



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 03:55 AM UTC

PDB ID : 5OQM / pdb_00005oqm
EMDB ID : EMD-3850
Title : STRUCTURE OF YEAST TRANSCRIPTION PRE-INITIATION COM-
PLEX WITH TFIIF AND CORE MEDIATOR
Authors : Schilbach, S.; Hantsche, M.; Tegunov, D.; Dienemann, C.; Wigge, C.; Urlaub,
H.; Cramer, P.
Deposited on : 2017-08-13
Resolution : 5.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

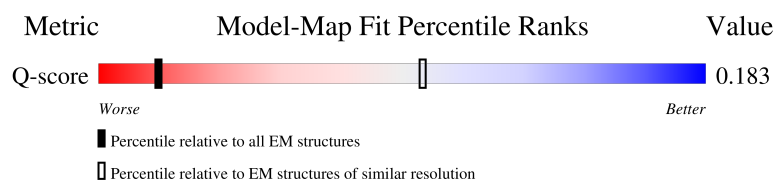
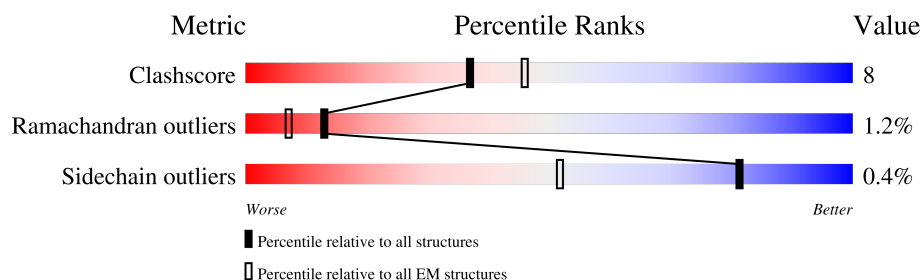
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 5.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



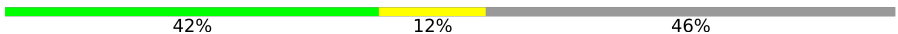
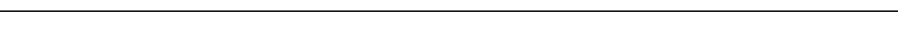
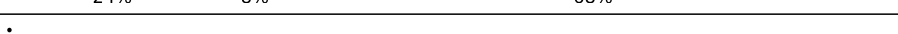
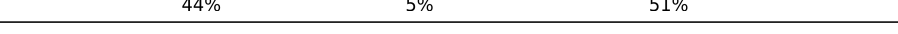
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	511 (5.30 - 6.30)

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	1733	
2	B	1224	
3	C	318	
4	D	221	

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	345	
14	N	106	
15	O	240	
16	Q	747	
17	R	400	
18	T	106	
19	U	286	
20	V	122	
21	W	541	
22	X	328	
23	0	778	
24	1	510	
25	2	553	
26	3	321	
27	4	333	
28	5	72	
29	6	461	

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Mol	Chain	Length	Quality of chain
30	7	843	
31	Z	43	
32	a	295	
33	b	223	
34	c	115	
35	d	687	
36	e	307	
37	f	210	
38	g	121	
39	h	300	
40	i	223	
41	j	149	
42	k	157	
43	l	745	
44	m	220	
45	n	140	
46	o	151	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
49	SF4	0	901	-	-	X	-

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 79757 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1398	Total	C	N	O	S	0	0
			10997	6931	1927	2078	61		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1152	Total	C	N	O	S	0	0
			9178	5807	1608	1708	55		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	262	Total	C	N	O	S	0	0
			2061	1299	343	406	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	157	Total	C	N	O	S	0	0
			1253	779	220	252	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	213	Total	C	N	O	S	0	0
			1744	1107	308	318	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	83	Total	C	N	O	S	0	0
			670	428	114	125	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	136	Total	C	N	O	S	0	0
			1089	686	184	215	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			944	581	172	181	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	112	Total	C	N	O	S	0	0
			904	580	154	168	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	279	Total	C	N	O	S	0	0
			2175	1382	373	403	17		

- Molecule 14 is a DNA chain called NONTEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	76	Total	C	N	O	P	0	0
			1533	747	288	422	76		

- Molecule 15 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	180	Total	C	N	O	S	0	0
			1416	921	242	247	6		

- Molecule 16 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	148	Total	C	N	O	S	0	0
			1144	733	195	212	4		

- Molecule 17 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	190	Total	C	N	O	S	0	0
			1303	812	238	246	7		

- Molecule 18 is a DNA chain called TEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	72	Total	C	N	O	P	0	0
			1440	706	254	408	72		

- Molecule 19 is a protein called Transcription initiation factor IIA large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	92	Total	C	N	O	S	0	0
			757	474	130	150	3		

- Molecule 20 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	100	Total	C	N	O	S	0	0
			782	492	130	156	4		

- Molecule 21 is a protein called Transcription factor TFIIE subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	258	Total	C	N	O	S	0	0
			1825	1147	321	351	6		

- Molecule 22 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	160	Total	C	N	O	S	0	0
			1004	620	184	196	4		

- Molecule 23 is a protein called General transcription and DNA repair factor IIIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	0	698	Total	C	N	O	S	0	0
			4844	3051	856	907	30		

- Molecule 24 is a protein called General transcription and DNA repair factor IIIH subunit TFB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1	491	Total	C	N	O	S	0	0
			3060	1893	570	590	7		

- Molecule 25 is a protein called General transcription and DNA repair factor IIIH subunit TFB2.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	2	395	Total	C	N	O	0	0
			2160	1317	413	430		

- Molecule 26 is a protein called RNA polymerase II transcription factor B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	3	138	Total	C	N	O	S	0	0
			860	533	160	160	7		

- Molecule 27 is a protein called General transcription and DNA repair factor IIIH subunit TFB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4	297	Total	C	N	O	S	0	0
			1475	877	297	297	4		

- Molecule 28 is a protein called General transcription and DNA repair factor IIH subunit TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	66	Total	C	N	O	S	0	0
			498	314	89	93	2		

- Molecule 29 is a protein called General transcription and DNA repair factor IIH subunit SSL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	6	335	Total	C	N	O	S	0	0
			2197	1355	399	422	21		

- Molecule 30 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	7	408	Total	C	N	O	S	0	0
			3148	2000	557	572	19		

- Molecule 31 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	Z	43	Total	C	N	O	0	0
			215	129	43	43		

- Molecule 32 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	a	149	Total	C	N	O	0	0
			741	443	149	149		

- Molecule 33 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	b	158	Total	C	N	O	0	0
			839	511	161	167		

- Molecule 34 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	99	Total	C	N	O	S	0	0
			809	506	137	163	3		

- Molecule 35 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	442	Total	C	N	O	S	0	0
			3065	1942	539	577	7		

- Molecule 36 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	232	Total	C	N	O	S	0	0
			1822	1161	297	355	9		

- Molecule 37 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	203	Total	C	N	O	S	0	0
			1560	987	263	305	5		

- Molecule 38 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	85	Total	C	N	O	S	1	0
			667	420	110	133	4		

- Molecule 39 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	131	Total	C	N	O	S	0	0
			654	392	131	131			

- Molecule 40 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	136	Total	C	N	O	S	0	0
			1096	704	190	197	5		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
i	14	SER	-	insertion	UNP Q08278
i	16	THR	PRO	conflict	UNP Q08278
i	17	SER	PRO	conflict	UNP Q08278
i	19	SER	PRO	conflict	UNP Q08278

- Molecule 41 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	j	66	Total	C	N	O	0	0
			328	196	66	66		

- Molecule 42 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	k	127	Total	C	N	O	0	0
			630	376	127	127		

- Molecule 43 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	l	471	Total	C	N	O	0	0
			2344	1402	471	471		

- Molecule 44 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	m	103	Total	C	N	O	0	0
			512	306	103	103		

- Molecule 45 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	136	Total	C	N	O	S	0	0
			999	623	171	201	4		

- Molecule 46 is a protein called Mediator of RNA polymerase II transcription subunit 31, Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	99	Total	C	N	O	S	0	0
			760	499	121	136	4		

- Molecule 47 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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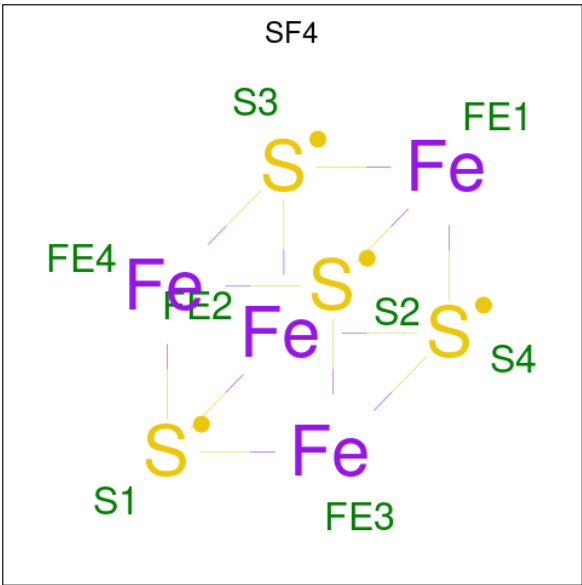
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Mol	Chain	Residues	Atoms		AltConf
47	B	1	Total 1	Zn 1	0
47	C	1	Total 1	Zn 1	0
47	I	2	Total 2	Zn 2	0
47	J	1	Total 1	Zn 1	0
47	L	1	Total 1	Zn 1	0
47	M	1	Total 1	Zn 1	0
47	W	1	Total 1	Zn 1	0
47	3	2	Total 2	Zn 2	0
47	4	1	Total 1	Zn 1	0
47	6	3	Total 3	Zn 3	0

- Molecule 48 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 49 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

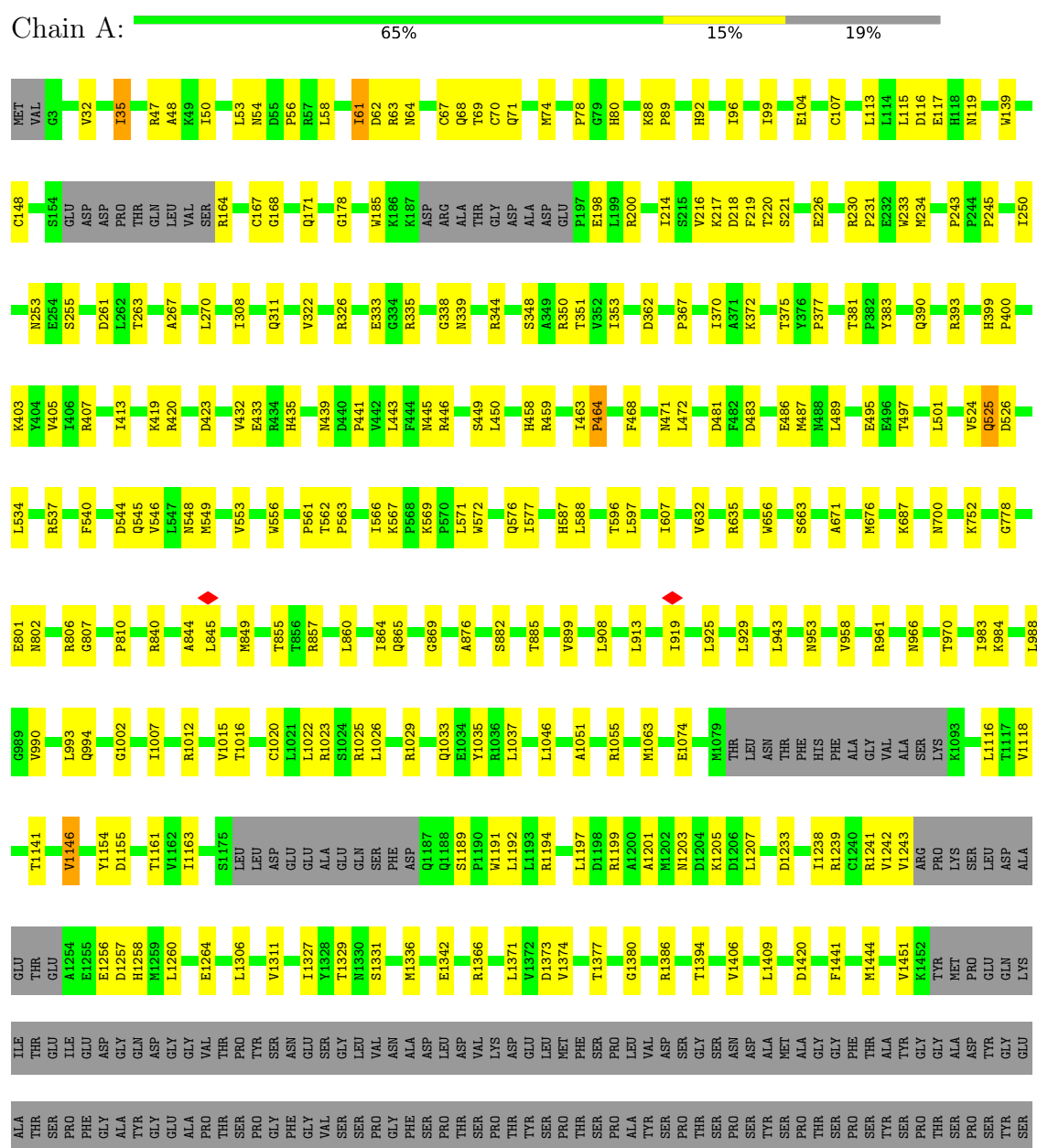


Mol	Chain	Residues	Atoms			AltConf
49	0	1	Total	Fe	S	0
			8	4	4	

3 Residue-property plots

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

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



SER ASN GLU ASP VAL THR MET MET THR GLN ALA GLU GLN ASP ASP PRO TYR SER ASN ALA ALA SER GLN MET GLY ASN THR SER GLY TYR ASP ASP ASN ALA THR

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

Chain D:  62% 9% 29%

MET ASN VAL SER THR SER THR PHE GLN THR ALA GLU ARG ASP ARG LEU LYS VAL SER GLU GLU ASN A24 N51 E54 A55 R56 L57 E61 A52 L63 R66 K76 HIS LYS LYS LYS HIS LEU LYS HIS GLU ASN ALA ASN ASP GLU THR THR VAL GLU ASP GLU

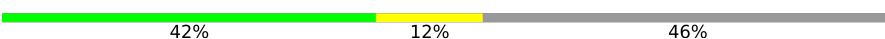
ASP ASP ASP LEU ASP ASP VAL ASP ASP ALA ASP ASP ASP PHE MET HIS GLU T118 L123 L130 L141 Q146 R155 D156 Q157 E158 T159 V160 Q165 S169 H173 E176 G181 Y221

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

Chain E:  87% 12% .

MET ASP Q3 R17 R26 G27 Y28 E36 K56 M57 M58 A62 H63 P64 G76 S77 L78 F82 C83 D84 Q106 V124 P125 S126 I127 I132 E133 N136 E137 I144 L156 Q179 R180 A181 G189 K197 R200 R215

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

Chain F:  42% 12% 46%

MET SER ASP TYR GLU ALA PHE ASN ASP GLY GLN ASN ASN PHE PHE VAL GLU HIS PHE SER ASP GLU THR TYR GLU LYS PRO GLN PHE LYS ASP GLY THR THR ASP ALA GLY LYS THR ILE VAL THR GLY ASN GLY PRO ASP PHE GLN

HIS GLU GLN ILE ARG ARG LYS THR LEU LYS K72 K76 R79 T82 P83 Y84 R92 R97 K123 E124 E127 V133 I134 R135 R136 F143 E144 D145 W146 S147 L151 D154 LEU

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

Chain G:  68% 32%

H1 I4 S8 L9 N10 P20 R21 R22 K23 Q24 Y25 L26 Y44 I45 L46 C47 V48 P63 T64 D65 G66 F70 W71 V72 V77 V78 K83 C84 S93 C94 S95 Q96 H97 G98 F99 E100 V101 Q102 K107 V110 T111 K112 H113 L114 L119 N122 A123

N126 P127 P128 S129 Y130 T133 I139 I143 R144 V145 K146 I147 G149 I157 I160 G161 S162 I163 K164 E165 A170 I171

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

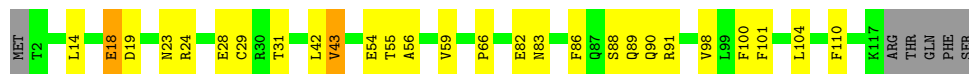
Chain H:  70% 23% 7%

MET S2 L5 F6 D7 D8 I9 G18 R19 Y20 I28 I42 M43 V44 P48 T56 V57 T58 I59 A60 S61 N64 L65 L66 ASP THR PRO ALA ASP ASP SER A75 Q83 L89 A90 Y93 V96 A101 Y102 K103 T112 Y115 Y129

L132 N133 N134 L142 L143 I144 R145

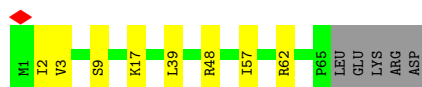
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I: 



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

Chain J: 



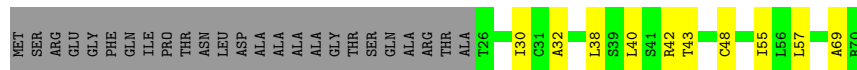
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K: 



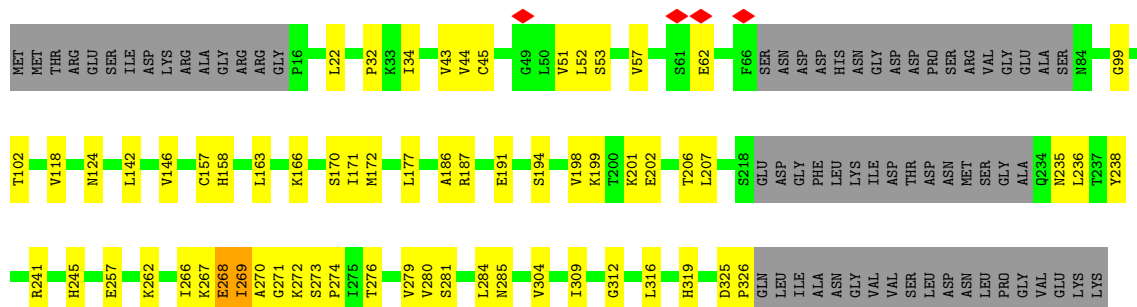
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 



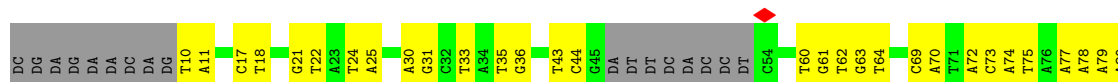
- Molecule 13: Transcription initiation factor IIB

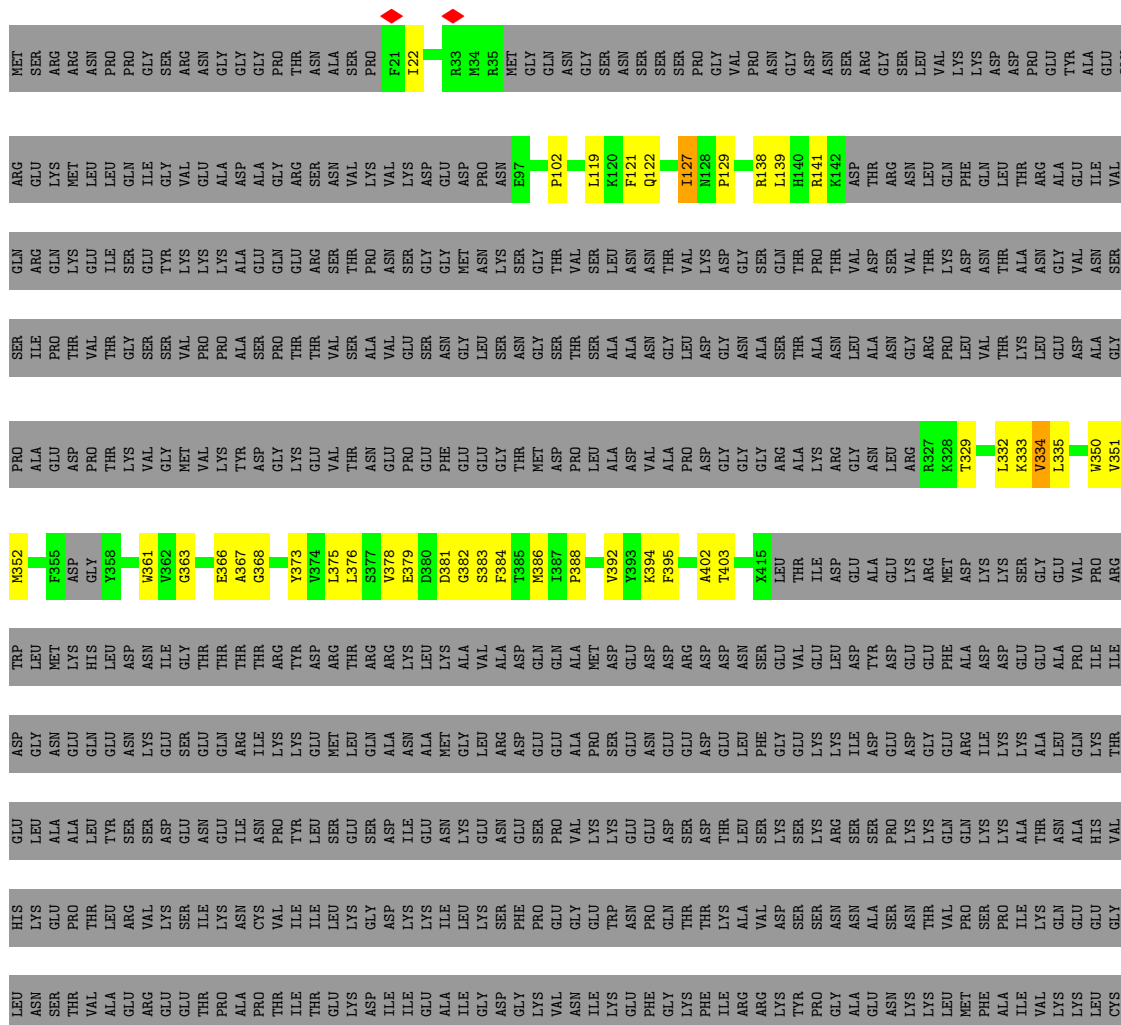
Chain M: 

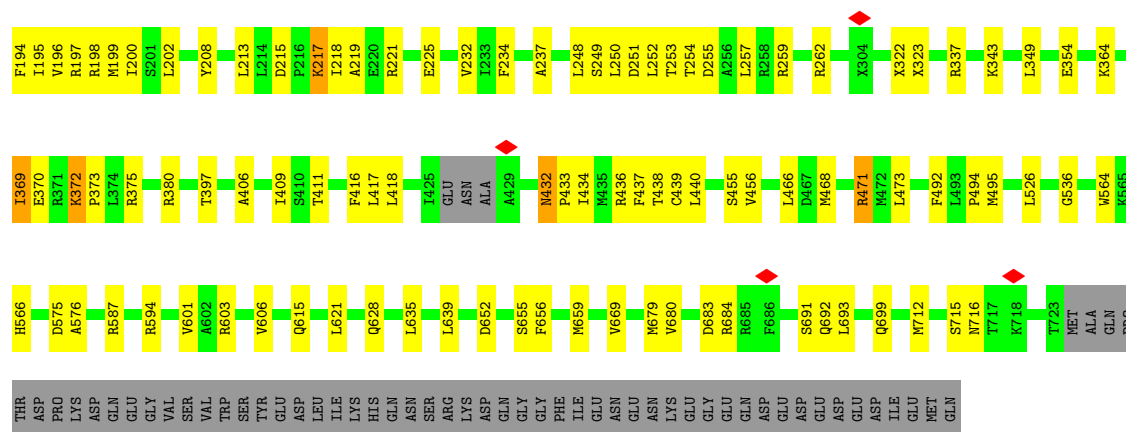


- Molecule 14: NONTEMPLATE DNA

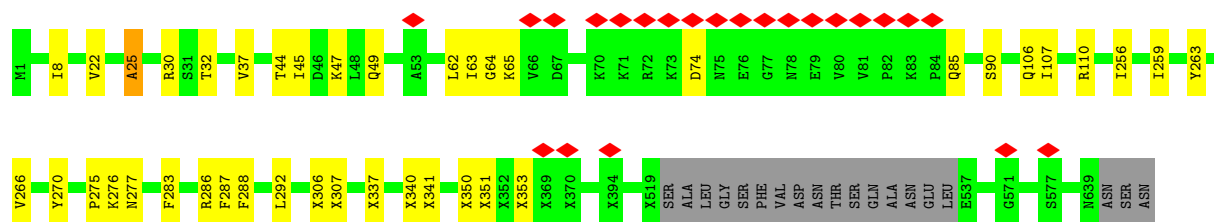
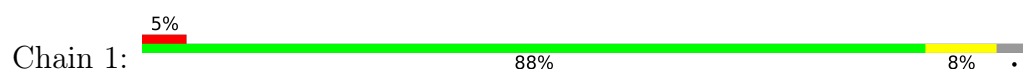
Chain N: 



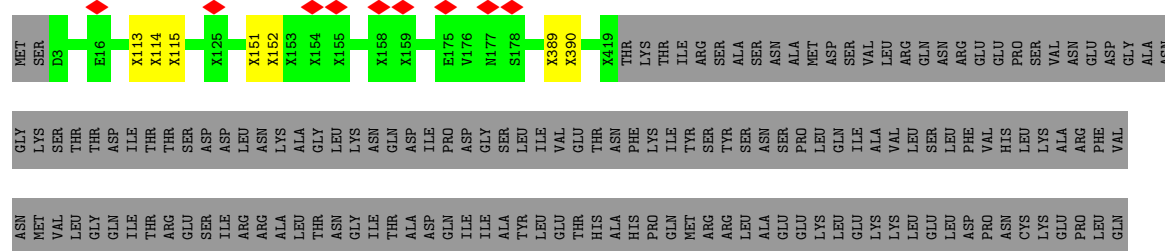




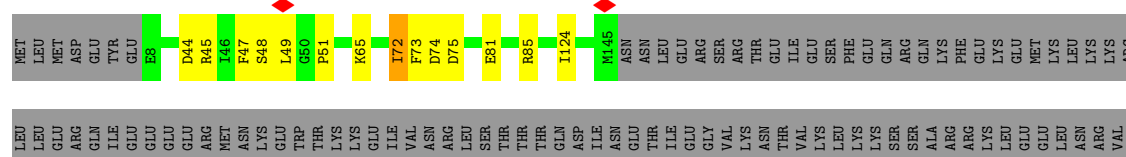
• Molecule 24: General transcription and DNA repair factor IIH subunit TFB1



• Molecule 25: General transcription and DNA repair factor IIH subunit TFB2



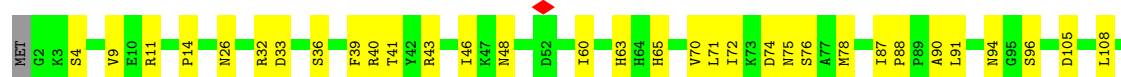
• Molecule 26: RNA polymerase II transcription factor B subunit 3





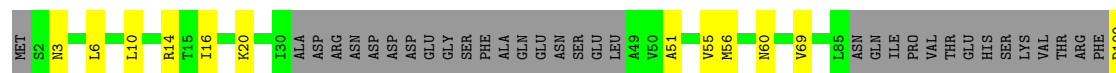
- Molecule 37: Mediator of RNA polymerase II transcription subunit 20

Chain f: 74% 22% .



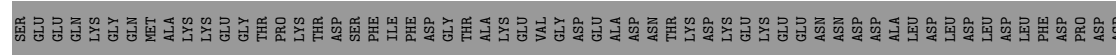
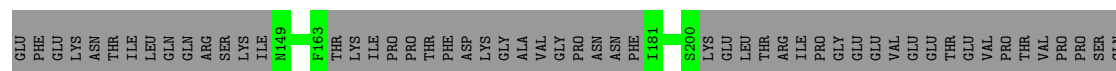
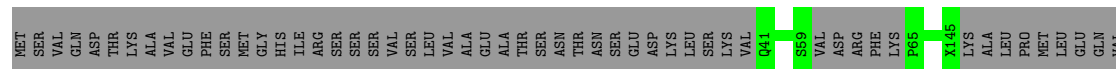
- Molecule 38: Mediator of RNA polymerase II transcription subunit 22

Chain g: 56% 14% 30%



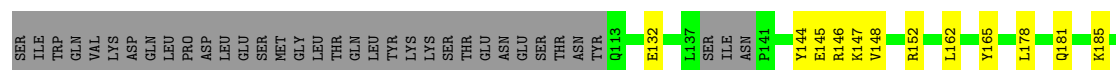
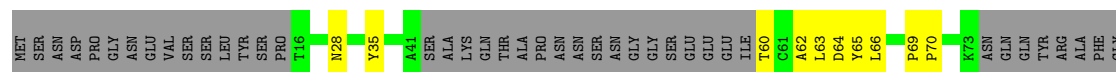
- Molecule 39: Mediator of RNA polymerase II transcription subunit 4

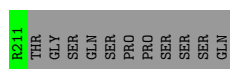
Chain h: 44% 56%



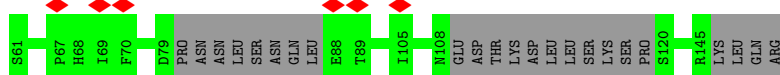
- Molecule 40: Mediator of RNA polymerase II transcription subunit 7

Chain i: 51% 10% 39%

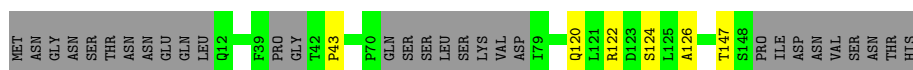
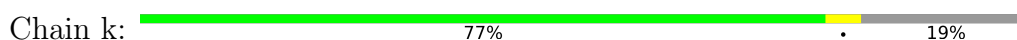




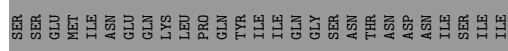
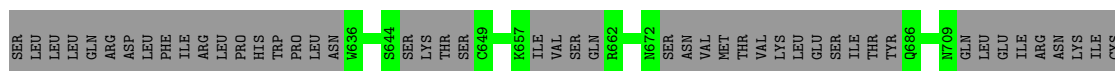
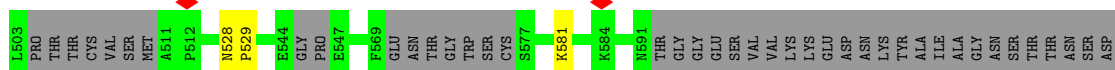
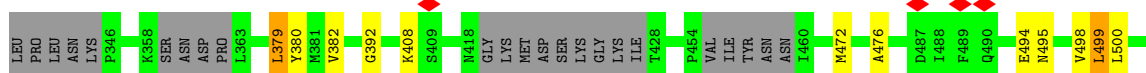
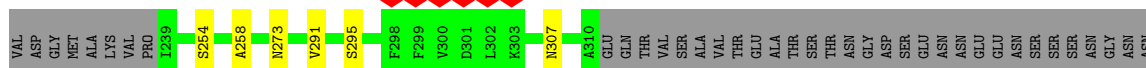
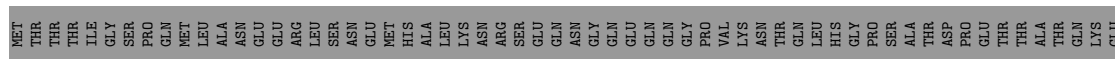
- Molecule 41: Mediator of RNA polymerase II transcription subunit 9



- Molecule 42: Mediator of RNA polymerase II transcription subunit 10

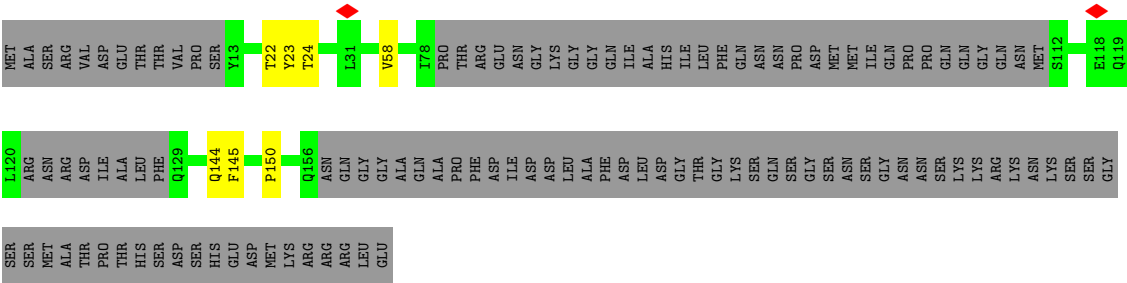


- Molecule 43: Mediator of RNA polymerase II transcription subunit 14

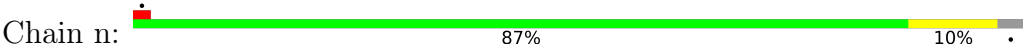


- Molecule 44: Mediator of RNA polymerase II transcription subunit 19

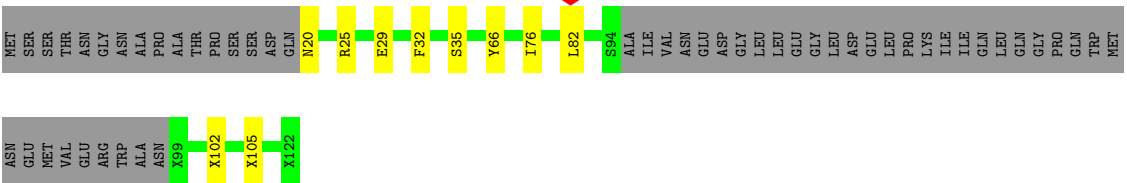




- Molecule 45: Mediator of RNA polymerase II transcription subunit 21



- Molecule 46: Mediator of RNA polymerase II transcription subunit 31, Mediator of RNA polymerase II transcription subunit 31



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	16000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.700	Depositor
Minimum map value	-0.340	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	479.5, 479.5, 479.5	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SF4, 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	0.12	0/11192	0.30	2/15128 (0.0%)
2	B	0.11	0/9357	0.27	0/12618
3	C	0.09	0/2099	0.24	0/2845
4	D	0.08	0/1262	0.22	0/1693
5	E	0.11	0/1780	0.32	2/2395 (0.1%)
6	F	0.10	0/682	0.26	0/922
7	G	0.10	0/1368	0.24	0/1844
8	H	0.11	0/1107	0.28	0/1499
9	I	0.11	0/962	0.32	0/1295
10	J	0.14	0/541	0.33	0/727
11	K	0.08	0/922	0.21	0/1244
12	L	0.14	0/360	0.43	0/478
13	M	0.12	0/2204	0.30	0/2963
14	N	0.20	0/1724	0.45	0/2614
15	O	0.12	0/1443	0.28	0/1942
16	Q	0.16	0/1108	0.40	0/1495
17	R	0.13	0/1312	0.33	0/1777
18	T	0.19	0/1614	0.40	0/2442
19	U	0.08	0/766	0.25	0/1032
20	V	0.08	0/789	0.23	0/1066
21	W	0.11	0/1566	0.26	0/2117
22	X	0.11	0/1013	0.33	0/1385
23	0	0.14	0/4739	0.37	0/6431
24	1	0.22	0/2198	0.36	0/2983
25	2	0.11	0/1631	0.30	0/2243
26	3	0.11	0/870	0.32	0/1190
27	4	0.19	0/1282	0.49	2/1780 (0.1%)
28	5	0.13	0/502	0.43	0/677
29	6	0.16	0/1996	0.33	0/2713
30	7	0.10	0/2980	0.27	0/4019
32	a	0.15	0/737	0.38	0/1023
33	b	0.09	0/841	0.26	0/1166

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
34	c	0.09	0/817	0.21	0/1096
35	d	0.16	0/3089	0.36	1/4188 (0.0%)
36	e	0.08	0/1854	0.22	0/2509
37	f	0.08	0/1584	0.22	0/2145
38	g	0.08	0/665	0.20	0/894
39	h	0.24	0/570	0.22	0/791
40	i	0.30	0/1112	0.42	0/1494
41	j	0.41	0/325	0.53	0/449
42	k	0.16	0/627	0.38	0/870
43	l	0.13	0/2328	0.37	2/3227 (0.1%)
44	m	0.11	0/509	0.30	0/706
45	n	0.15	0/1005	0.24	0/1357
46	o	0.16	0/661	0.33	0/902
All	All	0.14	0/78093	0.32	9/106374 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	d	607	ASP	N-CA-C	-9.50	100.92	111.28
5	E	127	ILE	CA-C-N	6.62	124.43	119.66
5	E	127	ILE	C-N-CA	6.62	124.43	119.66
1	A	1146	VAL	CA-C-N	-6.31	114.37	122.77
1	A	1146	VAL	C-N-CA	-6.31	114.37	122.77
43	l	380	TYR	CA-C-N	-6.02	112.70	120.65
43	l	380	TYR	C-N-CA	-6.02	112.70	120.65
27	4	288	ILE	CA-C-N	-5.24	113.51	120.63
27	4	288	ILE	C-N-CA	-5.24	113.51	120.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10997	0	11080	184	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	9178	0	9195	171	0
3	C	2061	0	2029	55	0
4	D	1253	0	1275	13	0
5	E	1744	0	1771	16	0
6	F	670	0	690	12	0
7	G	1340	0	1357	34	0
8	H	1089	0	1062	22	0
9	I	944	0	899	29	0
10	J	532	0	542	5	0
11	K	904	0	911	14	0
12	L	358	0	381	7	0
13	M	2175	0	2283	43	0
14	N	1533	0	860	32	0
15	O	1416	0	1493	22	0
16	Q	1144	0	1021	29	0
17	R	1303	0	1110	29	0
18	T	1440	0	820	30	0
19	U	757	0	747	13	0
20	V	782	0	790	11	0
21	W	1825	0	1546	28	0
22	X	1004	0	730	8	0
23	0	4844	0	4241	85	0
24	1	3060	0	2050	26	0
25	2	2160	0	1075	13	0
26	3	860	0	620	11	0
27	4	1475	0	624	11	0
28	5	498	0	506	12	0
29	6	2197	0	1738	15	0
30	7	3148	0	3002	69	0
31	Z	215	0	49	5	0
32	a	741	0	298	2	0
33	b	839	0	424	5	0
34	c	809	0	807	19	0
35	d	3065	0	2684	55	0
36	e	1822	0	1825	36	0
37	f	1560	0	1573	51	0
38	g	667	0	678	17	0
39	h	654	0	268	0	0
40	i	1096	0	1110	16	0
41	j	328	0	130	0	0
42	k	630	0	265	3	0
43	l	2344	0	979	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	m	512	0	212	1	0
45	n	999	0	925	7	0
46	o	760	0	656	6	0
47	3	2	0	0	0	0
47	4	1	0	0	0	0
47	6	3	0	0	0	0
47	A	2	0	0	0	0
47	B	1	0	0	0	0
47	C	1	0	0	0	0
47	I	2	0	0	0	0
47	J	1	0	0	0	0
47	L	1	0	0	0	0
47	M	1	0	0	0	0
47	W	1	0	0	0	0
48	A	1	0	0	0	0
49	0	8	0	0	3	0
All	All	79757	0	69331	1132	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 8.

All (1132) 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)
43:l:495:ASN:O	43:l:499:LEU:HA	1.50	1.12
9:I:54:GLU:O	9:I:89:GLN:N	1.93	1.02
3:C:85:ASP:OD1	37:f:146:THR:HG21	1.60	0.99
19:U:242:ASN:HA	19:U:268:THR:O	1.62	0.99
31:Z:31:UNK:HA	31:Z:41:UNK:CB	1.93	0.97
3:C:260:LEU:HD22	37:f:14:PRO:CB	1.95	0.96
1:A:70:CYS:SG	1:A:80:HIS:NE2	2.40	0.95
3:C:260:LEU:CD2	37:f:14:PRO:HB3	1.96	0.95
31:Z:30:UNK:O	31:Z:41:UNK:CB	2.18	0.91
17:R:98:ASN:HB3	17:R:103:LYS:O	1.71	0.91
9:I:54:GLU:HB3	9:I:88:SER:OG	1.72	0.90
16:Q:138:ARG:O	16:Q:352:MET:HA	1.72	0.89
17:R:106:LEU:O	17:R:119:GLU:HA	1.72	0.89
3:C:89:GLU:HB2	37:f:43:ARG:NH1	1.90	0.86
23:0:594:ARG:NH1	29:6:241:THR:O	2.08	0.85
2:B:70:ILE:HD11	16:Q:333:LYS:HB2	1.59	0.84
3:C:260:LEU:HD21	37:f:14:PRO:HB3	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:54:GLU:HA	9:I:90:GLN:H	1.43	0.84
3:C:85:ASP:OD1	37:f:146:THR:CG2	2.26	0.83
3:C:11:ARG:NH1	3:C:209:TYR:OH	2.12	0.82
9:I:54:GLU:CB	9:I:88:SER:OG	2.27	0.82
23:0:252:LEU:O	23:0:434:ILE:HA	1.78	0.82
21:W:14:LYS:O	21:W:18:ARG:HB2	1.79	0.81
23:0:191:CYS:HG	49:0:901:SF4:FE4	0.95	0.81
25:2:151:UNK:O	25:2:152:UNK:CB	2.29	0.81
18:T:30:DT:H2''	18:T:31:DT:H72	1.61	0.81
43:l:379:LEU:O	43:l:382:VAL:N	2.15	0.80
21:W:149:CYS:O	21:W:153:ASP:N	2.16	0.79
16:Q:376:LEU:HD21	16:Q:386:MET:HE3	1.65	0.79
3:C:260:LEU:HD22	37:f:14:PRO:HB2	1.66	0.78
23:0:635:LEU:O	23:0:639:LEU:HB2	1.83	0.78
2:B:835:GLN:HA	2:B:1013:ASN:ND2	1.99	0.77
24:1:64:GLY:HA3	24:1:85:GLN:O	1.83	0.77
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.65	0.77
30:7:672:GLN:HE21	30:7:722:ARG:HH12	1.31	0.77
1:A:1141:THR:HG23	1:A:1205:LYS:HD3	1.67	0.77
4:D:57:LEU:O	4:D:61:GLU:HB2	1.84	0.77
1:A:78:PRO:O	2:B:1205:GLN:NE2	2.18	0.76
1:A:419:LYS:NZ	36:e:57:GLN:OE1	2.17	0.76
35:d:609:LEU:HB2	38:g:108:LEU:HD13	1.67	0.76
2:B:839:MET:HG2	2:B:1012:ILE:HG22	1.66	0.76
18:T:77:DT:H2'	18:T:78:DA:H8	1.47	0.76
3:C:84:ARG:HG3	37:f:146:THR:HG21	1.68	0.75
25:2:114:UNK:O	25:2:115:UNK:CB	2.35	0.75
24:1:350:UNK:O	24:1:351:UNK:CB	2.35	0.75
25:2:113:UNK:O	25:2:114:UNK:CB	2.34	0.74
23:0:323:UNK:CB	23:0:380:ARG:NH2	2.51	0.74
11:K:20:LYS:HB2	11:K:34:THR:HB	1.67	0.74
3:C:75:MET:O	3:C:246:ARG:NH2	2.21	0.74
1:A:1055:ARG:NH1	6:F:154:ASP:O	2.20	0.73
8:H:56:THR:O	8:H:144:ILE:HA	1.86	0.73
38:g:6:LEU:O	38:g:10:LEU:HB2	1.89	0.73
1:A:441:PRO:HA	1:A:458:HIS:O	1.88	0.73
9:I:101:PHE:HB2	9:I:110:PHE:O	1.89	0.73
27:4:289:CYS:HB2	27:4:294:CYS:H	1.54	0.72
3:C:56:THR:HG22	3:C:147:LEU:HD21	1.70	0.72
12:L:32:ALA:HB2	12:L:55:ILE:HB	1.70	0.72
21:W:149:CYS:HB2	21:W:156:LEU:HD21	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:279:VAL:HG11	13:M:304:VAL:HG11	1.70	0.72
2:B:835:GLN:HA	2:B:1013:ASN:HD22	1.55	0.72
16:Q:127:ILE:HG22	16:Q:129:PRO:HD3	1.70	0.71
34:c:66:LEU:HD13	38:g:14:ARG:HH22	1.55	0.71
25:2:389:UNK:O	25:2:390:UNK:CB	2.39	0.71
23:0:526:LEU:HD22	23:0:621:LEU:HD21	1.73	0.71
35:d:461:ASN:HB3	35:d:464:LYS:HB3	1.73	0.71
3:C:89:GLU:CB	37:f:43:ARG:NH1	2.53	0.70
7:G:10:ASN:HA	7:G:70:PHE:O	1.92	0.70
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.73	0.70
9:I:19:ASP:HB3	9:I:24:ARG:O	1.92	0.69
13:M:99:GLY:H	13:M:102:THR:HG21	1.58	0.69
1:A:524:VAL:HG12	1:A:525:GLN:HG2	1.75	0.69
16:Q:375:LEU:O	16:Q:386:MET:HA	1.91	0.69
18:T:82:DT:H2'	18:T:83:DA:C8	2.28	0.69
14:N:63:DG:H2''	14:N:64:DT:C5	2.28	0.69
30:7:672:GLN:HE21	30:7:722:ARG:NH1	1.91	0.69
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.72	0.69
24:1:256:ILE:HD13	24:1:259:ILE:HD11	1.75	0.69
7:G:101:VAL:HG21	7:G:145:VAL:HG21	1.73	0.69
30:7:558:TRP:HE1	30:7:735:VAL:HB	1.57	0.68
8:H:96:VAL:HA	8:H:142:LEU:O	1.93	0.68
13:M:34:ILE:HG22	13:M:45:CYS:HA	1.75	0.68
30:7:592:GLN:HE22	30:7:749:ALA:H	1.41	0.68
13:M:236:LEU:HD11	13:M:257:GLU:HG3	1.74	0.68
3:C:260:LEU:CD2	37:f:14:PRO:CB	2.59	0.68
1:A:35:ILE:HG22	1:A:270:LEU:HD11	1.75	0.68
1:A:61:ILE:HG22	1:A:62:ASP:H	1.59	0.68
3:C:18:VAL:HG21	3:C:240:VAL:HG21	1.76	0.67
23:0:364:LYS:HZ2	23:0:369:ILE:H	1.43	0.67
3:C:84:ARG:HG3	37:f:146:THR:CG2	2.23	0.67
1:A:1146:VAL:HG23	1:A:1197:LEU:HD22	1.77	0.67
30:7:376:ASN:HD21	30:7:380:ARG:HB3	1.58	0.67
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.75	0.67
1:A:807:GLY:HA3	2:B:728:ARG:HH21	1.60	0.67
3:C:85:ASP:OD1	37:f:146:THR:OG1	2.11	0.67
26:3:51:PRO:HD3	26:3:65:LYS:HE3	1.77	0.67
35:d:608:LYS:HG3	38:g:105:GLU:HA	1.77	0.67
2:B:825:VAL:HA	2:B:1010:LEU:O	1.93	0.67
23:0:712:MET:O	23:0:716:ASN:ND2	2.27	0.67
24:1:47:LYS:HB2	24:1:63:ILE:HD12	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:64:SER:HA	17:R:216:GLY:HA2	1.77	0.67
2:B:373:ARG:HG3	2:B:566:LEU:HD23	1.75	0.67
1:A:446:ARG:HD2	1:A:487:MET:HE2	1.77	0.66
12:L:38:LEU:HD21	12:L:48:CYS:HA	1.77	0.66
23:O:669:VAL:HG21	23:O:679:MET:HB2	1.77	0.66
1:A:1451:VAL:HG12	7:G:20:PRO:HB3	1.76	0.66
13:M:157:CYS:SG	13:M:158:HIS:N	2.68	0.66
16:Q:121:PHE:HB2	17:R:131:ASN:HB3	1.78	0.66
13:M:267:LYS:HE2	13:M:270:ALA:HB2	1.78	0.66
29:6:221:LEU:HD13	29:6:230:ARG:HB3	1.78	0.66
2:B:67:SER:HB2	2:B:92:PHE:H	1.61	0.65
2:B:770:GLN:NE2	2:B:982:SER:O	2.29	0.65
2:B:383:ASN:O	2:B:387:LEU:HB2	1.96	0.65
36:e:229:ILE:O	36:e:255:ALA:HA	1.95	0.65
1:A:107:CYS:SG	1:A:171:GLN:NE2	2.70	0.65
36:e:230:LEU:HA	36:e:254:LYS:O	1.96	0.65
2:B:1171:VAL:HA	2:B:1181:GLU:O	1.97	0.65
18:T:19:DC:H2"	18:T:20:DT:H72	1.79	0.65
2:B:826:ALA:HB3	2:B:1011:ILE:HG12	1.79	0.65
3:C:79:GLN:CB	37:f:11:ARG:HH22	2.09	0.65
2:B:822:ASN:O	10:J:48:ARG:NH1	2.30	0.64
15:O:170:ILE:HD13	15:O:234:LEU:HD22	1.78	0.64
34:c:30:VAL:O	34:c:34:PHE:CB	2.46	0.64
43:l:254:SER:O	43:l:258:ALA:HB2	1.97	0.64
1:A:178:GLY:HA2	1:A:311:GLN:HE22	1.63	0.64
30:7:656:LYS:HZ1	30:7:686:ARG:HH21	1.46	0.64
37:f:138:ARG:NH1	37:f:156:GLN:OE1	2.29	0.64
36:e:163:PRO:HA	36:e:190:ILE:O	1.98	0.64
3:C:11:ARG:NH2	3:C:19:ASP:OD2	2.30	0.64
23:O:248:LEU:HD13	23:O:416:PHE:HE1	1.63	0.64
1:A:69:THR:HG23	1:A:80:HIS:CD2	2.32	0.64
35:d:619:ILE:HB	35:d:631:LEU:O	1.98	0.64
21:W:413:PHE:HB3	24:1:49:GLN:HB3	1.78	0.64
33:b:203:LYS:HD3	36:e:295:SER:HA	1.80	0.64
38:g:16:ILE:O	38:g:20:LYS:HB3	1.98	0.64
2:B:115:GLN:NE2	2:B:787:VAL:O	2.31	0.64
4:D:173:HIS:HB3	4:D:176:GLU:HG3	1.80	0.64
23:O:253:THR:O	23:O:255:ASP:N	2.26	0.64
1:A:1329:THR:HG22	1:A:1331:SER:H	1.62	0.64
3:C:13:ALA:HA	3:C:18:VAL:HG22	1.80	0.64
23:O:191:CYS:SG	49:O:901:SF4:FE4	1.90	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:8:ILE:HB	24:1:90:SER:HB2	1.77	0.63
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.80	0.63
7:G:114:LEU:HD23	7:G:162:SER:HB3	1.81	0.63
13:M:274:PRO:HD2	15:O:188:GLU:HG2	1.81	0.63
30:7:558:TRP:HB3	30:7:711:LYS:HE2	1.81	0.63
1:A:70:CYS:SG	1:A:80:HIS:CE1	2.91	0.63
23:0:248:LEU:HB2	23:0:439:CYS:HB3	1.79	0.63
34:c:62:SER:O	34:c:66:LEU:HB2	1.99	0.63
43:l:472:MET:O	43:l:476:ALA:HB2	1.97	0.63
2:B:911:ILE:HD11	2:B:941:LEU:HD12	1.81	0.62
23:0:603:ARG:NH1	23:0:628:GLN:HG3	2.13	0.62
3:C:85:ASP:OD1	37:f:146:THR:CB	2.46	0.62
43:l:494:GLU:HA	43:l:500:LEU:O	1.99	0.62
1:A:860:LEU:HD11	1:A:1394:THR:HA	1.80	0.62
17:R:126:LYS:HB3	17:R:221:GLU:HB2	1.79	0.62
21:W:178:GLN:NE2	22:X:254:CYS:SG	2.73	0.62
35:d:519:THR:HG22	35:d:533:LEU:HD11	1.82	0.62
1:A:68:GLN:O	1:A:71:GLN:NE2	2.33	0.62
23:0:251:ASP:OD1	23:0:436:ARG:NE	2.32	0.62
25:2:483:TRP:NE1	28:5:36:ASP:OD2	2.31	0.62
2:B:490:SER:O	2:B:494:HIS:HB2	2.00	0.62
2:B:944:THR:HG21	2:B:1122:ARG:HH12	1.63	0.62
30:7:560:PRO:HD2	30:7:586:THR:HG21	1.80	0.62
30:7:604:LYS:NZ	30:7:650:ASN:OD1	2.32	0.62
1:A:544:ASP:HB2	11:K:47:ARG:HH12	1.65	0.62
13:M:163:LEU:O	13:M:166:LYS:NZ	2.33	0.62
1:A:1189:SER:N	1:A:1242:VAL:O	2.31	0.62
2:B:25:ILE:HA	2:B:655:LYS:HE3	1.82	0.62
19:U:259:LYS:HA	19:U:281:VAL:O	2.00	0.62
23:0:217:LYS:HG3	23:0:218:ILE:HG12	1.81	0.62
13:M:118:VAL:HG22	13:M:124:ASN:HD21	1.65	0.61
1:A:1199:ARG:O	1:A:1203:ASN:ND2	2.33	0.61
7:G:96:GLN:NE2	21:W:146:GLU:OE2	2.33	0.61
35:d:448:GLU:HA	35:d:539:ILE:HD11	1.81	0.61
1:A:562:THR:O	1:A:576:GLN:NE2	2.34	0.61
3:C:25:VAL:HG13	3:C:29:MET:HB3	1.83	0.61
23:0:257:LEU:HB3	23:0:343:LYS:NZ	2.16	0.61
23:0:495:MET:SD	23:0:684:ARG:NH2	2.73	0.61
27:4:289:CYS:HB3	27:4:292:CYS:SG	2.40	0.61
27:4:305:CYS:O	27:4:307:ALA:N	2.34	0.61
2:B:249:ARG:HG2	2:B:415:GLN:HE22	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:84:ARG:HE	37:f:146:THR:HG22	1.65	0.61
34:c:13:LEU:HD21	34:c:69:GLU:HG2	1.82	0.61
36:e:228:LEU:HD21	36:e:278:LEU:HD22	1.81	0.61
23:0:257:LEU:HB3	23:0:343:LYS:HZ3	1.65	0.61
27:4:87:TYR:O	27:4:89:UNK:N	2.34	0.61
1:A:32:VAL:HG12	2:B:1183:LYS:HE2	1.81	0.61
16:Q:373:TYR:OH	17:R:72:ARG:NH2	2.34	0.61
30:7:565:PHE:O	30:7:569:TYR:HB2	2.01	0.61
30:7:673:ILE:HG12	30:7:708:LEU:HD12	1.82	0.61
30:7:656:LYS:NZ	30:7:686:ARG:HH21	1.98	0.61
37:f:36:SER:O	37:f:63:HIS:HB2	2.01	0.61
3:C:40:GLU:OE1	3:C:254:LYS:NZ	2.23	0.60
25:2:456:GLY:HA3	25:2:493:ILE:O	2.01	0.60
27:4:285:VAL:HA	29:6:322:UNK:O	2.00	0.60
2:B:193:LYS:HB3	2:B:787:VAL:HG21	1.83	0.60
36:e:231:GLU:HB2	36:e:254:LYS:HB3	1.83	0.60
1:A:671:ALA:HB3	1:A:676:MET:HE2	1.83	0.60
30:7:631:THR:HB	30:7:636:ARG:HE	1.66	0.60
1:A:481:ASP:O	1:A:483:ASP:OD1	2.20	0.60
1:A:185:TRP:HB2	1:A:198:GLU:O	2.02	0.60
3:C:84:ARG:NE	37:f:146:THR:HG22	2.16	0.60
14:N:30:DA:H2'	14:N:31:DG:C8	2.36	0.60
1:A:115:LEU:O	1:A:164:ARG:NH1	2.35	0.60
4:D:57:LEU:O	4:D:61:GLU:CB	2.50	0.60
40:i:65:TYR:O	46:o:25:ARG:NH2	2.34	0.60
43:l:107:LEU:O	43:l:111:MET:CB	2.50	0.60
30:7:672:GLN:HE22	30:7:686:ARG:HH22	1.48	0.60
35:d:514:VAL:HG11	35:d:610:LEU:HD11	1.83	0.60
1:A:1257:ASP:OD1	1:A:1258:HIS:N	2.35	0.60
1:A:1444:MET:HE2	6:F:135:ARG:HH21	1.65	0.60
8:H:129:TYR:O	8:H:133:ASN:ND2	2.35	0.60
30:7:493:VAL:O	30:7:495:ALA:N	2.35	0.60
35:d:442:MET:HE3	35:d:478:LEU:HB2	1.83	0.60
1:A:537:ARG:HD2	8:H:20:TYR:CZ	2.37	0.59
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.83	0.59
3:C:22:LEU:O	3:C:228:PHE:HB2	2.02	0.59
23:0:322:UNK:CB	23:0:380:ARG:HH12	2.14	0.59
1:A:483:ASP:OD1	1:A:483:ASP:N	2.35	0.59
4:D:66:ARG:NH2	7:G:47:CYS:SG	2.75	0.59
18:T:77:DT:H2'	18:T:78:DA:C8	2.34	0.59
13:M:281:SER:O	13:M:285:ASN:ND2	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.84	0.59
13:M:22:LEU:HB3	13:M:52:LEU:HD23	1.83	0.59
14:N:82:DA:H4'	30:7:676:HIS:HE1	1.66	0.59
23:0:364:LYS:NZ	23:0:370:GLU:H	1.99	0.59
2:B:919:SER:HB2	2:B:922:GLU:HB2	1.84	0.59
7:G:4:ILE:HG12	7:G:77:VAL:HG22	1.84	0.59
31:Z:31:UNK:CA	31:Z:41:UNK:CB	2.77	0.59
34:c:30:VAL:O	34:c:34:PHE:HB2	2.03	0.59
38:g:16:ILE:O	38:g:20:LYS:CB	2.50	0.59
2:B:287:ARG:NH2	2:B:294:ASP:OD1	2.36	0.59
2:B:298:LEU:HD23	2:B:311:LEU:HD22	1.84	0.59
3:C:54:ASN:HD21	3:C:63:ILE:HD12	1.68	0.59
8:H:101:ALA:HA	8:H:115:TYR:O	2.02	0.59
16:Q:139:LEU:HA	16:Q:351:VAL:O	2.02	0.59
30:7:680:ARG:HB3	30:7:722:ARG:HB2	1.84	0.59
2:B:969:ARG:NH2	3:C:60:ASP:OD2	2.36	0.59
11:K:49:GLU:OE2	11:K:97:LYS:NZ	2.35	0.58
18:T:30:DT:OP1	30:7:657:VAL:HA	2.03	0.58
23:0:354:GLU:HB2	23:0:418:LEU:HB2	1.84	0.58
2:B:1106:ARG:NH2	2:B:1110:PRO:O	2.34	0.58
3:C:73:GLN:HE21	3:C:74:SER:H	1.50	0.58
19:U:244:MET:HG3	19:U:267:VAL:HG22	1.85	0.58
1:A:1342:GLU:OE1	5:E:200:ARG:NH2	2.35	0.58
18:T:31:DT:H2'	18:T:32:DA:C8	2.38	0.58
23:0:364:LYS:HZ2	23:0:369:ILE:N	2.02	0.58
17:R:104:ILE:HD11	17:R:122:LEU:HD22	1.86	0.58
19:U:246:CYS:HB3	19:U:265:GLY:HA3	1.85	0.58
22:X:200:VAL:HG12	22:X:201:THR:HG23	1.85	0.58
1:A:333:GLU:OE1	2:B:1129:ARG:NH2	2.37	0.58
1:A:390:GLN:OE1	1:A:393:ARG:NH2	2.37	0.58
1:A:419:LYS:NZ	36:e:57:GLN:CD	2.61	0.58
7:G:84:GLY:CA	7:G:147:ILE:O	2.52	0.58
29:6:264:LEU:HD22	29:6:300:LEU:HD13	1.85	0.58
36:e:11:ILE:O	36:e:250:GLY:HA3	2.03	0.58
9:I:19:ASP:O	9:I:23:ASN:HA	2.04	0.58
16:Q:141:ARG:HA	16:Q:350:TRP:HA	1.85	0.58
17:R:104:ILE:HD11	17:R:122:LEU:HB3	1.86	0.58
29:6:291:LEU:HD22	29:6:297:LEU:HD13	1.86	0.58
1:A:420:ARG:HA	36:e:60:GLU:HG3	1.86	0.58
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.86	0.58
35:d:457:VAL:HG22	35:d:467:ILE:HG23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:d:604:ARG:O	35:d:607:ASP:N	2.37	0.58
1:A:250:ILE:HD13	13:M:62:GLU:HG3	1.85	0.57
1:A:348:SER:HA	1:A:489:LEU:O	2.04	0.57
2:B:858:SER:HA	2:B:966:VAL:O	2.04	0.57
9:I:82:GLU:HG2	9:I:104:LEU:HD12	1.85	0.57
11:K:29:ASN:ND2	11:K:78:THR:O	2.37	0.57
23:O:168:GLU:HG2	23:O:199:MET:HE1	1.86	0.57
37:f:135:LEU:HD22	37:f:166:LYS:HB3	1.86	0.57
8:H:65:LEU:HD21	8:H:89:LEU:HD13	1.86	0.57
34:c:24:LEU:HD11	38:g:69:VAL:HG11	1.86	0.57
36:e:7:LEU:HG	36:e:275:LEU:HD23	1.86	0.57
2:B:872:GLU:HG2	2:B:916:THR:HG22	1.85	0.57
38:g:103:GLN:O	38:g:107:LEU:HB2	2.04	0.57
1:A:1146:VAL:HG12	1:A:1201:ALA:HB1	1.85	0.57
36:e:76:ILE:HG23	36:e:80:MET:HB3	1.86	0.57
1:A:326:ARG:HG2	1:A:1406:VAL:HG11	1.86	0.57
2:B:881:ASN:O	2:B:933:SER:OG	2.23	0.57
35:d:604:ARG:O	35:d:607:ASP:HB3	2.03	0.57
7:G:8:SER:HA	7:G:72:VAL:O	2.05	0.57
30:7:474:UNK:O	30:7:478:UNK:CB	2.51	0.57
1:A:687:LYS:NZ	1:A:801:GLU:OE1	2.38	0.57
23:O:337:ARG:NH2	26:3:74:ASP:OD2	2.38	0.57
27:4:267:UNK:O	27:4:268:UNK:CB	2.51	0.57
43:l:93:ALA:O	43:l:97:ARG:CB	2.53	0.57
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.68	0.57
18:T:41:DC:H2''	18:T:42:DA:C8	2.39	0.57
3:C:5:GLY:O	3:C:24:ASN:ND2	2.36	0.57
7:G:84:GLY:HA2	7:G:147:ILE:O	2.05	0.57
13:M:284:LEU:HD22	13:M:316:LEU:HG	1.86	0.57
30:7:490:VAL:H	30:7:514:THR:HB	1.70	0.56
19:U:262:LEU:HB2	19:U:279:ALA:HB3	1.86	0.56
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.05	0.56
17:R:98:ASN:CB	17:R:103:LYS:O	2.50	0.56
24:1:283:PHE:O	24:1:287:PHE:HB3	2.06	0.56
26:3:44:ASP:O	26:3:48:SER:OG	2.23	0.56
37:f:4:SER:HA	37:f:155:LEU:O	2.05	0.56
1:A:544:ASP:O	1:A:548:ASN:ND2	2.38	0.56
2:B:984:HIS:NE2	2:B:1028:GLU:OE1	2.32	0.56
2:B:1009:ASP:OD2	10:J:48:ARG:NH2	2.38	0.56
9:I:55:THR:HG22	9:I:100:PHE:CD2	2.40	0.56
14:N:43:DT:H1'	14:N:44:DC:H5'	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:LEU:HG	1:A:501:LEU:HD21	1.87	0.56
7:G:138:THR:HG22	7:G:139:ILE:H	1.70	0.56
17:R:67:GLN:HB3	17:R:219:CYS:HB2	1.87	0.56
23:0:76:MET:HB2	24:1:341:UNK:HA	1.88	0.56
35:d:518:LYS:O	35:d:522:SER:CB	2.53	0.56
37:f:41:THR:HB	37:f:120:GLN:HB3	1.88	0.56
37:f:72:ILE:HA	37:f:76:SER:O	2.05	0.56
1:A:335:ARG:HH22	2:B:1114:LEU:HD11	1.69	0.56
7:G:84:GLY:N	7:G:147:ILE:O	2.39	0.56
23:0:468:MET:SD	23:0:468:MET:N	2.79	0.56
27:4:290:SER:C	27:4:292:CYS:H	2.14	0.56
3:C:84:ARG:CD	37:f:146:THR:HG22	2.36	0.56
36:e:5:LEU:O	36:e:256:TYR:HA	2.06	0.56
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.38	0.56
3:C:79:GLN:CB	37:f:11:ARG:NH2	2.69	0.56
3:C:242:GLN:O	3:C:246:ARG:HB2	2.06	0.56
11:K:36:GLU:OE1	11:K:70:ARG:NH1	2.39	0.56
29:6:175:ARG:NH1	29:6:176:ASN:OD1	2.38	0.56
40:i:62:ALA:HA	40:i:65:TYR:HD2	1.71	0.56
1:A:261:ASP:HB3	1:A:322:VAL:HG13	1.88	0.56
2:B:794:ASN:HA	2:B:854:LEU:O	2.06	0.56
5:E:17:ARG:HH12	5:E:36:GLU:HA	1.71	0.56
16:Q:122:GLN:HB2	16:Q:394:LYS:HE3	1.87	0.56
24:1:288:PHE:O	24:1:292:LEU:CB	2.53	0.56
18:T:19:DC:C2'	18:T:20:DT:H72	2.35	0.55
5:E:28:TYR:HA	5:E:64:PRO:HA	1.86	0.55
13:M:177:LEU:HD22	13:M:207:LEU:HD11	1.87	0.55
36:e:257:ILE:HD12	36:e:271:THR:HG23	1.88	0.55
1:A:445:ASN:OD1	1:A:449:SER:OG	2.21	0.55
2:B:785:TYR:O	2:B:967:ARG:NH1	2.32	0.55
1:A:62:ASP:O	1:A:64:ASN:N	2.35	0.55
1:A:545:GLN:HG2	1:A:549:MET:HE3	1.88	0.55
13:M:241:ARG:O	13:M:245:HIS:ND1	2.35	0.55
22:X:202:PHE:HE1	24:1:32:THR:O	1.89	0.55
29:6:154:ILE:HD13	29:6:197:LYS:NZ	2.22	0.55
30:7:698:ASP:HB2	30:7:701:PHE:HB2	1.89	0.55
2:B:71:LEU:HD21	2:B:436:VAL:HG11	1.88	0.55
2:B:118:ARG:NH2	2:B:202:TYR:OH	2.38	0.55
3:C:73:GLN:NE2	3:C:237:SER:O	2.38	0.55
13:M:34:ILE:HG21	13:M:52:LEU:HD22	1.87	0.55
1:A:908:LEU:HA	1:A:1029:ARG:HH22	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:112:ILE:HG23	8:H:132:LEU:HD12	1.89	0.55
9:I:54:GLU:HG2	9:I:90:GLN:HB3	1.89	0.55
19:U:30:ILE:HG23	19:U:31:ASP:H	1.71	0.55
28:5:13:ASP:OD1	28:5:15:SER:OG	2.23	0.55
1:A:185:TRP:HZ3	1:A:200:ARG:HB2	1.72	0.55
1:A:899:VAL:H	1:A:929:LEU:HD11	1.72	0.55
13:M:274:PRO:HD2	15:O:188:GLU:CG	2.36	0.55
23:0:114:LEU:HD21	23:0:196:VAL:HG21	1.88	0.55
1:A:845:LEU:HD11	1:A:1371:LEU:HD23	1.89	0.55
23:0:36:GLY:HA2	23:0:455:SER:H	1.72	0.55
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.72	0.55
12:L:30:ILE:HB	12:L:57:LEU:HB2	1.88	0.55
15:O:74:VAL:HG21	15:O:136:SER:HB3	1.88	0.55
23:0:575:ASP:OD1	23:0:576:ALA:N	2.40	0.55
37:f:46:ILE:HG22	37:f:48:ASN:H	1.72	0.55
33:b:203:LYS:O	33:b:207:THR:OG1	2.21	0.54
24:1:64:GLY:CA	24:1:85:GLN:O	2.53	0.54
2:B:347:LYS:O	2:B:351:TYR:HB2	2.07	0.54
4:D:141:LEU:HD13	7:G:46:LEU:HB3	1.88	0.54
15:O:205:LEU:HB2	15:O:213:VAL:HB	1.90	0.54
14:N:60:DT:H2''	14:N:61:DG:C8	2.42	0.54
36:e:234:LYS:NZ	36:e:250:GLY:O	2.36	0.54
2:B:298:LEU:HG	2:B:314:LEU:HD13	1.89	0.54
29:6:154:ILE:HD13	29:6:197:LYS:HZ2	1.73	0.54
36:e:167:GLN:NE2	37:f:96:SER:O	2.41	0.54
2:B:211:VAL:O	2:B:480:SER:HA	2.07	0.54
1:A:1386:ARG:CZ	18:T:53:DG:H5''	2.37	0.54
2:B:278:GLN:HB2	2:B:337:ARG:HD2	1.88	0.54
9:I:29:CYS:SG	9:I:31:THR:OG1	2.66	0.54
13:M:43:VAL:HG12	13:M:53:SER:HB3	1.90	0.54
13:M:202:GLU:OE2	13:M:206:THR:OG1	2.24	0.54
30:7:515:ALA:HB1	30:7:692:ARG:NH1	2.23	0.54
2:B:303:TYR:HD1	2:B:571:PRO:HB3	1.73	0.54
7:G:160:ILE:HD11	21:W:137:VAL:HG21	1.90	0.54
23:0:587:ARG:HH11	23:0:615:GLN:HB2	1.73	0.54
35:d:627:LYS:HG2	35:d:653:THR:HG23	1.89	0.54
1:A:1155:ASP:OD2	1:A:1241:ARG:NH2	2.39	0.54
3:C:6:PRO:HB3	3:C:25:VAL:HG23	1.90	0.54
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.90	0.54
1:A:115:LEU:HD22	1:A:119:ASN:HD22	1.73	0.54
2:B:429:PHE:CZ	16:Q:332:LEU:HB2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:47:CYS:SG	7:G:48:VAL:N	2.81	0.54
1:A:588:LEU:HD13	1:A:632:VAL:HG21	1.89	0.53
1:A:1441:PHE:O	6:F:92:ARG:NH1	2.41	0.53
18:T:32:DA:H5''	30:7:440:UNK:CB	2.38	0.53
24:1:22:VAL:HG23	24:1:25:ALA:H	1.74	0.53
30:7:690:ILE:O	30:7:694:LYS:NZ	2.41	0.53
1:A:700:ASN:HB2	9:I:98:VAL:HG22	1.91	0.53
1:A:778:GLY:HA3	2:B:516:ASN:HB2	1.88	0.53
2:B:923:GLU:HB3	2:B:925:LEU:HG	1.91	0.53
2:B:1106:ARG:HH11	2:B:1126:GLY:HA2	1.74	0.53
2:B:833:TYR:HB2	2:B:840:ILE:HD11	1.90	0.53
5:E:76:GLY:N	5:E:106:GLN:OE1	2.39	0.53
21:W:14:LYS:NZ	21:W:30:ASP:OD1	2.41	0.53
24:1:266:VAL:HG22	24:1:287:PHE:HZ	1.74	0.53
36:e:228:LEU:HA	36:e:257:ILE:HG12	1.88	0.53
13:M:276:THR:HA	13:M:279:VAL:HG12	1.91	0.53
1:A:48:ALA:HB3	1:A:56:PRO:HD3	1.90	0.53
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.90	0.53
10:J:2:ILE:HD13	10:J:57:ILE:HG21	1.90	0.53
46:o:102:UNK:O	46:o:105:UNK:N	2.42	0.53
2:B:1060:ARG:NH1	3:C:200:GLU:O	2.42	0.53
24:1:44:THR:HA	24:1:65:LYS:HE2	1.91	0.53
2:B:1187:ASN:ND2	2:B:1190:ASP:O	2.39	0.53
14:N:77:DA:H2''	14:N:78:DA:O5'	2.09	0.53
14:N:82:DA:H4'	30:7:676:HIS:CE1	2.44	0.53
24:1:283:PHE:O	24:1:287:PHE:CB	2.56	0.53
30:7:407:VAL:HG22	30:7:484:PHE:HB3	1.91	0.53
38:g:56:MET:O	38:g:60:ASN:ND2	2.42	0.53
2:B:445:LYS:NZ	17:R:267:GLY:O	2.36	0.53
2:B:1042:GLY:HA2	16:Q:22:ILE:HA	1.90	0.53
17:R:105:THR:HA	17:R:120:TYR:O	2.09	0.53
17:R:127:LYS:HA	17:R:220:HIS:CE1	2.43	0.53
23:0:492:PHE:HE2	23:0:715:SER:HB3	1.73	0.53
35:d:438:GLU:OE2	35:d:509:ARG:NH2	2.38	0.53
16:Q:366:GLU:HB3	16:Q:392:VAL:HG13	1.90	0.53
23:0:322:UNK:C	23:0:380:ARG:HH12	2.21	0.53
26:3:81:GLU:O	26:3:85:ARG:CB	2.57	0.53
1:A:423:ASP:OD2	36:e:184:THR:HG21	2.08	0.52
15:O:113:ALA:HA	15:O:122:VAL:O	2.09	0.52
20:V:71:PHE:HA	20:V:75:VAL:O	2.09	0.52
23:0:471:ARG:HA	23:0:471:ARG:HH11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:0:601:VAL:HG12	23:0:603:ARG:H	1.74	0.52
23:0:603:ARG:HH12	23:0:628:GLN:HG3	1.73	0.52
2:B:862:GLN:OE1	2:B:957:ASN:ND2	2.42	0.52
23:0:221:ARG:HG2	23:0:225:GLU:OE2	2.09	0.52
29:6:269:GLN:HB3	29:6:274:LYS:NZ	2.23	0.52
37:f:60:ILE:HD13	37:f:201:ALA:HB1	1.92	0.52
2:B:128:LEU:HB2	2:B:168:GLY:O	2.09	0.52
9:I:56:ALA:O	9:I:89:GLN:HG3	2.08	0.52
30:7:490:VAL:HG23	30:7:514:THR:HB	1.92	0.52
34:c:24:LEU:HD23	35:d:295:PHE:HA	1.90	0.52
1:A:226:GLU:HA	1:A:230:ARG:HE	1.74	0.52
2:B:458:LYS:O	2:B:462:ALA:HB2	2.09	0.52
4:D:51:ASN:HD22	4:D:181:GLY:HA3	1.74	0.52
13:M:199:LYS:O	13:M:201:LYS:N	2.42	0.52
35:d:479:LEU:HD12	35:d:483:ASP:HB2	1.92	0.52
16:Q:366:GLU:O	16:Q:368:GLY:N	2.43	0.52
2:B:342:GLY:O	2:B:344:LYS:N	2.41	0.52
2:B:1091:TYR:HE2	2:B:1093:GLN:HE21	1.58	0.52
3:C:34:ARG:HB3	3:C:230:MET:HE1	1.92	0.52
5:E:62:ALA:HB3	5:E:78:LEU:HB3	1.90	0.52
30:7:585:PRO:HG3	30:7:759:LEU:HD23	1.91	0.52
34:c:109:LEU:HD12	38:g:107:LEU:HD12	1.92	0.52
1:A:88:LYS:HD3	1:A:89:PRO:HD2	1.92	0.52
1:A:1154:TYR:HE2	9:I:18:GLU:HB2	1.75	0.52
2:B:806:THR:HG23	2:B:1045:SER:HA	1.91	0.52
2:B:1060:ARG:HH12	3:C:202:PRO:HD3	1.75	0.52
28:5:16:ILE:HD13	28:5:19:LEU:HD12	1.92	0.52
30:7:448:UNK:C	30:7:450:UNK:H	2.23	0.52
35:d:518:LYS:O	35:d:522:SER:HB3	2.09	0.52
35:d:604:ARG:C	35:d:607:ASP:H	2.18	0.52
2:B:757:PRO:HD3	2:B:983:ARG:HE	1.75	0.51
2:B:55:VAL:HA	2:B:59:LEU:HD13	1.90	0.51
2:B:791:THR:HG22	2:B:792:MET:HG3	1.91	0.51
3:C:100:THR:OG1	3:C:102:GLN:NE2	2.43	0.51
5:E:26:ARG:HH12	5:E:189:GLY:HA3	1.74	0.51
35:d:595:ASN:HD21	36:e:32:LEU:HA	1.75	0.51
2:B:376:PHE:HD2	2:B:566:LEU:HG	1.75	0.51
2:B:826:ALA:O	2:B:1011:ILE:HA	2.10	0.51
3:C:35:ARG:NH2	11:K:39:ASP:OD2	2.41	0.51
22:X:193:LEU:HA	22:X:196:LEU:HD12	1.91	0.51
23:0:77:SER:HB3	24:1:337:UNK:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:0:208:TYR:HE2	23:0:213:LEU:HB2	1.75	0.51
35:d:604:ARG:O	35:d:607:ASP:CB	2.58	0.51
2:B:345:LYS:HA	2:B:348:ARG:HG2	1.91	0.51
3:C:89:GLU:HB2	37:f:43:ARG:HH11	1.74	0.51
16:Q:334:VAL:HG12	16:Q:335:LEU:H	1.76	0.51
30:7:672:GLN:NE2	30:7:722:ARG:HH12	2.06	0.51
2:B:737:THR:OG1	9:I:66:PRO:O	2.27	0.51
24:1:106:GLN:HB3	24:1:286:ARG:NH1	2.26	0.51
2:B:771:SER:O	2:B:775:LYS:NZ	2.44	0.51
13:M:280:VAL:HG12	13:M:309:ILE:HA	1.92	0.51
17:R:63:ARG:C	17:R:65:ASN:H	2.18	0.51
2:B:43:LEU:O	2:B:496:ARG:NH1	2.41	0.51
23:0:194:PHE:HD1	23:0:197:ARG:HH21	1.59	0.51
23:0:250:LEU:HB3	23:0:437:PHE:CE2	2.46	0.51
30:7:576:LYS:HB2	30:7:576:LYS:NZ	2.26	0.51
1:A:534:LEU:HD11	1:A:577:ILE:HD11	1.93	0.51
1:A:840:ARG:O	1:A:844:ALA:HB2	2.11	0.51
2:B:22:SER:O	2:B:654:ARG:NH2	2.44	0.51
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.93	0.51
3:C:19:ASP:HB2	3:C:231:ASN:HD22	1.76	0.51
11:K:61:TYR:HA	11:K:72:LYS:O	2.11	0.51
15:O:115:ILE:HD13	15:O:143:ILE:HD11	1.92	0.51
28:5:54:LEU:HA	28:5:57:LEU:HG	1.93	0.51
40:i:145:GLU:O	40:i:148:VAL:HG22	2.10	0.51
2:B:102:VAL:O	2:B:109:THR:HA	2.12	0.51
15:O:206:ILE:HD13	15:O:234:LEU:HD21	1.93	0.51
23:0:106:LEU:HD11	23:0:196:VAL:HG22	1.93	0.51
30:7:373:MET:SD	30:7:373:MET:N	2.84	0.51
2:B:1028:GLU:O	2:B:1032:SER:OG	2.26	0.50
25:2:459:TYR:OH	25:2:498:ASN:OD1	2.21	0.50
34:c:30:VAL:O	34:c:34:PHE:HB3	2.10	0.50
35:d:467:ILE:HB	35:d:474:PHE:HB2	1.93	0.50
9:I:55:THR:HG22	9:I:100:PHE:CE2	2.47	0.50
23:0:466:LEU:H	23:0:466:LEU:HD23	1.75	0.50
1:A:63:ARG:HA	1:A:74:MET:HG2	1.92	0.50
2:B:755:ILE:O	2:B:983:ARG:NE	2.45	0.50
3:C:79:GLN:HA	37:f:11:ARG:HH22	1.75	0.50
3:C:222:LYS:H	3:C:222:LYS:HD3	1.76	0.50
1:A:752:LYS:HG3	2:B:1015:HIS:HB3	1.92	0.50
8:H:142:LEU:HG	8:H:144:ILE:HD11	1.92	0.50
21:W:99:LYS:HG2	21:W:186:LEU:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:VAL:HB	1:A:556:TRP:HB2	1.92	0.50
2:B:641:GLU:HB2	2:B:652:LYS:HE2	1.93	0.50
9:I:54:GLU:HA	9:I:90:GLN:N	2.21	0.50
1:A:1020:CYS:SG	1:A:1023:ARG:NH2	2.85	0.50
2:B:413:LEU:HD21	2:B:461:LEU:HD11	1.93	0.50
20:V:62:VAL:HG22	20:V:85:VAL:HG22	1.92	0.50
1:A:864:ILE:HG22	1:A:865:GLN:HG3	1.93	0.50
1:A:1116:LEU:HD11	1:A:1311:VAL:HG23	1.94	0.50
9:I:86:PHE:O	9:I:100:PHE:HB2	2.12	0.50
15:O:202:ILE:HD11	15:O:222:GLU:HB3	1.94	0.50
16:Q:119:LEU:HD12	17:R:133:TYR:HB2	1.93	0.50
7:G:111:THR:HB	7:G:114:LEU:HD13	1.92	0.50
8:H:8:ASP:OD1	8:H:9:ILE:N	2.44	0.50
24:1:351:UNK:O	24:1:353:UNK:N	2.45	0.50
36:e:196:LYS:NZ	37:f:74:ASP:O	2.45	0.50
37:f:40:ARG:NH1	37:f:105:ASP:OD2	2.45	0.50
1:A:961:ARG:NH1	1:A:1035:TYR:OH	2.44	0.50
1:A:984:LYS:O	1:A:988:LEU:HB2	2.12	0.50
7:G:95:SER:OG	7:G:98:GLY:O	2.23	0.50
13:M:187:ARG:HH11	13:M:241:ARG:HH21	1.59	0.50
15:O:93:GLU:OE2	15:O:105:ARG:NH1	2.45	0.50
23:0:372:LYS:N	23:0:373:PRO:HD3	2.27	0.50
1:A:540:PHE:HB3	1:A:571:LEU:HD23	1.94	0.49
5:E:56:LYS:NZ	5:E:84:ASP:OD2	2.43	0.49
17:R:73:LEU:HD23	17:R:78:ALA:HA	1.92	0.49
29:6:133:SER:H	29:6:136:MET:HG2	1.76	0.49
30:7:548:HIS:HB2	30:7:697:ASN:HA	1.93	0.49
6:F:82:THR:HG22	6:F:84:TYR:H	1.76	0.49
16:Q:352:MET:HG3	16:Q:361:TRP:HB2	1.94	0.49
1:A:99:ILE:HG12	1:A:234:MET:HE3	1.94	0.49
2:B:63:ILE:O	2:B:67:SER:HB3	2.13	0.49
2:B:766:ARG:HE	2:B:1020:ARG:HB3	1.77	0.49
17:R:263:MET:O	17:R:266:THR:OG1	2.28	0.49
21:W:24:SER:HA	21:W:27:LEU:HD22	1.94	0.49
36:e:167:GLN:HA	36:e:186:ALA:O	2.12	0.49
1:A:1029:ARG:O	1:A:1033:GLN:HB3	2.12	0.49
1:A:1386:ARG:NH2	18:T:53:DG:H5"	2.26	0.49
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.94	0.49
14:N:33:DT:O2	18:T:75:DG:N2	2.46	0.49
23:0:432:ASN:O	23:0:434:ILE:HG13	2.12	0.49
1:A:419:LYS:HZ3	36:e:57:GLN:CD	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:GLY:O	2:B:405:ARG:NH1	2.41	0.49
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.93	0.49
30:7:551:ASN:O	30:7:703:ALA:HB3	2.12	0.49
34:c:63:THR:HG22	38:g:14:ARG:HD3	1.93	0.49
1:A:966:ASN:O	1:A:970:THR:OG1	2.25	0.49
1:A:1191:TRP:CZ3	9:I:43:VAL:HG21	2.48	0.49
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.12	0.49
2:B:87:LYS:HB2	2:B:137:TYR:HB2	1.93	0.49
3:C:185:LYS:HE2	3:C:213:PRO:HB3	1.93	0.49
40:i:165:TYR:HD2	45:n:5:LEU:HD13	1.78	0.49
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	1.93	0.49
1:A:1199:ARG:NH1	1:A:1233:ASP:O	2.45	0.49
16:Q:363:GLY:HA2	16:Q:395:PHE:HA	1.95	0.49
21:W:77:PRO:O	21:W:79:SER:N	2.46	0.49
24:1:276:LYS:H	24:1:276:LYS:HD3	1.77	0.49
30:7:691:LEU:HA	30:7:694:LYS:NZ	2.27	0.49
33:b:120:PRO:O	33:b:124:GLU:CB	2.60	0.49
1:A:869:GLY:HA3	1:A:1366:ARG:HD2	1.93	0.49
2:B:226:PHE:HD1	2:B:395:GLN:HE21	1.60	0.49
9:I:14:LEU:HA	9:I:28:GLU:O	2.13	0.49
19:U:283:ALA:HB1	20:V:66:LEU:HB2	1.94	0.49
24:1:306:UNK:O	24:1:307:UNK:CB	2.60	0.49
43:l:291:VAL:O	43:l:307:ASN:HA	2.13	0.49
1:A:495:GLU:OE1	1:A:495:GLU:N	2.46	0.49
1:A:597:LEU:HD13	8:H:103:LYS:HD3	1.94	0.49
2:B:793:ALA:O	2:B:855:PHE:HA	2.13	0.49
22:X:273:GLU:HG2	22:X:276:ARG:HH11	1.77	0.49
26:3:45:ARG:O	26:3:49:LEU:HG	2.12	0.49
37:f:88:PRO:HD2	37:f:91:LEU:HD12	1.94	0.49
1:A:446:ARG:O	1:A:449:SER:OG	2.31	0.49
1:A:526:ASP:OD1	2:B:1015:HIS:ND1	2.45	0.49
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.95	0.49
14:N:24:DT:H2''	14:N:25:DA:N7	2.27	0.49
28:5:33:GLU:HB2	28:5:41:LEU:HB3	1.95	0.49
35:d:511:LEU:HD13	35:d:541:ILE:HA	1.94	0.49
1:A:63:ARG:HH11	13:M:57:VAL:HG22	1.76	0.48
6:F:133:VAL:HA	6:F:147:SER:HA	1.95	0.48
8:H:89:LEU:HG	8:H:90:ALA:H	1.78	0.48
9:I:19:ASP:CB	9:I:24:ARG:O	2.60	0.48
11:K:32:VAL:HG22	11:K:74:ARG:HG2	1.94	0.48
14:N:78:DA:H4'	14:N:79:DA:OP1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:30:DT:H2"	18:T:31:DT:C7	2.38	0.48
40:i:60:THR:OG1	40:i:64:ASP:OD2	2.23	0.48
1:A:481:ASP:C	1:A:483:ASP:OD1	2.56	0.48
16:Q:381:ASP:OD1	16:Q:382:GLY:N	2.42	0.48
17:R:73:LEU:HD23	17:R:78:ALA:CA	2.43	0.48
27:4:290:SER:N	27:4:292:CYS:SG	2.86	0.48
36:e:60:GLU:OE1	36:e:299:ARG:NH2	2.39	0.48
11:K:24:ASP:HB2	11:K:32:VAL:HG23	1.95	0.48
36:e:189:ILE:HG13	37:f:87:ILE:HG12	1.96	0.48
38:g:51:ALA:O	38:g:55:VAL:HG23	2.12	0.48
4:D:54:GLU:HB2	4:D:160:VAL:HG11	1.95	0.48
8:H:26:ILE:HG13	8:H:42:ILE:HD12	1.95	0.48
30:7:553:GLN:HB2	30:7:703:ALA:O	2.13	0.48
1:A:69:THR:HG23	1:A:80:HIS:NE2	2.28	0.48
2:B:810:GLU:HB2	2:B:815:ARG:HH12	1.79	0.48
2:B:931:TYR:O	2:B:933:SER:N	2.43	0.48
15:O:95:ASN:N	15:O:95:ASN:OD1	2.47	0.48
31:Z:22:UNK:O	31:Z:26:UNK:CB	2.62	0.48
35:d:642:ASN:ND2	43:l:529:PRO:O	2.46	0.48
13:M:267:LYS:HG3	13:M:268:GLU:H	1.78	0.48
23:0:323:UNK:CB	23:0:380:ARG:HH22	2.26	0.48
13:M:118:VAL:HG22	13:M:124:ASN:ND2	2.28	0.48
23:0:234:PHE:HB3	23:0:237:ALA:HB2	1.95	0.48
40:i:162:LEU:HD13	45:n:9:GLN:HE22	1.79	0.48
23:0:322:UNK:CA	23:0:380:ARG:HH12	2.27	0.48
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.79	0.48
1:A:810:PRO:HG2	2:B:705:MET:HE2	1.95	0.48
7:G:119:LEU:HD11	7:G:130:TYR:HB3	1.95	0.48
15:O:214:LEU:HD22	15:O:223:ILE:HG23	1.96	0.48
21:W:118:GLU:HB2	26:3:49:LEU:HD22	1.96	0.48
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.95	0.47
1:A:1336:MET:HE2	1:A:1380:GLY:HA2	1.96	0.47
18:T:46:DC:H2"	18:T:47:DA:C8	2.49	0.47
21:W:176:MET:HA	21:W:179:ILE:HG22	1.95	0.47
35:d:550:ARG:NH2	35:d:554:TYR:OH	2.41	0.47
40:i:178:LEU:HB2	45:n:97:LEU:HD13	1.95	0.47
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.96	0.47
34:c:105:LEU:HB3	38:g:107:LEU:HD21	1.95	0.47
36:e:69:GLU:HG3	37:f:90:ALA:HB1	1.96	0.47
1:A:139:TRP:HH2	14:N:60:DT:OP1	1.98	0.47
2:B:70:ILE:HG22	2:B:89:GLU:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:171:ARG:HB2	15:O:237:PHE:HB3	1.96	0.47
37:f:39:PHE:HD2	37:f:122:ILE:HD13	1.78	0.47
1:A:864:ILE:HG12	1:A:1374:VAL:HG22	1.97	0.47
2:B:458:LYS:O	2:B:462:ALA:CB	2.63	0.47
3:C:79:GLN:CA	37:f:11:ARG:HH22	2.27	0.47
16:Q:102:PRO:HA	17:R:94:LYS:HA	1.97	0.47
17:R:69:TRP:CD1	17:R:219:CYS:HB3	2.49	0.47
23:O:156:CYS:SG	23:O:157:GLU:N	2.87	0.47
29:6:251:ILE:HG12	29:6:276:LEU:HD13	1.95	0.47
34:c:48:PHE:O	34:c:52:VAL:HG23	2.15	0.47
37:f:9:VAL:HB	37:f:151:LEU:HB3	1.96	0.47
2:B:861:ASP:OD1	2:B:862:GLN:N	2.48	0.47
5:E:156:LEU:HD11	5:E:197:LYS:HB2	1.96	0.47
23:O:259:ARG:HG2	23:O:262:ARG:HH21	1.78	0.47
35:d:441:LEU:HD21	35:d:508:LEU:HB3	1.96	0.47
36:e:11:ILE:HG21	36:e:19:LEU:HD22	1.97	0.47
46:o:29:GLU:OE1	46:o:66:TYR:OH	2.31	0.47
1:A:481:ASP:OD2	1:A:483:ASP:OD2	2.31	0.47
5:E:179:GLN:HG2	5:E:181:ALA:H	1.78	0.47
13:M:312:GLY:O	13:M:316:LEU:HB2	2.14	0.47
17:R:122:LEU:HD21	17:R:222:CYS:HB3	1.97	0.47
23:O:257:LEU:HD13	23:O:343:LYS:HG2	1.96	0.47
26:3:47:PHE:HB2	26:3:65:LYS:HG2	1.96	0.47
30:7:608:PHE:HE2	30:7:670:LEU:HB3	1.79	0.47
1:A:381:THR:HG23	1:A:383:TYR:H	1.78	0.47
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.96	0.47
2:B:398:ARG:H	2:B:398:ARG:HD2	1.80	0.47
13:M:268:GLU:C	13:M:270:ALA:H	2.23	0.47
20:V:60:LEU:HA	20:V:86:THR:O	2.15	0.47
21:W:74:GLU:CB	21:W:82:VAL:O	2.63	0.47
23:O:417:LEU:O	23:O:438:THR:HB	2.14	0.47
30:7:495:ALA:HB3	30:7:498:PHE:CD1	2.50	0.47
7:G:123:ALA:HA	7:G:128:PRO:HB3	1.97	0.47
9:I:54:GLU:CG	9:I:88:SER:OG	2.62	0.47
11:K:17:SER:H	11:K:20:LYS:HZ1	1.62	0.47
25:2:453:THR:HG22	28:5:10:VAL:HG22	1.95	0.47
28:5:55:ASN:HA	28:5:58:LEU:HG	1.96	0.47
35:d:535:VAL:O	35:d:539:ILE:N	2.48	0.47
1:A:58:LEU:HA	1:A:80:HIS:HB2	1.96	0.47
2:B:810:GLU:HG3	2:B:815:ARG:HH22	1.79	0.47
21:W:117:SER:O	26:3:49:LEU:HD13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:7:410:LEU:HB3	30:7:457:TYR:CZ	2.50	0.47
9:I:88:SER:O	9:I:91:ARG:NH1	2.47	0.47
15:O:94:TYR:CZ	15:O:96:PRO:HG3	2.50	0.47
16:Q:402:ALA:O	16:Q:403:THR:HG23	2.15	0.47
1:A:990:VAL:HG12	1:A:994:GLN:HE21	1.80	0.46
2:B:336:ARG:HD2	2:B:348:ARG:NH1	2.30	0.46
4:D:123:LEU:HD21	4:D:146:GLN:HA	1.97	0.46
21:W:77:PRO:C	21:W:79:SER:H	2.23	0.46
31:Z:30:UNK:C	31:Z:41:UNK:CB	2.93	0.46
32:a:122:GLU:HA	32:a:123:PRO:HA	1.64	0.46
1:A:471:ASN:OD1	1:A:472:LEU:N	2.48	0.46
1:A:882:SER:O	1:A:1025:ARG:NH2	2.43	0.46
1:A:1012:ARG:O	1:A:1016:THR:OG1	2.30	0.46
6:F:76:LYS:HA	6:F:79:ARG:HE	1.79	0.46
30:7:406:SER:HA	30:7:451:UNK:CB	2.45	0.46
37:f:70:VAL:HA	37:f:78:MET:O	2.15	0.46
1:A:806:ARG:HD2	2:B:728:ARG:HA	1.97	0.46
2:B:194:GLU:HA	2:B:784:ASN:HD22	1.80	0.46
2:B:364:ILE:HG22	2:B:365:THR:HG22	1.96	0.46
7:G:44:TYR:OH	7:G:157:ILE:O	2.28	0.46
17:R:97:ILE:HA	17:R:104:ILE:HG22	1.97	0.46
28:5:8:ALA:HB3	28:5:42:VAL:O	2.15	0.46
29:6:211:GLN:HE22	29:6:245:GLY:C	2.23	0.46
30:7:534:LYS:HD2	30:7:537:GLU:OE2	2.15	0.46
43:l:472:MET:O	43:l:476:ALA:CB	2.63	0.46
2:B:363:HIS:CD2	2:B:364:ILE:HG13	2.49	0.46
30:7:565:PHE:HE2	30:7:763:VAL:HG21	1.81	0.46
30:7:659:ASP:HB3	30:7:686:ARG:HG3	1.96	0.46
1:A:308:ILE:HG23	1:A:311:GLN:HB2	1.97	0.46
18:T:30:DT:C2'	18:T:31:DT:H72	2.38	0.46
18:T:48:DC:C2	18:T:49:DA:C8	3.04	0.46
20:V:72:CYS:O	20:V:75:VAL:HB	2.15	0.46
36:e:85:LEU:HA	36:e:89:ILE:HD11	1.97	0.46
40:i:144:TYR:O	40:i:148:VAL:HG13	2.15	0.46
10:J:17:LYS:HB3	10:J:39:LEU:HD13	1.96	0.46
18:T:71:DC:H2''	18:T:72:DA:C8	2.50	0.46
22:X:218:ASP:HA	22:X:221:ILE:HD12	1.97	0.46
35:d:208:LEU:O	35:d:212:ASN:CB	2.64	0.46
1:A:596:THR:HG22	1:A:597:LEU:H	1.80	0.46
1:A:1012:ARG:HH21	1:A:1015:VAL:HG11	1.81	0.46
2:B:933:SER:OG	2:B:934:LYS:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1004:GLU:OE1	2:B:1064:TYR:OH	2.27	0.46
14:N:21:DG:H1'	14:N:22:DT:H5'	1.98	0.46
23:0:494:PRO:HB2	23:0:699:GLN:HE22	1.80	0.46
1:A:561:PRO:HB2	1:A:576:GLN:HE21	1.80	0.46
2:B:634:TYR:HA	2:B:694:ASP:HA	1.98	0.46
2:B:1172:ILE:HD11	2:B:1183:LYS:HD2	1.98	0.46
9:I:54:GLU:HB3	9:I:88:SER:CB	2.46	0.46
18:T:40:DA:H2''	18:T:41:DC:H5'	1.97	0.46
23:0:133:CYS:HA	49:0:901:SF4:S4	2.56	0.46
23:0:564:TRP:O	23:0:566:HIS:N	2.40	0.46
30:7:495:ALA:HB3	30:7:498:PHE:HD1	1.80	0.46
40:i:28:ASN:HB3	40:i:66:LEU:HD11	1.97	0.46
1:A:481:ASP:CG	1:A:483:ASP:OD1	2.59	0.46
1:A:563:PRO:HG2	1:A:566:ILE:HG13	1.98	0.46
2:B:301:ILE:O	2:B:383:ASN:ND2	2.49	0.46
23:0:372:LYS:HD3	23:0:375:ARG:NH1	2.31	0.46
1:A:993:LEU:HD13	1:A:1046:LEU:HD22	1.98	0.46
3:C:29:MET:HE1	11:K:97:LYS:HE3	1.97	0.46
19:U:38:LEU:O	19:U:42:TRP:HB2	2.15	0.46
21:W:18:ARG:CZ	22:X:250:GLY:H	2.28	0.46
30:7:719:SER:O	30:7:723:GLN:HG2	2.16	0.46
35:d:639:ASN:O	35:d:641:CYS:N	2.48	0.46
1:A:855:THR:HG21	1:A:857:ARG:HH21	1.81	0.45
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.81	0.45
2:B:824:ILE:HD13	2:B:1089:PRO:HB3	1.98	0.45
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.98	0.45
25:2:466:GLN:OE1	25:2:466:GLN:N	2.47	0.45
34:c:74:ASP:OD2	38:g:3:ASN:ND2	2.49	0.45
35:d:457:VAL:HG13	35:d:467:ILE:HG12	1.97	0.45
18:T:33:DT:OP1	30:7:467:UNK:CB	2.64	0.45
23:0:70:ILE:HB	23:0:232:VAL:HA	1.96	0.45
26:3:72:ILE:H	26:3:72:ILE:HG13	1.62	0.45
30:7:554:CYS:HB2	30:7:733:PHE:HA	1.97	0.45
40:i:181:GLN:O	40:i:185:LYS:HG2	2.16	0.45
1:A:53:LEU:HD21	1:A:267:ALA:HB2	1.99	0.45
2:B:314:LEU:O	2:B:318:VAL:HG23	2.16	0.45
5:E:58:MET:HE2	5:E:82:PHE:HE2	1.80	0.45
7:G:21:ARG:HG3	7:G:25:TYR:HE2	1.81	0.45
1:A:587:HIS:HA	1:A:607:ILE:O	2.16	0.45
3:C:79:GLN:HB2	37:f:11:ARG:NH2	2.30	0.45
4:D:158:GLU:OE1	4:D:158:GLU:N	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:61:DG:C2	18:T:47:DA:C2	3.05	0.45
23:0:652:ASP:O	23:0:656:PHE:HB3	2.16	0.45
24:1:45:ILE:HD12	24:1:62:LEU:HB3	1.97	0.45
35:d:504:MET:O	35:d:508:LEU:HG	2.15	0.45
35:d:608:LYS:HG3	38:g:105:GLU:CA	2.45	0.45
4:D:165:GLN:O	4:D:169:SER:OG	2.32	0.45
21:W:171:LYS:O	21:W:175:LEU:HB2	2.16	0.45
23:0:77:SER:C	23:0:81:LYS:HZ3	2.24	0.45
23:0:171:LEU:HD22	23:0:199:MET:HG2	1.99	0.45
29:6:427:TYR:O	29:6:435:GLU:HA	2.16	0.45
36:e:195:GLY:HA3	37:f:76:SER:HA	1.98	0.45
45:n:34:ARG:O	45:n:36:THR:N	2.50	0.45
1:A:92:HIS:O	1:A:96:ILE:HG13	2.17	0.45
1:A:419:LYS:HZ2	36:e:57:GLN:CD	2.25	0.45
1:A:1191:TRP:CD1	1:A:1256:GLU:HB2	2.52	0.45
2:B:249:ARG:HG2	2:B:415:GLN:NE2	2.29	0.45
2:B:924:GLU:H	2:B:928:ARG:HD2	1.79	0.45
6:F:135:ARG:HA	6:F:144:GLU:O	2.16	0.45
9:I:83:ASN:HA	9:I:104:LEU:HG	1.99	0.45
24:1:107:ILE:HD12	24:1:110:ARG:HH11	1.81	0.45
30:7:573:THR:HA	30:7:577:ARG:HD2	1.97	0.45
35:d:442:MET:HE1	35:d:476:ILE:HG22	1.99	0.45
35:d:448:GLU:HG3	35:d:539:ILE:HG13	1.98	0.45
37:f:36:SER:OG	37:f:125:ASP:OD1	2.32	0.45
1:A:463:ILE:HD12	1:A:464:PRO:O	2.17	0.45
2:B:290:GLY:HA2	2:B:327:ARG:HD2	1.98	0.45
2:B:737:THR:HB	9:I:66:PRO:CB	2.47	0.45
12:L:43:THR:HG22	12:L:43:THR:O	2.16	0.45
21:W:24:SER:HA	21:W:27:LEU:HB2	1.98	0.45
33:b:201:VAL:HG22	36:e:246:ILE:HG22	1.99	0.45
1:A:216:VAL:O	1:A:220:THR:OG1	2.27	0.45
1:A:849:MET:HE3	1:A:1063:MET:HE1	1.98	0.45
1:A:1146:VAL:HG11	1:A:1207:LEU:CD1	2.47	0.45
2:B:238:ALA:HB2	2:B:385:LEU:HD13	1.99	0.45
14:N:79:DA:H1'	14:N:80:DA:H5'	1.98	0.45
16:Q:379:GLU:OE2	16:Q:383:SER:OG	2.35	0.45
21:W:179:ILE:HD12	21:W:182:ILE:HD12	1.97	0.45
30:7:561:MET:SD	30:7:584:ASN:ND2	2.90	0.45
46:o:32:PHE:O	46:o:35:SER:OG	2.28	0.45
7:G:23:LYS:O	7:G:26:LEU:HB2	2.16	0.45
23:0:364:LYS:HZ2	23:0:370:GLU:H	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:462:PHE:HE1	25:2:471:LEU:HD12	1.82	0.45
30:7:556:GLU:HG2	30:7:707:SER:HB3	1.98	0.45
35:d:562:ILE:HD13	35:d:619:ILE:HD11	1.99	0.45
1:A:350:ARG:HA	1:A:487:MET:O	2.17	0.45
1:A:439:ASN:HA	1:A:459:ARG:HG3	1.99	0.45
7:G:165:GLU:HG2	26:3:65:LYS:NZ	2.31	0.45
8:H:5:LEU:HD22	8:H:134:ASN:HB3	1.99	0.45
23:0:106:LEU:HD22	23:0:199:MET:HB3	1.99	0.45
23:0:215:ASP:H	23:0:219:ALA:HB2	1.81	0.45
16:Q:352:MET:CG	16:Q:361:TRP:HB2	2.47	0.44
17:R:133:TYR:CD1	17:R:217:THR:HG22	2.52	0.44
30:7:392:LYS:HD3	30:7:513:LEU:HB3	2.00	0.44
1:A:231:PRO:HA	1:A:234:MET:HE2	1.99	0.44
2:B:859:TYR:OH	2:B:945:GLU:OE1	2.35	0.44
2:B:867:GLY:C	2:B:869:SER:H	2.25	0.44
15:O:76:LEU:HD13	15:O:143:ILE:HG21	1.99	0.44
15:O:202:ILE:HG13	15:O:226:ALA:HB2	1.98	0.44
15:O:227:PHE:HA	15:O:230:ILE:HG22	1.99	0.44
20:V:61:THR:HB	20:V:86:THR:HB	1.98	0.44
21:W:169:GLN:NE2	21:W:173:ASN:OD1	2.45	0.44
23:0:196:VAL:O	23:0:200:ILE:HG12	2.17	0.44
24:1:263:TYR:HB2	24:1:266:VAL:HG23	1.98	0.44
1:A:104:GLU:OE1	1:A:139:TRP:NE1	2.47	0.44
1:A:367:PRO:HD2	1:A:370:ILE:HD12	1.98	0.44
2:B:663:ALA:O	2:B:667:GLN:HB2	2.17	0.44
7:G:64:THR:C	7:G:66:GLY:H	2.25	0.44
21:W:40:GLU:OE2	21:W:51:LYS:NZ	2.41	0.44
29:6:176:ASN:HA	29:6:206:GLY:HA3	2.00	0.44
33:b:122:VAL:O	33:b:126:MET:CB	2.65	0.44
34:c:33:ILE:HD12	34:c:51:HIS:HD2	1.83	0.44
20:V:23:LEU:HD13	20:V:37:ALA:HB1	1.99	0.44
21:W:152:CYS:O	21:W:154:GLU:HG3	2.17	0.44
2:B:499:ASN:OD1	2:B:500:THR:N	2.50	0.44
43:l:254:SER:O	43:l:258:ALA:CB	2.64	0.44
21:W:44:LYS:NZ	21:W:49:ILE:O	2.50	0.44
27:4:290:SER:C	27:4:292:CYS:N	2.76	0.44
28:5:62:ILE:HA	30:7:717:TYR:CZ	2.53	0.44
44:m:22:THR:O	44:m:24:THR:N	2.51	0.44
2:B:281:PRO:HD2	2:B:284:ILE:HD12	2.00	0.44
2:B:412:LEU:HB3	2:B:466:TRP:CE2	2.53	0.44
13:M:44:VAL:HG22	13:M:51:VAL:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:166:LYS:HB3	13:M:170:SER:HB3	2.00	0.44
23:O:199:MET:HE2	23:O:202:LEU:HD22	1.99	0.44
34:c:38:LYS:HA	34:c:38:LYS:HD2	1.81	0.44
35:d:442:MET:HG2	35:d:478:LEU:HD22	1.99	0.44
46:o:76:ILE:HG13	46:o:82:LEU:HD11	2.00	0.44
2:B:273:LEU:HD12	2:B:280:ILE:HD12	2.00	0.44
13:M:262:LYS:O	13:M:266:ILE:HG13	2.17	0.44
18:T:75:DG:H1'	18:T:76:DC:H5'	1.98	0.44
29:6:262:LYS:HE2	29:6:264:LEU:HD21	1.99	0.44
1:A:1051:ALA:O	1:A:1055:ARG:HG2	2.18	0.44
2:B:195:CYS:HB3	2:B:782:LEU:HD22	2.00	0.44
3:C:92:CYS:C	3:C:94:LYS:H	2.26	0.44
6:F:123:LYS:NZ	6:F:127:GLU:OE2	2.51	0.44
14:N:72:DA:H5'	14:N:72:DA:C8	2.53	0.44
19:U:260:CYS:HB2	19:U:281:VAL:HB	1.99	0.44
1:A:362:ASP:OD2	1:A:459:ARG:NH1	2.51	0.43
1:A:882:SER:OG	1:A:953:ASN:ND2	2.51	0.43
4:D:63:LEU:HD13	4:D:130:LEU:HD13	1.99	0.43
7:G:95:SER:O	7:G:130:TYR:OH	2.35	0.43
7:G:102:GLN:HE22	7:G:107:LYS:HE2	1.83	0.43
14:N:73:DC:H2''	14:N:74:DA:C8	2.52	0.43
23:O:197:ARG:HG3	23:O:221:ARG:NH1	2.33	0.43
35:d:638:PRO:HD3	35:d:644:LEU:HG	2.00	0.43
1:A:116:ASP:OD1	1:A:117:GLU:N	2.43	0.43
1:A:339:ASN:HB3	2:B:1199:ALA:HB1	2.00	0.43
1:A:351:THR:O	1:A:486:GLU:HA	2.18	0.43
1:A:1035:TYR:HB3	1:A:1037:LEU:HG	2.01	0.43
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.99	0.43
2:B:954:VAL:HG11	2:B:962:LYS:HE3	1.98	0.43
9:I:54:GLU:CA	9:I:88:SER:OG	2.66	0.43
14:N:69:DC:H2''	14:N:70:DA:C8	2.53	0.43
14:N:83:DT:H2''	14:N:84:DC:C5	2.54	0.43
21:W:99:LYS:HE3	22:X:278:LEU:HD13	2.00	0.43
30:7:459:MET:O	30:7:462:ASN:ND2	2.51	0.43
35:d:543:ARG:HH12	35:d:639:ASN:HB2	1.82	0.43
36:e:66:LEU:HA	36:e:165:SER:O	2.18	0.43
1:A:405:VAL:HG13	1:A:432:VAL:HG22	2.01	0.43
1:A:407:ARG:HH11	1:A:413:ILE:HD11	1.83	0.43
13:M:198:VAL:HG12	13:M:198:VAL:O	2.18	0.43
13:M:267:LYS:CG	13:M:268:GLU:H	2.31	0.43
14:N:60:DT:H2''	14:N:61:DG:H8	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:9:VAL:HG13	20:V:51:THR:HG21	1.99	0.43
30:7:608:PHE:CG	30:7:686:ARG:NH1	2.87	0.43
1:A:925:LEU:HD22	1:A:983:ILE:HB	2.01	0.43
2:B:223:VAL:HG22	2:B:240:ILE:HD12	1.99	0.43
13:M:325:ASP:HB3	13:M:326:PRO:HD3	2.00	0.43
14:N:77:DA:H4'	14:N:78:DA:OP1	2.18	0.43
19:U:267:VAL:HG12	19:U:269:ILE:HG13	2.01	0.43
23:0:232:VAL:HB	23:0:456:VAL:HG13	1.99	0.43
23:0:432:ASN:O	23:0:434:ILE:N	2.52	0.43
30:7:495:ALA:O	30:7:499:ARG:HG2	2.18	0.43
32:a:114:GLU:O	32:a:130:LYS:HA	2.17	0.43
35:d:464:LYS:HG3	35:d:477:GLU:HG2	2.00	0.43
46:o:20:ASN:OD1	46:o:20:ASN:N	2.52	0.43
1:A:377:PRO:HB3	1:A:433:GLU:HG2	2.00	0.43
1:A:1146:VAL:HG11	1:A:1207:LEU:HD12	2.00	0.43
13:M:171:ILE:H	13:M:171:ILE:HG13	1.66	0.43
14:N:74:DA:H1'	14:N:75:DT:H5''	2.00	0.43
23:0:217:LYS:NZ	23:0:218:ILE:HD11	2.34	0.43
35:d:510:LEU:O	35:d:514:VAL:HG23	2.18	0.43
36:e:219:GLY:HA3	36:e:233:GLN:HA	2.00	0.43
37:f:195:ASN:HD22	37:f:196:GLU:N	2.17	0.43
40:i:147:LYS:HA	40:i:147:LYS:HD2	1.90	0.43
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.99	0.43
2:B:376:PHE:HE2	2:B:567:GLU:HA	1.84	0.43
7:G:97:HIS:O	7:G:112:LYS:N	2.51	0.43
17:R:258:THR:O	17:R:260:GLY:N	2.42	0.43
30:7:382:GLY:HA3	30:7:535:LEU:HG	2.00	0.43
1:A:167:CYS:SG	1:A:168:GLY:N	2.92	0.43
1:A:546:VAL:HG21	1:A:572:TRP:HB2	1.99	0.43
2:B:393:LYS:NZ	2:B:621:GLU:OE1	2.46	0.43
2:B:1073:TYR:CE1	2:B:1080:LYS:HG2	2.53	0.43
7:G:143:ILE:HG13	7:G:170:ALA:HA	2.01	0.43
8:H:5:LEU:HD11	8:H:61:SER:HB3	2.00	0.43
13:M:187:ARG:NH1	13:M:241:ARG:HH21	2.17	0.43
23:0:416:PHE:CE2	23:0:437:PHE:HB2	2.54	0.43
36:e:37:LEU:HD11	36:e:214:GLN:HE21	1.84	0.43
40:i:35:TYR:HB2	40:i:63:LEU:HD23	2.01	0.43
1:A:113:LEU:HD11	1:A:218:ASP:HA	2.01	0.43
2:B:276:ILE:HA	2:B:338:GLY:HA3	1.99	0.43
2:B:1058:LEU:O	2:B:1062:HIS:ND1	2.50	0.43
2:B:1074:ASN:OD1	2:B:1075:GLY:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:64:ASN:OD1	8:H:65:LEU:N	2.52	0.43
19:U:253:ARG:HD2	19:U:258:TRP:CZ2	2.54	0.43
30:7:515:ALA:HB1	30:7:692:ARG:HH12	1.83	0.43
37:f:94:ASN:ND2	37:f:96:SER:OG	2.51	0.43
5:E:144:ILE:H	5:E:144:ILE:HG13	1.71	0.43
17:R:262:THR:O	17:R:266:THR:HG23	2.19	0.43
18:T:80:DT:H6	18:T:80:DT:H2'	1.70	0.43
24:1:266:VAL:O	24:1:270:TYR:HB2	2.19	0.43
25:2:480:VAL:HG11	25:2:497:GLY:HA3	2.00	0.43
26:3:44:ASP:O	26:3:48:SER:CB	2.67	0.43
30:7:387:PRO:HB3	30:7:692:ARG:HD3	2.01	0.43
1:A:253:ASN:C	1:A:255:SER:H	2.26	0.43
1:A:399:HIS:HB3	1:A:400:PRO:HD3	2.00	0.43
2:B:205:ILE:O	2:B:208:SER:OG	2.34	0.43
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.84	0.43
16:Q:388:PRO:HB2	17:R:82:ARG:NH1	2.34	0.43
45:n:18:GLN:HB3	45:n:66:ILE:HG12	2.01	0.43
1:A:849:MET:SD	1:A:849:MET:N	2.92	0.42
1:A:1386:ARG:NH1	18:T:53:DG:H5''	2.34	0.42
12:L:38:LEU:HD23	12:L:40:LEU:HD23	2.01	0.42
15:O:199:LYS:HA	15:O:200:PRO:HA	1.85	0.42
35:d:394:PHE:HB3	35:d:403:TYR:HB3	2.01	0.42
1:A:372:LYS:HA	1:A:435:HIS:HD2	1.84	0.42
14:N:17:DC:H1'	14:N:18:DT:H5'	2.01	0.42
17:R:105:THR:OG1	17:R:106:LEU:N	2.52	0.42
35:d:651:ALA:HB3	35:d:658:VAL:H	1.84	0.42
1:A:1260:LEU:O	1:A:1264:GLU:HG3	2.19	0.42
3:C:262:LEU:HD22	11:K:87:LEU:HD23	2.01	0.42
13:M:235:ASN:CG	13:M:274:PRO:HB2	2.44	0.42
14:N:33:DT:C2	18:T:75:DG:N2	2.87	0.42
15:O:94:TYR:O	20:V:71:PHE:HD2	2.02	0.42
28:5:44:PRO:HA	28:5:47:VAL:HG23	2.01	0.42
30:7:583:MET:HE1	30:7:621:LYS:NZ	2.35	0.42
35:d:563:LYS:HA	35:d:567:LEU:HD13	2.01	0.42
35:d:604:ARG:HA	35:d:607:ASP:HB2	1.99	0.42
40:i:146:ARG:H	40:i:146:ARG:HD2	1.84	0.42
1:A:148:CYS:O	1:A:168:GLY:HA2	2.19	0.42
1:A:362:ASP:O	1:A:458:HIS:ND1	2.51	0.42
1:A:375:THR:HB	1:A:403:LYS:HD3	2.00	0.42
1:A:443:LEU:HD21	1:A:501:LEU:HD11	2.00	0.42
15:O:108:GLU:HA	15:O:109:PRO:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:24:DA:H2'	18:T:25:DT:H71	2.02	0.42
40:i:148:VAL:O	40:i:152:ARG:HG2	2.19	0.42
1:A:913:LEU:HD11	1:A:919:ILE:HG13	2.02	0.42
2:B:186:GLU:OE2	10:J:62:ARG:NH1	2.52	0.42
2:B:474:SER:O	2:B:476:ARG:N	2.52	0.42
2:B:487:THR:HG23	2:B:490:SER:H	1.85	0.42
13:M:142:LEU:HD23	13:M:146:VAL:HG11	2.01	0.42
18:T:93:DT:H2''	18:T:94:DG:C8	2.55	0.42
42:k:122:ARG:O	42:k:126:ALA:HB2	2.20	0.42
2:B:283:VAL:O	2:B:287:ARG:HG2	2.19	0.42
7:G:98:GLY:HA3	7:G:110:VAL:O	2.20	0.42
14:N:43:DT:H2''	14:N:44:DC:H5'	2.01	0.42
18:T:33:DT:H2''	18:T:34:DG:C8	2.55	0.42
30:7:372:LYS:HB3	30:7:380:ARG:HH12	1.85	0.42
30:7:379:ALA:H	30:7:508:HIS:CE1	2.37	0.42
42:k:120:GLN:O	42:k:124:SER:CB	2.68	0.42
45:n:4:ARG:HE	45:n:80:LEU:HD23	1.85	0.42
8:H:18:GLY:C	8:H:20:TYR:H	2.27	0.42
34:c:21:CYS:O	34:c:25:GLN:HG2	2.20	0.42
1:A:74:MET:O	2:B:1116:ARG:NH2	2.48	0.42
2:B:884:ARG:HG3	2:B:935:ARG:HE	1.84	0.42
2:B:950:ASP:HB2	2:B:969:ARG:HG2	2.02	0.42
14:N:80:DA:OP2	30:7:495:ALA:HB2	2.20	0.42
23:0:114:LEU:HA	23:0:182:LEU:HD21	2.01	0.42
24:1:30:ARG:HA	24:1:37:VAL:HG12	2.02	0.42
37:f:71:LEU:HD21	37:f:108:LEU:HD11	2.01	0.42
2:B:279:ASP:OD1	2:B:279:ASP:N	2.50	0.42
2:B:451:LYS:O	2:B:455:SER:HB2	2.20	0.42
14:N:43:DT:C1'	14:N:44:DC:H5'	2.50	0.42
21:W:9:VAL:HG22	21:W:189:ILE:HD13	2.01	0.42
28:5:7:GLY:HA3	28:5:41:LEU:HD11	2.01	0.42
6:F:97:ARG:NE	6:F:124:GLU:OE1	2.39	0.42
8:H:7:ASP:OD1	8:H:58:THR:OG1	2.37	0.42
13:M:191:GLU:O	13:M:194:SER:OG	2.30	0.42
14:N:10:DT:H2''	14:N:11:DA:N7	2.35	0.42
15:O:151:LYS:HG2	15:O:153:THR:HG23	2.02	0.42
23:0:372:LYS:N	23:0:373:PRO:CD	2.83	0.42
35:d:522:SER:O	35:d:527:PRO:HG3	2.20	0.42
37:f:135:LEU:HB2	37:f:166:LYS:HD3	2.01	0.42
1:A:54:ASN:OD1	1:A:54:ASN:N	2.52	0.41
3:C:19:ASP:HA	3:C:231:ASN:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:146:TRP:HB3	6:F:151:LEU:HD21	2.02	0.41
14:N:61:DG:H2''	14:N:62:DT:C6	2.55	0.41
23:0:635:LEU:O	23:0:639:LEU:CB	2.62	0.41
23:0:692:GLN:HG3	23:0:693:LEU:HG	2.01	0.41
27:4:226:GLN:O	27:4:230:ALA:CB	2.68	0.41
35:d:635:LEU:HD13	35:d:645:ILE:HG13	2.01	0.41
40:i:132:GLU:HB2	40:i:147:LYS:HE2	2.01	0.41
1:A:1022:LEU:O	1:A:1026:LEU:HB2	2.20	0.41
7:G:83:LYS:HG2	7:G:149:GLY:HA2	2.01	0.41
30:7:497:MET:HG3	30:7:498:PHE:N	2.35	0.41
35:d:626:HIS:ND1	35:d:627:LYS:HG3	2.35	0.41
37:f:32:ARG:HG2	37:f:33:ASP:H	1.85	0.41
6:F:136:ARG:O	6:F:143:PHE:HA	2.21	0.41
21:W:26:VAL:HA	21:W:29:LEU:HB3	2.01	0.41
23:0:621:LEU:HA	23:0:680:VAL:HG23	2.02	0.41
37:f:63:HIS:C	37:f:65:HIS:H	2.29	0.41
1:A:53:LEU:HD23	1:A:263:THR:HG22	2.03	0.41
1:A:230:ARG:HB2	1:A:233:TRP:CG	2.55	0.41
1:A:1191:TRP:CZ3	1:A:1257:ASP:HB3	2.55	0.41
3:C:68:GLY:HA3	12:L:69:ALA:HB1	2.01	0.41
14:N:80:DA:H1'	14:N:81:DT:H5'	2.02	0.41
16:Q:376:LEU:HB2	17:R:69:TRP:HB2	2.01	0.41
34:c:93:GLN:HG2	34:c:95:THR:H	1.85	0.41
35:d:466:ILE:HG22	35:d:475:GLU:HG2	2.02	0.41
35:d:562:ILE:HD11	35:d:633:LEU:HD22	2.02	0.41
1:A:348:SER:HB2	2:B:1128:LEU:HD12	2.01	0.41
2:B:54:PHE:O	2:B:58:THR:HB	2.21	0.41
2:B:793:ALA:HB3	2:B:856:PHE:HB2	2.02	0.41
13:M:269:ILE:HG23	13:M:272:LYS:HE3	2.03	0.41
14:N:35:DT:H2''	14:N:36:DG:C8	2.56	0.41
20:V:34:ALA:C	20:V:36:LEU:H	2.29	0.41
27:4:87:TYR:O	27:4:88:PRO:C	2.63	0.41
30:7:410:LEU:HB3	30:7:457:TYR:CE1	2.56	0.41
1:A:663:SER:OG	2:B:1084:GLN:O	2.25	0.41
2:B:70:ILE:HG21	16:Q:335:LEU:HD21	2.01	0.41
2:B:70:ILE:HG12	16:Q:335:LEU:HD21	2.03	0.41
2:B:778:MET:HA	2:B:1096:ARG:HH12	1.86	0.41
2:B:895:ASP:OD2	12:L:42:ARG:NH2	2.54	0.41
7:G:122:ASN:HB3	7:G:129:SER:O	2.21	0.41
16:Q:139:LEU:HD23	17:R:212:THR:HG21	2.03	0.41
23:0:198:ARG:HA	23:0:198:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:7:582:ILE:HG23	30:7:673:ILE:HG22	2.03	0.41
30:7:609:SER:HB2	30:7:615:LEU:HD13	2.02	0.41
37:f:195:ASN:ND2	37:f:197:ILE:HG22	2.35	0.41
2:B:1171:VAL:HG22	2:B:1182:CYS:HB2	2.03	0.41
5:E:136:ASN:OD1	5:E:137:GLU:N	2.54	0.41
11:K:58:PHE:HB3	11:K:76:GLN:HB3	2.01	0.41
13:M:171:ILE:HD12	13:M:172:MET:HG3	2.03	0.41
13:M:268:GLU:OE1	13:M:319:HIS:NE2	2.38	0.41
16:Q:378:VAL:HG22	16:Q:384:PHE:CD1	2.56	0.41
18:T:96:DT:H6	18:T:96:DT:H2'	1.73	0.41
23:0:492:PHE:CE2	23:0:715:SER:HB3	2.53	0.41
30:7:519:ARG:HE	30:7:682:GLN:HE22	1.67	0.41
1:A:481:ASP:N	1:A:481:ASP:OD1	2.52	0.41
2:B:910:VAL:HA	2:B:940:PRO:HA	2.01	0.41
2:B:1183:LYS:HE3	2:B:1183:LYS:HB3	1.83	0.41
5:E:58:MET:HE2	5:E:82:PHE:CE2	2.55	0.41
6:F:76:LYS:HB3	6:F:79:ARG:HH21	1.85	0.41
23:0:659:MET:HE1	23:0:691:SER:HA	2.03	0.41
30:7:457:TYR:HB3	30:7:497:MET:HE2	2.02	0.41
36:e:196:LYS:NZ	37:f:75:ASN:HB2	2.35	0.41
36:e:292:ASP:OD1	36:e:293:ARG:N	2.54	0.41
42:k:122:ARG:O	42:k:126:ALA:CB	2.69	0.41
1:A:1194:ARG:HA	1:A:1238:ILE:O	2.20	0.41
2:B:259:TYR:HE1	2:B:270:LYS:HB2	1.85	0.41
4:D:165:GLN:HE21	4:D:165:GLN:HB3	1.68	0.41
5:E:124:VAL:H	5:E:125:PRO:HD2	1.85	0.41
7:G:93:SER:OG	7:G:100:GLU:OE1	2.39	0.41
9:I:55:THR:CG2	9:I:100:PHE:CE2	3.03	0.41
13:M:186:ALA:HB1	13:M:238:TYR:CZ	2.56	0.41
15:O:71:VAL:HG13	15:O:124:THR:HB	2.03	0.41
19:U:264:ASP:OD1	19:U:277:GLN:NE2	2.54	0.41
20:V:61:THR:O	20:V:85:VAL:HA	2.21	0.41
23:0:259:ARG:HH22	23:0:397:THR:HB	1.85	0.41
23:0:655:SER:O	23:0:659:MET:HB2	2.20	0.41
25:2:483:TRP:CZ2	28:5:35:LEU:HB3	2.55	0.41
35:d:518:LYS:O	35:d:522:SER:HB2	2.20	0.41
35:d:639:ASN:N	35:d:639:ASN:OD1	2.53	0.41
38:g:103:GLN:O	38:g:107:LEU:CB	2.68	0.41
1:A:1420:ASP:OD1	1:A:1420:ASP:N	2.54	0.41
2:B:1135:ARG:HG3	2:B:1147:LEU:HD11	2.03	0.41
21:W:140:LEU:HD22	21:W:147:PHE:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:0:155:LEU:O	23:0:156:CYS:HB2	2.21	0.41
25:2:465:SER:O	25:2:469:ASN:ND2	2.32	0.41
36:e:41:TRP:CD1	36:e:66:LEU:HD13	2.55	0.41
37:f:26:ASN:O	37:f:26:ASN:ND2	2.54	0.41
1:A:635:ARG:NH2	1:A:876:ALA:O	2.54	0.40
2:B:26:THR:OG1	2:B:27:ALA:N	2.54	0.40
2:B:102:VAL:HG23	2:B:112:LEU:HB2	2.03	0.40
3:C:14:SER:OG	3:C:17:ASN:O	2.32	0.40
5:E:26:ARG:NH2	5:E:133:GLU:OE1	2.54	0.40
7:G:45:ILE:HA	7:G:78:VAL:HG12	2.02	0.40
7:G:126:ASN:HA	7:G:127:PRO:HA	1.96	0.40
23:0:257:LEU:O	23:0:343:LYS:NZ	2.53	0.40
24:1:340:UNK:O	24:1:341:UNK:CB	2.69	0.40
34:c:6:ILE:O	34:c:10:LEU:HB2	2.21	0.40
35:d:394:PHE:CD1	35:d:405:LEU:HA	2.57	0.40
1:A:497:THR:O	1:A:501:LEU:HB2	2.20	0.40
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.36	0.40
2:B:443:ASN:HD22	2:B:446:LEU:HG	1.86	0.40
2:B:649:LYS:HZ1	2:B:738:PHE:HD2	1.70	0.40
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.56	0.40
8:H:56:THR:HB	8:H:145:ARG:HG2	2.03	0.40
8:H:93:TYR:CG	8:H:143:LEU:HB3	2.56	0.40
14:N:73:DC:H2"	14:N:74:DA:N7	2.36	0.40
23:0:195:ILE:O	23:0:199:MET:HB2	2.21	0.40
35:d:480:SER:OG	35:d:481:LEU:N	2.53	0.40
45:n:94:ILE:HG22	45:n:98:GLN:HE21	1.85	0.40
1:A:214:ILE:HG22	1:A:219:PHE:HD2	1.87	0.40
1:A:217:LYS:O	1:A:221:SER:OG	2.33	0.40
1:A:802:ASN:HA	1:A:806:ARG:HH21	1.87	0.40
1:A:885:THR:HB	1:A:943:LEU:HD12	2.03	0.40
2:B:26:THR:HG23	2:B:29:ASP:H	1.86	0.40
2:B:780:VAL:HG22	2:B:795:ILE:HG23	2.04	0.40
3:C:255:VAL:HG21	11:K:94:ILE:HG21	2.04	0.40
4:D:56:ARG:HH22	4:D:155:ARG:HE	1.68	0.40
18:T:96:DT:H2"	18:T:97:DA:C8	2.56	0.40
23:0:406:ALA:HA	23:0:409:ILE:HG12	2.02	0.40
30:7:575:ARG:HB2	30:7:578:MET:HE2	2.04	0.40
35:d:441:LEU:HB2	35:d:512:LEU:HD22	2.04	0.40
1:A:139:TRP:CH2	14:N:60:DT:OP1	2.75	0.40
8:H:90:ALA:HB1	8:H:96:VAL:HG21	2.03	0.40
9:I:54:GLU:HG2	9:I:88:SER:OG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:f:4:SER:O	37:f:203:GLN:NE2	2.53	0.40
38:g:100:ASP:O	38:g:104:ILE:HG13	2.22	0.40
40:i:69:PRO:HA	40:i:70:PRO:HD3	1.98	0.40
1:A:450:LEU:HD12	1:A:1074:GLU:HG2	2.03	0.40
2:B:230:ALA:C	2:B:232:SER:H	2.30	0.40
23:0:117:HIS:N	23:0:118:PRO:HD2	2.36	0.40
34:c:98:MET:HB2	35:d:513:VAL:HG11	2.03	0.40
35:d:396:LYS:HB2	35:d:403:TYR:CE2	2.57	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	1386/1733 (80%)	1298 (94%)	77 (6%)	11 (1%)	16	54
2	B	1136/1224 (93%)	1064 (94%)	62 (6%)	10 (1%)	14	50
3	C	260/318 (82%)	236 (91%)	20 (8%)	4 (2%)	8	39
4	D	153/221 (69%)	145 (95%)	7 (5%)	1 (1%)	18	56
5	E	211/215 (98%)	202 (96%)	8 (4%)	1 (0%)	24	63
6	F	81/155 (52%)	79 (98%)	2 (2%)	0	100	100
7	G	169/171 (99%)	155 (92%)	13 (8%)	1 (1%)	21	59
8	H	132/146 (90%)	117 (89%)	12 (9%)	3 (2%)	5	27
9	I	114/122 (93%)	99 (87%)	15 (13%)	0	100	100
10	J	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	3	21
11	K	110/120 (92%)	109 (99%)	1 (1%)	0	100	100
12	L	43/70 (61%)	37 (86%)	6 (14%)	0	100	100
13	M	273/345 (79%)	252 (92%)	16 (6%)	5 (2%)	6	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	O	178/240 (74%)	164 (92%)	13 (7%)	1 (1%)	21	59
16	Q	129/747 (17%)	111 (86%)	15 (12%)	3 (2%)	5	27
17	R	176/400 (44%)	160 (91%)	15 (8%)	1 (1%)	21	59
19	U	88/286 (31%)	82 (93%)	4 (4%)	2 (2%)	5	27
20	V	96/122 (79%)	92 (96%)	3 (3%)	1 (1%)	12	48
21	W	198/541 (37%)	189 (96%)	6 (3%)	3 (2%)	8	39
22	X	156/328 (48%)	129 (83%)	23 (15%)	4 (3%)	4	25
23	0	659/778 (85%)	590 (90%)	54 (8%)	15 (2%)	5	27
24	1	309/510 (61%)	297 (96%)	8 (3%)	4 (1%)	9	41
25	2	284/553 (51%)	266 (94%)	17 (6%)	1 (0%)	30	67
26	3	136/321 (42%)	114 (84%)	19 (14%)	3 (2%)	5	28
27	4	257/333 (77%)	231 (90%)	17 (7%)	9 (4%)	3	20
28	5	64/72 (89%)	59 (92%)	5 (8%)	0	100	100
29	6	289/461 (63%)	260 (90%)	26 (9%)	3 (1%)	12	48
30	7	361/843 (43%)	333 (92%)	23 (6%)	5 (1%)	9	40
32	a	141/295 (48%)	132 (94%)	6 (4%)	3 (2%)	5	29
33	b	154/223 (69%)	147 (96%)	6 (4%)	1 (1%)	21	59
34	c	95/115 (83%)	90 (95%)	5 (5%)	0	100	100
35	d	422/687 (61%)	387 (92%)	30 (7%)	5 (1%)	10	43
36	e	226/307 (74%)	212 (94%)	14 (6%)	0	100	100
37	f	199/210 (95%)	182 (92%)	16 (8%)	1 (0%)	24	63
38	g	79/121 (65%)	79 (100%)	0	0	100	100
39	h	107/300 (36%)	106 (99%)	1 (1%)	0	100	100
40	i	128/223 (57%)	122 (95%)	6 (5%)	0	100	100
41	j	60/149 (40%)	56 (93%)	4 (7%)	0	100	100
42	k	121/157 (77%)	111 (92%)	8 (7%)	2 (2%)	7	36
43	l	439/745 (59%)	402 (92%)	27 (6%)	10 (2%)	5	27
44	m	97/220 (44%)	82 (84%)	10 (10%)	5 (5%)	1	14
45	n	134/140 (96%)	126 (94%)	6 (4%)	2 (2%)	8	39
46	o	73/151 (48%)	69 (94%)	4 (6%)	0	100	100
All	All	9986/15488 (64%)	9231 (92%)	633 (6%)	122 (1%)	13	43

All (122) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	Q	127	ILE
21	W	77	PRO
23	0	156	CYS
23	0	254	THR
27	4	88	PRO
27	4	290	SER
43	l	499	LEU
44	m	58	VAL
2	B	830	TYR
2	B	933	SER
7	G	63	PRO
13	M	269	ILE
21	W	78	ASN
22	X	251	ASN
23	0	349	LEU
24	1	275	PRO
26	3	124	ILE
30	7	461	ALA
35	d	370	PRO
35	d	571	PRO
43	l	273	ASN
45	n	35	LEU
2	B	277	LYS
2	B	475	SER
3	C	214	ASN
8	H	60	ALA
13	M	268	GLU
19	U	255	LYS
22	X	152	SER
23	0	62	HIS
23	0	217	LYS
23	0	471	ARG
24	1	25	ALA
24	1	74	ASP
27	4	87	TYR
27	4	170	THR
27	4	291	VAL
27	4	307	ALA
29	6	244	PRO
30	7	494	PRO
30	7	550	ALA
30	7	696	ARG

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Mol	Chain	Res	Type
32	a	119	SER
33	b	60	PRO
43	l	295	SER
44	m	23	TYR
44	m	150	PRO
1	A	47	ARG
1	A	67	CYS
1	A	567	LYS
1	A	958	VAL
2	B	364	ILE
2	B	957	ASN
3	C	93	ASP
4	D	156	ASP
8	H	83	GLN
10	J	9	SER
19	U	264	ASP
20	V	6	TYR
23	0	432	ASN
23	0	683	ASP
24	1	277	ASN
25	2	451	VAL
27	4	115	TYR
27	4	305	CYS
27	4	306	PRO
29	6	451	CYS
30	7	667	ALA
32	a	11	TRP
32	a	123	PRO
42	k	147	THR
43	l	581	LYS
1	A	35	ILE
1	A	50	ILE
1	A	525	GLN
1	A	569	LYS
2	B	339	THR
2	B	705	MET
3	C	236	GLY
5	E	124	VAL
10	J	3	VAL
13	M	271	GLY
22	X	240	THR
23	0	249	SER

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Mol	Chain	Res	Type
23	0	433	PRO
23	0	473	LEU
23	0	606	VAL
26	3	75	ASP
29	6	286	SER
35	d	541	ILE
37	f	181	GLU
43	l	209	LEU
43	l	379	LEU
43	l	392	GLY
43	l	408	LYS
44	m	144	GLN
44	m	145	PHE
1	A	464	PRO
2	B	1046	PRO
13	M	273	SER
16	Q	329	THR
16	Q	367	ALA
21	W	410	GLU
26	3	73	PHE
35	d	317	SER
45	n	39	GLU
15	O	147	GLY
22	X	205	ILE
23	0	536	GLY
42	k	43	PRO
43	l	498	VAL
2	B	343	ILE
8	H	59	ILE
23	0	372	LYS
1	A	61	ILE
3	C	182	PRO
17	R	215	VAL
1	A	1327	ILE
13	M	32	PRO
23	0	369	ILE
35	d	397	ILE
43	l	528	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1221/1520 (80%)	1221 (100%)	0	100	100
2	B	1000/1061 (94%)	998 (100%)	2 (0%)	87	86
3	C	230/274 (84%)	229 (100%)	1 (0%)	84	84
4	D	139/200 (70%)	139 (100%)	0	100	100
5	E	195/197 (99%)	195 (100%)	0	100	100
6	F	73/137 (53%)	73 (100%)	0	100	100
7	G	152/152 (100%)	151 (99%)	1 (1%)	76	81
8	H	119/128 (93%)	119 (100%)	0	100	100
9	I	110/116 (95%)	106 (96%)	4 (4%)	31	52
10	J	60/65 (92%)	60 (100%)	0	100	100
11	K	97/102 (95%)	97 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100
13	M	245/299 (82%)	245 (100%)	0	100	100
15	O	152/205 (74%)	152 (100%)	0	100	100
16	Q	109/641 (17%)	108 (99%)	1 (1%)	70	78
17	R	107/363 (30%)	107 (100%)	0	100	100
19	U	84/260 (32%)	84 (100%)	0	100	100
20	V	90/108 (83%)	90 (100%)	0	100	100
21	W	161/429 (38%)	161 (100%)	0	100	100
22	X	62/295 (21%)	62 (100%)	0	100	100
23	0	413/677 (61%)	410 (99%)	3 (1%)	76	81
24	1	179/306 (58%)	179 (100%)	0	100	100
25	2	53/407 (13%)	53 (100%)	0	100	100
26	3	53/303 (18%)	52 (98%)	1 (2%)	50	66
27	4	4/260 (2%)	3 (75%)	1 (25%)	0	4
28	5	53/66 (80%)	52 (98%)	1 (2%)	50	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	6	173/378 (46%)	173 (100%)	0	100	100
30	7	315/695 (45%)	311 (99%)	4 (1%)	61	73
33	b	15/207 (7%)	15 (100%)	0	100	100
34	c	93/108 (86%)	93 (100%)	0	100	100
35	d	256/642 (40%)	253 (99%)	3 (1%)	63	75
36	e	210/280 (75%)	209 (100%)	1 (0%)	81	83
37	f	172/178 (97%)	171 (99%)	1 (1%)	78	82
38	g	75/113 (66%)	75 (100%)	0	100	100
40	i	118/209 (56%)	118 (100%)	0	100	100
45	n	96/132 (73%)	95 (99%)	1 (1%)	68	77
46	o	73/117 (62%)	73 (100%)	0	100	100
All	All	6797/11687 (58%)	6772 (100%)	25 (0%)	81	84

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	70	ILE
2	B	1170	THR
3	C	95	CYS
7	G	163	ILE
9	I	18	GLU
9	I	42	LEU
9	I	43	VAL
9	I	59	VAL
16	Q	334	VAL
23	0	133	CYS
23	0	411	THR
23	0	440	LEU
26	3	72	ILE
27	4	292	CYS
28	5	54	LEU
30	7	492	VAL
30	7	701	PHE
30	7	715	GLU
30	7	737	THR
35	d	397	ILE
35	d	540	LEU
35	d	608	LYS

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Mol	Chain	Res	Type
36	e	70	VAL
37	f	195	ASN
45	n	110	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (147) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	68	GLN
1	A	256	GLN
1	A	311	GLN
1	A	313	GLN
1	A	339	ASN
1	A	363	GLN
1	A	399	HIS
1	A	488	ASN
1	A	517	ASN
1	A	525	GLN
1	A	576	GLN
1	A	589	GLN
1	A	640	GLN
1	A	698	GLN
1	A	723	ASN
1	A	745	GLN
1	A	760	GLN
1	A	767	GLN
1	A	881	GLN
1	A	953	ASN
1	A	965	GLN
1	A	968	GLN
1	A	994	GLN
1	A	1040	GLN
1	A	1130	GLN
1	A	1140	HIS
1	A	1258	HIS
1	A	1265	ASN
1	A	1330	ASN
1	A	1367	HIS
1	A	1427	ASN
2	B	47	GLN
2	B	73	GLN
2	B	103	ASN

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Mol	Chain	Res	Type
2	B	224	GLN
2	B	415	GLN
2	B	433	GLN
2	B	516	ASN
2	B	573	GLN
2	B	587	HIS
2	B	657	HIS
2	B	667	GLN
2	B	784	ASN
2	B	800	GLN
2	B	958	GLN
2	B	1093	GLN
2	B	1193	GLN
2	B	1211	ASN
3	C	73	GLN
3	C	79	GLN
3	C	102	GLN
3	C	184	ASN
3	C	206	ASN
3	C	224	GLN
3	C	231	ASN
3	C	242	GLN
4	D	157	GLN
4	D	165	GLN
4	D	179	GLN
4	D	216	ASN
5	E	54	GLN
7	G	96	GLN
7	G	102	GLN
7	G	153	GLN
8	H	35	GLN
8	H	83	GLN
9	I	60	GLN
9	I	89	GLN
9	I	108	HIS
10	J	53	HIS
11	K	89	ASN
11	K	112	GLN
13	M	90	ASN
13	M	114	GLN
13	M	193	GLN
15	O	158	GLN

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Mol	Chain	Res	Type
16	Q	117	HIS
16	Q	359	ASN
17	R	138	GLN
19	U	33	GLN
19	U	272	ASN
19	U	280	GLN
20	V	55	ASN
20	V	84	GLN
21	W	11	ASN
21	W	107	GLN
21	W	178	GLN
22	X	216	GLN
22	X	223	GLN
22	X	267	GLN
22	X	279	GLN
23	0	651	ASN
23	0	699	GLN
23	0	716	ASN
24	1	38	HIS
24	1	85	GLN
24	1	188	ASN
24	1	258	ASN
28	5	11	GLN
28	5	22	GLN
29	6	184	GLN
29	6	211	GLN
29	6	212	ASN
29	6	269	GLN
29	6	302	ASN
30	7	423	GLN
30	7	462	ASN
30	7	491	HIS
30	7	508	HIS
30	7	551	ASN
30	7	553	GLN
30	7	584	ASN
30	7	592	GLN
30	7	641	GLN
30	7	644	GLN
30	7	648	GLN
30	7	672	GLN
30	7	676	HIS

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Mol	Chain	Res	Type
30	7	682	GLN
30	7	685	GLN
34	c	25	GLN
34	c	51	HIS
35	d	502	ASN
35	d	595	ASN
35	d	626	HIS
35	d	642	ASN
35	d	646	HIS
35	d	656	ASN
35	d	683	GLN
36	e	4	GLN
36	e	214	GLN
36	e	258	ASN
36	e	269	ASN
37	f	26	ASN
37	f	68	GLN
37	f	94	ASN
37	f	173	HIS
37	f	195	ASN
38	g	60	ASN
40	i	150	ASN
40	i	159	HIS
45	n	9	GLN
45	n	98	GLN
46	o	20	ASN
46	o	34	GLN
46	o	56	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 17 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
49	SF4	0	901	23	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	SF4	0	901	23	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	0	901	SF4	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
24	1	3
21	W	2
25	2	1
27	4	1
39	h	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	394:UNK	C	465:UNK	N	84.00
1	W	289:UNK	C	349:UNK	N	45.11
1	1	121:ARG	C	168:UNK	N	38.20
1	2	281:ASP	C	380:UNK	N	36.23
1	W	194:ILE	C	259:UNK	N	35.82
1	4	97:UNK	C	103:UNK	N	15.93
1	1	353:UNK	C	369:UNK	N	14.71
1	h	125:LEU	C	130:UNK	N	5.44

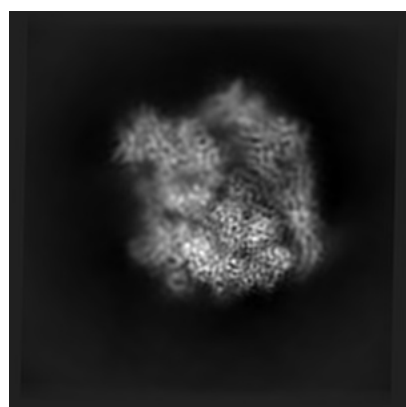
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3850. These allow visual inspection of the internal detail of the map and identification of artifacts.

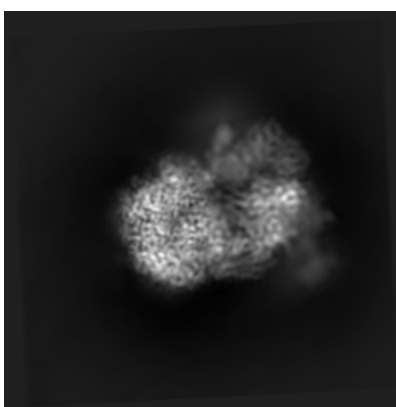
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

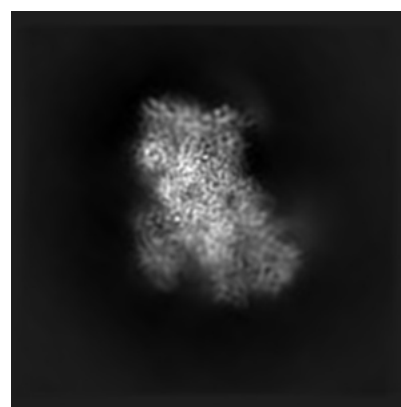
6.1.1 Primary map



X



Y

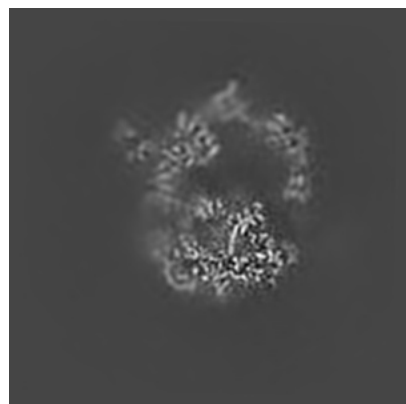


Z

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

6.2 Central slices [i](#)

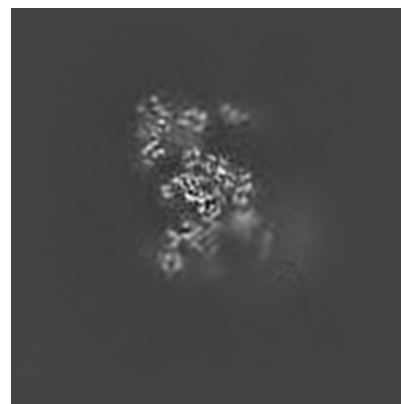
6.2.1 Primary map



X Index: 175



Y Index: 175

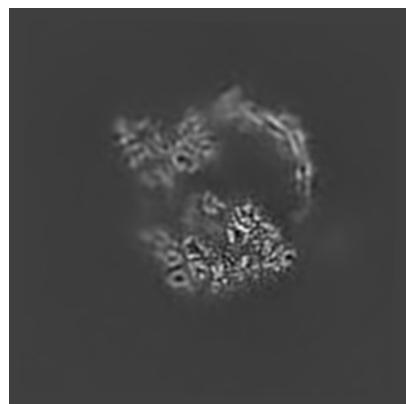


Z Index: 175

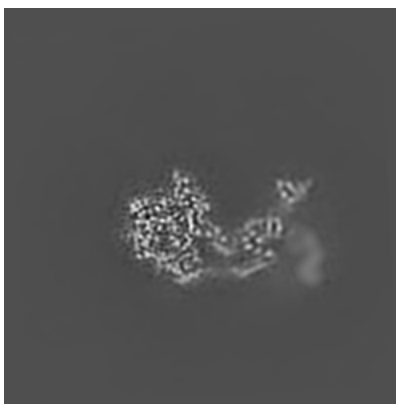
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

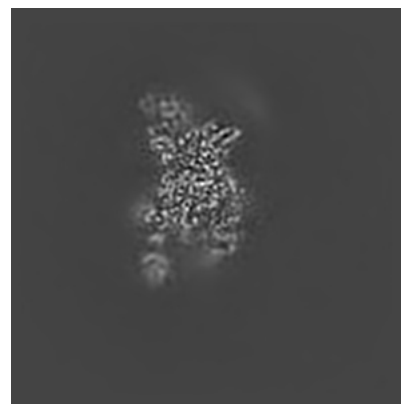
6.3.1 Primary map



X Index: 182



Y Index: 217

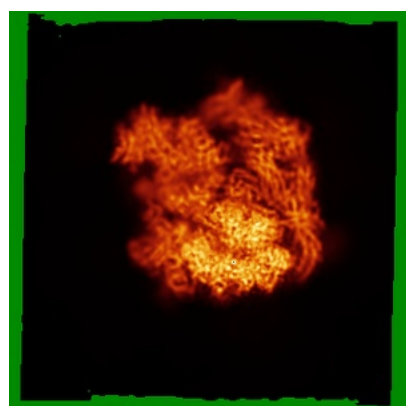


Z Index: 130

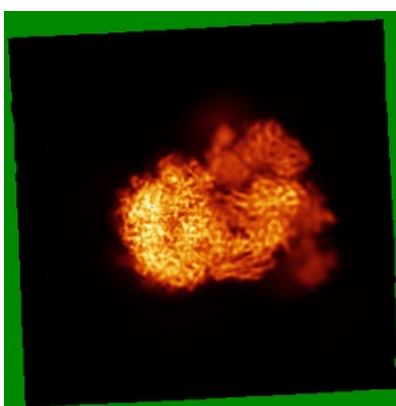
The images above show the largest variance slices of the map in three orthogonal directions.

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

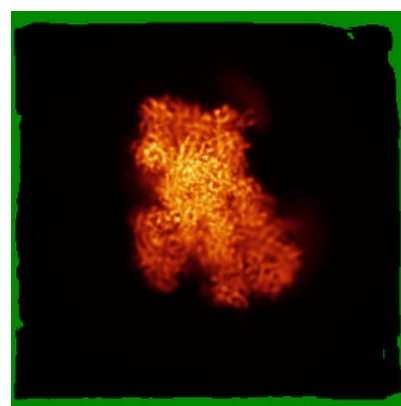
6.4.1 Primary map



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

This section was not generated.

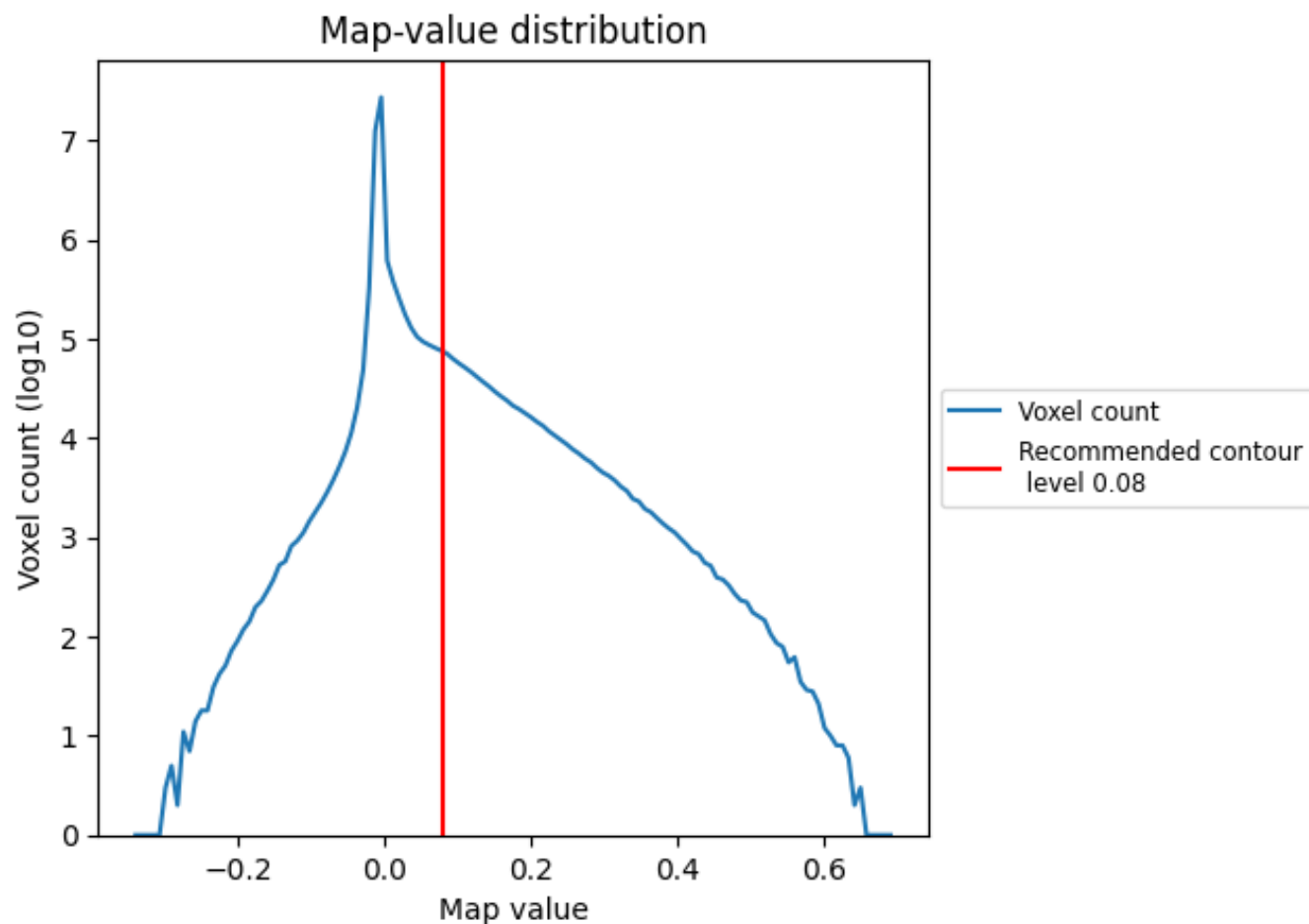
6.6 Mask visualisation

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

7 Map analysis [i](#)

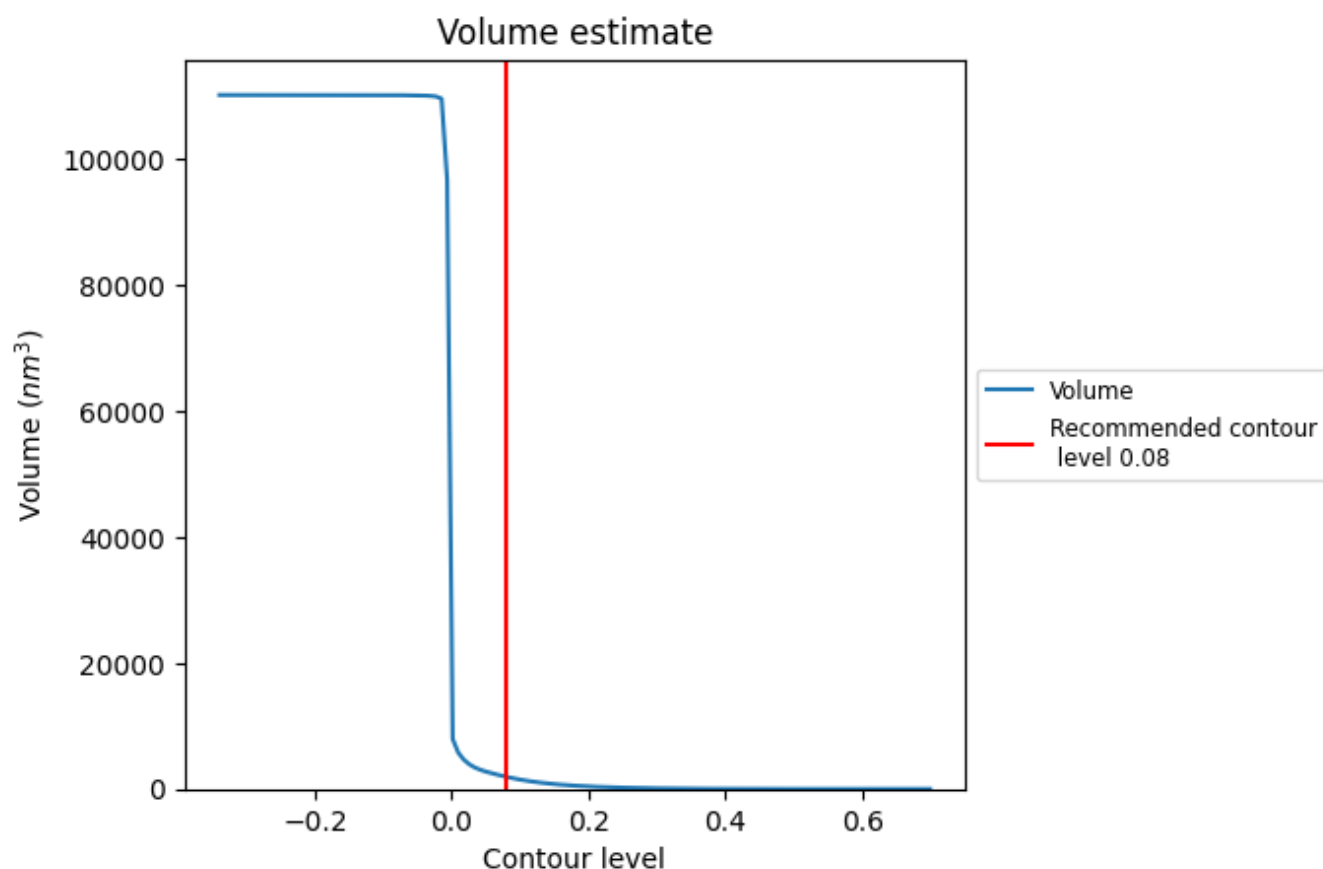
This section contains the results of statistical analysis of the map.

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.

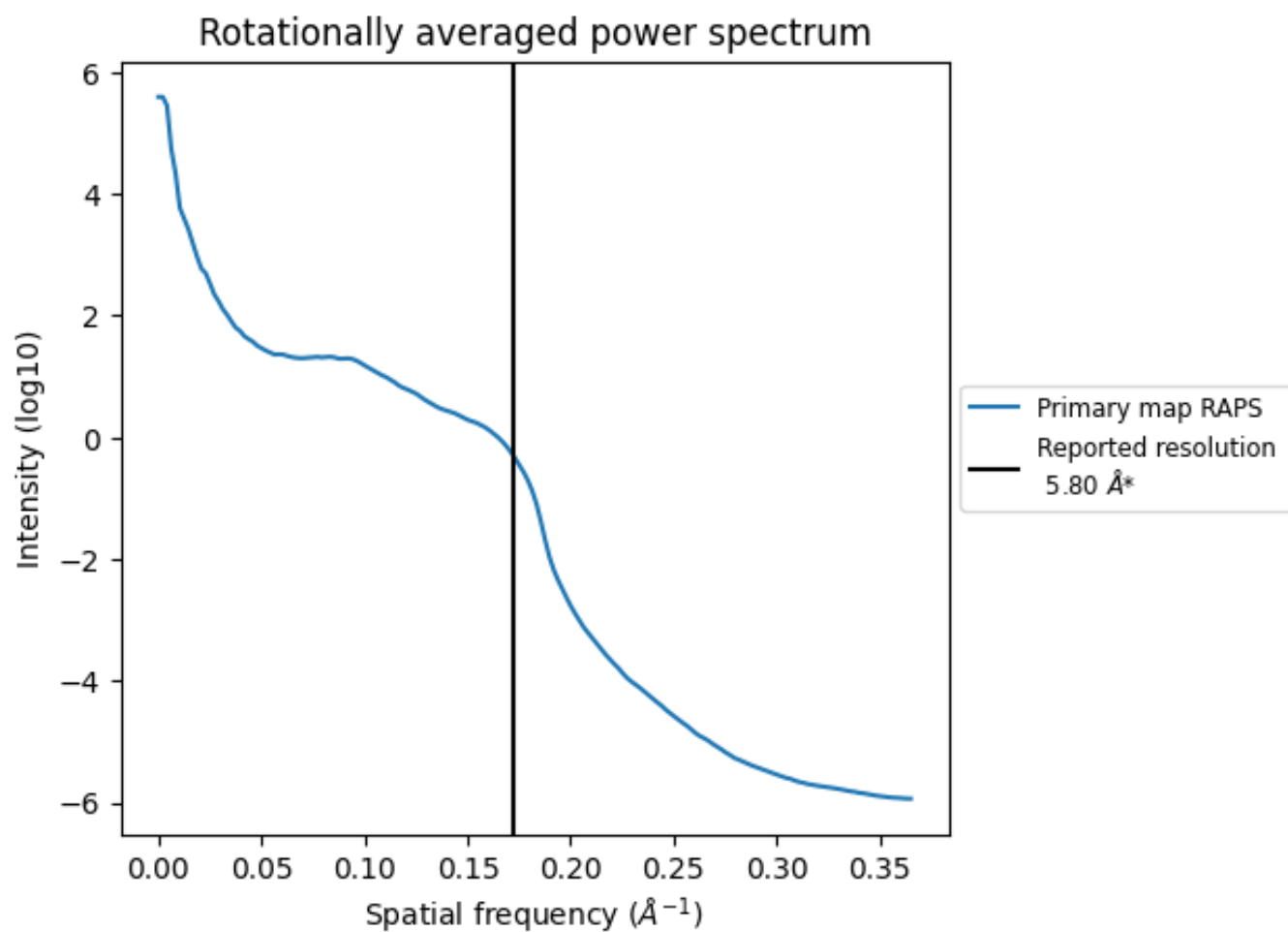
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1922 nm^3 ; this corresponds to an approximate mass of 1736 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.172 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-3850 and PDB model 5OQM. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)

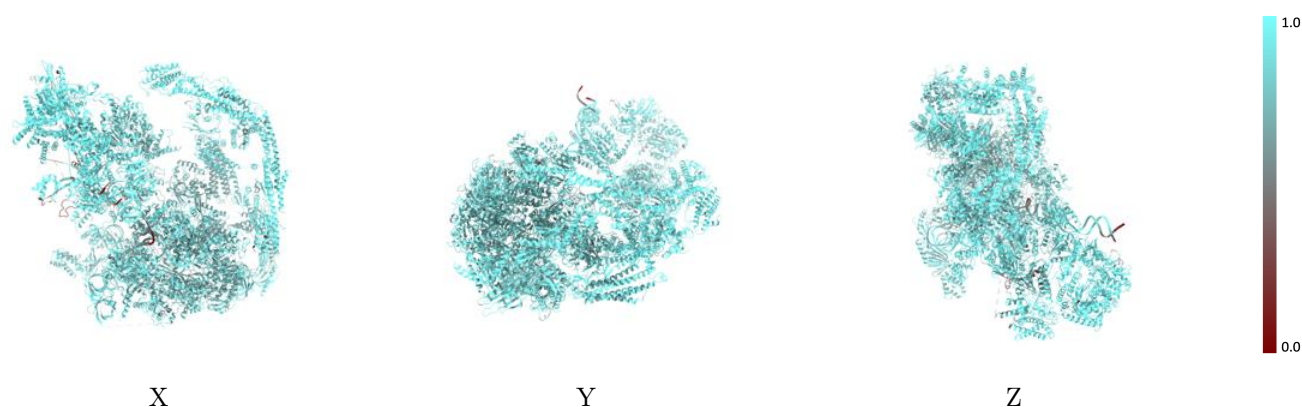
This section was not generated.

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



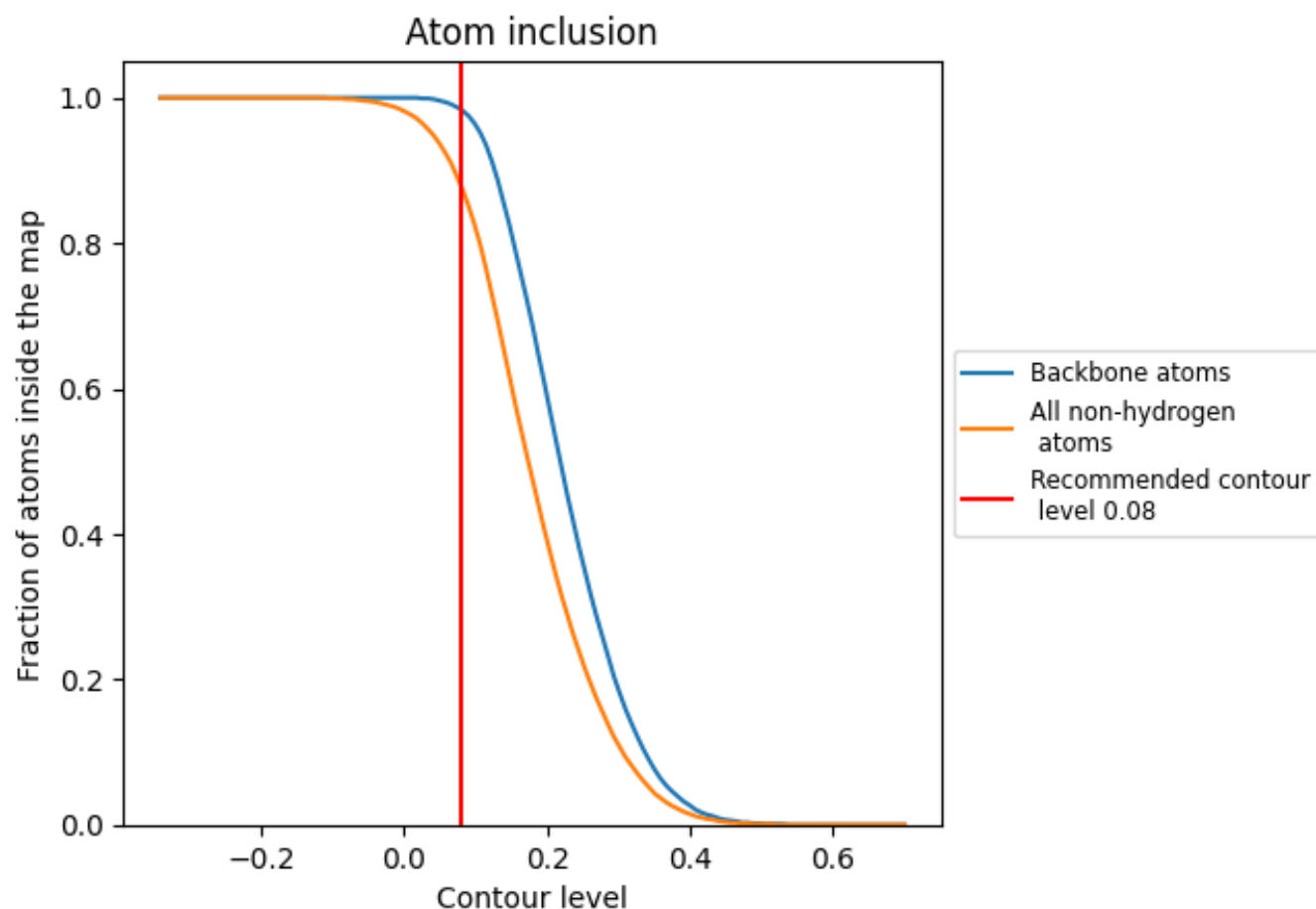
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8790	 0.1830
0	 0.9060	 0.1670
1	 0.8850	 0.1810
2	 0.9460	 0.1890
3	 0.9330	 0.1940
4	 0.9610	 0.2140
5	 0.9020	 0.1230
6	 0.9050	 0.1750
7	 0.9540	 0.1340
A	 0.8400	 0.1930
B	 0.8370	 0.1900
C	 0.8560	 0.2160
D	 0.8310	 0.1700
E	 0.8840	 0.1950
F	 0.8670	 0.2250
G	 0.8630	 0.1950
H	 0.8450	 0.1890
I	 0.8920	 0.1850
J	 0.8470	 0.2000
K	 0.8330	 0.1960
L	 0.8610	 0.2160
M	 0.8050	 0.1650
N	 0.9030	 0.1940
O	 0.8980	 0.1520
Q	 0.8660	 0.1600
R	 0.9190	 0.2040
T	 0.8420	 0.1780
U	 0.8910	 0.1450
V	 0.8970	 0.1560
W	 0.8470	 0.1630
X	 0.9160	 0.1890
Z	 0.9810	 0.2250
a	 0.9870	 0.2400
b	 0.9570	 0.2420
c	 0.8420	 0.1340



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Chain	Atom inclusion	Q-score
d	 0.8820	 0.1750
e	 0.8390	 0.1810
f	 0.8400	 0.1880
g	 0.8190	 0.1460
h	 0.9800	 0.2510
i	 0.9090	 0.1670
j	 0.8900	 0.2320
k	 0.9970	 0.2120
l	 0.9580	 0.2150
m	 0.9730	 0.1220
n	 0.8820	 0.1530
o	 0.8750	 0.1490