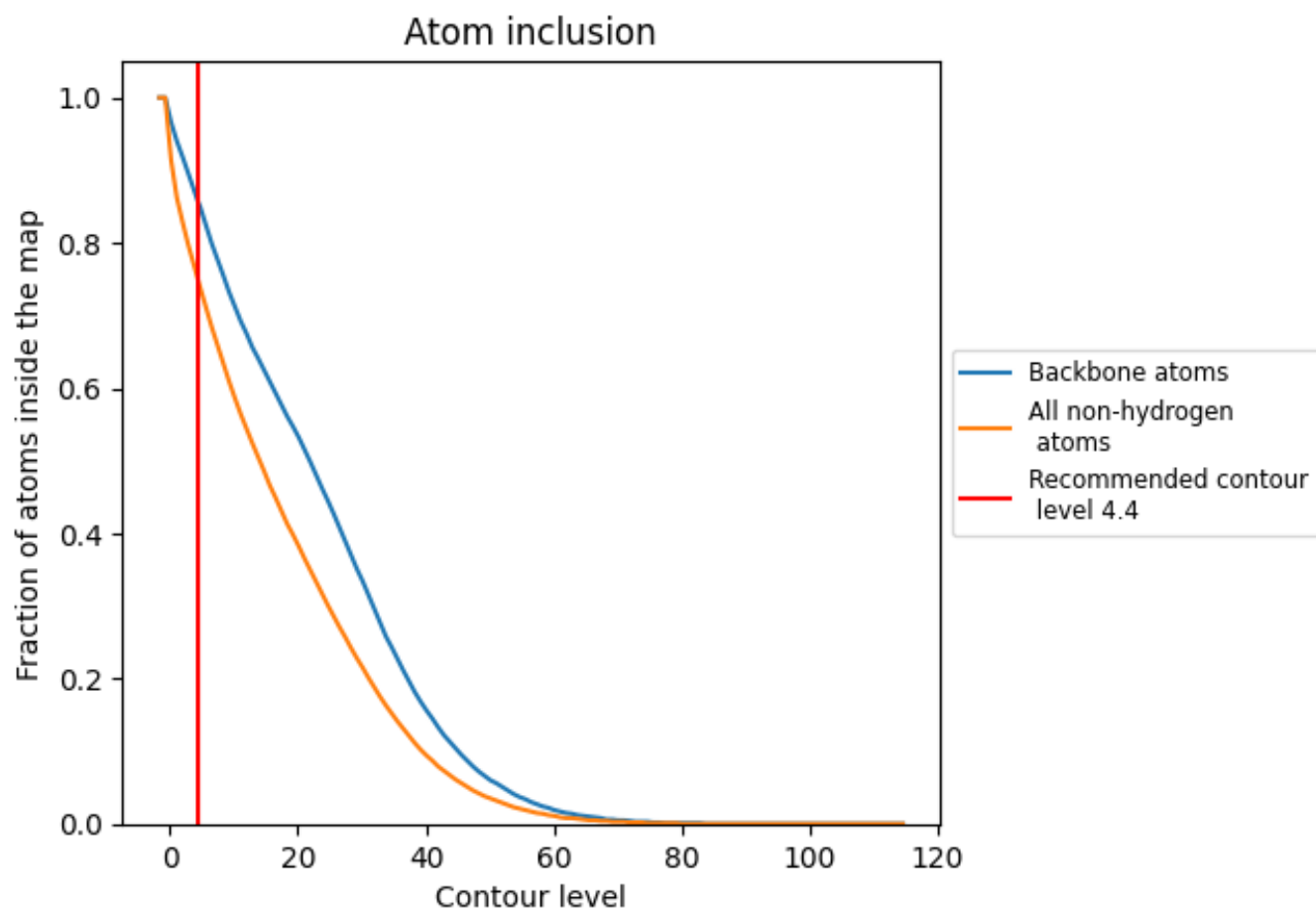
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.4).















































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 75% 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 (4.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7490	 0.4360
A	 0.7920	 0.4980
B	 0.8130	 0.5090
C	 0.8510	 0.5400
D	 0.1360	 -0.0040
E	 0.7950	 0.4840
F	 0.8290	 0.5120
G	 0.3060	 0.1540
H	 0.8190	 0.5180
I	 0.6570	 0.3880
J	 0.8870	 0.5680
K	 0.8580	 0.5480
L	 0.7290	 0.4390
M	 0.8910	 0.4930
N	 0.6400	 0.2460
T	 0.7120	 0.3270
a	 0.8710	 0.5110
b	 0.8450	 0.4820
c	 0.5360	 0.3050
d	 0.3510	 0.1260
e	 0.7330	 0.3740
f	 0.6370	 0.3180
g	 0.6310	 0.2400

