



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 03:54 AM UTC

PDB ID : 8TQW / pdb_00008tqw
EMDB ID : EMD-41565
Title : Structure of human transcriptional Mediator complex
Authors : Chen, S.F.; Chao, T.C.; Kim, H.J.; Tang, H.C.; Khadka, S.; Li, T.; Murakami, K.; Boyer, T.G.; Tsai, K.L.
Deposited on : 2023-08-08
Resolution : 8.20 Å(reported)

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

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A user guide is available at

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

The types of validation reports are described at

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

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

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

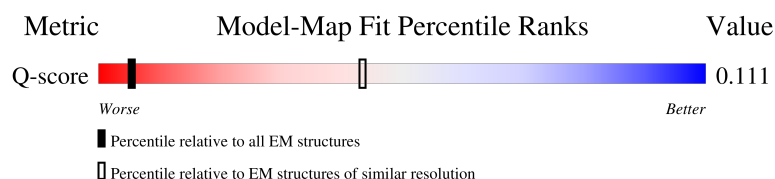
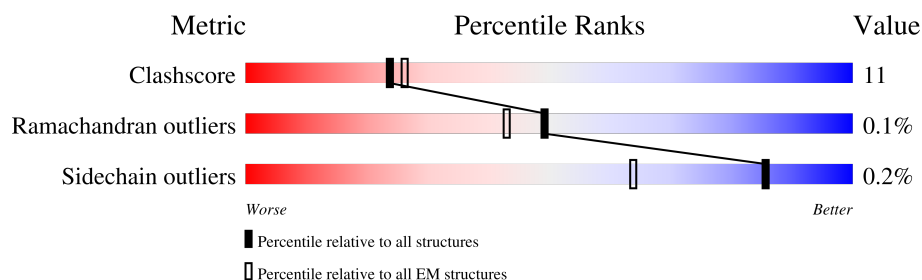
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

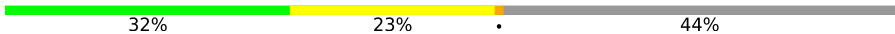
The reported resolution of this entry is 8.20 Å.

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.



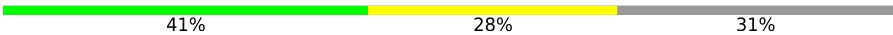
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	337 (7.70 - 8.70)

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	0	311	
2	1	178	
3	2	200	
4	3	178	

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Mol	Chain	Length	Quality of chain
5	4	131	 57% 29% 14%
6	A	1581	 18% 11% 70%
7	B	20	 65% 35%
8	D	110	 41% 28% 31%

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 83816 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 Mediator of RNA polymerase II transcription subunit 27.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	267	Total	C	N	O	S	0	0
			2159	1373	384	390	12		

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 28.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	99	Total	C	N	O	S	0	0
			817	511	143	160	3		

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 29.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	115	Total	C	N	O	S	0	0
			899	563	155	172	9		

- Molecule 4 is a protein called Mediator of RNA polymerase II transcription subunit 30.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	122	Total	C	N	O	S	0	0
			1022	639	187	189	7		

- Molecule 5 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	113	Total	C	N	O	S	0	0
			986	642	171	168	5		

- Molecule 6 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	467	Total	C	N	O	S	0	0
			3578	2278	613	663	24		

- Molecule 7 is a protein called Unknown Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	B	20	Total	C	N	O	0	0
			100	60	20	20		

- Molecule 8 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	158	Total	C	N	O	S	0	0
			1268	791	228	243	6		

- Molecule 9 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	166	Total	C	N	O	S	0	0
			1363	882	234	242	5		

- Molecule 10 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	161	Total	C	N	O	S	0	0
			1348	856	239	243	10		

- Molecule 11 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	181	Total	C	N	O	S	0	0
			1422	888	250	280	4		

- Molecule 12 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	73	Total	C	N	O	S	0	0
			605	382	107	110	6		

- Molecule 13 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	122	Total	C	N	O	S	0	0
			840	527	151	159	3		

- Molecule 14 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	112	Total	C	N	O	S	0	0
			879	537	163	175	4		

- Molecule 15 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	1017	Total	C	N	O	S	0	0
			7772	4958	1365	1407	42		

- Molecule 16 is a protein called Mediator of RNA polymerase II transcription subunit 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	157	Total	C	N	O	S	0	0
			1226	783	213	223	7		

- Molecule 17 is a protein called Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	753	Total	C	N	O	S	0	0
			5875	3742	1008	1077	48		

- Molecule 18 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	546	Total	C	N	O	S	0	0
			4319	2732	773	794	20		

- Molecule 19 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	191	Total	C	N	O	S	0	0
			1532	971	270	276	15		

- Molecule 20 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	75	Total	C	N	O	S	0	0
			517	328	87	100	2		

- Molecule 21 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	193	Total	C	N	O	S	0	0
			1499	955	247	280	17		

- Molecule 22 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	121	Total	C	N	O	S	0	0
			918	570	153	190	5		

- Molecule 23 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	130	Total	C	N	O	S	0	0
			1063	656	181	222	4		

- Molecule 24 is a protein called Mediator of RNA polymerase II transcription subunit 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	1334	Total	C	N	O	S	0	0
			10774	6967	1827	1909	71		

- Molecule 25 is a protein called Mediator of RNA polymerase II transcription subunit 24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	897	Total	C	N	O	S	0	0
			7061	4524	1190	1293	54		

- Molecule 26 is a protein called Cyclin-dependent kinase 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	313	Total	C	N	O	S	0	0
			2561	1663	439	442	17		

- Molecule 27 is a protein called Cyclin-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	262	Total	C	N	O	S	1	0
			2196	1442	358	379	17		

- Molecule 28 is a protein called Mediator of RNA polymerase II transcription subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	1452	Total	C	N	O	S	0	0
			11499	7270	2009	2147	73		

- Molecule 29 is a protein called Mediator of RNA polymerase II transcription subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	969	Total	C	N	O	S	0	0
			7714	4945	1310	1393	66		

- Molecule 30 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
30	0	1	Total	Zn	0
			1	1	
30	P	1	Total	Zn	0
			1	1	
30	c	1	Total	Zn	0
			1	1	
30	d	1	Total	Zn	0
			1	1	

L79	
L82	
A83	
L84	
N85	
Q86	
Q87	
K88	
I89	
H90	
H91	
E97	
V100	
D104	
S105	
D106	
I107	
Q108	
Q109	
L110	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6348	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.063	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.004	Depositor
Map size ($\text{\AA}$)	727.04004, 727.04004, 727.04004	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.272, 2.272, 2.272	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0	0.16	0/2201	0.48	1/2972 (0.0%)
2	1	0.30	0/825	0.61	1/1107 (0.1%)
3	2	0.20	0/911	0.49	0/1229
4	3	0.18	0/1029	0.48	0/1378
5	4	0.18	0/1013	0.44	0/1364
6	A	0.28	0/3653	0.55	0/4961
8	D	0.24	0/1281	0.53	0/1718
9	F	0.24	0/1400	0.54	0/1902
10	G	0.23	0/1374	0.59	1/1847 (0.1%)
11	H	0.19	0/1441	0.51	2/1946 (0.1%)
12	I	0.24	0/612	0.70	1/815 (0.1%)
13	J	0.21	0/849	0.50	0/1150
14	K	0.17	0/885	0.49	0/1190
15	N	0.27	0/7923	0.61	4/10761 (0.0%)
16	O	0.21	0/1261	0.55	0/1731
17	P	0.18	0/6001	0.48	1/8151 (0.0%)
18	Q	0.17	0/4400	0.47	1/5941 (0.0%)
19	R	0.17	0/1562	0.44	0/2101
20	S	0.23	0/524	0.59	0/709
21	T	0.18	0/1530	0.51	0/2066
22	U	0.18	0/927	0.43	0/1257
23	V	0.17	0/1072	0.44	0/1440
24	W	0.17	0/11056	0.42	0/15023
25	X	0.19	0/7191	0.48	0/9728
26	a	0.20	0/2627	0.50	2/3542 (0.1%)
27	b	0.18	0/2253	0.46	0/3051
28	c	0.18	0/11719	0.46	0/15850
29	d	0.19	0/7895	0.50	3/10703 (0.0%)
All	All	0.20	0/85415	0.50	17/115633 (0.0%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	368	LYS	CA-C-N	9.14	129.56	120.52
15	N	368	LYS	C-N-CA	9.14	129.56	120.52
29	d	337	VAL	N-CA-C	8.51	119.30	110.62
29	d	1136	ASN	N-CA-C	7.91	119.90	111.28
26	a	340	LEU	CA-C-N	6.60	128.09	119.84
26	a	340	LEU	C-N-CA	6.60	128.09	119.84
12	I	109	LEU	N-CA-C	-6.35	98.07	108.41
17	P	402	MET	N-CA-C	6.09	118.00	111.36
1	0	129	ASN	CB-CA-C	-5.86	109.81	116.54
29	d	1135	GLY	N-CA-C	5.72	119.60	112.73
10	G	107	GLU	N-CA-C	-5.71	105.14	111.36
2	1	135	LYS	N-CA-C	-5.52	105.35	111.36
15	N	154	ILE	CB-CA-C	-5.45	108.57	114.35
15	N	187	GLU	N-CA-C	-5.38	108.49	114.62
11	H	98	PRO	CA-C-N	5.09	131.13	121.97
11	H	98	PRO	C-N-CA	5.09	131.13	121.97
18	Q	35	SER	N-CA-C	5.04	116.84	110.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	2159	0	2176	39	0
2	1	817	0	818	72	0
3	2	899	0	908	14	0
4	3	1022	0	1054	28	0
5	4	986	0	965	28	0
6	A	3578	0	3522	149	0
7	B	100	0	23	4	0
8	D	1268	0	1305	59	0
9	F	1363	0	1344	22	0
10	G	1348	0	1373	77	0
11	H	1422	0	1440	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	I	605	0	628	33	0
13	J	840	0	718	39	0
14	K	879	0	886	7	0
15	N	7772	0	7557	353	0
16	O	1226	0	1217	21	0
17	P	5875	0	5968	150	0
18	Q	4319	0	4403	117	0
19	R	1532	0	1542	28	0
20	S	517	0	432	27	0
21	T	1499	0	1484	38	0
22	U	918	0	905	12	0
23	V	1063	0	1051	48	0
24	W	10774	0	10838	197	0
25	X	7061	0	7223	130	0
26	a	2561	0	2578	60	0
27	b	2196	0	2233	21	0
28	c	11499	0	11504	153	0
29	d	7714	0	7627	151	0
30	0	1	0	0	0	0
30	P	1	0	0	0	0
30	c	1	0	0	0	0
30	d	1	0	0	0	0
All	All	83816	0	83722	1828	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 11.

All (1828) 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)
26:a:340:LEU:HD21	29:d:1622:VAL:CG2	1.33	1.53
26:a:340:LEU:CD2	29:d:1622:VAL:HG21	1.56	1.34
26:a:338:ASP:HB3	26:a:339:PRO:CD	1.62	1.29
15:N:375:ASP:CB	15:N:376:PRO:HD3	1.67	1.22
2:1:115:VAL:HG22	4:3:142:ILE:HD11	1.29	1.14
8:D:86:GLN:CD	12:I:106:GLY:HA2	1.72	1.14
12:I:109:LEU:CD2	12:I:114:GLN:HE21	1.60	1.14
12:I:140:MET:O	22:U:117:LYS:HD3	1.44	1.14
29:d:1133:LYS:CG	29:d:1222:ARG:HH21	1.60	1.14
10:G:104:LYS:HD3	20:S:72:PRO:HG3	1.19	1.13
10:G:98:ARG:O	20:S:78:THR:HG22	1.47	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:a:340:LEU:HG	26:a:341:PRO:HD2	1.14	1.11
10:G:104:LYS:CD	20:S:72:PRO:HG3	1.78	1.11
8:D:86:GLN:OE1	12:I:106:GLY:HA2	1.51	1.11
15:N:375:ASP:HB3	15:N:376:PRO:HD3	1.25	1.11
6:A:22:ARG:CB	8:D:39:VAL:HB	1.80	1.11
15:N:149:LEU:HD12	15:N:150:PRO:HD2	1.15	1.09
15:N:375:ASP:HB2	15:N:376:PRO:CD	1.82	1.09
15:N:308:LEU:HD13	15:N:370:LEU:HD11	1.30	1.09
26:a:340:LEU:CD2	29:d:1622:VAL:CG2	2.21	1.09
15:N:375:ASP:CB	15:N:376:PRO:CD	2.29	1.09
26:a:340:LEU:HD21	29:d:1622:VAL:HG22	1.30	1.08
6:A:278:HIS:ND1	6:A:279:PRO:HD2	1.69	1.07
18:Q:216:PHE:HE1	18:Q:218:HIS:CB	1.68	1.07
15:N:374:HIS:CE1	15:N:379:PRO:HG2	1.88	1.06
10:G:90:LEU:CD2	13:J:109:LEU:HD13	1.87	1.03
18:Q:216:PHE:CE1	18:Q:218:HIS:HB3	1.94	1.03
26:a:338:ASP:CB	26:a:339:PRO:CD	2.33	1.03
10:G:90:LEU:HD21	13:J:109:LEU:HD13	1.36	1.03
2:1:128:LEU:HD13	23:V:133:GLU:CB	1.88	1.03
26:a:338:ASP:CB	26:a:339:PRO:HD3	1.89	1.02
18:Q:216:PHE:CE1	18:Q:218:HIS:CB	2.42	1.02
10:G:97:ILE:HG13	13:J:102:MET:SD	2.00	1.00
15:N:358:THR:HG23	15:N:375:ASP:OD2	1.61	0.99
21:T:187:ALA:O	21:T:191:VAL:HG23	1.61	0.99
2:1:89:ARG:HD3	18:Q:544:MET:HG2	1.44	0.99
2:1:128:LEU:HD13	23:V:133:GLU:HB2	1.03	0.99
18:Q:215:LEU:HD23	18:Q:215:LEU:H	1.27	0.98
8:D:30:LEU:HD13	12:I:99:LYS:HB3	1.41	0.98
26:a:340:LEU:CG	26:a:341:PRO:HD2	1.94	0.98
29:d:1133:LYS:CG	29:d:1222:ARG:NH2	2.28	0.96
10:G:101:GLY:HA2	15:N:128:LEU:CD2	1.96	0.96
25:X:274:GLN:HE21	25:X:276:ILE:HD11	1.31	0.96
26:a:307:LYS:CD	26:a:337:GLU:HG3	1.96	0.95
25:X:274:GLN:NE2	25:X:276:ILE:HD11	1.82	0.95
15:N:308:LEU:HD13	15:N:370:LEU:CD1	1.96	0.94
26:a:81:LEU:HD23	29:d:1735:LEU:HD22	1.45	0.94
10:G:90:LEU:HD21	13:J:109:LEU:CD1	1.96	0.94
15:N:703:ARG:NH2	18:Q:614:LYS:HG3	1.82	0.94
15:N:643:HIS:CD2	18:Q:560:ILE:HG12	2.02	0.94
26:a:338:ASP:HB3	26:a:339:PRO:HD3	0.95	0.94
15:N:149:LEU:CD1	15:N:150:PRO:HD2	1.97	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:128:LEU:CD1	23:V:133:GLU:HB2	1.95	0.93
15:N:374:HIS:HB2	15:N:378:LEU:HD23	1.50	0.93
12:I:109:LEU:HD21	12:I:114:GLN:HE21	1.31	0.92
3:2:155:LEU:N	3:2:160:TYR:HH	1.68	0.92
10:G:90:LEU:CD2	13:J:109:LEU:CD1	2.48	0.92
15:N:374:HIS:CG	15:N:379:PRO:HD3	2.04	0.92
29:d:1373:VAL:O	29:d:1416:MET:SD	2.29	0.91
10:G:104:LYS:HD3	20:S:72:PRO:CG	1.98	0.91
26:a:307:LYS:HD3	26:a:337:GLU:HG3	1.51	0.91
2:1:115:VAL:CG2	4:3:142:ILE:HD11	2.00	0.90
26:a:340:LEU:HD21	29:d:1622:VAL:HG21	0.92	0.90
10:G:96:LEU:HB2	13:J:102:MET:HE1	1.53	0.90
15:N:374:HIS:CG	15:N:379:PRO:CD	2.56	0.89
20:S:109:LEU:O	20:S:113:PRO:CD	2.20	0.89
2:1:101:GLN:CG	4:3:114:LEU:HD21	2.03	0.89
23:V:119:LEU:O	23:V:123:ILE:HG12	1.73	0.89
10:G:101:GLY:HA2	15:N:128:LEU:HD23	1.55	0.88
15:N:375:ASP:HB2	15:N:376:PRO:HD3	1.46	0.88
2:1:101:GLN:HG3	4:3:114:LEU:HD21	1.55	0.87
15:N:149:LEU:HD12	15:N:150:PRO:CD	2.02	0.87
29:d:1133:LYS:CE	29:d:1222:ARG:HH21	1.88	0.86
2:1:125:LYS:HE2	23:V:137:SER:HB2	1.58	0.86
18:Q:216:PHE:CE1	18:Q:218:HIS:HB2	2.10	0.86
29:d:1133:LYS:HG2	29:d:1222:ARG:NH2	1.89	0.86
2:1:125:LYS:HE2	23:V:137:SER:CB	2.06	0.85
17:P:402:MET:SD	17:P:461:MET:HE2	2.16	0.85
6:A:278:HIS:CE1	6:A:279:PRO:HD2	2.12	0.85
26:a:340:LEU:CG	29:d:1622:VAL:HG21	2.07	0.85
2:1:135:LYS:HG2	2:1:139:TRP:HZ3	1.42	0.84
18:Q:472:GLU:HA	18:Q:497:ILE:O	1.78	0.83
10:G:131:ALA:HB1	15:N:154:ILE:HD11	1.60	0.82
15:N:374:HIS:CE1	15:N:379:PRO:CG	2.61	0.82
2:1:146:ILE:HG12	23:V:115:LYS:HE3	1.62	0.82
12:I:109:LEU:CD2	12:I:114:GLN:NE2	2.42	0.81
18:Q:216:PHE:HE1	18:Q:218:HIS:HB3	1.35	0.81
6:A:278:HIS:CG	6:A:279:PRO:HD2	2.15	0.81
29:d:1133:LYS:NZ	29:d:1222:ARG:NH2	2.28	0.81
2:1:146:ILE:HD11	23:V:115:LYS:HD2	1.64	0.80
26:a:340:LEU:CD1	29:d:1622:VAL:HG21	2.10	0.80
26:a:71:ARG:HH12	29:d:1734:THR:HA	1.47	0.80
15:N:375:ASP:HB2	15:N:376:PRO:HD2	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:382:ASP:HB2	15:N:386:VAL:H	1.46	0.79
26:a:340:LEU:HG	26:a:341:PRO:CD	2.06	0.79
26:a:81:LEU:CD2	29:d:1735:LEU:HD22	2.11	0.79
8:D:109:GLN:HE22	10:G:174:ASP:HB3	1.47	0.79
15:N:372:ILE:H	15:N:372:ILE:HD13	1.48	0.78
17:P:393:ILE:HG21	17:P:402:MET:HE3	1.65	0.78
26:a:71:ARG:NH1	29:d:1734:THR:HA	1.99	0.78
29:d:1133:LYS:HG3	29:d:1222:ARG:NH2	1.99	0.78
2:1:139:TRP:HZ2	23:V:122:GLU:HB3	1.50	0.77
15:N:361:ILE:HB	15:N:370:LEU:HD23	1.67	0.77
8:D:30:LEU:HD13	12:I:99:LYS:CB	2.15	0.77
15:N:145:VAL:O	15:N:148:ARG:HG2	1.85	0.77
15:N:374:HIS:CD2	15:N:379:PRO:HD2	2.19	0.77
26:a:340:LEU:HD11	29:d:1622:VAL:HG21	1.66	0.77
29:d:1133:LYS:HG3	29:d:1222:ARG:HH21	1.49	0.77
20:S:109:LEU:O	20:S:113:PRO:CG	2.33	0.76
18:Q:216:PHE:CD1	18:Q:218:HIS:HB3	2.19	0.76
10:G:90:LEU:HD21	13:J:109:LEU:CB	2.15	0.76
8:D:83:ALA:HB1	12:I:102:SER:HB3	1.65	0.76
15:N:361:ILE:HD12	15:N:370:LEU:HD23	1.67	0.76
10:G:90:LEU:HD21	13:J:109:LEU:HB3	1.68	0.75
1:0:127:LEU:HD23	2:1:74:ARG:HG3	1.66	0.75
2:1:143:LEU:HD21	23:V:119:LEU:HG	1.67	0.75
15:N:591:PHE:CD1	24:W:25:MET:HE2	2.21	0.75
10:G:96:LEU:HB3	15:N:129:PHE:CE1	2.21	0.75
15:N:703:ARG:HH22	18:Q:614:LYS:HG3	1.49	0.75
15:N:361:ILE:HB	15:N:370:LEU:CD2	2.16	0.75
15:N:453:HIS:HB2	15:N:466:MET:HB2	1.68	0.75
11:H:19:VAL:HG21	18:Q:113:TYR:HB2	1.68	0.75
15:N:135:ARG:HD2	15:N:135:ARG:C	2.13	0.74
18:Q:215:LEU:H	18:Q:215:LEU:CD2	1.98	0.74
15:N:374:HIS:ND1	15:N:379:PRO:CD	2.49	0.74
6:A:459:ASN:ND2	6:A:484:SER:O	2.20	0.74
12:I:140:MET:O	22:U:117:LYS:CD	2.31	0.74
25:X:585:ILE:HD11	25:X:623:TRP:HB3	1.69	0.74
29:d:1374:LEU:HA	29:d:1416:MET:SD	2.27	0.74
3:2:121:ARG:HH12	15:N:907:LEU:HD21	1.52	0.73
8:D:86:GLN:OE1	12:I:106:GLY:CA	2.33	0.73
13:J:127:ILE:HG13	20:S:65:PHE:CE1	2.22	0.73
6:A:347:GLU:HG3	6:A:422:GLY:HA3	1.68	0.73
6:A:22:ARG:CB	8:D:39:VAL:CB	2.62	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:30:ASN:HB2	8:D:182:MET:HE1	1.71	0.73
24:W:396:MET:O	24:W:399:PHE:HB3	1.88	0.72
29:d:1133:LYS:HG2	29:d:1222:ARG:HH21	1.43	0.72
5:4:43:PHE:HB2	5:4:85:ARG:HB3	1.72	0.72
15:N:372:ILE:HD13	15:N:372:ILE:N	2.04	0.72
6:A:149:GLU:HG3	6:A:152:LYS:HD2	1.70	0.72
15:N:358:THR:HG23	15:N:375:ASP:CG	2.14	0.72
15:N:737:ARG:HH21	15:N:743:ARG:HH11	1.37	0.72
17:P:640:ARG:HG2	17:P:642:GLY:H	1.54	0.72
15:N:916:LEU:HB2	15:N:924:ILE:HB	1.71	0.72
1:0:306:HIS:H	1:0:309:CYS:HB2	1.54	0.72
10:G:96:LEU:CB	13:J:102:MET:HE1	2.20	0.72
21:T:46:TYR:HB2	21:T:63:MET:HB2	1.72	0.71
25:X:644:ARG:HH21	25:X:684:GLN:H	1.39	0.71
15:N:823:GLN:NE2	15:N:832:HIS:O	2.23	0.71
25:X:772:PHE:HB3	25:X:779:VAL:HG21	1.73	0.71
2:1:139:TRP:CZ2	23:V:122:GLU:HB3	2.25	0.71
15:N:371:GLN:OE1	15:N:373:PHE:HE2	1.73	0.71
6:A:455:GLN:NE2	6:A:460:ASP:OD1	2.24	0.70
12:I:109:LEU:HD23	12:I:114:GLN:HE21	1.52	0.70
15:N:245:TRP:O	15:N:279:GLN:NE2	2.25	0.70
17:P:403:ALA:HB2	17:P:461:MET:HE1	1.73	0.70
25:X:792:LEU:HD22	25:X:911:ILE:HD11	1.73	0.69
10:G:90:LEU:HD23	13:J:109:LEU:HD13	1.72	0.69
6:A:208:VAL:HG12	6:A:222:LEU:HD13	1.74	0.69
6:A:460:ASP:OD2	25:X:11:LEU:HD11	1.92	0.69
10:G:96:LEU:HB3	15:N:129:PHE:HE1	1.56	0.69
23:V:130:LEU:C	23:V:130:LEU:HD13	2.18	0.69
6:A:77:MET:SD	6:A:145:LYS:NZ	2.66	0.69
5:4:17:ARG:NH2	5:4:54:TYR:OH	2.26	0.69
5:4:28:LEU:HG	5:4:34:LEU:HD21	1.75	0.69
15:N:374:HIS:CG	15:N:379:PRO:HD2	2.28	0.69
20:S:65:PHE:HB3	20:S:68:MET:HE2	1.73	0.69
20:S:109:LEU:O	20:S:113:PRO:HG2	1.92	0.69
15:N:374:HIS:ND1	15:N:379:PRO:HD3	2.06	0.69
15:N:530:ILE:HB	15:N:588:LEU:HD21	1.74	0.69
28:c:413:PHE:CZ	29:d:339:PRO:HB2	2.28	0.68
24:W:931:LYS:HB3	24:W:935:GLU:HB2	1.75	0.68
13:J:82:LYS:HG2	20:S:96:PHE:HB3	1.74	0.68
21:T:186:PRO:O	21:T:190:MET:HG2	1.93	0.68
6:A:278:HIS:CG	6:A:279:PRO:CD	2.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:d:1133:LYS:CE	29:d:1222:ARG:NH2	2.56	0.68
8:D:76:PHE:HA	8:D:79:LEU:HD13	1.75	0.68
18:Q:215:LEU:HD23	18:Q:215:LEU:N	2.07	0.68
8:D:152:ALA:CB	15:N:154:ILE:HA	2.24	0.68
15:N:853:HIS:O	15:N:856:GLN:NE2	2.24	0.68
1:O:258:MET:HE3	1:O:260:ASP:HB3	1.74	0.68
8:D:152:ALA:HB2	15:N:154:ILE:HA	1.76	0.68
15:N:684:LEU:HB2	15:N:708:CYS:HB3	1.76	0.67
19:R:130:VAL:HB	19:R:149:PHE:HB2	1.77	0.67
29:d:1896:CYS:HB2	29:d:1899:CYS:SG	2.35	0.67
15:N:676:ASP:OD2	18:Q:593:MET:HB2	1.93	0.67
29:d:1133:LYS:CD	29:d:1222:ARG:HH21	2.07	0.67
6:A:181:GLU:HA	6:A:184:LEU:HD12	1.76	0.67
21:T:79:PHE:HB2	21:T:82:GLY:H	1.60	0.67
19:R:60:LEU:HB3	19:R:68:PHE:HB3	1.77	0.67
2:1:128:LEU:HD11	23:V:129:GLU:OE1	1.94	0.67
9:F:174:ARG:NH1	15:N:265:LEU:O	2.27	0.67
18:Q:216:PHE:CD2	18:Q:306:GLU:HG2	2.29	0.67
2:1:125:LYS:HA	23:V:133:GLU:OE2	1.94	0.67
25:X:743:TRP:O	25:X:747:ASN:ND2	2.27	0.67
17:P:219:ALA:HB3	17:P:291:SER:HB3	1.77	0.67
5:4:78:LEU:HD22	15:N:178:ILE:HG13	1.77	0.66
8:D:27:ARG:NH1	12:I:103:THR:HB	2.10	0.66
22:U:127:GLN:HA	22:U:130:LEU:HD23	1.77	0.66
15:N:375:ASP:HB3	15:N:376:PRO:CD	2.10	0.66
6:A:476:SER:OG	6:A:478:LYS:NZ	2.28	0.66
2:1:125:LYS:HE2	23:V:137:SER:HB3	1.78	0.66
1:O:112:LYS:HD3	1:O:115:ASN:HD22	1.61	0.66
6:A:460:ASP:CG	25:X:11:LEU:HD21	2.21	0.66
15:N:356:LYS:O	15:N:375:ASP:HB2	1.96	0.66
15:N:935:ALA:HB1	15:N:1174:PRO:HB2	1.77	0.66
2:1:101:GLN:HG2	4:3:114:LEU:HD21	1.76	0.66
6:A:265:VAL:HA	6:A:300:PRO:HA	1.78	0.66
6:A:315:ARG:NH2	6:A:389:GLN:OE1	2.28	0.66
10:G:109:LEU:HD22	15:N:135:ARG:CZ	2.25	0.66
12:I:109:LEU:HD23	12:I:114:GLN:CG	2.26	0.66
10:G:64:ILE:HG12	10:G:117:VAL:HG11	1.78	0.65
29:d:1107:VAL:HG11	29:d:1128:ALA:HB3	1.78	0.65
6:A:305:LEU:HB2	6:A:396:ILE:HB	1.79	0.65
17:P:96:LEU:HB2	17:P:108:TRP:HB2	1.77	0.65
17:P:583:ILE:HD12	17:P:599:LEU:HD22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:471:LEU:HD22	17:P:499:MET:HE1	1.78	0.65
18:Q:496:ASN:HB3	18:Q:503:ARG:HB2	1.79	0.65
26:a:336:LEU:HA	26:a:340:LEU:HD12	1.79	0.65
9:F:171:ILE:HG13	9:F:173:GLN:H	1.60	0.65
15:N:245:TRP:H	15:N:282:LEU:HD22	1.62	0.65
17:P:231:ALA:HB2	17:P:283:LEU:HD13	1.78	0.65
24:W:1071:LEU:HA	24:W:1074:ARG:HE	1.60	0.65
10:G:101:GLY:CA	15:N:128:LEU:CD2	2.75	0.65
28:c:510:TRP:HD1	28:c:516:ARG:HH21	1.45	0.65
6:A:310:PRO:HB2	6:A:392:LEU:HB3	1.79	0.64
9:F:129:ALA:HB1	18:Q:98:VAL:HG23	1.78	0.64
15:N:858:MET:HE1	15:N:867:GLN:HB3	1.79	0.64
17:P:60:ARG:HG2	17:P:80:HIS:HB2	1.78	0.64
17:P:634:ASN:HB3	17:P:640:ARG:HH21	1.62	0.64
25:X:765:VAL:HG21	25:X:808:ALA:HB1	1.80	0.64
17:P:282:HIS:HB2	17:P:297:CYS:HB3	1.79	0.64
15:N:135:ARG:HD2	15:N:135:ARG:O	1.97	0.64
15:N:355:HIS:HB3	15:N:377:PRO:HG3	1.80	0.64
15:N:707:ASP:OD2	16:O:684:ARG:NH1	2.30	0.64
6:A:371:GLN:HB2	6:A:436:GLY:HA3	1.78	0.64
17:P:62:ILE:HB	17:P:76:ILE:HB	1.80	0.64
29:d:2132:PHE:O	29:d:2136:GLN:NE2	2.31	0.64
10:G:101:GLY:HA2	15:N:128:LEU:HD21	1.75	0.64
10:G:87:ILE:HD12	13:J:124:TYR:CD1	2.33	0.64
15:N:591:PHE:HD1	24:W:25:MET:HE2	1.61	0.64
18:Q:607:SER:H	18:Q:610:LEU:HD12	1.63	0.64
21:T:112:THR:HG22	21:T:129:VAL:HG22	1.79	0.64
6:A:171:THR:O	6:A:175:LEU:N	2.30	0.63
15:N:796:ILE:O	15:N:816:LYS:NZ	2.31	0.63
15:N:707:ASP:CG	16:O:684:ARG:HH11	2.06	0.63
29:d:1411:LEU:HG	29:d:1411:LEU:O	1.98	0.63
1:O:39:MET:HB2	1:O:48:ARG:HE	1.64	0.63
2:1:115:VAL:HG22	4:3:142:ILE:CD1	2.18	0.63
10:G:101:GLY:CA	15:N:128:LEU:HD23	2.27	0.63
8:D:26:THR:N	8:D:86:GLN:HE22	1.94	0.63
15:N:154:ILE:N	15:N:155:PRO:HD2	2.14	0.63
15:N:374:HIS:CE1	15:N:379:PRO:CD	2.81	0.63
28:c:1694:LEU:HG	28:c:1696:PRO:HD2	1.80	0.63
10:G:104:LYS:HD2	20:S:72:PRO:HG3	1.79	0.63
17:P:402:MET:SD	17:P:461:MET:CE	2.87	0.63
18:Q:461:GLN:HB2	18:Q:478:LEU:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:853:MET:HA	24:W:857:TYR:HB2	1.80	0.63
13:J:31:PRO:HA	28:c:624:LEU:HD11	1.80	0.63
15:N:421:ARG:NH1	15:N:429:SER:OG	2.26	0.63
28:c:1738:TYR:HB3	29:d:1820:ILE:HG12	1.81	0.63
2:1:128:LEU:HD11	23:V:129:GLU:CD	2.23	0.62
8:D:132:LEU:HD22	22:U:108:VAL:HG22	1.80	0.62
10:G:96:LEU:O	15:N:129:PHE:CZ	2.52	0.62
17:P:141:VAL:HA	17:P:161:ARG:HH22	1.63	0.62
26:a:338:ASP:CB	26:a:339:PRO:HD2	2.28	0.62
28:c:243:MET:HG3	28:c:249:LEU:HD22	1.81	0.62
15:N:372:ILE:O	15:N:372:ILE:HG12	1.98	0.62
15:N:667:PRO:HG2	15:N:686:LYS:HB3	1.81	0.62
15:N:1337:GLN:HA	15:N:1355:PRO:HA	1.80	0.62
17:P:548:HIS:HB3	17:P:732:LEU:HB3	1.80	0.62
25:X:792:LEU:HD21	25:X:907:LEU:HD23	1.80	0.62
6:A:168:LYS:HD3	6:A:169:LEU:HD12	1.81	0.62
13:J:72:ASP:OD1	15:N:98:ARG:NH1	2.33	0.62
24:W:373:MET:HG3	24:W:425:MET:HB2	1.80	0.62
26:a:85:PHE:HB2	26:a:94:TRP:HB2	1.82	0.62
29:d:1373:VAL:HB	29:d:1415:ILE:HG13	1.82	0.62
4:3:44:ILE:HD12	4:3:92:LEU:HD13	1.81	0.62
6:A:488:ILE:HG23	6:A:515:ALA:HB2	1.82	0.62
15:N:455:PHE:HB2	15:N:464:GLN:HB2	1.82	0.62
15:N:553:GLU:HB3	15:N:567:LYS:HB2	1.81	0.62
17:P:64:ILE:HB	17:P:74:HIS:HB3	1.82	0.62
21:T:76:PHE:CE2	21:T:190:MET:HE2	2.35	0.62
9:F:49:VAL:HG23	9:F:50:VAL:HG23	1.81	0.62
23:V:130:LEU:HD13	23:V:130:LEU:O	1.99	0.62
24:W:767:TRP:HD1	24:W:768:LYS:HG3	1.62	0.62
25:X:779:VAL:HA	25:X:782:VAL:HG12	1.81	0.62
28:c:1432:ILE:O	28:c:1440:GLN:NE2	2.33	0.62
2:1:143:LEU:HG	23:V:119:LEU:HD11	1.82	0.61
17:P:488:TRP:NE1	17:P:529:MET:SD	2.73	0.61
8:D:124:ALA:O	8:D:127:GLN:NE2	2.32	0.61
23:V:100:GLN:HG3	23:V:101:ARG:HE	1.64	0.61
18:Q:494:GLN:HB3	18:Q:505:VAL:HB	1.81	0.61
28:c:364:CYS:HB2	29:d:340:GLN:NE2	2.16	0.61
6:A:183:ASP:HA	6:A:186:LYS:HD2	1.83	0.61
24:W:958:ASN:HD21	24:W:961:LEU:HD23	1.65	0.61
6:A:163:LEU:HB2	6:A:170:LYS:HG2	1.82	0.61
15:N:441:PRO:HA	15:N:451:CYS:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:643:HIS:HB2	18:Q:560:ILE:HG23	1.82	0.61
17:P:393:ILE:CG2	17:P:402:MET:HE3	2.29	0.61
18:Q:18:GLN:HE21	18:Q:18:GLN:HA	1.65	0.61
29:d:32:LYS:HB3	29:d:103:GLU:HB3	1.82	0.61
25:X:585:ILE:HD12	25:X:624:LEU:HG	1.83	0.61
28:c:530:GLU:HB3	28:c:608:VAL:HG22	1.82	0.61
6:A:64:THR:HA	6:A:67:LYS:HG2	1.83	0.61
10:G:109:LEU:HD13	15:N:135:ARG:HG3	1.82	0.61
17:P:286:LEU:HD11	17:P:396:ARG:HG3	1.81	0.61
25:X:274:GLN:HG3	25:X:276:ILE:HG13	1.80	0.61
17:P:220:PHE:H	17:P:289:ASP:HA	1.65	0.61
17:P:640:ARG:HB3	17:P:643:HIS:HB3	1.82	0.61
29:d:1920:GLN:HG3	29:d:2097:LYS:HZ3	1.65	0.61
6:A:186:LYS:O	6:A:190:MET:N	2.29	0.60
15:N:587:LEU:HD12	15:N:589:GLN:HE22	1.64	0.60
17:P:626:LEU:HD11	17:P:724:LEU:HD22	1.82	0.60
18:Q:18:GLN:HA	18:Q:18:GLN:NE2	2.16	0.60
6:A:420:LEU:HD23	6:A:502:MET:O	2.01	0.60
17:P:12:MET:N	17:P:458:SER:OG	2.33	0.60
24:W:585:ILE:HA	24:W:589:LEU:HB2	1.82	0.60
7:B:8:UNK:O	7:B:12:UNK:N	2.34	0.60
15:N:825:ASN:OD1	15:N:832:HIS:ND1	2.28	0.60
24:W:247:THR:O	24:W:249:ARG:NH1	2.34	0.60
2:1:93:CYS:HA	2:1:96:LEU:HB2	1.83	0.60
12:I:109:LEU:HD23	12:I:114:GLN:HG3	1.82	0.60
16:O:735:LEU:HD21	24:W:73:PRO:HB2	1.83	0.60
18:Q:576:GLY:O	18:Q:619:ARG:NH2	2.34	0.60
24:W:698:THR:O	24:W:1223:GLN:NE2	2.35	0.60
5:4:21:GLU:HB3	5:4:58:TRP:HH2	1.66	0.60
8:D:156:SER:HB2	8:D:161:VAL:HG12	1.83	0.60
15:N:247:LEU:HD13	15:N:278:VAL:HG11	1.83	0.60
15:N:1251:VAL:HA	15:N:1263:LEU:HA	1.83	0.60
15:N:197:GLN:OE1	15:N:200:ARG:NH1	2.34	0.60
15:N:387:GLU:O	15:N:391:LYS:NZ	2.35	0.60
1:0:127:LEU:CD2	2:1:74:ARG:HG3	2.31	0.60
1:0:282:GLN:NE2	1:0:304:ALA:O	2.34	0.60
6:A:379:ASP:OD1	6:A:386:ARG:NH1	2.34	0.60
15:N:1218:ARG:HG2	15:N:1219:HIS:CD2	2.37	0.60
28:c:246:ASP:HB3	28:c:248:MET:HB2	1.84	0.60
29:d:1133:LYS:NZ	29:d:1222:ARG:HH21	1.95	0.60
6:A:443:CYS:SG	6:A:451:SER:OG	2.60	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:107:ILE:HG22	12:I:107:ILE:O	2.00	0.60
26:a:333:PRO:O	26:a:337:GLU:HG2	2.02	0.60
8:D:82:LEU:HA	8:D:85:ASN:HB2	1.84	0.60
15:N:458:LEU:HD11	18:Q:325:ILE:HG22	1.83	0.60
15:N:530:ILE:HD12	15:N:533:LEU:HD12	1.81	0.60
25:X:955:LEU:HD11	25:X:968:LEU:HB2	1.84	0.59
8:D:34:LEU:HD13	12:I:96:GLU:HG2	1.82	0.59
12:I:95:GLN:HB3	12:I:99:LYS:HZ2	1.67	0.59
19:R:52:LEU:HB2	19:R:132:LYS:HD3	1.84	0.59
6:A:208:VAL:CG1	6:A:222:LEU:HD13	2.31	0.59
6:A:408:LEU:HA	6:A:411:ILE:HD12	1.85	0.59
28:c:1636:ARG:HD3	28:c:1639:LEU:HD21	1.83	0.59
2:1:88:ALA:O	2:1:91:THR:OG1	2.20	0.59
6:A:304:PHE:HB2	6:A:306:LYS:HZ2	1.68	0.59
15:N:186:ILE:HG23	15:N:186:ILE:O	2.01	0.59
15:N:457:ASP:OD1	15:N:462:MET:N	2.35	0.59
17:P:697:TRP:O	17:P:701:ARG:N	2.34	0.59
21:T:129:VAL:HG11	21:T:200:ILE:HD13	1.84	0.59
24:W:559:LEU:HD11	24:W:563:LEU:HD23	1.85	0.59
15:N:711:ARG:HD2	18:Q:549:LEU:HD23	1.83	0.59
21:T:76:PHE:CD2	21:T:190:MET:HE2	2.37	0.59
6:A:376:LEU:HA	6:A:442:VAL:HB	1.85	0.59
15:N:690:CYS:SG	15:N:691:LYS:N	2.76	0.59
22:U:118:ILE:O	22:U:122:LEU:N	2.33	0.59
6:A:305:LEU:HD11	6:A:404:VAL:HG23	1.84	0.59
15:N:725:VAL:HA	15:N:744:HIS:HA	1.84	0.59
25:X:134:CYS:SG	25:X:164:ARG:NH2	2.76	0.59
15:N:444:GLU:H	15:N:562:THR:HB	1.68	0.59
15:N:660:GLU:HA	15:N:663:ASN:HB2	1.85	0.59
17:P:527:LEU:HD13	17:P:550:LYS:HZ3	1.68	0.59
24:W:727:TRP:HB2	24:W:747:ASN:HD21	1.67	0.59
28:c:1096:LEU:HB3	28:c:1150:ALA:HB2	1.85	0.59
29:d:1095:ILE:HB	29:d:1870:HIS:HB2	1.84	0.59
2:1:119:ARG:NH1	4:3:141:GLU:OE2	2.33	0.59
15:N:540:ILE:HB	15:N:550:ILE:HB	1.84	0.59
28:c:611:HIS:HA	28:c:614:TYR:HB3	1.85	0.59
29:d:1820:ILE:HD12	29:d:1843:LEU:HD23	1.85	0.59
2:1:118:LEU:O	2:1:122:LEU:N	2.36	0.59
2:1:123:GLN:O	2:1:127:ALA:N	2.36	0.59
17:P:186:GLY:H	17:P:210:ARG:HG3	1.66	0.59
28:c:930:LEU:HD11	28:c:937:LEU:HD22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:c:1451:LEU:HB3	28:c:1502:SER:HB2	1.84	0.59
11:H:97:VAL:HG11	11:H:108:HIS:HE2	1.68	0.58
15:N:506:LYS:O	15:N:510:LYS:NZ	2.29	0.58
17:P:214:ALA:N	17:P:231:ALA:O	2.36	0.58
29:d:11:SER:N	29:d:1951:THR:HG1	2.00	0.58
23:V:117:ILE:HG12	23:V:120:ARG:HH21	1.69	0.58
17:P:688:LEU:HB2	17:P:691:ARG:HH21	1.67	0.58
20:S:109:LEU:O	20:S:113:PRO:HD2	2.03	0.58
25:X:979:ARG:HH12	25:X:983:ALA:HB2	1.67	0.58
26:a:129:LYS:HD2	26:a:335:PHE:HA	1.83	0.58
25:X:554:VAL:HG11	25:X:583:ALA:HB3	1.84	0.58
6:A:179:SER:OG	6:A:270:ILE:O	2.21	0.58
9:F:174:ARG:HA	9:F:177:VAL:HB	1.86	0.58
17:P:261:PRO:HD2	17:P:337:LEU:HD12	1.85	0.58
29:d:1732:VAL:CG1	29:d:1734:THR:CG2	2.81	0.58
15:N:779:CYS:HA	15:N:782:GLU:HB2	1.85	0.58
18:Q:203:ILE:HG23	18:Q:224:VAL:HB	1.85	0.58
25:X:773:CYS:HA	25:X:776:MET:HB3	1.84	0.58
28:c:246:ASP:O	28:c:1646:ARG:NH1	2.37	0.58
15:N:726:PHE:O	15:N:743:ARG:N	2.37	0.58
10:G:25:ASN:HD22	10:G:32:PRO:HB3	1.68	0.58
18:Q:381:GLU:HA	18:Q:384:LYS:HG2	1.86	0.58
18:Q:425:GLU:HG2	18:Q:430:LYS:HE3	1.84	0.58
25:X:821:TYR:HH	25:X:942:SER:N	2.02	0.58
15:N:711:ARG:CD	18:Q:549:LEU:HD23	2.34	0.58
15:N:804:ASN:OD1	15:N:807:LYS:N	2.29	0.58
17:P:309:TRP:HB3	17:P:339:TRP:HB3	1.85	0.58
28:c:1392:GLN:HA	28:c:1395:GLU:HB2	1.86	0.58
29:d:1732:VAL:HG12	29:d:1734:THR:CG2	2.34	0.58
6:A:288:PHE:HD1	6:A:296:SER:H	1.51	0.58
15:N:657:LEU:HD23	15:N:682:ILE:HD12	1.85	0.58
17:P:743:GLN:HB3	17:P:746:GLN:HB2	1.86	0.58
23:V:118:THR:O	23:V:122:GLU:HG3	2.04	0.58
28:c:1178:HIS:HA	28:c:1181:LYS:HG2	1.85	0.58
17:P:212:ARG:NH1	17:P:232:ASP:O	2.37	0.57
18:Q:216:PHE:HE1	18:Q:218:HIS:HB2	1.48	0.57
15:N:340:TRP:HZ2	15:N:405:VAL:HG13	1.68	0.57
15:N:534:SER:O	15:N:537:LYS:NZ	2.33	0.57
15:N:568:TYR:HB2	15:N:591:PHE:HB2	1.85	0.57
15:N:802:VAL:H	15:N:809:ILE:HG22	1.68	0.57
24:W:753:ARG:NH2	24:W:832:TYR:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:d:1449:LEU:HD21	29:d:1665:GLY:HA3	1.86	0.57
2:1:101:GLN:HG3	4:3:114:LEU:CD2	2.29	0.57
15:N:359:ILE:HD12	15:N:372:ILE:HG22	1.86	0.57
24:W:339:ILE:HD11	24:W:575:GLU:HB2	1.87	0.57
24:W:1102:ALA:O	24:W:1106:HIS:ND1	2.37	0.57
29:d:1885:LEU:HD13	29:d:1888:LEU:HD21	1.86	0.57
6:A:318:VAL:HA	6:A:329:LEU:HD13	1.86	0.57
6:A:386:ARG:HH11	6:A:387:SER:H	1.51	0.57
11:H:70:LEU:HD11	11:H:72:ARG:HH21	1.69	0.57
15:N:452:LEU:HD11	15:N:465:LEU:HB3	1.86	0.57
15:N:507:GLN:NE2	15:N:508:SER:OG	2.36	0.57
19:R:17:ASN:ND2	19:R:104:ASN:OD1	2.36	0.57
24:W:57:GLU:O	24:W:60:ILE:HB	2.04	0.57
25:X:796:SER:O	25:X:799:HIS:ND1	2.37	0.57
28:c:1621:GLN:HE21	28:c:1639:LEU:HD13	1.69	0.57
2:1:113:GLU:OE2	4:3:31:ALA:HB3	2.04	0.57
15:N:530:ILE:HD11	15:N:551:VAL:HG11	1.87	0.57
15:N:683:ARG:HA	15:N:709:THR:HA	1.86	0.57
17:P:377:TYR:H	17:P:459:PRO:HB3	1.68	0.57
24:W:696:HIS:HB2	24:W:736:PRO:HG3	1.85	0.57
28:c:523:MET:HE1	28:c:887:SER:HB3	1.86	0.57
6:A:66:GLN:HE22	12:I:73:ILE:CD1	2.16	0.57
13:J:127:ILE:HG13	20:S:65:PHE:HE1	1.69	0.57
15:N:683:ARG:HD2	16:O:684:ARG:HG3	1.86	0.57
24:W:1154:THR:HG21	24:W:1218:HIS:HB2	1.85	0.57
28:c:1202:SER:HA	28:c:1205:ARG:HE	1.69	0.57
29:d:1107:VAL:HG21	29:d:1128:ALA:H	1.70	0.57
6:A:84:ILE:HD11	6:A:147:PHE:HB3	1.87	0.57
6:A:502:MET:O	6:A:502:MET:HG2	2.05	0.57
17:P:737:GLY:O	17:P:741:ARG:NH1	2.38	0.57
27:b:32:LEU:HD23	27:b:36:GLU:HB3	1.85	0.57
29:d:1790:LEU:HD11	29:d:1860:VAL:HG23	1.87	0.57
14:K:19:ARG:NH2	14:K:55:SER:OG	2.38	0.57
15:N:361:ILE:HD12	15:N:370:LEU:CD2	2.34	0.57
23:V:90:ASP:HB3	23:V:92:PRO:HD3	1.85	0.57
24:W:176:CYS:O	24:W:1330:ARG:NH2	2.37	0.57
24:W:332:GLN:NE2	24:W:575:GLU:OE2	2.37	0.57
15:N:279:GLN:O	15:N:283:PHE:N	2.35	0.57
17:P:668:LEU:HD23	17:P:669:LYS:HG2	1.85	0.57
15:N:676:ASP:OD2	18:Q:593:MET:CB	2.53	0.57
24:W:467:LEU:HD12	24:W:474:ILE:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:126:TYR:HA	10:G:129:HIS:HB3	1.86	0.56
15:N:819:SER:N	15:N:836:GLY:O	2.37	0.56
15:N:927:TYR:HB2	15:N:935:ALA:HB3	1.87	0.56
16:O:673:SER:OG	16:O:674:ILE:N	2.38	0.56
20:S:65:PHE:HB3	20:S:68:MET:CE	2.33	0.56
28:c:1451:LEU:O	28:c:1455:GLN:NE2	2.38	0.56
29:d:1133:LYS:HZ3	29:d:1222:ARG:NH2	2.02	0.56
6:A:498:VAL:HA	6:A:502:MET:HA	1.87	0.56
14:K:78:PRO:HA	18:Q:195:LYS:HD3	1.86	0.56
24:W:666:THR:HA	24:W:669:LEU:HB2	1.87	0.56
5:4:77:GLU:HA	5:4:80:GLN:HG2	1.86	0.56
13:J:95:VAL:HG11	15:N:122:LEU:HD22	1.86	0.56
15:N:475:LEU:HA	15:N:478:MET:HE2	1.86	0.56
15:N:887:THR:O	15:N:903:CYS:N	2.39	0.56
17:P:821:GLN:HA	17:P:824:ILE:HB	1.87	0.56
26:a:202:PRO:HG3	26:a:255:ILE:HD13	1.85	0.56
28:c:601:CYS:SG	28:c:842:HIS:NE2	2.78	0.56
1:0:211:ARG:NH1	1:0:212:THR:O	2.39	0.56
19:R:111:SER:OG	19:R:112:GLU:N	2.37	0.56
6:A:364:TYR:HB3	6:A:430:LEU:HD23	1.87	0.56
6:A:459:ASN:ND2	6:A:485:ASP:OD1	2.38	0.56
18:Q:336:PHE:HB2	18:Q:339:LEU:HB3	1.88	0.56
22:U:118:ILE:HA	22:U:121:ALA:HB3	1.87	0.56
28:c:1071:VAL:HG21	28:c:1127:SER:HB2	1.88	0.56
29:d:237:LYS:NZ	29:d:242:ILE:O	2.39	0.56
24:W:467:LEU:HD11	24:W:491:PRO:HB3	1.88	0.56
24:W:867:LEU:HD12	24:W:966:VAL:HG22	1.88	0.56
25:X:905:PHE:HA	25:X:908:ILE:HD12	1.87	0.56
17:P:579:ARG:HD2	17:P:600:LYS:HE3	1.88	0.56
24:W:384:ILE:HG23	24:W:385:GLN:HG2	1.88	0.56
25:X:294:ILE:HD13	25:X:351:ALA:HA	1.87	0.56
29:d:1640:VAL:HG22	29:d:1686:SER:HB3	1.86	0.56
10:G:96:LEU:HD21	15:N:132:THR:HG21	1.88	0.56
13:J:75:ARG:HD2	13:J:79:LEU:HD22	1.87	0.56
21:T:28:LEU:HD12	21:T:31:LEU:HD12	1.87	0.56
25:X:43:ALA:HA	25:X:46:LEU:HD12	1.86	0.56
25:X:284:GLU:HA	25:X:287:LYS:HG2	1.88	0.56
28:c:247:GLY:HA2	28:c:1644:GLN:HE21	1.69	0.56
15:N:669:GLN:HG3	15:N:685:LEU:HD21	1.88	0.56
15:N:717:ASN:HD21	18:Q:552:SER:HA	1.71	0.56
17:P:436:LEU:HD13	17:P:443:LEU:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:104:HIS:HA	5:4:110:ARG:HH22	1.71	0.56
6:A:489:CYS:HA	6:A:514:LYS:HD3	1.88	0.56
10:G:96:LEU:HB2	13:J:102:MET:CE	2.33	0.56
19:R:95:ASP:O	19:R:98:ARG:NH1	2.39	0.56
25:X:505:GLN:HB3	25:X:672:ARG:HE	1.71	0.56
6:A:446:SER:HB3	6:A:449:ARG:HE	1.71	0.55
7:B:11:UNK:O	7:B:15:UNK:N	2.40	0.55
15:N:471:ASP:N	15:N:471:ASP:OD1	2.36	0.55
24:W:308:VAL:HG22	24:W:334:LEU:HD21	1.88	0.55
24:W:985:GLU:HA	24:W:1025:LYS:HG2	1.86	0.55
27:b:207:VAL:HG13	28:c:72:ASN:HD22	1.71	0.55
25:X:506:THR:OG1	25:X:672:ARG:NH2	2.38	0.55
28:c:474:SER:O	28:c:483:ARG:NH2	2.40	0.55
4:3:88:LEU:HA	4:3:91:LYS:HG2	1.89	0.55
8:D:86:GLN:CD	12:I:106:GLY:CA	2.65	0.55
17:P:781:HIS:O	17:P:784:ARG:NH2	2.40	0.55
18:Q:209:TYR:C	18:Q:214:SER:OG	2.50	0.55
24:W:516:ALA:HA	24:W:558:ALA:HB3	1.88	0.55
28:c:413:PHE:HZ	29:d:339:PRO:HB2	1.71	0.55
29:d:1457:ARG:HA	29:d:1673:MET:HE1	1.89	0.55
10:G:84:SER:O	10:G:88:ASN:ND2	2.38	0.55
15:N:804:ASN:HD21	15:N:807:LYS:HB2	1.70	0.55
21:T:119:TYR:O	21:T:122:PHE:HB2	2.07	0.55
24:W:1082:LYS:HG3	24:W:1084:PRO:HD2	1.86	0.55
29:d:338:ASP:OD1	29:d:338:ASP:N	2.33	0.55
25:X:610:LYS:O	25:X:659:TYR:OH	2.24	0.55
15:N:374:HIS:ND1	15:N:379:PRO:CG	2.70	0.55
19:R:34:SER:O	19:R:37:HIS:HB2	2.07	0.55
24:W:294:LYS:NZ	24:W:344:PHE:O	2.39	0.55
24:W:886:ILE:HG21	24:W:970:VAL:HG11	1.87	0.55
25:X:912:LEU:HD22	25:X:954:GLU:HB3	1.88	0.55
28:c:1338:ASN:ND2	28:c:1380:GLU:OE2	2.40	0.55
29:d:1799:ASP:HB2	29:d:1801:ARG:HG2	1.89	0.55
8:D:30:LEU:HD22	12:I:99:LYS:HG2	1.89	0.55
10:G:131:ALA:HB1	15:N:154:ILE:CD1	2.34	0.55
2:1:143:LEU:HD21	23:V:119:LEU:CG	2.36	0.55
11:H:8:LEU:HG	11:H:69:PRO:HG3	1.89	0.55
15:N:279:GLN:HA	15:N:282:LEU:HB2	1.87	0.55
15:N:371:GLN:CD	15:N:373:PHE:HE2	2.15	0.55
17:P:750:LEU:HA	17:P:754:ARG:HH21	1.72	0.55
18:Q:216:PHE:CE2	18:Q:306:GLU:HG3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:145:VAL:HG22	19:R:169:VAL:HG13	1.89	0.55
27:b:46:ASN:OD1	27:b:185:ARG:NH2	2.40	0.55
29:d:1732:VAL:CG1	29:d:1734:THR:HG23	2.37	0.55
15:N:535:LYS:NZ	15:N:536:ASN:OD1	2.39	0.55
15:N:711:ARG:HD3	18:Q:549:LEU:HB3	1.88	0.55
17:P:312:ARG:O	17:P:340:ARG:NH2	2.40	0.55
20:S:112:LEU:HB3	20:S:113:PRO:HD3	1.88	0.55
25:X:251:GLU:HG3	25:X:263:LEU:HD13	1.89	0.55
25:X:539:ILE:HG12	25:X:629:ARG:HG2	1.87	0.55
28:c:527:LYS:HA	28:c:530:GLU:HG2	1.88	0.55
29:d:1809:ASP:HB2	29:d:1814:LEU:HG	1.89	0.55
10:G:96:LEU:O	15:N:129:PHE:HZ	1.89	0.54
17:P:364:THR:OG1	17:P:367:ASP:HB2	2.07	0.54
18:Q:5:ARG:HG3	18:Q:7:VAL:HG13	1.89	0.54
24:W:213:ARG:NH1	25:X:759:GLU:OE1	2.38	0.54
28:c:120:LEU:O	28:c:155:ARG:NE	2.40	0.54
6:A:288:PHE:HB2	6:A:296:SER:HB2	1.89	0.54
8:D:174:ARG:NH1	8:D:176:TYR:OH	2.40	0.54
10:G:97:ILE:CG1	13:J:102:MET:SD	2.86	0.54
24:W:941:VAL:HG12	24:W:943:PRO:HD2	1.89	0.54
25:X:135:THR:HG22	25:X:161:CYS:HB3	1.88	0.54
25:X:472:ASN:HD22	25:X:525:PHE:HB2	1.72	0.54
28:c:519:ARG:HH22	28:c:521:ARG:HH21	1.55	0.54
28:c:877:PHE:HA	28:c:880:MET:HE1	1.88	0.54
1:O:133:LEU:HG	1:O:135:ARG:HH12	1.72	0.54
8:D:186:LEU:HB3	8:D:190:MET:HE3	1.89	0.54
9:F:61:ASN:OD1	9:F:86:ARG:NH2	2.40	0.54
15:N:217:VAL:HA	15:N:222:VAL:HA	1.89	0.54
15:N:443:LEU:HG	15:N:500:LEU:HD23	1.89	0.54
18:Q:489:LYS:O	18:Q:507:ARG:NH1	2.40	0.54
1:O:260:ASP:OD2	1:O:264:ARG:NH2	2.41	0.54
15:N:250:LEU:HD22	15:N:271:ILE:HG23	1.88	0.54
24:W:1153:ILE:HG12	24:W:1161:TRP:HB3	1.89	0.54
29:d:11:SER:N	29:d:1951:THR:OG1	2.41	0.54
29:d:1395:ILE:HG21	29:d:1711:LEU:HB3	1.89	0.54
29:d:1416:MET:HE1	29:d:1418:VAL:HG13	1.88	0.54
12:I:109:LEU:HD23	12:I:114:GLN:NE2	2.16	0.54
15:N:376:PRO:HB2	15:N:377:PRO:HD3	1.88	0.54
19:R:150:ARG:HB2	19:R:163:LEU:HD12	1.89	0.54
25:X:472:ASN:HA	25:X:475:THR:HG22	1.88	0.54
9:F:80:ILE:O	9:F:82:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:761:LYS:HA	15:N:764:GLU:HB2	1.89	0.54
17:P:131:ILE:HA	17:P:183:THR:HA	1.89	0.54
17:P:359:LEU:HD22	17:P:378:PRO:HG2	1.90	0.54
17:P:656:ARG:HG2	17:P:693:LEU:HD13	1.90	0.54
27:b:171:MET:O	27:b:209:GLN:NE2	2.41	0.54
1:0:241:LYS:NZ	1:0:295:THR:OG1	2.39	0.54
3:2:185:VAL:HG12	3:2:186:THR:HG23	1.89	0.54
6:A:322:GLN:HG2	6:A:329:LEU:H	1.73	0.54
8:D:97:GLU:HA	8:D:100:VAL:HG22	1.90	0.54
15:N:358:THR:CG2	15:N:375:ASP:OD2	2.47	0.54
18:Q:138:LYS:HB3	18:Q:143:THR:HG21	1.89	0.54
24:W:373:MET:O	24:W:377:LEU:N	2.38	0.54
24:W:688:ILE:HD11	24:W:719:ILE:HG21	1.89	0.54
26:a:330:MET:SD	26:a:331:GLN:NE2	2.81	0.54
6:A:210:TYR:HB3	6:A:223:LYS:HB2	1.90	0.54
15:N:683:ARG:HD2	16:O:684:ARG:CG	2.38	0.54
17:P:248:VAL:HA	17:P:253:CYS:HA	1.89	0.54
17:P:796:LYS:NZ	17:P:824:ILE:O	2.41	0.54
25:X:113:LYS:HG3	25:X:116:GLU:H	1.71	0.54
25:X:657:GLN:O	25:X:662:ARG:NH2	2.41	0.54
26:a:1:MET:N	27:b:80:SER:O	2.41	0.54
28:c:1593:THR:O	28:c:1609:ASN:N	2.41	0.54
18:Q:216:PHE:CD2	18:Q:306:GLU:CG	2.90	0.54
9:F:65:GLY:O	9:F:86:ARG:NH1	2.42	0.53
15:N:356:LYS:H	15:N:376:PRO:HD2	1.72	0.53
24:W:581:ILE:HA	24:W:584:PHE:HB2	1.90	0.53
24:W:732:LEU:HG	24:W:740:GLN:HG2	1.89	0.53
24:W:978:LEU:O	24:W:981:SER:OG	2.22	0.53
24:W:1127:LEU:O	24:W:1131:LEU:N	2.31	0.53
28:c:1419:SER:HB2	28:c:1422:ARG:HH21	1.74	0.53
29:d:1126:PHE:HE1	29:d:1131:ASN:HD22	1.56	0.53
15:N:882:ILE:HG23	15:N:916:LEU:HD21	1.90	0.53
15:N:925:ASP:HB3	15:N:927:TYR:HE1	1.73	0.53
15:N:942:SER:OG	15:N:945:ASP:O	2.25	0.53
25:X:783:LEU:HA	25:X:787:ILE:HD12	1.90	0.53
26:a:60:SER:H	26:a:63:ALA:HB3	1.72	0.53
5:4:28:LEU:HD11	5:4:76:LEU:HD13	1.91	0.53
15:N:1316:CYS:O	15:N:1320:MET:N	2.36	0.53
17:P:595:VAL:HG12	17:P:599:LEU:HD21	1.90	0.53
22:U:3:ASP:O	22:U:6:THR:OG1	2.25	0.53
24:W:148:ILE:O	24:W:198:HIS:NE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:501:GLY:HA3	24:W:517:SER:HB3	1.90	0.53
24:W:1050:LYS:O	24:W:1054:ASN:ND2	2.41	0.53
4:3:92:LEU:HA	4:3:95:VAL:HG22	1.90	0.53
15:N:808:LEU:HB3	15:N:822:ILE:HB	1.90	0.53
21:T:47:HIS:O	21:T:103:GLN:N	2.41	0.53
15:N:376:PRO:HD2	15:N:377:PRO:CD	2.37	0.53
18:Q:589:GLY:O	18:Q:591:LYS:NZ	2.42	0.53
19:R:156:ASN:HD22	19:R:156:ASN:C	2.14	0.53
29:d:1290:GLN:HE22	29:d:1303:GLY:HA2	1.73	0.53
2:1:139:TRP:HD1	23:V:119:LEU:HD13	1.74	0.53
15:N:493:ILE:HA	15:N:496:LEU:HB2	1.91	0.53
2:1:89:ARG:HD3	18:Q:544:MET:CG	2.29	0.53
8:D:104:ASP:OD2	8:D:108:GLN:NE2	2.42	0.53
17:P:359:LEU:HD13	17:P:378:PRO:HB2	1.90	0.53
15:N:737:ARG:NH1	15:N:803:TYR:O	2.42	0.53
21:T:116:ARG:HD2	21:T:125:LYS:HZ3	1.74	0.53
6:A:208:VAL:HG12	6:A:222:LEU:CD1	2.38	0.53
15:N:458:LEU:HD21	18:Q:325:ILE:CG2	2.39	0.53
18:Q:404:ARG:HH21	18:Q:421:LEU:HD21	1.74	0.53
24:W:296:ARG:NH2	24:W:348:SER:OG	2.42	0.53
25:X:414:GLU:HG3	25:X:415:PRO:HD3	1.90	0.53
28:c:604:ILE:HD13	28:c:740:ILE:HG12	1.89	0.53
8:D:118:GLU:HG2	22:U:122:LEU:HD12	1.89	0.53
15:N:675:GLY:HA3	18:Q:622:PHE:CE1	2.44	0.53
15:N:700:ALA:O	15:N:704:SER:N	2.41	0.53
27:b:156:TYR:OH	27:b:181:ASN:OD1	2.27	0.53
28:c:88:ASP:HB3	28:c:1703:GLY:HA3	1.90	0.53
8:D:39:VAL:HA	8:D:42:ARG:HD2	1.91	0.52
15:N:376:PRO:N	15:N:377:PRO:CD	2.72	0.52
2:1:69:ASP:N	2:1:71:GLU:OE1	2.42	0.52
6:A:187:MET:HB3	6:A:208:VAL:HG21	1.90	0.52
6:A:206:GLY:O	6:A:412:ARG:NH1	2.42	0.52
15:N:703:ARG:HH22	18:Q:614:LYS:CG	2.20	0.52
17:P:208:ARG:NH2	25:X:680:GLN:O	2.42	0.52
25:X:408:GLN:HA	25:X:411:LEU:HB2	1.91	0.52
28:c:828:ASP:N	28:c:828:ASP:OD1	2.43	0.52
1:0:211:ARG:HH11	1:0:212:THR:H	1.58	0.52
15:N:678:PHE:HE1	18:Q:581:SER:HB2	1.75	0.52
15:N:845:SER:OG	15:N:846:ASN:N	2.41	0.52
15:N:1212:GLY:HA2	15:N:1215:ILE:HG22	1.91	0.52
17:P:402:MET:HE1	17:P:461:MET:HE1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:50:ARG:NH1	23:V:53:GLN:OE1	2.43	0.52
24:W:349:PHE:HD2	24:W:391:ASP:HB3	1.73	0.52
25:X:179:HIS:ND1	25:X:225:ILE:O	2.43	0.52
29:d:1133:LYS:HG3	29:d:1222:ARG:CZ	2.40	0.52
1:O:40:ARG:HA	17:P:790:CYS:HB3	1.90	0.52
15:N:806:ARG:HH12	15:N:824:TRP:H	1.58	0.52
17:P:738:LEU:HB3	17:P:742:LEU:HD23	1.90	0.52
18:Q:152:SER:OG	23:V:61:MET:SD	2.68	0.52
24:W:234:SER:HB2	24:W:660:GLU:HB3	1.91	0.52
25:X:424:MET:HE1	25:X:435:LEU:HD13	1.91	0.52
28:c:247:GLY:HA3	28:c:1646:ARG:HH12	1.73	0.52
6:A:178:GLN:HA	6:A:181:GLU:HB2	1.90	0.52
15:N:334:CYS:HB2	15:N:360:LYS:HG2	1.90	0.52
15:N:465:LEU:HD12	15:N:478:MET:HG3	1.91	0.52
21:T:66:MET:HE1	21:T:190:MET:CE	2.39	0.52
28:c:1545:ASP:O	28:c:1548:GLN:NE2	2.39	0.52
2:1:56:PHE:CE2	3:2:185:VAL:HG21	2.44	0.52
8:D:117:ALA:HB1	10:G:163:MET:SD	2.49	0.52
15:N:541:LYS:HE2	15:N:547:GLN:H	1.74	0.52
24:W:27:MET:N	24:W:27:MET:SD	2.83	0.52
24:W:1216:TRP:O	24:W:1258:ARG:NH1	2.42	0.52
28:c:21:PRO:HB2	28:c:24:VAL:HB	1.90	0.52
8:D:106:ASP:OD1	8:D:109:GLN:NE2	2.42	0.52
13:J:61:ILE:O	15:N:50:ARG:N	2.42	0.52
15:N:192:LEU:HD23	15:N:195:LEU:HD12	1.92	0.52
15:N:445:PRO:O	15:N:504:ARG:NH2	2.43	0.52
15:N:480:LYS:O	15:N:484:ASP:N	2.41	0.52
21:T:136:ARG:NH1	21:T:205:GLN:O	2.43	0.52
6:A:398:PHE:HB2	6:A:403:ARG:HB2	1.91	0.52
8:D:127:GLN:OE1	10:G:152:ARG:NH2	2.43	0.52
14:K:76:GLY:O	14:K:77:GLN:NE2	2.43	0.52
15:N:308:LEU:CD1	15:N:370:LEU:HD11	2.21	0.52
15:N:370:LEU:O	15:N:392:ILE:HD11	2.10	0.52
15:N:639:LYS:CE	18:Q:562:SER:HA	2.39	0.52
24:W:793:LEU:HG	24:W:803:ILE:HG12	1.92	0.52
25:X:352:ASP:OD2	25:X:389:ARG:NH1	2.43	0.52
6:A:317:PHE:HA	6:A:320:LYS:HD2	1.91	0.52
15:N:457:ASP:OD1	15:N:457:ASP:N	2.42	0.52
18:Q:224:VAL:HG22	18:Q:245:VAL:HG12	1.91	0.52
18:Q:546:TRP:HA	18:Q:574:PRO:HD3	1.90	0.52
24:W:1046:ASP:OD1	24:W:1046:ASP:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:633:LEU:HA	25:X:636:ARG:HD2	1.92	0.52
6:A:357:LEU:HD13	6:A:427:ARG:HH21	1.75	0.52
10:G:43:MET:HE3	10:G:45:PHE:HB2	1.92	0.52
15:N:751:ASN:ND2	15:N:755:GLU:O	2.43	0.52
17:P:310:SER:OG	17:P:312:ARG:NH1	2.43	0.52
28:c:1148:ARG:NH2	28:c:1149:CYS:SG	2.83	0.52
6:A:187:MET:HB3	6:A:208:VAL:CG2	2.40	0.51
17:P:483:VAL:HG13	17:P:484:THR:HG23	1.91	0.51
24:W:735:PHE:O	24:W:740:GLN:NE2	2.43	0.51
25:X:558:VAL:O	25:X:562:ASN:ND2	2.43	0.51
25:X:637:GLU:HA	25:X:640:LEU:HD12	1.92	0.51
29:d:1962:VAL:HG12	29:d:2066:GLY:HA3	1.92	0.51
15:N:376:PRO:HD2	15:N:377:PRO:HD2	1.91	0.51
15:N:403:ASP:O	15:N:407:ALA:N	2.38	0.51
18:Q:226:LYS:NZ	18:Q:242:PRO:O	2.43	0.51
25:X:162:LEU:HD21	25:X:211:LEU:HD22	1.91	0.51
25:X:530:GLN:HG3	25:X:531:THR:HG23	1.92	0.51
2:1:139:TRP:HE1	23:V:122:GLU:HB2	1.75	0.51
15:N:372:ILE:N	15:N:372:ILE:CD1	2.73	0.51
15:N:680:HIS:CD2	18:Q:557:LEU:HD11	2.45	0.51
15:N:737:ARG:HH22	15:N:805:TYR:HE1	1.58	0.51
15:N:1177:LEU:HD23	15:N:1181:ALA:HB3	1.92	0.51
21:T:36:GLN:OE1	21:T:118:GLN:NE2	2.43	0.51
24:W:188:ARG:NH1	24:W:193:GLU:OE2	2.43	0.51
26:a:82:GLN:HA	29:d:1733:LYS:NZ	2.26	0.51
29:d:1794:TYR:HD2	29:d:1803:ILE:HD11	1.76	0.51
6:A:379:ASP:HA	6:A:387:SER:HB3	1.92	0.51
10:G:51:CYS:HB3	10:G:54:LEU:HD21	1.92	0.51
15:N:781:LEU:HD12	15:N:782:GLU:HG3	1.91	0.51
16:O:636:HIS:HE1	17:P:616:GLN:HG2	1.76	0.51
1:0:137:ALA:H	18:Q:486:GLN:HG3	1.74	0.51
6:A:343:ILE:HA	6:A:346:PHE:HB3	1.92	0.51
15:N:918:PHE:N	15:N:922:TYR:O	2.44	0.51
17:P:218:ILE:HG12	17:P:228:VAL:HG12	1.92	0.51
17:P:663:ARG:NH2	17:P:684:ASP:OD2	2.44	0.51
24:W:1049:LEU:HA	24:W:1053:MET:HE1	1.93	0.51
27:b:57:LEU:HD22	27:b:61:VAL:HG21	1.93	0.51
29:d:29:LYS:HG2	29:d:106:VAL:HG12	1.93	0.51
6:A:338:PRO:HA	6:A:389:GLN:HA	1.92	0.51
15:N:806:ARG:NH2	15:N:824:TRP:O	2.34	0.51
21:T:66:MET:HE1	21:T:190:MET:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:a:77:ASN:ND2	26:a:137:ASP:OD1	2.40	0.51
10:G:90:LEU:HD21	13:J:109:LEU:CG	2.41	0.51
15:N:707:ASP:CG	16:O:684:ARG:NH1	2.69	0.51
19:R:82:PRO:HG2	19:R:109:ALA:HB1	1.92	0.51
24:W:271:ARG:HH12	24:W:307:LEU:HA	1.75	0.51
24:W:1018:ASP:OD1	24:W:1018:ASP:N	2.43	0.51
25:X:737:HIS:HB2	25:X:831:ARG:HD3	1.92	0.51
25:X:776:MET:HA	25:X:779:VAL:HG22	1.91	0.51
28:c:519:ARG:HH11	28:c:522:ALA:HB2	1.75	0.51
3:2:123:ALA:HA	3:2:126:CYS:HB2	1.92	0.51
15:N:384:LYS:O	15:N:388:ARG:N	2.39	0.51
17:P:702:ASP:HB3	17:P:705:PRO:HB3	1.92	0.51
26:a:71:ARG:CZ	29:d:1734:THR:HA	2.40	0.51
29:d:1198:ASN:HD22	29:d:1198:ASN:C	2.17	0.51
2:1:71:GLU:HG3	2:1:74:ARG:HH21	1.76	0.51
2:1:128:LEU:O	2:1:132:HIS:N	2.30	0.51
11:H:155:SER:O	11:H:159:ARG:NH1	2.43	0.51
15:N:445:PRO:HG2	15:N:635:CYS:HB3	1.93	0.51
15:N:507:GLN:NE2	15:N:636:ALA:O	2.44	0.51
15:N:589:GLN:HA	24:W:26:PHE:HE1	1.75	0.51
24:W:569:ARG:NH2	24:W:912:TRP:O	2.44	0.51
25:X:498:LEU:HD22	25:X:665:ILE:HG23	1.93	0.51
25:X:612:LYS:HD2	25:X:656:LEU:HD21	1.92	0.51
25:X:628:VAL:HG11	25:X:677:VAL:HG13	1.93	0.51
25:X:753:LEU:HD22	25:X:800:SER:HB2	1.92	0.51
28:c:1504:TYR:O	28:c:1508:HIS:ND1	2.44	0.51
29:d:1855:SER:O	29:d:1855:SER:OG	2.29	0.51
15:N:683:ARG:HH11	15:N:685:LEU:HD23	1.76	0.51
15:N:723:GLU:HG2	15:N:744:HIS:HB2	1.92	0.51
18:Q:103:ARG:HE	18:Q:106:LEU:HD22	1.76	0.51
21:T:116:ARG:HA	21:T:124:VAL:O	2.11	0.51
28:c:1537:LEU:HA	28:c:1540:VAL:HG22	1.93	0.51
28:c:1731:ARG:NH1	29:d:1752:ASP:O	2.44	0.51
29:d:1130:MET:SD	29:d:1130:MET:C	2.94	0.51
29:d:1263:PRO:HA	29:d:1266:LYS:HE3	1.92	0.51
29:d:1411:LEU:H	29:d:1411:LEU:HD23	1.75	0.51
1:0:18:ILE:HD12	1:0:21:ILE:HD11	1.93	0.50
6:A:81:LEU:HD11	6:A:142:LEU:HD11	1.92	0.50
21:T:28:LEU:O	21:T:32:GLY:N	2.41	0.50
24:W:1034:LEU:HD13	24:W:1038:ARG:HH11	1.75	0.50
25:X:282:VAL:HG21	25:X:334:VAL:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:c:499:ASP:OD1	28:c:499:ASP:N	2.43	0.50
8:D:79:LEU:O	8:D:83:ALA:N	2.40	0.50
17:P:588:THR:OG1	17:P:701:ARG:NH1	2.43	0.50
24:W:803:ILE:HB	24:W:940:GLN:HE22	1.77	0.50
6:A:258:THR:H	6:A:306:LYS:NZ	2.09	0.50
15:N:121:PHE:HE1	15:N:125:GLN:HE21	1.57	0.50
15:N:154:ILE:N	15:N:155:PRO:CD	2.74	0.50
15:N:225:ARG:HE	15:N:227:GLU:HG3	1.77	0.50
15:N:376:PRO:CD	15:N:377:PRO:CD	2.89	0.50
24:W:1172:ILE:O	24:W:1244:GLN:NE2	2.44	0.50
27:b:42:ILE:HD13	27:b:241:TRP:HE1	1.76	0.50
5:4:29:ALA:HB2	5:4:72:CYS:HB3	1.94	0.50
6:A:506:VAL:HG22	6:A:509:ARG:HH22	1.77	0.50
19:R:129:PHE:HB2	19:R:148:ILE:HG23	1.93	0.50
24:W:891:LEU:O	24:W:897:ARG:NH2	2.43	0.50
24:W:964:LEU:HD13	24:W:994:LEU:HG	1.93	0.50
25:X:274:GLN:CD	25:X:276:ILE:HD11	2.35	0.50
28:c:785:LYS:HB3	28:c:866:HIS:HB2	1.93	0.50
2:1:128:LEU:HB3	23:V:133:GLU:HG2	1.93	0.50
10:G:100:PRO:O	15:N:128:LEU:HD23	2.10	0.50
15:N:536:ASN:HB3	15:N:554:MET:HE3	1.93	0.50
17:P:345:THR:HB	17:P:400:GLN:HA	1.93	0.50
2:1:89:ARG:CD	18:Q:544:MET:HG2	2.30	0.50
6:A:320:LYS:HB3	6:A:410:LEU:HD13	1.94	0.50
15:N:545:LEU:HD12	15:N:652:MET:HG3	1.93	0.50
17:P:311:LEU:HD13	17:P:339:TRP:CE2	2.47	0.50
17:P:585:THR:HA	17:P:697:TRP:HH2	1.77	0.50
18:Q:397:SER:HB2	19:R:73:ARG:HH21	1.77	0.50
21:T:184:TYR:OH	21:T:192:GLN:OE1	2.30	0.50
24:W:506:ARG:HH22	24:W:557:VAL:HG13	1.75	0.50
24:W:1047:THR:HA	24:W:1050:LYS:HD2	1.94	0.50
25:X:517:ARG:HG2	25:X:523:PRO:HD3	1.94	0.50
8:D:109:GLN:NE2	10:G:174:ASP:HB3	2.22	0.50
25:X:951:THR:HA	25:X:954:GLU:HG2	1.93	0.50
29:d:1411:LEU:HD21	29:d:1414:GLY:HA2	1.94	0.50
8:D:104:ASP:HA	8:D:107:ILE:HD12	1.94	0.50
10:G:145:GLN:HA	10:G:148:GLU:HG3	1.94	0.50
21:T:38:THR:HG22	21:T:115:THR:HG22	1.94	0.50
24:W:94:PRO:HG2	24:W:128:GLY:HA3	1.94	0.50
25:X:274:GLN:CG	25:X:276:ILE:HD11	2.41	0.50
2:1:143:LEU:CD2	23:V:119:LEU:HG	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:168:LEU:HD23	10:G:171:LEU:HD13	1.94	0.50
15:N:722:ALA:O	15:N:747:LEU:N	2.43	0.50
24:W:700:PHE:HA	24:W:1222:GLY:HA3	1.94	0.50
25:X:271:LYS:HG3	25:X:276:ILE:HB	1.94	0.50
26:a:186:PRO:HG2	26:a:189:ASP:HB2	1.94	0.50
1:0:201:ILE:HD13	1:0:228:LEU:HD22	1.93	0.49
2:1:125:LYS:CE	23:V:137:SER:HB2	2.34	0.49
5:4:19:GLN:NE2	8:D:190:MET:SD	2.85	0.49
8:D:129:LYS:HD3	8:D:132:LEU:HD12	1.94	0.49
15:N:712:LEU:O	18:Q:550:SER:HA	2.11	0.49
17:P:60:ARG:O	17:P:78:SER:OG	2.30	0.49
17:P:220:PHE:HD1	17:P:289:ASP:HA	1.77	0.49
4:3:136:SER:O	4:3:139:ARG:NE	2.45	0.49
5:4:40:ARG:NH1	10:G:17:TYR:OH	2.45	0.49
6:A:188:ALA:O	6:A:202:LYS:NZ	2.45	0.49
6:A:343:ILE:O	6:A:347:GLU:N	2.45	0.49
9:F:169:SER:OG	15:N:263:ARG:NH2	2.45	0.49
15:N:221:ARG:HB3	15:N:233:THR:HB	1.93	0.49
15:N:376:PRO:CB	15:N:377:PRO:HD3	2.42	0.49
15:N:937:ARG:HE	15:N:943:LEU:HG	1.76	0.49
15:N:1301:ALA:O	15:N:1305:LEU:N	2.43	0.49
17:P:12:MET:N	17:P:458:SER:HG	2.09	0.49
24:W:16:GLU:OE1	24:W:19:GLU:N	2.44	0.49
24:W:620:ARG:NH2	24:W:652:LEU:O	2.45	0.49
24:W:797:LEU:HA	24:W:801:ASP:H	1.78	0.49
27:b:196:MET:HG2	27:b:226:LYS:HE2	1.92	0.49
28:c:778:ILE:O	28:c:851:ASN:ND2	2.45	0.49
6:A:441:GLU:OE1	6:A:453:SER:OG	2.30	0.49
10:G:90:LEU:CD2	13:J:109:LEU:HD12	2.36	0.49
10:G:90:LEU:HD23	13:J:109:LEU:CD1	2.34	0.49
10:G:109:LEU:HD22	15:N:135:ARG:NE	2.26	0.49
10:G:143:LYS:HA	10:G:146:ARG:HE	1.77	0.49
11:H:140:ILE:HG21	18:Q:146:LEU:HA	1.92	0.49
17:P:106:LYS:HE2	17:P:123:GLY:HA3	1.95	0.49
18:Q:366:ASP:N	18:Q:366:ASP:OD1	2.43	0.49
19:R:40:ARG:HH12	23:V:98:ILE:HD11	1.78	0.49
24:W:1203:MET:HG3	24:W:1205:CYS:H	1.78	0.49
2:1:132:HIS:O	2:1:136:LEU:N	2.40	0.49
15:N:722:ALA:HB3	15:N:747:LEU:HB2	1.93	0.49
17:P:14:ASP:O	17:P:456:ARG:N	2.40	0.49
17:P:182:VAL:HG23	17:P:218:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:21:TYR:HB2	19:R:173:VAL:HB	1.95	0.49
24:W:238:CYS:HG	24:W:240:SER:HG	1.59	0.49
24:W:1295:CYS:HA	24:W:1298:LEU:HD12	1.93	0.49
8:D:87:GLY:O	8:D:91:HIS:ND1	2.38	0.49
15:N:361:ILE:CD1	15:N:370:LEU:HD23	2.40	0.49
17:P:535:LYS:HD3	17:P:541:VAL:HG23	1.93	0.49
19:R:58:PHE:HB3	19:R:123:PHE:HD2	1.77	0.49
24:W:863:ASP:HB2	24:W:966:VAL:HG21	1.93	0.49
24:W:866:ILE:HG23	24:W:886:ILE:HD12	1.93	0.49
24:W:981:SER:HB3	24:W:1022:LEU:HD22	1.93	0.49
25:X:363:LEU:HD12	25:X:364:LEU:HG	1.95	0.49
28:c:1455:GLN:O	28:c:1465:ARG:NH2	2.44	0.49
29:d:1679:PRO:HA	29:d:1682:LYS:HG2	1.95	0.49
18:Q:595:GLN:NE2	18:Q:619:ARG:O	2.46	0.49
28:c:1042:SER:O	28:c:1049:ASN:ND2	2.45	0.49
28:c:1341:ARG:HG2	28:c:1385:ALA:HB2	1.94	0.49
28:c:1588:VAL:HA	28:c:1591:ASN:HB2	1.93	0.49
29:d:1618:ASP:HB2	29:d:1621:LYS:HB2	1.95	0.49
29:d:2121:LEU:HA	29:d:2129:VAL:HG12	1.94	0.49
10:G:91:ASP:OD2	13:J:124:TYR:OH	2.26	0.49
12:I:86:ASP:OD1	12:I:86:ASP:N	2.45	0.49
13:J:75:ARG:HA	20:S:102:LYS:HG2	1.94	0.49
15:N:946:ASN:HD21	15:N:1169:TRP:CD1	2.31	0.49
18:Q:197:ARG:HH22	18:Q:221:THR:HG22	1.77	0.49
24:W:144:LYS:O	24:W:147:THR:OG1	2.25	0.49
29:d:1675:GLN:HG3	29:d:1676:THR:HG23	1.93	0.49
5:4:23:GLU:O	5:4:27:CYS:N	2.36	0.49
5:4:107:HIS:CE1	15:N:168:ARG:HE	2.31	0.49
6:A:258:THR:H	6:A:306:LYS:HZ1	1.60	0.49
6:A:320:LYS:HD3	6:A:410:LEU:HD22	1.95	0.49
15:N:247:LEU:HB3	15:N:275:HIS:CD2	2.48	0.49
15:N:918:PHE:HB3	15:N:922:TYR:HB2	1.95	0.49
17:P:100:ASP:N	17:P:100:ASP:OD1	2.44	0.49
23:V:130:LEU:C	23:V:130:LEU:CD1	2.86	0.49
24:W:882:CYS:HA	24:W:885:ILE:HD12	1.95	0.49
26:a:259:MET:HE1	26:a:293:LEU:HD22	1.95	0.49
28:c:1376:ASN:HA	28:c:1379:LEU:HB2	1.95	0.49
29:d:1229:CYS:HB3	29:d:1257:LYS:HA	1.95	0.49
15:N:280:SER:O	15:N:284:ALA:N	2.45	0.49
15:N:917:ALA:HA	15:N:923:CYS:HA	1.94	0.49
17:P:204:GLU:OE2	25:X:704:LYS:NZ	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:d:1844:TRP:HZ3	29:d:1879:LEU:HB3	1.77	0.49
15:N:548:TYR:CG	15:N:652:MET:HE1	2.48	0.49
15:N:666:ILE:O	15:N:668:HIS:ND1	2.32	0.49
15:N:699:LYS:O	15:N:703:ARG:N	2.44	0.49
24:W:561:PRO:HA	24:W:564:VAL:HG22	1.95	0.49
28:c:1391:GLN:O	28:c:1395:GLU:N	2.45	0.49
29:d:96:HIS:ND1	29:d:98:ASP:OD1	2.45	0.49
29:d:1732:VAL:HG12	29:d:1734:THR:HG22	1.94	0.49
5:4:46:LYS:HA	5:4:49:VAL:HG22	1.94	0.48
17:P:432:LYS:N	17:P:446:ILE:O	2.43	0.48
17:P:582:GLU:HA	17:P:585:THR:HG22	1.94	0.48
21:T:40:CYS:HA	21:T:112:THR:O	2.14	0.48
24:W:794:TRP:HA	24:W:797:LEU:HG	1.95	0.48
24:W:816:ALA:HA	24:W:819:LEU:HB2	1.95	0.48
25:X:629:ARG:O	25:X:636:ARG:NH2	2.46	0.48
28:c:769:HIS:O	28:c:773:LYS:N	2.43	0.48
2:1:80:CYS:SG	2:1:81:ILE:N	2.85	0.48
3:2:160:TYR:HA	3:2:163:VAL:HG22	1.95	0.48
8:D:112:LYS:HA	8:D:115:LYS:HG2	1.94	0.48
20:S:112:LEU:N	20:S:113:PRO:CD	2.76	0.48
25:X:314:PRO:HB3	25:X:370:GLN:HG3	1.95	0.48
25:X:757:ARG:HE	25:X:760:HIS:CE1	2.32	0.48
28:c:1121:ASP:OD1	28:c:1121:ASP:N	2.45	0.48
5:4:21:GLU:HB3	5:4:58:TRP:CH2	2.48	0.48
6:A:208:VAL:HG12	6:A:222:LEU:HD22	1.95	0.48
6:A:363:PHE:HB2	6:A:374:TYR:HB2	1.94	0.48
6:A:426:LYS:HE3	6:A:505:PRO:HG2	1.94	0.48
15:N:193:HIS:HA	15:N:196:ASN:HB2	1.96	0.48
17:P:71:TRP:HB2	17:P:753:GLY:H	1.78	0.48
17:P:699:CYS:O	17:P:707:SER:OG	2.30	0.48
25:X:303:LEU:HD12	25:X:410:ILE:HD11	1.95	0.48
2:1:135:LYS:HG2	2:1:139:TRP:CZ3	2.34	0.48
7:B:7:UNK:O	7:B:11:UNK:N	2.46	0.48
15:N:849:ASN:HA	15:N:852:LEU:HB2	1.95	0.48
17:P:489:TRP:HH2	17:P:739:VAL:HB	1.76	0.48
24:W:726:ASN:HD22	24:W:750:GLN:HG2	1.79	0.48
24:W:966:VAL:HA	24:W:969:ILE:HG22	1.95	0.48
24:W:1252:VAL:HG12	24:W:1256:LEU:HG	1.94	0.48
28:c:1165:SER:O	28:c:1169:ALA:N	2.46	0.48
29:d:2154:SER:OG	29:d:2155:CYS:N	2.45	0.48
5:4:22:LEU:HD11	5:4:66:TYR:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:72:PHE:HB3	10:G:74:HIS:CE1	2.49	0.48
10:G:162:GLU:O	10:G:166:ASN:ND2	2.47	0.48
15:N:493:ILE:O	15:N:497:LYS:N	2.46	0.48
17:P:14:ASP:HB2	17:P:456:ARG:HB2	1.95	0.48
18:Q:595:GLN:HG2	18:Q:619:ARG:HB2	1.95	0.48
24:W:503:GLY:HA2	24:W:506:ARG:HH21	1.78	0.48
24:W:1210:ALA:O	24:W:1213:HIS:HB2	2.14	0.48
24:W:1241:THR:HG23	24:W:1243:PHE:H	1.78	0.48
25:X:274:GLN:HG3	25:X:276:ILE:CG1	2.42	0.48
26:a:71:ARG:NH2	27:b:13:GLN:OE1	2.45	0.48
26:a:307:LYS:HE2	26:a:337:GLU:CG	2.42	0.48
28:c:620:SER:OG	28:c:621:ARG:NH1	2.47	0.48
28:c:850:ARG:HA	28:c:853:LEU:HB3	1.95	0.48
28:c:1321:MET:HG3	28:c:1324:ILE:HD12	1.95	0.48
1:0:49:GLU:OE2	1:0:50:LYS:NZ	2.41	0.48
4:3:83:ARG:NH1	4:3:84:GLN:OE1	2.44	0.48
6:A:210:TYR:H	6:A:223:LYS:H	1.61	0.48
15:N:555:LEU:O	15:N:565:SER:N	2.45	0.48
15:N:806:ARG:HG3	15:N:807:LYS:HD2	1.96	0.48
26:a:27:VAL:HG22	26:a:356:ARG:HD2	1.95	0.48
29:d:1337:LEU:HD11	29:d:1768:PRO:HD3	1.96	0.48
29:d:1367:ARG:HE	29:d:1638:ALA:HB2	1.78	0.48
2:1:101:GLN:HG2	2:1:105:GLN:HE22	1.78	0.48
10:G:136:ARG:O	10:G:139:MET:HG3	2.14	0.48
15:N:330:HIS:ND1	15:N:334:CYS:SG	2.84	0.48
15:N:592:LYS:HG2	24:W:25:MET:CE	2.42	0.48
15:N:929:ARG:HE	16:O:655:THR:HG21	1.78	0.48
15:N:1224:ILE:O	15:N:1230:GLN:N	2.47	0.48
24:W:523:LEU:O	24:W:569:ARG:NH1	2.44	0.48
25:X:169:LEU:HD13	25:X:221:LEU:HD22	1.95	0.48
26:a:338:ASP:HB2	26:a:339:PRO:HD2	1.95	0.48
28:c:196:GLU:OE2	28:c:197:GLN:NE2	2.46	0.48
15:N:320:TRP:HB3	15:N:322:ASP:H	1.79	0.48
15:N:495:GLN:HA	15:N:498:PHE:CD2	2.48	0.48
17:P:39:TRP:HE1	17:P:43:ASN:HA	1.79	0.48
17:P:825:LYS:NZ	17:P:826:ASN:OD1	2.39	0.48
19:R:32:LEU:HD21	19:R:145:VAL:HG11	1.96	0.48
24:W:507:ILE:HD12	24:W:508:PRO:HD2	1.95	0.48
28:c:931:ARG:NH2	28:c:1213:ASN:OD1	2.47	0.48
29:d:54:LEU:HG	29:d:1075:LEU:HD21	1.96	0.48
2:1:143:LEU:HD21	23:V:119:LEU:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:81:ASN:ND2	3:2:100:GLN:O	2.42	0.48
6:A:367:LEU:HD13	6:A:509:ARG:HH11	1.78	0.48
11:H:30:ILE:HG23	18:Q:99:ARG:HH12	1.78	0.48
17:P:592:ILE:HG21	17:P:686:MET:HE1	1.95	0.48
17:P:742:LEU:HD13	17:P:748:LEU:HD23	1.96	0.48
24:W:469:MET:HE2	24:W:527:LEU:HD22	1.95	0.48
28:c:583:ASP:N	28:c:583:ASP:OD1	2.46	0.48
5:4:23:GLU:HA	5:4:26:GLN:HB2	1.95	0.48
6:A:208:VAL:CG1	6:A:222:LEU:CD1	2.92	0.48
6:A:462:LEU:HB2	25:X:52:ILE:HG21	1.96	0.48
15:N:301:LEU:HD11	15:N:366:VAL:HG23	1.94	0.48
15:N:807:LYS:HG3	15:N:823:GLN:HB3	1.95	0.48
18:Q:329:ASN:HB3	18:Q:345:LEU:HB3	1.96	0.48
24:W:1005:LEU:HD22	24:W:1026:LEU:HD21	1.96	0.48
24:W:1090:CYS:SG	24:W:1091:ASP:N	2.86	0.48
25:X:193:GLU:HA	25:X:196:LEU:HB3	1.95	0.48
29:d:239:PHE:HD2	29:d:1071:LEU:HD11	1.79	0.48
29:d:1142:LEU:HB2	29:d:1800:GLN:HG3	1.96	0.48
29:d:1732:VAL:HG12	29:d:1734:THR:HG23	1.96	0.48
1:0:163:ASP:OD1	1:0:182:ARG:NH2	2.44	0.47
4:3:167:ILE:HA	4:3:170:ILE:HG22	1.95	0.47
10:G:131:ALA:CB	15:N:154:ILE:HD11	2.36	0.47
10:G:134:THR:HA	10:G:137:VAL:HG22	1.96	0.47
17:P:311:LEU:HD11	17:P:337:LEU:HB3	1.96	0.47
17:P:358:LYS:HB3	17:P:438:TRP:HE3	1.78	0.47
24:W:1322:LYS:O	24:W:1326:LYS:N	2.45	0.47
6:A:187:MET:HA	6:A:190:MET:HB3	1.97	0.47
24:W:755:ASN:O	24:W:759:ASN:ND2	2.47	0.47
28:c:1451:LEU:HD21	28:c:1475:LEU:HD22	1.97	0.47
6:A:222:LEU:HB2	6:A:255:ALA:HB3	1.96	0.47
8:D:136:GLU:O	8:D:140:LYS:NZ	2.47	0.47
9:F:42:ASP:N	9:F:42:ASP:OD1	2.46	0.47
17:P:355:ALA:HB3	17:P:383:ALA:HB3	1.96	0.47
22:U:109:TYR:HA	22:U:112:ASP:HB2	1.97	0.47
24:W:534:HIS:HA	24:W:537:MET:HG3	1.96	0.47
24:W:655:ALA:HA	24:W:1000:ARG:HD2	1.96	0.47
24:W:834:PHE:HB2	24:W:885:ILE:HD11	1.97	0.47
28:c:106:THR:OG1	28:c:135:ILE:O	2.33	0.47
28:c:146:LEU:HD11	28:c:159:LEU:HD23	1.95	0.47
28:c:451:PHE:O	28:c:455:ARG:N	2.47	0.47
29:d:28:ILE:HG22	29:d:107:TRP:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:375:PHE:O	6:A:442:VAL:N	2.47	0.47
15:N:202:ARG:NH2	15:N:243:VAL:O	2.47	0.47
17:P:655:LEU:HD23	17:P:658:LEU:HD21	1.96	0.47
19:R:184:ASP:OD1	19:R:185:ASP:N	2.47	0.47
1:O:30:ARG:NH2	1:O:33:ASP:OD2	2.48	0.47
4:3:45:VAL:O	4:3:48:THR:OG1	2.23	0.47
6:A:496:LYS:O	6:A:500:ARG:N	2.47	0.47
6:A:498:VAL:O	6:A:502:MET:N	2.47	0.47
8:D:44:LEU:HA	8:D:47:MET:HG3	1.95	0.47
15:N:794:LEU:HA	15:N:797:PHE:HB3	1.95	0.47
15:N:1214:VAL:HG22	15:N:1217:ARG:HH21	1.79	0.47
24:W:101:LEU:HD13	24:W:118:THR:HG23	1.95	0.47
24:W:374:TRP:O	24:W:377:LEU:HB3	2.15	0.47
24:W:1064:ASP:OD1	24:W:1064:ASP:N	2.42	0.47
24:W:1273:ALA:O	24:W:1277:MET:HG3	2.15	0.47
17:P:402:MET:SD	17:P:402:MET:C	2.97	0.47
29:d:345:TRP:O	29:d:349:SER:OG	2.30	0.47
29:d:1879:LEU:O	29:d:1884:ASN:ND2	2.47	0.47
2:1:128:LEU:HD11	23:V:129:GLU:OE2	2.14	0.47
6:A:278:HIS:ND1	6:A:279:PRO:CD	2.58	0.47
6:A:464:CYS:HB3	6:A:480:TYR:HB2	1.96	0.47
8:D:154:ARG:HE	8:D:155:ILE:HG23	1.80	0.47
10:G:152:ARG:HA	10:G:155:LYS:HE3	1.95	0.47
11:H:9:GLU:HA	11:H:12:LEU:HG	1.96	0.47
15:N:234:LEU:HD11	15:N:247:LEU:HD12	1.97	0.47
15:N:440:VAL:O	15:N:452:LEU:N	2.46	0.47
18:Q:454:ARG:NH2	18:Q:522:GLN:OE1	2.46	0.47
21:T:129:VAL:HG11	21:T:200:ILE:HG21	1.97	0.47
24:W:1318:ILE:HD11	24:W:1329:LEU:HD22	1.96	0.47
25:X:273:MET:SD	25:X:934:CYS:SG	3.12	0.47
27:b:250:MET:HB2	27:b:254:LEU:HD13	1.95	0.47
28:c:429:LYS:NZ	28:c:433:GLN:OE1	2.44	0.47
29:d:17:CYS:SG	29:d:18:ASN:N	2.88	0.47
29:d:55:SER:OG	29:d:59:ARG:NH2	2.48	0.47
29:d:270:LEU:HA	29:d:275:ARG:HA	1.96	0.47
29:d:1917:MET:HE3	29:d:1918:GLU:H	1.79	0.47
1:O:295:THR:O	1:O:297:ARG:NH1	2.47	0.47
2:1:92:GLU:O	2:1:96:LEU:N	2.37	0.47
6:A:313:VAL:HG12	6:A:414:GLN:HG2	1.97	0.47
6:A:503:SER:O	6:A:507:THR:HG23	2.15	0.47
13:J:85:LEU:HD13	20:S:93:TYR:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:782:GLU:HG2	15:N:785:ARG:HH22	1.80	0.47
17:P:565:ARG:NH1	17:P:566:PRO:O	2.47	0.47
24:W:173:ARG:O	24:W:1328:ARG:NH1	2.46	0.47
25:X:274:GLN:O	25:X:276:ILE:HG13	2.14	0.47
25:X:297:PRO:HG2	25:X:301:GLU:HG3	1.96	0.47
4:3:162:GLN:HB3	14:K:103:LYS:HE3	1.96	0.47
6:A:462:LEU:HD12	25:X:52:ILE:HB	1.97	0.47
6:A:498:VAL:HG13	6:A:502:MET:HA	1.97	0.47
8:D:180:LEU:HD12	8:D:181:GLU:HG2	1.97	0.47
10:G:127:ARG:HH22	22:U:1:MET:H1	1.62	0.47
15:N:269:MET:SD	15:N:270:GLN:NE2	2.88	0.47
15:N:402:ILE:O	15:N:406:HIS:N	2.42	0.47
17:P:30:CYS:HB2	17:P:52:ARG:HG2	1.96	0.47
17:P:345:THR:OG1	17:P:346:ASN:N	2.48	0.47
25:X:169:LEU:O	25:X:175:ARG:NH1	2.48	0.47
28:c:150:THR:O	29:d:1390:ARG:NH1	2.43	0.47
29:d:1277:ASP:N	29:d:1277:ASP:OD1	2.47	0.47
6:A:386:ARG:HD2	6:A:386:ARG:HA	1.60	0.47
15:N:371:GLN:OE1	15:N:373:PHE:CE2	2.61	0.47
15:N:643:HIS:CG	18:Q:560:ILE:HG12	2.48	0.47
27:b:221:SER:OG	28:c:16:ARG:NH1	2.47	0.47
29:d:1859:ARG:HD3	29:d:2121:LEU:HD12	1.96	0.47
2:1:60:VAL:HG11	3:2:182:ALA:HB2	1.98	0.46
6:A:187:MET:CB	6:A:208:VAL:HG21	2.45	0.46
6:A:386:ARG:NH2	6:A:389:GLN:HE21	2.12	0.46
8:D:28:GLU:OE1	12:I:107:ILE:HD12	2.14	0.46
10:G:100:PRO:C	15:N:128:LEU:HD23	2.41	0.46
15:N:574:ASN:HB2	15:N:583:ALA:HA	1.97	0.46
18:Q:42:ARG:HH21	18:Q:46:ARG:HB3	1.80	0.46
19:R:107:ASP:O	21:T:90:ASN:ND2	2.48	0.46
21:T:154:TRP:HZ2	21:T:171:GLY:HA2	1.80	0.46
24:W:153:SER:HA	25:X:916:THR:HA	1.96	0.46
24:W:408:TYR:OH	24:W:452:ARG:NH1	2.40	0.46
24:W:975:LEU:HD22	24:W:1016:LEU:HD21	1.97	0.46
25:X:666:MET:HA	25:X:669:ILE:HD12	1.97	0.46
26:a:340:LEU:CD2	26:a:341:PRO:HD2	2.43	0.46
28:c:961:ARG:HE	28:c:972:LEU:HD12	1.80	0.46
28:c:1715:ALA:HB3	28:c:1718:GLU:HB2	1.97	0.46
29:d:59:ARG:HD2	29:d:94:LEU:HA	1.97	0.46
6:A:59:VAL:HG11	8:D:52:ARG:HD3	1.96	0.46
15:N:224:PHE:HD2	15:N:234:LEU:HD13	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:499:TRP:HA	15:N:502:GLN:HB2	1.96	0.46
17:P:63:HIS:HB3	17:P:73:LEU:HD21	1.98	0.46
20:S:109:LEU:O	20:S:113:PRO:HD3	2.10	0.46
24:W:349:PHE:HA	24:W:352:MET:HE2	1.97	0.46
25:X:543:ASP:HA	25:X:548:ARG:HH12	1.80	0.46
26:a:306:SER:O	26:a:310:HIS:ND1	2.44	0.46
26:a:340:LEU:HD11	29:d:1622:VAL:CG2	2.39	0.46
29:d:1663:THR:H	29:d:2173:MET:HE1	1.79	0.46
1:O:200:VAL:HG22	1:O:214:VAL:HG23	1.97	0.46
15:N:149:LEU:HD21	15:N:152:PHE:HZ	1.81	0.46
15:N:158:ILE:O	15:N:162:THR:OG1	2.31	0.46
24:W:188:ARG:NH2	24:W:256:LEU:O	2.48	0.46
24:W:708:GLN:HA	24:W:713:LYS:HD2	1.98	0.46
24:W:891:LEU:HD23	24:W:897:ARG:HD3	1.98	0.46
28:c:843:GLN:O	28:c:847:GLN:N	2.45	0.46
15:N:521:GLN:NE2	21:T:30:MET:SD	2.88	0.46
15:N:886:PRO:HD2	15:N:904:PHE:HD2	1.80	0.46
23:V:35:GLU:HB3	23:V:64:ARG:HD3	1.98	0.46
24:W:831:VAL:O	24:W:835:SER:OG	2.26	0.46
24:W:1308:ASP:OD1	24:W:1308:ASP:N	2.49	0.46
28:c:97:ASN:OD1	28:c:101:ASN:ND2	2.49	0.46
1:O:73:LEU:HD13	1:O:76:LEU:HD21	1.96	0.46
1:O:121:ALA:HB2	4:3:60:LEU:HD23	1.97	0.46
10:G:154:GLN:HA	10:G:157:LEU:HG	1.97	0.46
11:H:61:LYS:HD2	23:V:53:GLN:HG3	1.98	0.46
15:N:268:SER:HA	15:N:271:ILE:HD12	1.98	0.46
15:N:818:SER:OG	15:N:846:ASN:ND2	2.46	0.46
17:P:102:ASP:H	17:P:130:PRO:HA	1.79	0.46
17:P:180:ILE:HG22	17:P:190:VAL:HG13	1.97	0.46
21:T:191:VAL:O	21:T:194:MET:HG3	2.14	0.46
24:W:623:LEU:HD23	24:W:627:LEU:HD23	1.97	0.46
25:X:975:LEU:HB3	25:X:978:GLY:H	1.80	0.46
28:c:310:ASP:OD1	28:c:310:ASP:N	2.46	0.46
28:c:524:VAL:O	28:c:528:LEU:N	2.46	0.46
29:d:1917:MET:HE2	29:d:2096:LEU:HD12	1.98	0.46
2:1:100:LEU:HD12	2:1:103:SER:HB3	1.96	0.46
2:1:128:LEU:HD13	23:V:133:GLU:CG	2.44	0.46
3:2:96:ASP:N	3:2:96:ASP:OD1	2.44	0.46
3:2:120:LEU:O	3:2:124:HIS:N	2.45	0.46
5:4:61:PRO:HA	5:4:64:ALA:HB3	1.96	0.46
11:H:65:HIS:HB2	23:V:48:VAL:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:183:ILE:HG13	18:Q:46:ARG:CZ	2.46	0.46
15:N:791:PRO:HB2	15:N:793:HIS:CE1	2.51	0.46
24:W:701:PHE:CG	24:W:736:PRO:HB3	2.50	0.46
24:W:732:LEU:HD12	24:W:735:PHE:HD2	1.81	0.46
28:c:302:THR:HG23	28:c:397:LEU:HB2	1.97	0.46
6:A:177:LEU:HD22	6:A:259:ILE:HG12	1.97	0.46
15:N:683:ARG:HE	16:O:684:ARG:HG2	1.79	0.46
17:P:626:LEU:HD22	17:P:727:PRO:HD3	1.98	0.46
24:W:448:PRO:HG2	24:W:451:LEU:HB3	1.96	0.46
25:X:222:ILE:HD12	25:X:225:ILE:HD12	1.97	0.46
25:X:491:LEU:HD23	25:X:491:LEU:HA	1.77	0.46
25:X:831:ARG:HA	25:X:834:LYS:HD2	1.96	0.46
6:A:190:MET:SD	6:A:191:TYR:N	2.88	0.46
15:N:221:ARG:HB2	15:N:223:LYS:HE2	1.98	0.46
17:P:615:GLN:O	17:P:619:GLN:N	2.47	0.46
28:c:1425:VAL:HA	28:c:1428:VAL:HG12	1.98	0.46
1:O:269:TRP:HA	1:O:302:LEU:HD21	1.98	0.46
8:D:73:ASP:OD2	12:I:66:LEU:HD22	2.16	0.46
17:P:735:SER:O	17:P:741:ARG:NH1	2.38	0.46
24:W:57:GLU:OE2	24:W:61:GLN:NE2	2.41	0.46
25:X:757:ARG:HB2	25:X:760:HIS:HB2	1.96	0.46
6:A:340:TYR:CD1	6:A:376:LEU:HB3	2.51	0.46
9:F:171:ILE:HG13	9:F:173:GLN:N	2.29	0.46
15:N:480:LYS:HA	15:N:483:ASN:HB2	1.97	0.46
15:N:783:PHE:O	15:N:787:LEU:N	2.48	0.46
24:W:122:VAL:HA	24:W:125:ILE:HG12	1.98	0.46
24:W:283:VAL:HA	24:W:286:MET:HE2	1.98	0.46
24:W:859:ILE:HG13	24:W:934:PHE:HE1	1.81	0.46
25:X:534:PRO:HB3	25:X:539:ILE:HD12	1.97	0.46
28:c:138:LYS:HE2	28:c:140:GLU:HB2	1.98	0.46
28:c:477:LEU:HD12	28:c:480:LEU:HD12	1.97	0.46
28:c:1136:ILE:HB	28:c:1141:LEU:HD12	1.96	0.46
28:c:1300:LEU:HD11	28:c:1307:LEU:HD12	1.98	0.46
28:c:1367:ILE:HG13	28:c:1368:LYS:HD3	1.98	0.46
8:D:34:LEU:CD1	12:I:96:GLU:HG2	2.47	0.45
15:N:386:VAL:O	15:N:390:MET:HG2	2.16	0.45
16:O:674:ILE:HB	16:O:678:LEU:HD11	1.98	0.45
17:P:383:ALA:HA	17:P:393:ILE:HD12	1.98	0.45
26:a:71:ARG:NH2	29:d:1734:THR:HA	2.31	0.45
28:c:1379:LEU:HD23	28:c:1382:ILE:HD11	1.97	0.45
28:c:1494:GLU:OE2	28:c:1495:GLN:NE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:68:ASN:ND2	16:O:615:GLN:OE1	2.46	0.45
1:0:231:TRP:HZ2	18:Q:467:ILE:HG22	1.81	0.45
6:A:321:LEU:HG	6:A:407:ILE:HD12	1.98	0.45
15:N:340:TRP:CZ2	15:N:405:VAL:HG13	2.50	0.45
15:N:468:TYR:OH	18:Q:515:SER:HB2	2.16	0.45
24:W:796:MET:O	24:W:800:THR:OG1	2.26	0.45
25:X:562:ASN:O	25:X:604:LYS:NZ	2.50	0.45
25:X:968:LEU:HD11	25:X:985:ALA:HB1	1.97	0.45
29:d:61:LEU:O	29:d:129:ARG:NH1	2.49	0.45
2:1:139:TRP:CD1	23:V:119:LEU:HD13	2.51	0.45
6:A:190:MET:O	6:A:194:ALA:N	2.47	0.45
15:N:528:HIS:HE1	15:N:588:LEU:HG	1.81	0.45
16:O:700:ASN:O	25:X:915:ARG:NH2	2.42	0.45
17:P:471:LEU:HD12	17:P:506:LYS:HG3	1.98	0.45
17:P:827:CYS:SG	17:P:828:LEU:N	2.89	0.45
24:W:701:PHE:HB2	24:W:738:PRO:HD2	1.98	0.45
25:X:413:ALA:O	25:X:416:THR:OG1	2.30	0.45
25:X:697:TYR:HE1	25:X:727:ARG:HA	1.82	0.45
28:c:1061:VAL:HA	28:c:1070:ARG:HH12	1.81	0.45
1:0:79:LYS:HG2	3:2:60:TYR:HB3	1.98	0.45
15:N:821:SER:OG	15:N:834:SER:N	2.50	0.45
15:N:875:THR:HB	15:N:879:LEU:HD12	1.98	0.45
18:Q:597:PRO:HA	18:Q:619:ARG:HA	1.97	0.45
28:c:591:VAL:HA	28:c:594:PHE:HB3	1.98	0.45
2:1:121:GLU:HA	2:1:124:ARG:HG2	1.98	0.45
6:A:362:ARG:NH1	6:A:375:PHE:HB2	2.32	0.45
11:H:117:VAL:HA	11:H:120:GLN:HG3	1.98	0.45
15:N:300:CYS:O	15:N:304:GLN:N	2.47	0.45
15:N:770:TRP:O	15:N:774:ALA:N	2.46	0.45
28:c:780:LYS:NZ	28:c:817:ARG:O	2.36	0.45
5:4:109:SER:HB3	8:D:163:ALA:HB3	1.99	0.45
8:D:105:SER:HA	8:D:108:GLN:HB2	1.99	0.45
15:N:648:CYS:O	15:N:652:MET:HG2	2.16	0.45
16:O:723:LEU:HD13	16:O:725:VAL:HG23	1.98	0.45
18:Q:93:TRP:CG	18:Q:94:PRO:HD3	2.50	0.45
24:W:154:SER:HB2	25:X:917:ALA:H	1.82	0.45
25:X:172:THR:HG22	25:X:175:ARG:HH21	1.81	0.45
26:a:150:ARG:NH2	26:a:191:ASP:OD2	2.50	0.45
28:c:581:LEU:HG	28:c:593:PHE:HB2	1.97	0.45
28:c:1125:HIS:HA	28:c:1128:LEU:HB3	1.99	0.45
29:d:1338:LEU:O	29:d:1345:LEU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:134:LYS:NZ	18:Q:486:GLN:O	2.50	0.45
1:0:166:ILE:HG12	1:0:190:LEU:HD21	1.99	0.45
3:2:103:ASP:OD1	3:2:103:ASP:N	2.49	0.45
4:3:177:ARG:NH1	23:V:113:ASP:OD2	2.50	0.45
6:A:445:LEU:HD11	6:A:451:SER:HB3	1.99	0.45
9:F:178:ASP:HA	9:F:181:LEU:HB2	1.99	0.45
15:N:697:THR:HG22	15:N:781:LEU:HD21	1.99	0.45
24:W:214:PRO:HG3	24:W:1186:TYR:HE1	1.81	0.45
28:c:1584:ASP:O	28:c:1587:SER:OG	2.31	0.45
29:d:1730:THR:HG21	29:d:1744:MET:HE1	1.98	0.45
6:A:344:THR:HA	6:A:425:VAL:HG11	1.98	0.45
15:N:929:ARG:HB3	15:N:933:VAL:HB	1.99	0.45
17:P:439:THR:OG1	17:P:490:ASP:OD2	2.34	0.45
18:Q:311:LEU:HD21	18:Q:343:ILE:HG21	1.99	0.45
24:W:311:ALA:HA	24:W:314:ARG:HG2	1.99	0.45
24:W:418:GLN:O	24:W:421:HIS:HB2	2.17	0.45
25:X:672:ARG:NH1	25:X:694:THR:O	2.50	0.45
26:a:336:LEU:HD13	26:a:340:LEU:CD1	2.47	0.45
28:c:826:ALA:O	28:c:882:TYR:OH	2.34	0.45
3:2:76:LYS:HD2	3:2:76:LYS:HA	1.67	0.45
6:A:178:GLN:O	6:A:182:GLN:N	2.39	0.45
6:A:339:LEU:HD23	6:A:342:LEU:HD12	1.98	0.45
6:A:365:ALA:HB3	6:A:372:HIS:HB2	1.99	0.45
11:H:33:LEU:HD21	18:Q:95:TRP:HB3	1.97	0.45
15:N:376:PRO:CD	15:N:377:PRO:HD2	2.47	0.45
15:N:903:CYS:SG	15:N:904:PHE:N	2.90	0.45
15:N:1282:GLU:O	15:N:1286:GLU:N	2.42	0.45
24:W:201:LEU:HD23	24:W:205:VAL:HG11	1.98	0.45
25:X:746:ASN:O	25:X:750:LYS:NZ	2.39	0.45
28:c:362:LEU:HD13	28:c:365:ILE:HD11	1.98	0.45
28:c:863:MET:HE3	28:c:863:MET:HB3	1.81	0.45
6:A:174:TYR:HA	6:A:177:LEU:HB3	1.98	0.45
19:R:70:LEU:HD12	19:R:85:LEU:HB2	1.99	0.45
24:W:67:ILE:HG12	24:W:79:LEU:HD13	1.97	0.45
28:c:295:ARG:NE	28:c:376:ALA:O	2.51	0.45
28:c:858:SER:OG	28:c:863:MET:SD	2.72	0.45
29:d:235:GLU:HB3	29:d:1071:LEU:HD22	1.98	0.45
29:d:1133:LYS:HG3	29:d:1222:ARG:NE	2.32	0.45
15:N:376:PRO:N	15:N:377:PRO:HD2	2.32	0.44
17:P:652:LEU:HA	17:P:655:LEU:HD12	1.99	0.44
18:Q:138:LYS:HE3	18:Q:143:THR:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:370:ASP:OD1	24:W:370:ASP:N	2.50	0.44
24:W:1014:MET:HA	24:W:1017:ARG:HH21	1.82	0.44
26:a:340:LEU:CD2	29:d:1622:VAL:HG22	2.19	0.44
29:d:53:ILE:HB	29:d:78:ARG:HH21	1.81	0.44
29:d:1359:MET:O	29:d:1359:MET:HG2	2.17	0.44
29:d:1732:VAL:HG11	29:d:1734:THR:CG2	2.47	0.44
5:4:72:CYS:SG	5:4:73:LEU:N	2.90	0.44
8:D:125:VAL:HG11	22:U:115:LEU:HD11	1.99	0.44
11:H:65:HIS:HD2	23:V:48:VAL:HG22	1.82	0.44
15:N:637:PHE:CZ	18:Q:563:ILE:O	2.71	0.44
18:Q:259:VAL:HG12	18:Q:343:ILE:HG13	2.00	0.44
24:W:427:CYS:HA	24:W:430:ILE:HG22	1.99	0.44
25:X:128:LEU:HD13	25:X:131:LEU:HD12	1.99	0.44
25:X:905:PHE:HE2	25:X:946:PHE:HB2	1.82	0.44
29:d:2155:CYS:SG	29:d:2156:LEU:N	2.88	0.44
2:1:100:LEU:HD11	18:Q:631:GLU:OE1	2.17	0.44
15:N:361:ILE:CB	15:N:370:LEU:HD23	2.42	0.44
21:T:45:THR:HG22	21:T:108:SER:HB2	2.00	0.44
25:X:301:GLU:HA	25:X:304:LYS:HE3	1.98	0.44
28:c:1079:ALA:HB1	28:c:1138:ARG:HD2	1.99	0.44
28:c:1579:PHE:HA	28:c:1582:VAL:HG12	1.98	0.44
6:A:65:LEU:HD13	8:D:63:ASN:HD21	1.82	0.44
6:A:317:PHE:HA	6:A:320:LYS:HB2	1.98	0.44
8:D:104:ASP:O	8:D:108:GLN:N	2.47	0.44
15:N:528:HIS:CE1	15:N:588:LEU:HG	2.52	0.44
15:N:941:TYR:HD2	15:N:1172:SER:HB3	1.83	0.44
17:P:109:SER:OG	17:P:119:GLU:OE2	2.36	0.44
17:P:583:ILE:HG22	17:P:586:LYS:HE3	1.99	0.44
17:P:669:LYS:HD3	17:P:669:LYS:HA	1.75	0.44
21:T:118:GLN:HA	21:T:122:PHE:O	2.17	0.44
24:W:852:ASP:O	24:W:857:TYR:N	2.49	0.44
25:X:20:ASP:OD1	25:X:21:TYR:N	2.50	0.44
25:X:420:ILE:HA	25:X:423:THR:HG22	1.99	0.44
28:c:846:ALA:O	28:c:850:ARG:NH1	2.50	0.44
28:c:1001:LYS:HA	28:c:1001:LYS:HD2	1.80	0.44
10:G:83:MET:HE3	13:J:120:ASP:HB2	1.99	0.44
15:N:374:HIS:CB	15:N:379:PRO:HD3	2.47	0.44
15:N:534:SER:HB3	15:N:553:GLU:HG3	1.99	0.44
19:R:23:LEU:HD12	19:R:199:LEU:HB3	1.98	0.44
28:c:88:ASP:N	28:c:88:ASP:OD1	2.49	0.44
28:c:938:ILE:HD12	28:c:944:MET:HE2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:d:1111:ILE:HD12	29:d:1132:ARG:NH1	2.32	0.44
29:d:2079:ASP:N	29:d:2079:ASP:OD1	2.49	0.44
14:K:55:SER:HA	14:K:58:HIS:ND1	2.33	0.44
15:N:592:LYS:HG2	24:W:25:MET:HE1	1.98	0.44
16:O:758:SER:HB2	24:W:30:PRO:HD2	1.99	0.44
17:P:495:VAL:HB	17:P:536:LEU:HD23	1.99	0.44
19:R:23:LEU:HB3	19:R:199:LEU:HD22	1.99	0.44
24:W:205:VAL:HA	24:W:208:PHE:HB3	1.98	0.44
25:X:319:LYS:HA	25:X:322:LYS:HE2	2.00	0.44
25:X:633:LEU:HB2	25:X:680:GLN:HE22	1.83	0.44
27:b:178:ARG:HD3	28:c:59:ALA:HB3	2.00	0.44
28:c:983:SER:HA	28:c:986:LYS:HD3	2.00	0.44
28:c:1697:SER:HB2	28:c:1700:LEU:HB2	2.00	0.44
28:c:1708:VAL:HB	29:d:1346:VAL:HB	2.00	0.44
1:O:248:THR:HG21	18:Q:509:GLY:HA2	2.00	0.44
6:A:348:LEU:HD23	6:A:348:LEU:HA	1.84	0.44
10:G:67:LEU:HB2	20:S:66:TYR:CG	2.52	0.44
15:N:960:LYS:O	15:N:964:ASN:N	2.47	0.44
18:Q:223:GLU:HG2	18:Q:246:GLN:HB2	2.00	0.44
18:Q:514:LEU:HD22	18:Q:520:GLU:HB3	2.00	0.44
24:W:182:PHE:O	24:W:185:THR:OG1	2.35	0.44
24:W:382:GLY:HA2	24:W:534:HIS:HB2	2.00	0.44
24:W:546:ARG:HA	24:W:549:LYS:HE2	1.99	0.44
25:X:285:ILE:HG23	25:X:313:ILE:HD11	2.00	0.44
26:a:205:LEU:HB3	26:a:252:LEU:HD21	1.99	0.44
27:b:147:ASP:OD1	29:d:1734:THR:HB	2.17	0.44
28:c:1375:MET:O	28:c:1379:LEU:N	2.48	0.44
2:1:146:ILE:HD11	23:V:115:LYS:CD	2.41	0.44
6:A:509:ARG:O	6:A:513:ARG:N	2.45	0.44
9:F:9:ASN:HD21	9:F:11:LEU:HD12	1.83	0.44
10:G:109:LEU:HD22	15:N:135:ARG:NH2	2.33	0.44
11:H:16:LEU:HB2	18:Q:113:TYR:HD1	1.82	0.44
15:N:362:ASP:OD1	15:N:363:GLU:N	2.51	0.44
17:P:796:LYS:O	17:P:805:THR:OG1	2.34	0.44
18:Q:608:ASP:N	18:Q:608:ASP:OD1	2.51	0.44
24:W:108:GLU:HG2	24:W:110:GLU:H	1.83	0.44
24:W:763:GLU:HA	24:W:766:LYS:HB2	2.00	0.44
27:b:30:LYS:HA	27:b:30:LYS:HD3	1.69	0.44
28:c:78:ALA:HB1	28:c:82:ARG:HH12	1.83	0.44
29:d:1226:ARG:O	29:d:1230:ASN:N	2.45	0.44
29:d:2145:CYS:HA	29:d:2152:ARG:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:90:ARG:HA	4:3:90:ARG:HD3	1.83	0.44
9:F:185:ARG:HH22	15:N:299:PHE:HE1	1.66	0.44
12:I:109:LEU:HD21	12:I:114:GLN:NE2	2.15	0.44
15:N:642:ALA:HB1	18:Q:565:ASN:HD22	1.83	0.44
19:R:141:MET:HB2	19:R:171:LEU:HD11	1.99	0.44
21:T:161:LEU:HB3	21:T:169:THR:HG23	1.99	0.44
24:W:318:GLU:HG2	24:W:320:LYS:H	1.83	0.44
24:W:459:GLN:HB3	24:W:463:ARG:NH1	2.33	0.44
24:W:1005:LEU:HD11	24:W:1030:ILE:HG21	2.00	0.44
27:b:175:LEU:HD13	27:b:178:ARG:HD2	2.00	0.44
28:c:782:LEU:HD22	28:c:868:PRO:HB3	1.99	0.44
29:d:84:TRP:NE1	29:d:88:ASP:OD1	2.48	0.44
29:d:1416:MET:SD	29:d:1416:MET:C	3.01	0.44
9:F:50:VAL:HG12	9:F:51:LYS:HG3	2.00	0.43
9:F:68:TYR:HD1	9:F:83:LYS:HA	1.83	0.43
12:I:110:SER:O	12:I:114:GLN:N	2.48	0.43
15:N:499:TRP:O	15:N:503:GLN:N	2.34	0.43
24:W:653:ILE:HG21	24:W:686:ALA:HB1	2.00	0.43
25:X:274:GLN:HG3	25:X:274:GLN:O	2.17	0.43
28:c:859:PHE:HB2	28:c:867:LEU:HD21	2.00	0.43
28:c:1050:ARG:HE	28:c:1091:GLU:HG2	1.83	0.43
28:c:1555:THR:HG22	28:c:1616:LEU:HD13	1.99	0.43
29:d:338:ASP:CG	29:d:339:PRO:HD3	2.43	0.43
29:d:340:GLN:C	29:d:340:GLN:CD	2.86	0.43
1:O:179:HIS:ND1	1:O:191:LEU:O	2.43	0.43
1:O:269:TRP:O	1:O:272:SER:OG	2.36	0.43
4:3:107:ASP:HA	4:3:108:PRO:HD3	1.90	0.43
8:D:30:LEU:HD13	12:I:99:LYS:CG	2.48	0.43
11:H:34:GLU:OE2	18:Q:99:ARG:NH1	2.51	0.43
21:T:38:THR:HA	21:T:115:THR:HA	1.99	0.43
6:A:15:LYS:O	6:A:19:LEU:N	2.43	0.43
6:A:273:LEU:HD12	6:A:273:LEU:HA	1.78	0.43
6:A:339:LEU:HD12	6:A:388:LEU:HB3	2.00	0.43
11:H:59:LEU:HA	11:H:62:VAL:HG12	1.99	0.43
15:N:305:LEU:HD21	15:N:361:ILE:HG21	2.00	0.43
15:N:688:PRO:HA	15:N:689:PRO:HD3	1.88	0.43
15:N:1202:TYR:CD2	15:N:1292:PRO:HB2	2.53	0.43
16:O:768:SER:OG	16:O:769:VAL:N	2.50	0.43
17:P:361:ILE:C	17:P:363:LEU:H	2.26	0.43
17:P:479:GLU:OE2	17:P:513:ARG:NH2	2.50	0.43
18:Q:191:ARG:HA	18:Q:196:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:207:LEU:O	18:Q:299:GLN:NE2	2.39	0.43
25:X:789:PRO:O	25:X:793:THR:OG1	2.36	0.43
26:a:307:LYS:CE	26:a:337:GLU:HG3	2.47	0.43
28:c:29:PRO:HG2	28:c:30:LYS:HD2	2.00	0.43
28:c:1204:ASP:HA	28:c:1207:LEU:HG	1.99	0.43
6:A:375:PHE:HB3	6:A:441:GLU:HA	2.00	0.43
6:A:375:PHE:HD2	6:A:441:GLU:HG2	1.83	0.43
8:D:30:LEU:O	8:D:34:LEU:N	2.48	0.43
13:J:70:TYR:HB3	13:J:75:ARG:HB3	2.00	0.43
15:N:330:HIS:HB2	15:N:334:CYS:H	1.83	0.43
15:N:385:LEU:HD21	15:N:406:HIS:ND1	2.34	0.43
24:W:857:TYR:O	24:W:937:LEU:N	2.51	0.43
24:W:1013:GLU:O	24:W:1017:ARG:NE	2.46	0.43
25:X:329:ASP:N	25:X:329:ASP:OD1	2.51	0.43
28:c:621:ARG:HD3	28:c:621:ARG:HA	1.78	0.43
28:c:1050:ARG:HH21	28:c:1091:GLU:HG2	1.82	0.43
29:d:1834:SER:OG	29:d:1835:ALA:N	2.52	0.43
2:1:121:GLU:OE2	23:V:138:SER:HB3	2.19	0.43
6:A:345:GLN:HE22	6:A:392:LEU:HD11	1.82	0.43
6:A:361:MET:HE1	6:A:377:ASN:H	1.83	0.43
6:A:374:TYR:CE2	6:A:505:PRO:HG3	2.53	0.43
15:N:186:ILE:HD12	15:N:186:ILE:HA	1.90	0.43
15:N:637:PHE:HD2	15:N:639:LYS:HE3	1.84	0.43
15:N:885:LEU:HD21	15:N:1186:LEU:HD22	2.00	0.43
15:N:1292:PRO:HA	15:N:1294:PHE:CE2	2.53	0.43
17:P:286:LEU:O	17:P:356:LEU:HD13	2.18	0.43
18:Q:262:GLN:O	18:Q:340:GLN:NE2	2.51	0.43
18:Q:572:ALA:HA	18:Q:579:ALA:HA	1.99	0.43
24:W:750:GLN:HE22	24:W:874:HIS:HA	1.82	0.43
26:a:307:LYS:HE2	26:a:337:GLU:HG2	1.99	0.43
26:a:340:LEU:CG	26:a:341:PRO:CD	2.80	0.43
28:c:861:LEU:HD22	28:c:863:MET:HE1	2.00	0.43
29:d:1193:GLN:O	29:d:1197:THR:OG1	2.34	0.43
2:1:139:TRP:HA	2:1:142:VAL:HB	2.00	0.43
13:J:89:LEU:HG	20:S:84:ILE:HD12	1.99	0.43
17:P:375:GLN:HB2	17:P:465:LEU:HD11	1.99	0.43
17:P:690:PHE:HA	17:P:693:LEU:HG	2.00	0.43
18:Q:149:LYS:HD3	18:Q:149:LYS:HA	1.80	0.43
19:R:84:HIS:HD1	19:R:109:ALA:HB2	1.83	0.43
20:S:84:ILE:HG23	20:S:89:LEU:HB3	2.00	0.43
24:W:119:PHE:HA	24:W:122:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:327:SER:O	24:W:331:TRP:N	2.44	0.43
24:W:442:LYS:HE2	24:W:442:LYS:HB2	1.90	0.43
24:W:665:PHE:HE2	24:W:691:LEU:HD21	1.84	0.43
29:d:2138:ASN:O	29:d:2141:SER:OG	2.32	0.43
8:D:125:VAL:HA	8:D:128:ALA:HB3	1.99	0.43
13:J:77:PRO:HB3	15:N:105:TRP:CD1	2.53	0.43
15:N:420:LEU:HD13	15:N:427:GLU:HG2	2.01	0.43
17:P:40:SER:OG	17:P:41:CYS:N	2.51	0.43
17:P:560:LEU:HD13	17:P:563:LEU:HD13	2.00	0.43
25:X:258:GLY:O	25:X:312:LYS:NZ	2.50	0.43
3:2:122:LEU:O	3:2:126:CYS:N	2.48	0.43
5:4:37:LEU:HD12	5:4:42:TYR:HB2	2.00	0.43
6:A:88:ASN:HD21	6:A:151:SER:HA	1.83	0.43
6:A:148:ASP:OD1	6:A:148:ASP:N	2.51	0.43
9:F:171:ILE:HG12	9:F:174:ARG:HG2	1.99	0.43
15:N:372:ILE:HG13	15:N:390:MET:HA	2.00	0.43
15:N:807:LYS:HE3	15:N:823:GLN:HB2	2.01	0.43
15:N:903:CYS:HA	15:N:919:ARG:HG2	2.00	0.43
17:P:103:GLY:HA3	17:P:126:VAL:H	1.83	0.43
18:Q:414:ASP:OD1	21:T:71:TYR:OH	2.27	0.43
24:W:13:VAL:HB	24:W:75:ARG:HD2	2.01	0.43
24:W:576:ILE:O	24:W:580:GLY:N	2.51	0.43
25:X:135:THR:HG21	25:X:165:LEU:HD11	1.99	0.43
25:X:415:PRO:O	25:X:419:ASN:ND2	2.51	0.43
26:a:82:GLN:HA	29:d:1733:LYS:HZ3	1.84	0.43
27:b:7:GLN:HE22	29:d:1631:HIS:HB2	1.83	0.43
28:c:189:ILE:HA	28:c:192:LYS:HG2	2.00	0.43
2:1:119:ARG:HA	2:1:122:LEU:HB2	2.00	0.43
5:4:60:ASP:N	5:4:60:ASP:OD1	2.52	0.43
11:H:61:LYS:O	11:H:65:HIS:ND1	2.45	0.43
15:N:278:VAL:O	15:N:282:LEU:N	2.45	0.43
15:N:553:GLU:O	15:N:567:LYS:N	2.50	0.43
17:P:496:GLN:HB2	17:P:499:MET:HG2	2.01	0.43
18:Q:384:LYS:O	18:Q:388:SER:N	2.45	0.43
21:T:76:PHE:CE2	21:T:190:MET:CE	3.01	0.43
24:W:986:THR:O	24:W:990:HIS:ND1	2.49	0.43
24:W:1065:ASP:HA	24:W:1068:TYR:HD2	1.84	0.43
28:c:152:PRO:HG2	28:c:155:ARG:HD3	2.01	0.43
28:c:477:LEU:HA	28:c:480:LEU:HB2	2.00	0.43
28:c:1152:ILE:HG13	28:c:1153:PRO:HD3	2.00	0.43
29:d:1116:GLN:HB3	29:d:1117:GLU:H	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:d:1665:GLY:HA2	29:d:1668:ARG:HG3	2.01	0.43
6:A:321:LEU:HD22	6:A:329:LEU:HD12	2.01	0.43
8:D:118:GLU:O	8:D:122:ALA:N	2.43	0.43
15:N:455:PHE:N	15:N:464:GLN:O	2.39	0.43
15:N:725:VAL:HG23	15:N:744:HIS:HB3	2.00	0.43
18:Q:156:ALA:HB2	23:V:61:MET:HG2	2.00	0.43
24:W:366:ILE:HG22	24:W:369:ARG:HD3	2.01	0.43
24:W:1198:GLN:HA	25:X:723:TRP:CD1	2.54	0.43
29:d:1133:LYS:HE2	29:d:1222:ARG:NH2	2.33	0.43
6:A:177:LEU:O	6:A:181:GLU:N	2.45	0.42
8:D:173:ARG:HD2	8:D:173:ARG:HA	1.88	0.42
10:G:51:CYS:SG	10:G:52:ASP:N	2.92	0.42
15:N:372:ILE:HG13	15:N:389:ALA:O	2.19	0.42
18:Q:96:ASP:OD1	18:Q:97:SER:N	2.52	0.42
24:W:36:LYS:HD2	24:W:36:LYS:HA	1.81	0.42
24:W:73:PRO:HA	24:W:76:ILE:HB	2.00	0.42
25:X:894:ARG:HA	25:X:899:ARG:HH21	1.84	0.42
28:c:447:ALA:O	28:c:451:PHE:N	2.42	0.42
29:d:1198:ASN:HB3	29:d:1721:GLN:HG2	2.01	0.42
29:d:1664:LEU:HG	29:d:2173:MET:HE3	2.01	0.42
1:O:274:ILE:HG13	1:O:275:LYS:HD3	2.01	0.42
6:A:219:LEU:HD13	6:A:258:THR:HB	2.00	0.42
15:N:309:HIS:CE1	15:N:331:ALA:HA	2.54	0.42
17:P:376:PHE:HD1	17:P:473:HIS:HD2	1.65	0.42
19:R:58:PHE:HB3	19:R:123:PHE:HB3	2.01	0.42
24:W:366:ILE:HD12	24:W:402:LEU:HD12	2.00	0.42
25:X:606:THR:HG21	25:X:645:GLN:HB3	2.00	0.42
26:a:158:LEU:HD23	26:a:356:ARG:HH22	1.84	0.42
28:c:464:ASP:OD1	28:c:510:TRP:NE1	2.40	0.42
6:A:173:MET:O	6:A:177:LEU:N	2.45	0.42
6:A:314:SER:HB2	6:A:447:GLU:OE1	2.19	0.42
10:G:67:LEU:HD13	20:S:66:TYR:CZ	2.55	0.42
10:G:90:LEU:CD2	13:J:109:LEU:CB	2.92	0.42
15:N:941:TYR:OH	15:N:1168:SER:O	2.30	0.42
17:P:534:CYS:O	17:P:540:THR:OG1	2.28	0.42
17:P:544:VAL:HB	17:P:548:HIS:CE1	2.54	0.42
2:1:84:PHE:HA	2:1:87:ILE:HG22	2.00	0.42
9:F:69:ILE:HG22	9:F:82:ARG:HH21	1.83	0.42
15:N:102:LEU:HD23	15:N:102:LEU:HA	1.91	0.42
15:N:925:ASP:HB3	15:N:927:TYR:CE1	2.53	0.42
18:Q:202:LYS:HA	18:Q:202:LYS:HD3	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:506:ARG:HD3	24:W:506:ARG:HA	1.80	0.42
24:W:559:LEU:HD12	24:W:559:LEU:HA	1.91	0.42
24:W:1075:LEU:HD12	24:W:1075:LEU:HA	1.87	0.42
28:c:874:GLN:HA	28:c:877:PHE:HD2	1.83	0.42
28:c:969:ARG:O	28:c:973:ALA:N	2.50	0.42
5:4:17:ARG:CZ	5:4:21:GLU:HG3	2.50	0.42
10:G:91:ASP:OD1	13:J:124:TYR:OH	2.38	0.42
13:J:73:GLN:O	20:S:102:LYS:NZ	2.48	0.42
15:N:376:PRO:HD2	15:N:377:PRO:HD3	2.00	0.42
15:N:639:LYS:HE2	18:Q:562:SER:HA	2.00	0.42
15:N:820:ILE:HG22	15:N:835:LEU:HD23	2.01	0.42
17:P:402:MET:HE1	17:P:461:MET:CE	2.49	0.42
18:Q:384:LYS:HA	18:Q:384:LYS:HD3	1.73	0.42
24:W:452:ARG:HA	24:W:455:HIS:HB3	2.00	0.42
27:b:193:PRO:HA	27:b:194:PRO:HD3	1.88	0.42
2:1:86:ASP:O	2:1:90:GLN:NE2	2.42	0.42
6:A:191:TYR:CD2	6:A:202:LYS:HG2	2.54	0.42
10:G:78:LEU:HD23	10:G:119:VAL:HG23	2.01	0.42
10:G:100:PRO:HG2	15:N:125:GLN:OE1	2.20	0.42
13:J:80:TYR:HD2	15:N:105:TRP:HE1	1.68	0.42
15:N:370:LEU:HB2	15:N:392:ILE:HD11	2.01	0.42
15:N:703:ARG:HA	15:N:703:ARG:HD2	1.85	0.42
15:N:730:PRO:HG2	15:N:780:VAL:HG11	2.02	0.42
15:N:751:ASN:ND2	15:N:756:PRO:O	2.41	0.42
17:P:186:GLY:HA3	17:P:210:ARG:HA	2.02	0.42
18:Q:431:ILE:HD13	18:Q:431:ILE:HA	1.89	0.42
21:T:112:THR:HG23	21:T:197:PHE:HE1	1.84	0.42
24:W:126:ILE:HG21	24:W:169:TYR:HE2	1.83	0.42
28:c:431:ARG:HD2	28:c:1580:THR:HB	2.00	0.42
28:c:810:GLU:HA	28:c:813:GLN:HG2	2.01	0.42
29:d:1789:VAL:HG22	29:d:1859:ARG:HB2	2.01	0.42
1:0:36:LYS:HD2	16:O:643:VAL:HA	2.02	0.42
4:3:111:VAL:HG22	18:Q:651:LEU:HG	2.00	0.42
4:3:170:ILE:HD12	4:3:173:MET:HG3	2.01	0.42
6:A:172:LYS:HB3	6:A:299:LEU:HD21	2.02	0.42
10:G:56:ILE:HG23	10:G:57:ARG:HG2	2.01	0.42
15:N:223:LYS:HD3	15:N:233:THR:HG22	2.00	0.42
15:N:467:LEU:HB2	15:N:470:LEU:HD12	2.02	0.42
17:P:34:PRO:HA	17:P:432:LYS:HE3	2.01	0.42
24:W:236:ALA:HB2	24:W:663:PRO:HB3	2.01	0.42
24:W:253:LYS:HZ3	24:W:1257:GLN:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:196:LEU:HD11	25:X:223:ARG:HH11	1.85	0.42
25:X:452:LEU:HD13	25:X:507:TYR:HE2	1.85	0.42
26:a:202:PRO:HA	26:a:205:LEU:HB2	2.00	0.42
1:0:133:LEU:HD12	1:0:133:LEU:HA	1.91	0.42
2:1:119:ARG:HD3	2:1:122:LEU:HD12	2.01	0.42
14:K:32:ILE:HD13	14:K:35:LEU:HD21	2.02	0.42
15:N:195:LEU:HD23	15:N:198:ILE:HD11	2.02	0.42
15:N:683:ARG:CD	16:O:684:ARG:HG3	2.48	0.42
17:P:434:MET:N	17:P:434:MET:SD	2.93	0.42
17:P:524:THR:HG22	17:P:554:ILE:HD12	2.01	0.42
17:P:732:LEU:O	17:P:734:ALA:N	2.50	0.42
22:U:102:THR:HA	22:U:105:GLU:HG2	2.01	0.42
24:W:238:CYS:HB3	24:W:241:TRP:HD1	1.85	0.42
24:W:732:LEU:O	24:W:740:GLN:NE2	2.52	0.42
25:X:406:ASN:HA	25:X:409:LEU:HD12	2.02	0.42
28:c:1534:LYS:HA	28:c:1534:LYS:HD2	1.88	0.42
29:d:1352:LEU:HD12	29:d:2147:PRO:HG3	2.02	0.42
6:A:462:LEU:O	6:A:482:GLY:N	2.52	0.42
10:G:152:ARG:HA	10:G:155:LYS:HG2	2.00	0.42
15:N:202:ARG:NH1	15:N:241:PRO:O	2.50	0.42
15:N:313:LEU:HD23	15:N:313:LEU:HA	1.93	0.42
15:N:376:PRO:CD	15:N:377:PRO:HD3	2.50	0.42
15:N:1186:LEU:HD23	15:N:1207:LEU:HD13	2.01	0.42
17:P:143:LEU:HA	17:P:161:ARG:HA	2.02	0.42
25:X:274:GLN:HG3	25:X:276:ILE:CD1	2.50	0.42
28:c:1220:VAL:HG11	28:c:1295:ARG:HH12	1.85	0.42
1:0:68:ASN:HB3	1:0:72:ARG:HH12	1.84	0.42
9:F:67:GLU:OE1	9:F:86:ARG:NH1	2.53	0.42
10:G:91:ASP:CG	13:J:124:TYR:OH	2.63	0.42
15:N:1224:ILE:HD13	15:N:1224:ILE:HA	1.93	0.42
24:W:416:LYS:HB3	24:W:418:GLN:HG2	2.02	0.42
24:W:617:PRO:HA	24:W:620:ARG:HB2	2.02	0.42
25:X:517:ARG:HH21	25:X:523:PRO:HG3	1.85	0.42
26:a:307:LYS:HD2	26:a:337:GLU:HG3	1.93	0.42
29:d:1871:GLY:HA2	29:d:1874:LYS:HE2	2.01	0.42
2:1:135:LYS:HE2	2:1:139:TRP:CH2	2.55	0.41
6:A:354:PRO:HG2	6:A:355:ILE:HD12	2.02	0.41
11:H:19:VAL:O	11:H:23:LYS:HG2	2.20	0.41
15:N:236:VAL:HB	15:N:243:VAL:HG11	2.02	0.41
15:N:449:SER:HB3	18:Q:516:TYR:OH	2.20	0.41
17:P:531:ALA:HB1	17:P:548:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:540:THR:O	17:P:544:VAL:HG13	2.20	0.41
18:Q:598:ARG:NH2	18:Q:605:PRO:O	2.41	0.41
19:R:116:ASP:OD1	19:R:116:ASP:N	2.53	0.41
24:W:339:ILE:HA	24:W:342:VAL:HG12	2.01	0.41
24:W:982:LYS:O	24:W:985:GLU:HB2	2.20	0.41
25:X:320:LEU:O	25:X:324:SER:OG	2.33	0.41
26:a:160:MET:HG3	26:a:165:GLU:HG3	2.01	0.41
26:a:342:THR:OG1	26:a:344:ASP:O	2.30	0.41
28:c:297:LEU:O	28:c:301:CYS:N	2.47	0.41
28:c:1055:CYS:HB3	28:c:1116:ASN:HD21	1.85	0.41
29:d:1708:PRO:HB2	29:d:1709:GLN:H	1.61	0.41
2:1:135:LYS:CG	2:1:139:TRP:HZ3	2.23	0.41
5:4:103:LEU:O	5:4:110:ARG:NH1	2.36	0.41
9:F:84:GLN:HA	9:F:94:PRO:HA	2.02	0.41
15:N:343:GLN:H	15:N:343:GLN:HG3	1.68	0.41
15:N:812:TYR:HE1	15:N:820:ILE:HG23	1.85	0.41
17:P:310:SER:HB3	17:P:342:LEU:HD21	2.01	0.41
17:P:784:ARG:HA	17:P:784:ARG:HD3	1.77	0.41
18:Q:391:MET:SD	18:Q:391:MET:N	2.77	0.41
24:W:101:LEU:HD11	24:W:121:LEU:HD23	2.02	0.41
24:W:373:MET:O	24:W:376:LEU:HB3	2.19	0.41
24:W:552:HIS:CE1	24:W:591:THR:HB	2.55	0.41
24:W:714:ASP:OD1	24:W:714:ASP:N	2.51	0.41
29:d:1808:THR:HG23	29:d:2159:HIS:HB3	2.02	0.41
6:A:80:ARG:HH21	6:A:147:PHE:HB2	1.84	0.41
6:A:194:ALA:CB	6:A:280:VAL:HG23	2.50	0.41
6:A:366:ALA:HB3	6:A:428:THR:HB	2.02	0.41
6:A:503:SER:OG	6:A:506:VAL:HB	2.19	0.41
9:F:184:LEU:HD23	15:N:299:PHE:CE1	2.56	0.41
12:I:73:ILE:HA	12:I:76:MET:HG3	2.02	0.41
15:N:233:THR:HG23	15:N:249:LYS:HE3	2.01	0.41
15:N:806:ARG:HH12	15:N:824:TRP:N	2.16	0.41
17:P:503:LEU:HD23	17:P:533:LEU:HD11	2.01	0.41
18:Q:139:GLN:HB3	18:Q:142:GLN:HB2	2.01	0.41
19:R:108:ILE:HG12	21:T:90:ASN:HB3	2.01	0.41
24:W:378:GLN:HE22	24:W:532:THR:HG22	1.86	0.41
24:W:431:HIS:NE2	24:W:479:ASN:O	2.43	0.41
24:W:883:TYR:HB3	24:W:974:PHE:CE1	2.55	0.41
24:W:1176:SER:HA	24:W:1180:GLU:HB3	2.02	0.41
25:X:50:ALA:HB2	25:X:60:ILE:HG21	2.03	0.41
26:a:82:GLN:O	29:d:1733:LYS:NZ	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:a:168:ARG:HH21	26:a:343:SER:HB3	1.85	0.41
29:d:66:LEU:HB2	29:d:83:PHE:HB2	2.02	0.41
29:d:1411:LEU:HD23	29:d:1411:LEU:N	2.35	0.41
29:d:1820:ILE:HD13	29:d:1842:LYS:HB3	2.02	0.41
9:F:178:ASP:O	9:F:182:LEU:N	2.50	0.41
10:G:83:MET:HG3	13:J:120:ASP:HB2	2.02	0.41
15:N:1192:PRO:HD3	15:N:1209:ARG:CZ	2.51	0.41
17:P:402:MET:SD	17:P:402:MET:O	2.79	0.41
25:X:801:LEU:HD23	25:X:801:LEU:HA	1.95	0.41
28:c:510:TRP:CD1	28:c:516:ARG:HH21	2.30	0.41
28:c:1026:LEU:HD11	28:c:1053:PHE:HA	2.02	0.41
29:d:1762:PRO:HG2	29:d:1765:ILE:HG22	2.03	0.41
6:A:493:PHE:CD2	6:A:514:LYS:HD2	2.56	0.41
8:D:86:GLN:HB3	12:I:105:PRO:C	2.45	0.41
10:G:21:TYR:CE1	10:G:33:LYS:HD3	2.55	0.41
13:J:106:LYS:HA	13:J:109:LEU:HD12	2.03	0.41
15:N:328:ARG:NH1	15:N:336:SER:HB3	2.35	0.41
15:N:419:ILE:HD12	15:N:487:LYS:HD3	2.01	0.41
15:N:567:LYS:HB3	15:N:569:TYR:HE1	1.85	0.41
15:N:784:ALA:O	15:N:788:PRO:HD3	2.21	0.41
17:P:431:LEU:HA	17:P:447:ASP:HA	2.02	0.41
17:P:511:TYR:HB2	17:P:526:ILE:HD13	2.01	0.41
18:Q:226:LYS:HA	18:Q:243:LEU:HG	2.02	0.41
23:V:29:ILE:HD11	23:V:75:LEU:HD11	2.03	0.41
24:W:180:ALA:HB1	24:W:208:PHE:HE1	1.85	0.41
24:W:1238:ILE:O	24:W:1244:GLN:NE2	2.52	0.41
27:b:155:PRO:HG3	27:b:194:PRO:HB3	2.01	0.41
27:b:174:PRO:O	27:b:178:ARG:NE	2.53	0.41
29:d:67:GLY:O	29:d:125:ASN:ND2	2.50	0.41
1:0:103:LEU:HD12	1:0:107:LEU:HD23	2.03	0.41
2:1:125:LYS:CE	23:V:137:SER:CB	2.89	0.41
2:1:128:LEU:HD22	23:V:133:GLU:HG2	2.02	0.41
5:4:90:ASN:HB3	5:4:92:GLN:HG3	2.03	0.41
6:A:367:LEU:HD21	6:A:426:LYS:NZ	2.36	0.41
15:N:463:PHE:H	15:N:483:ASN:HD21	1.68	0.41
24:W:224:ARG:NH2	24:W:240:SER:O	2.53	0.41
24:W:1142:ILE:HD12	24:W:1145:TRP:HB2	2.02	0.41
25:X:101:MET:O	25:X:167:LYS:NZ	2.50	0.41
25:X:561:LEU:HD11	25:X:588:ILE:HD11	2.02	0.41
25:X:784:LEU:HG	25:X:904:LEU:HD22	2.01	0.41
28:c:1611:ARG:HA	28:c:1611:ARG:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:d:1898:MET:SD	29:d:1898:MET:N	2.92	0.41
2:1:71:GLU:HG3	2:1:74:ARG:NH2	2.35	0.41
2:1:128:LEU:HD23	2:1:132:HIS:HB2	2.02	0.41
10:G:112:LEU:HA	10:G:115:LEU:HD12	2.03	0.41
11:H:89:LEU:HD21	11:H:97:VAL:HB	2.02	0.41
13:J:79:LEU:O	13:J:82:LYS:HB2	2.19	0.41
15:N:159:ASP:O	15:N:163:THR:OG1	2.31	0.41
15:N:515:ILE:HD12	15:N:541:LYS:HB3	2.03	0.41
15:N:945:ASP:HB3	15:N:948:LYS:H	1.84	0.41
21:T:79:PHE:CD2	21:T:83:PRO:HD2	2.56	0.41
24:W:764:TYR:HD1	24:W:792:LEU:HD13	1.86	0.41
28:c:472:ASP:O	28:c:476:SER:N	2.54	0.41
29:d:1257:LYS:HB2	29:d:1257:LYS:HE2	1.90	0.41
6:A:156:GLY:O	6:A:160:LEU:N	2.52	0.41
6:A:177:LEU:HD13	6:A:259:ILE:HG23	2.03	0.41
6:A:269:PRO:HB2	6:A:271:ALA:O	2.21	0.41
15:N:386:VAL:HG13	15:N:390:MET:HE3	2.01	0.41
17:P:227:VAL:HB	17:P:291:SER:OG	2.21	0.41
17:P:286:LEU:O	17:P:356:LEU:HD22	2.20	0.41
17:P:301:GLN:O	17:P:350:ARG:NH1	2.54	0.41
17:P:627:TYR:HB2	17:P:726:ILE:HG23	2.02	0.41
19:R:191:GLU:HA	19:R:194:LYS:HG2	2.03	0.41
20:S:110:PRO:C	20:S:113:PRO:HD2	2.46	0.41
24:W:1313:GLN:HA	24:W:1316:LYS:HE2	2.02	0.41
28:c:259:LEU:HD13	28:c:296:ARG:HB3	2.03	0.41
28:c:460:LEU:HD22	28:c:510:TRP:CD1	2.56	0.41
28:c:602:GLU:O	28:c:606:HIS:ND1	2.54	0.41
28:c:1514:TRP:CE2	28:c:1569:THR:HA	2.56	0.41
29:d:1136:ASN:HD22	29:d:1223:VAL:HB	1.85	0.41
29:d:1416:MET:SD	29:d:1416:MET:O	2.79	0.41
2:1:137:ARG:HG3	2:1:140:GLN:NE2	2.36	0.41
4:3:170:ILE:HD12	4:3:170:ILE:HA	1.95	0.41
6:A:67:LYS:HD3	6:A:67:LYS:HA	1.79	0.41
6:A:280:VAL:O	6:A:280:VAL:HG22	2.21	0.41
6:A:370:GLN:HB2	6:A:509:ARG:HG2	2.02	0.41
6:A:491:ASP:HA	6:A:494:ILE:HG12	2.02	0.41
11:H:37:TYR:CZ	18:Q:94:PRO:HG2	2.55	0.41
11:H:93:THR:O	11:H:96:ARG:NE	2.54	0.41
15:N:385:LEU:HD23	15:N:385:LEU:HA	1.92	0.41
15:N:572:SER:HB3	15:N:586:LEU:HD12	2.03	0.41
15:N:824:TRP:CH2	15:N:829:GLN:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:1291:GLY:HA2	15:N:1292:PRO:HD3	1.91	0.41
16:O:636:HIS:CD2	17:P:786:HIS:H	2.38	0.41
16:O:764:PRO:O	16:O:767:HIS:ND1	2.42	0.41
17:P:66:ASP:HB2	17:P:799:THR:HG21	2.03	0.41
17:P:457:LEU:O	17:P:494:HIS:NE2	2.54	0.41
17:P:527:LEU:HD12	17:P:554:ILE:HD13	2.02	0.41
18:Q:591:LYS:HD3	18:Q:591:LYS:HA	1.87	0.41
20:S:103:GLU:O	20:S:107:ASN:HB2	2.21	0.41
23:V:104:GLN:O	23:V:107:THR:OG1	2.38	0.41
24:W:261:ASP:N	24:W:261:ASP:OD1	2.54	0.41
24:W:782:MET:SD	24:W:785:SER:HB3	2.60	0.41
25:X:180:ILE:O	25:X:979:ARG:NE	2.53	0.41
25:X:533:MET:SD	25:X:533:MET:N	2.94	0.41
26:a:98:ASP:N	26:a:98:ASP:OD1	2.54	0.41
28:c:243:MET:HE2	28:c:243:MET:HB2	1.94	0.41
28:c:727:ASP:OD1	28:c:727:ASP:N	2.54	0.41
28:c:949:GLU:HA	28:c:989:PHE:HE2	1.86	0.41
28:c:1375:MET:HE3	28:c:1375:MET:HB3	1.94	0.41
29:d:1133:LYS:HZ2	29:d:1222:ARG:NH2	2.12	0.41
6:A:339:LEU:HA	6:A:342:LEU:HD12	2.03	0.41
8:D:88:LYS:HD2	8:D:89:ILE:HG13	2.03	0.41
15:N:154:ILE:O	15:N:157:ALA:HB3	2.21	0.41
18:Q:331:ILE:HB	18:Q:343:ILE:HB	2.02	0.41
21:T:98:LEU:HB3	21:T:101:PHE:HD2	1.86	0.41
24:W:71:HIS:H	24:W:75:ARG:HH21	1.67	0.41
24:W:111:ARG:HB3	24:W:114:LEU:HB3	2.02	0.41
25:X:630:MET:SD	25:X:630:MET:N	2.91	0.41
28:c:1202:SER:O	28:c:1206:HIS:ND1	2.54	0.41
28:c:1647:ASP:OD1	28:c:1647:ASP:N	2.46	0.41
29:d:1960:ILE:HG13	29:d:2134:LEU:HD13	2.02	0.41
29:d:2068:PHE:HB3	29:d:2096:LEU:HB2	2.01	0.41
1:O:253:TYR:HB2	1:O:262:VAL:HG13	2.03	0.40
5:4:114:ARG:NH2	18:Q:28:GLU:OE2	2.53	0.40
6:A:192:TRP:HE3	6:A:202:LYS:HE3	1.86	0.40
6:A:221:ASN:HA	6:A:256:SER:HA	2.03	0.40
6:A:477:CYS:C	6:A:478:LYS:HD3	2.46	0.40
10:G:73:ASP:OD1	10:G:73:ASP:N	2.45	0.40
12:I:108:HIS:ND1	12:I:108:HIS:N	2.68	0.40
15:N:1281:LEU:HD21	15:N:1306:LEU:HD11	2.02	0.40
17:P:149:LYS:NZ	17:P:157:GLU:O	2.42	0.40
17:P:290:MET:SD	17:P:290:MET:O	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:780:ASP:O	17:P:784:ARG:NH1	2.54	0.40
17:P:783:ARG:HE	17:P:785:LEU:HD22	1.86	0.40
20:S:67:LEU:HD12	20:S:67:LEU:C	2.46	0.40
24:W:1013:GLU:HG3	24:W:1157:PRO:HG2	2.03	0.40
24:W:1062:VAL:HA	24:W:1063:PRO:HD3	1.91	0.40
25:X:97:LEU:HD23	25:X:100:ILE:HD12	2.03	0.40
27:b:159:LEU:HD11	27:b:176:ALA:HB1	2.02	0.40
28:c:1061:VAL:HG12	28:c:1070:ARG:HH12	1.86	0.40
14:K:94:LEU:HD23	14:K:94:LEU:HA	1.95	0.40
15:N:667:PRO:HB2	15:N:685:LEU:HB2	2.03	0.40
17:P:469:LEU:HD23	17:P:469:LEU:HA	1.85	0.40
18:Q:188:LEU:O	18:Q:191:ARG:NE	2.55	0.40
18:Q:247:ILE:HD11	18:Q:295:LEU:HD23	2.04	0.40
21:T:116:ARG:HB3	21:T:125:LYS:HD3	2.02	0.40
28:c:803:ASP:O	28:c:807:LEU:N	2.54	0.40
28:c:856:ILE:HA	28:c:859:PHE:HB3	2.03	0.40
29:d:1795:CYS:HB3	29:d:1865:LEU:HB3	2.03	0.40
4:3:78:LEU:HD23	4:3:78:LEU:HA	1.92	0.40
4:3:95:VAL:HA	4:3:98:LYS:HB2	2.03	0.40
4:3:168:TRP:HA	4:3:171:ASN:ND2	2.36	0.40
6:A:88:ASN:O	6:A:155:LYS:NZ	2.40	0.40
6:A:225:TYR:OH	6:A:502:MET:SD	2.76	0.40
6:A:262:THR:OG1	6:A:264:ALA:O	2.39	0.40
6:A:315:ARG:NH1	6:A:389:GLN:HB2	2.36	0.40
15:N:922:TYR:HE2	15:N:1215:ILE:HD13	1.86	0.40
17:P:439:THR:HB	17:P:477:LEU:HD23	2.03	0.40
21:T:43:CYS:HA	21:T:66:MET:HG2	2.03	0.40
25:X:25:ILE:HG22	25:X:29:LYS:HZ2	1.86	0.40
25:X:25:ILE:HG22	25:X:29:LYS:NZ	2.36	0.40
7:B:9:UNK:O	7:B:13:UNK:N	2.54	0.40
11:H:62:VAL:HA	11:H:65:HIS:HD1	1.86	0.40
15:N:918:PHE:HD2	15:N:922:TYR:HD2	1.68	0.40
15:N:923:CYS:SG	15:N:924:ILE:N	2.94	0.40
17:P:823:TRP:HZ2	17:P:828:LEU:HB2	1.86	0.40
18:Q:215:LEU:HG	18:Q:215:LEU:O	2.20	0.40
25:X:561:LEU:HD13	25:X:605:ILE:HG21	2.03	0.40
26:a:291:CYS:SG	26:a:292:SER:N	2.94	0.40
28:c:1508:HIS:CE1	28:c:1560:LEU:HD22	2.57	0.40
1:0:197:VAL:HG12	1:0:198:LEU:HG	2.04	0.40
2:1:97:GLN:CD	4:3:111:VAL:HG11	2.47	0.40
5:4:17:ARG:NE	5:4:21:GLU:HG3	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:47:MET:HA	8:D:50:ILE:HG12	2.04	0.40
12:I:109:LEU:CD2	12:I:109:LEU:O	2.70	0.40
15:N:77:SER:O	15:N:81:ARG:N	2.52	0.40
15:N:929:ARG:N	15:N:933:VAL:O	2.55	0.40
15:N:1211:LEU:O	15:N:1215:ILE:N	2.44	0.40
16:O:719:PRO:HA	16:O:720:PRO:HD3	1.92	0.40
17:P:88:GLU:HG2	17:P:288:ARG:HH22	1.86	0.40
24:W:781:SER:HB3	24:W:810:VAL:HG13	2.04	0.40
25:X:406:ASN:HA	25:X:409:LEU:HB2	2.04	0.40
28:c:116:TRP:HZ3	28:c:120:LEU:HD22	1.87	0.40
28:c:297:LEU:HD11	28:c:369:ILE:HG13	2.04	0.40
28:c:605:ARG:HH11	28:c:606:HIS:CD2	2.40	0.40
29:d:118:LEU:HD23	29:d:118:LEU:HA	1.95	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	0	261/311 (84%)	250 (96%)	11 (4%)	0	100	100
2	1	95/178 (53%)	92 (97%)	3 (3%)	0	100	100
3	2	111/200 (56%)	107 (96%)	4 (4%)	0	100	100
4	3	114/178 (64%)	112 (98%)	2 (2%)	0	100	100
5	4	111/131 (85%)	106 (96%)	5 (4%)	0	100	100
6	A	455/1581 (29%)	427 (94%)	27 (6%)	1 (0%)	43	78
8	D	154/110 (140%)	148 (96%)	6 (4%)	0	100	100
9	F	-	148 (91%)	14 (9%)	0	100	100
10	G	-	152 (96%)	7 (4%)	0	100	100
11	H	-	169 (96%)	7 (4%)	1 (1%)	21	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	I	-	66 (96%)	3 (4%)	0	100	100
13	J	-	119 (99%)	1 (1%)	0	100	100
14	K	-	108 (98%)	2 (2%)	0	100	100
15	N	-	358 (91%)	32 (8%)	3 (1%)	16	54
23	V	-	25 (100%)	0	0	100	100
24	W	-	1096 (96%)	47 (4%)	0	100	100
25	X	-	828 (94%)	49 (6%)	0	100	100
26	a	-	292 (97%)	8 (3%)	1 (0%)	36	72
27	b	-	258 (99%)	3 (1%)	0	100	100
28	c	-	1359 (96%)	63 (4%)	0	100	100
29	d	-	874 (95%)	49 (5%)	0	100	100
All	All	7443/2689 (277%)	7094 (95%)	343 (5%)	6 (0%)	49	83

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	N	375	ASP
26	a	338	ASP
11	H	99	VAL
6	A	208	VAL
15	N	153	ALA
15	N	186	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	241/280 (86%)	241 (100%)	0	100	100
2	1	94/152 (62%)	94 (100%)	0	100	100
3	2	102/163 (63%)	102 (100%)	0	100	100
4	3	116/155 (75%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	4	102/115 (89%)	102 (100%)	0	100	100
6	A	394/1391 (28%)	391 (99%)	3 (1%)	73	80
8	D	139/93 (150%)	139 (100%)	0	100	100
9	F	-	150 (100%)	0	100	100
10	G	-	153 (100%)	0	100	100
11	H	-	161 (100%)	0	100	100
12	I	-	68 (96%)	3 (4%)	26	48
13	J	-	66 (100%)	0	100	100
14	K	-	94 (100%)	0	100	100
15	N	-	808 (100%)	2 (0%)	87	87
16	O	-	141 (100%)	0	100	100
17	P	-	669 (100%)	1 (0%)	88	89
18	Q	-	487 (100%)	1 (0%)	87	87
19	R	-	168 (99%)	1 (1%)	78	83
20	S	-	43 (100%)	0	100	100
21	T	-	166 (100%)	0	100	100
22	U	-	98 (100%)	0	100	100
23	V	-	122 (100%)	0	100	100
24	W	-	1203 (100%)	0	100	100
25	X	-	789 (100%)	0	100	100
26	a	-	277 (100%)	0	100	100
27	b	-	241 (100%)	0	100	100
28	c	-	1282 (100%)	0	100	100
29	d	-	863 (99%)	6 (1%)	76	81
All	All	9251/2349 (394%)	9234 (100%)	17 (0%)	85	87

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	A	190	MET
6	A	208	VAL
6	A	502	MET
12	I	108	HIS
12	I	109	LEU

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Mol	Chain	Res	Type
12	I	110	SER
15	N	186	ILE
15	N	372	ILE
17	P	289	ASP
18	Q	215	LEU
19	R	156	ASN
29	d	338	ASP
29	d	1129	VAL
29	d	1198	ASN
29	d	1359	MET
29	d	1413	ASP
29	d	1735	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	41	ASN
1	0	64	ASN
1	0	115	ASN
1	0	118	GLN
1	0	129	ASN
1	0	130	GLN
1	0	138	ASN
1	0	237	GLN
1	0	254	GLN
1	0	289	GLN
2	1	70	GLN
2	1	79	GLN
2	1	109	GLN
2	1	132	HIS
2	1	138	HIS
2	1	140	GLN
3	2	129	GLN
4	3	53	GLN
4	3	79	GLN
4	3	81	ASN
5	4	26	GLN
8	D	64	GLN
8	D	85	ASN
8	D	108	GLN
8	D	109	GLN
10	G	25	ASN

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Mol	Chain	Res	Type
10	G	166	ASN
11	H	7	GLN
11	H	18	GLN
11	H	102	HIS
12	I	95	GLN
12	I	114	GLN
15	N	374	HIS
15	N	428	ASN
15	N	448	ASN
15	N	507	GLN
15	N	717	ASN
15	N	828	HIS
15	N	909	GLN
15	N	1219	HIS
16	O	700	ASN
16	O	742	GLN
16	O	750	GLN
16	O	762	GLN
17	P	225	ASN
17	P	282	HIS
17	P	301	GLN
17	P	609	ASN
17	P	751	GLN
18	Q	18	GLN
18	Q	227	ASN
18	Q	290	HIS
18	Q	300	ASN
18	Q	330	GLN
18	Q	340	GLN
18	Q	411	GLN
18	Q	482	GLN
18	Q	565	ASN
18	Q	634	ASN
19	R	90	GLN
19	R	127	HIS
19	R	156	ASN
21	T	118	GLN
22	U	13	ASN
22	U	21	ASN
22	U	56	GLN
24	W	53	GLN
24	W	113	GLN

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Mol	Chain	Res	Type
24	W	203	ASN
24	W	233	ASN
24	W	239	ASN
24	W	345	GLN
24	W	587	GLN
24	W	602	HIS
24	W	730	HIS
24	W	747	ASN
24	W	759	ASN
24	W	844	ASN
24	W	946	GLN
24	W	1095	ASN
24	W	1134	GLN
25	X	26	ASN
25	X	335	ASN
25	X	356	ASN
25	X	370	GLN
25	X	419	ASN
25	X	502	HIS
25	X	571	GLN
25	X	730	HIS
25	X	945	GLN
26	a	251	GLN
26	a	331	GLN
27	b	4	ASN
27	b	26	GLN
27	b	243	ASN
28	c	40	ASN
28	c	43	GLN
28	c	101	ASN
28	c	232	GLN
28	c	458	HIS
28	c	866	HIS
28	c	946	GLN
28	c	1014	ASN
28	c	1338	ASN
28	c	1369	GLN
28	c	1512	ASN
28	c	1530	HIS
28	c	1615	ASN
29	d	182	GLN
29	d	184	GLN

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Mol	Chain	Res	Type
29	d	287	GLN
29	d	1101	ASN
29	d	1131	ASN
29	d	1137	ASN
29	d	1800	GLN
29	d	1821	ASN
29	d	2101	HIS

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 ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

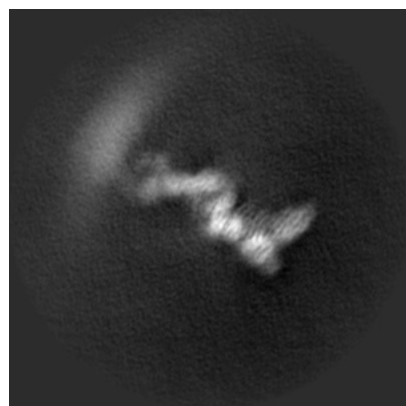
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41565. These allow visual inspection of the internal detail of the map and identification of artifacts.

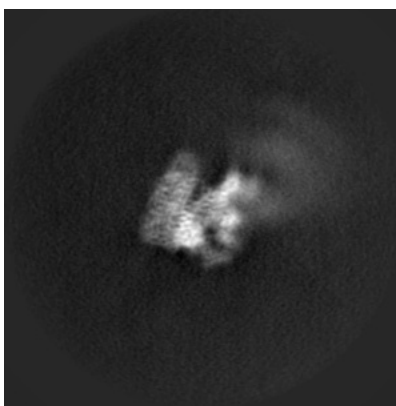
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

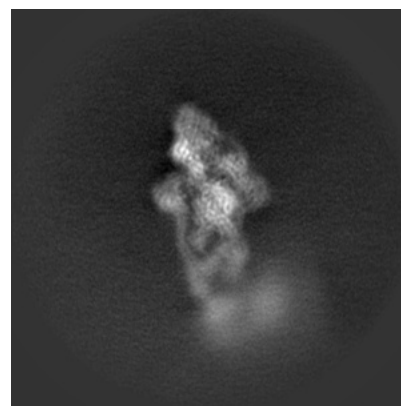
6.1.1 Primary map



X

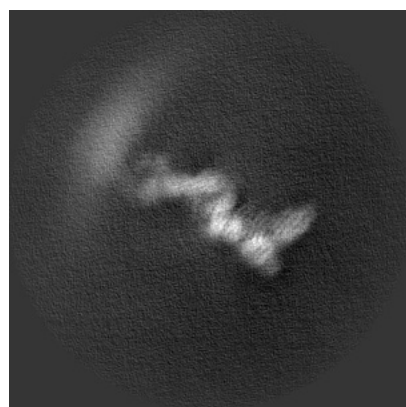


Y

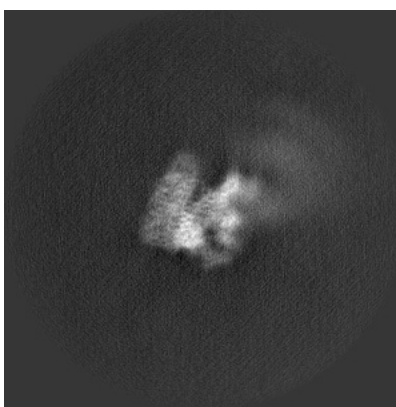


Z

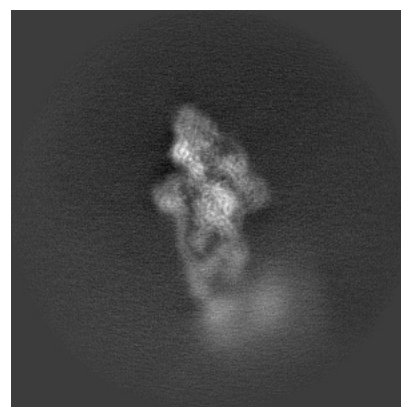
6.1.2 Raw map



X



Y

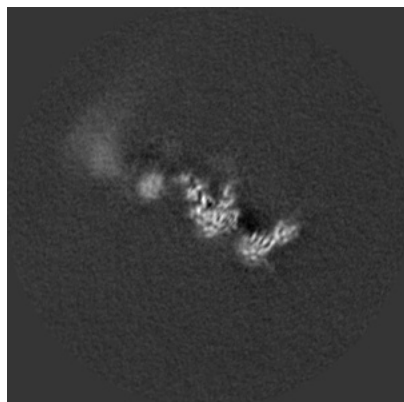


Z

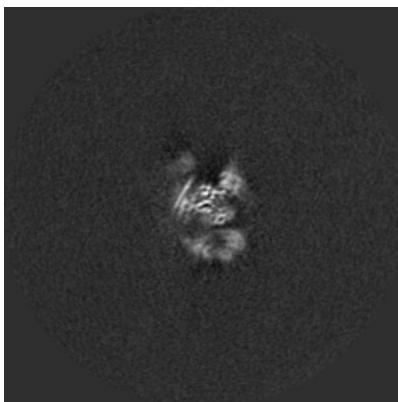
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

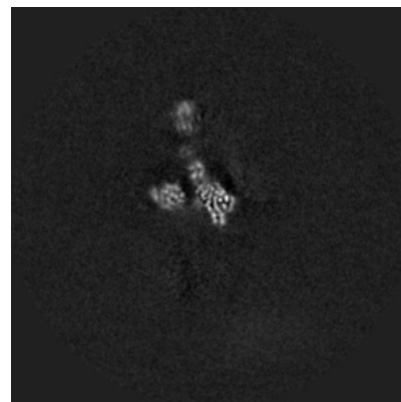
6.2.1 Primary map



X Index: 160

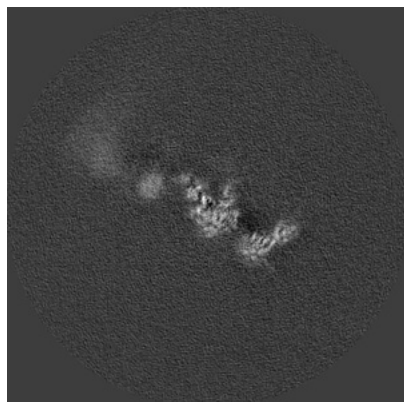


Y Index: 160

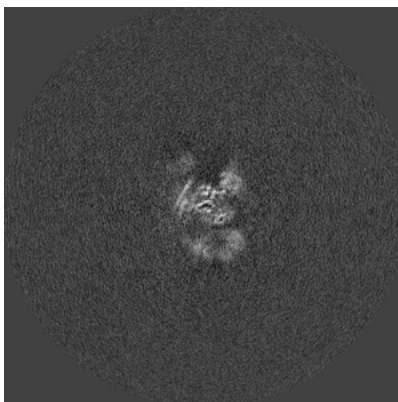


Z Index: 160

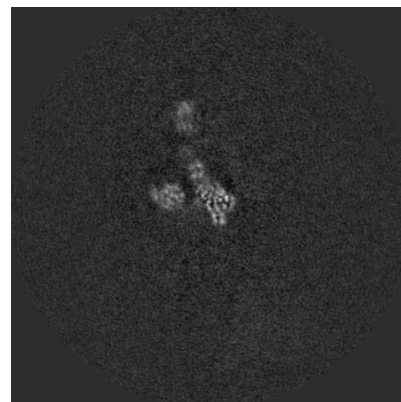
6.2.2 Raw map



X Index: 160



Y Index: 160

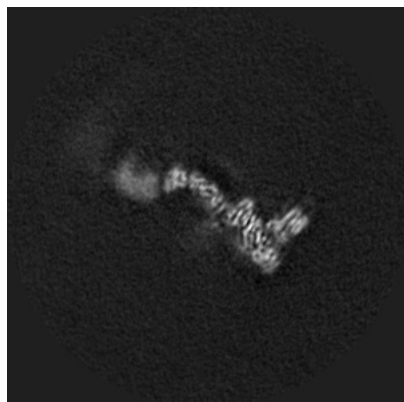


Z Index: 160

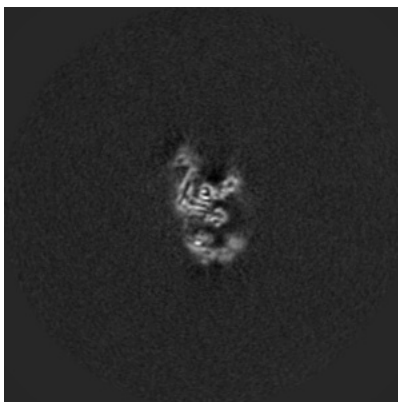
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

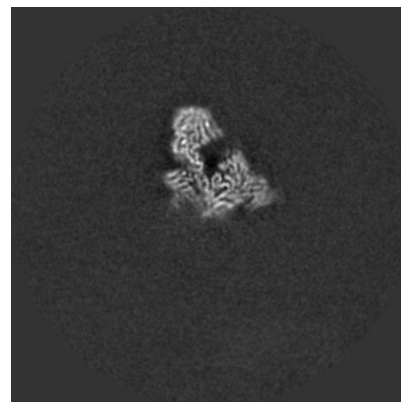
6.3.1 Primary map



X Index: 149

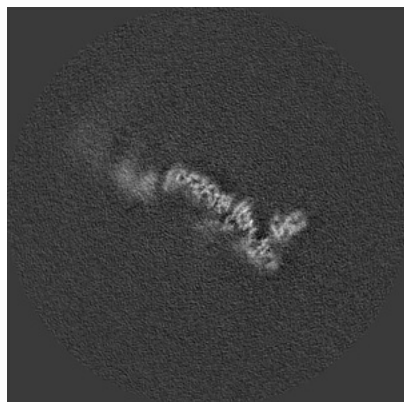


Y Index: 165

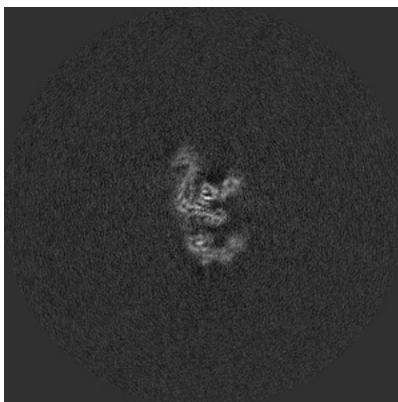


Z Index: 145

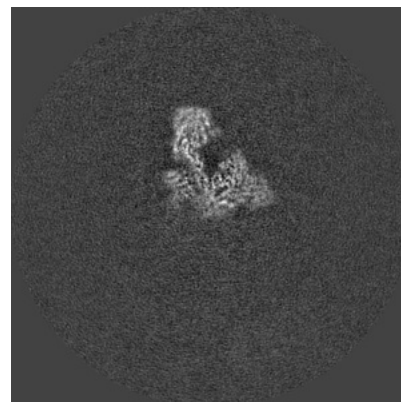
6.3.2 Raw map



X Index: 152



Y Index: 166



Z Index: 146

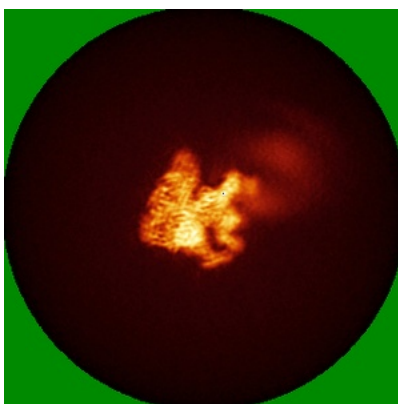
The images above show the largest variance slices of the map in three orthogonal directions.

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

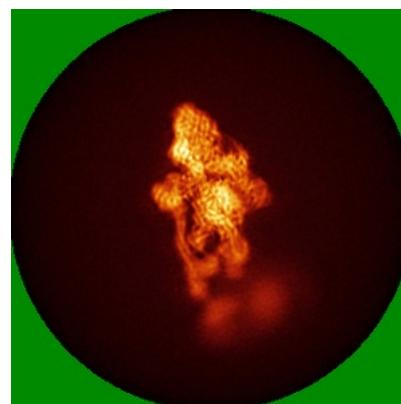
6.4.1 Primary map



X

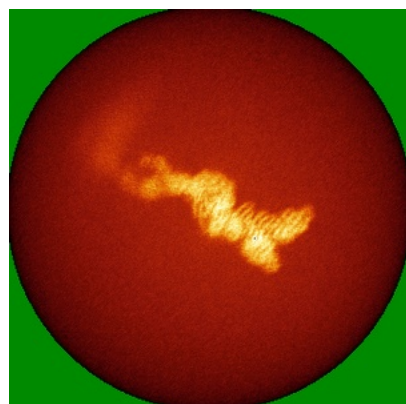


Y

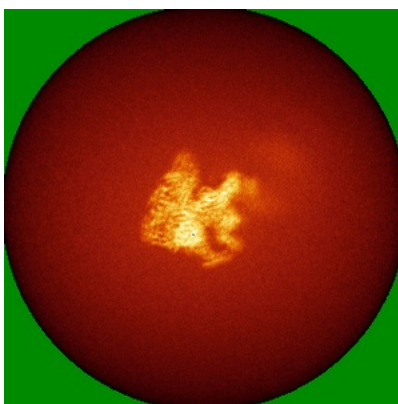


Z

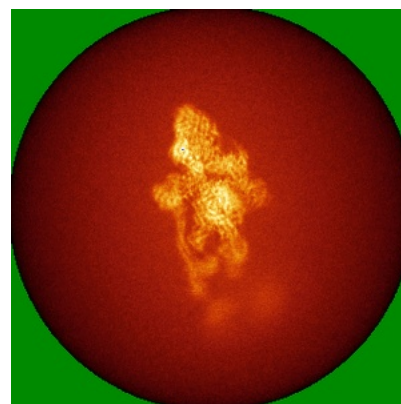
6.4.2 Raw map



X



Y

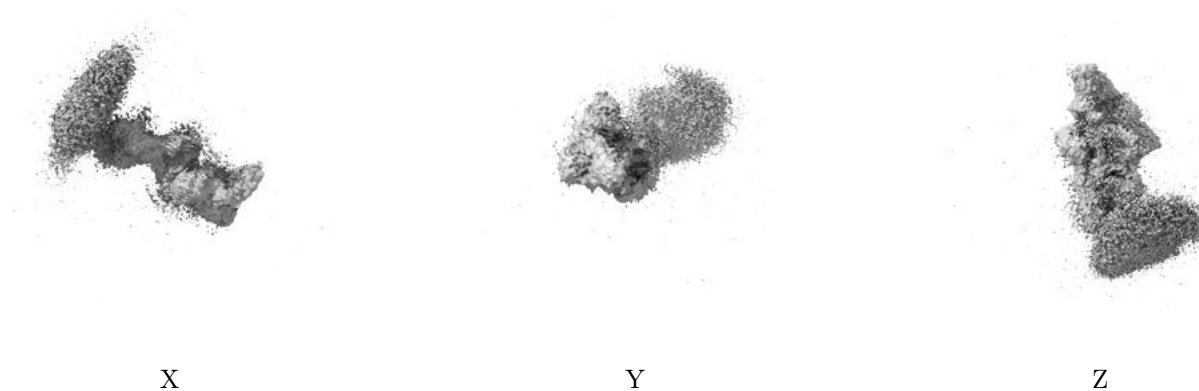


Z

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

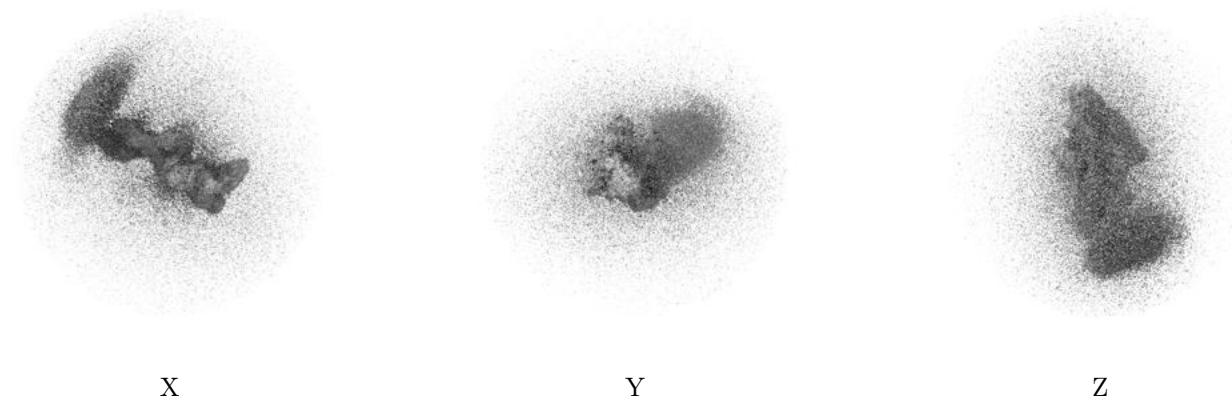
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

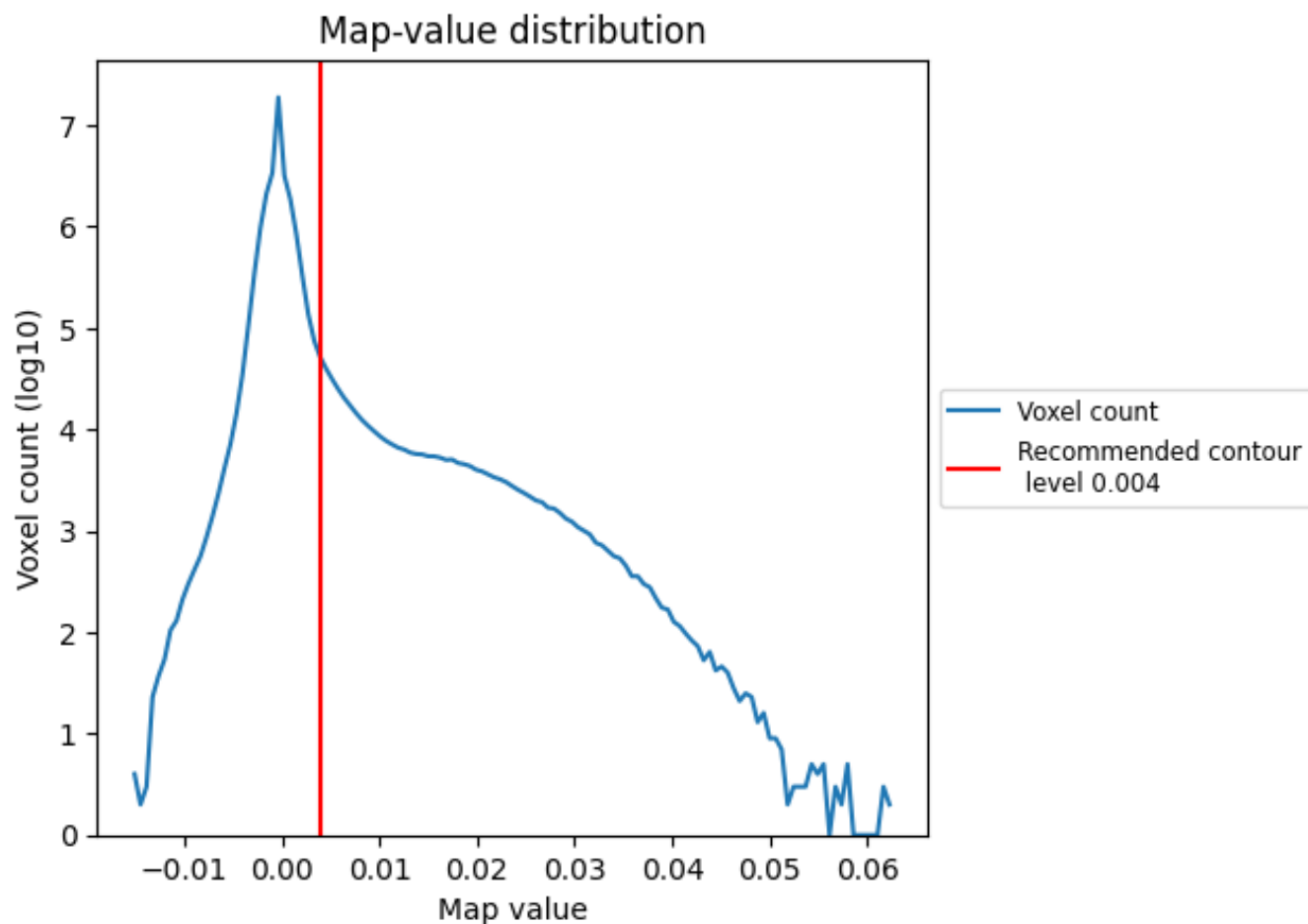
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

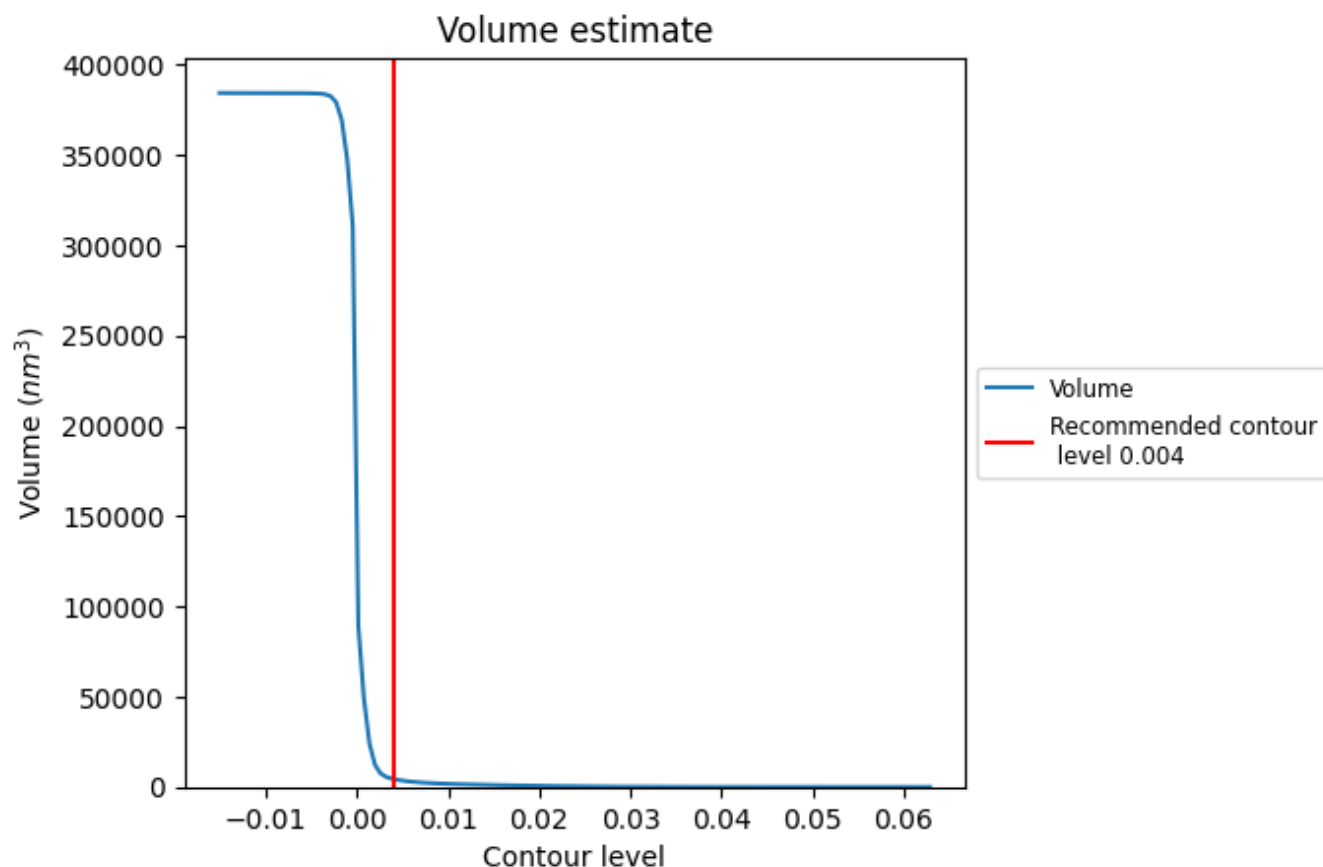
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

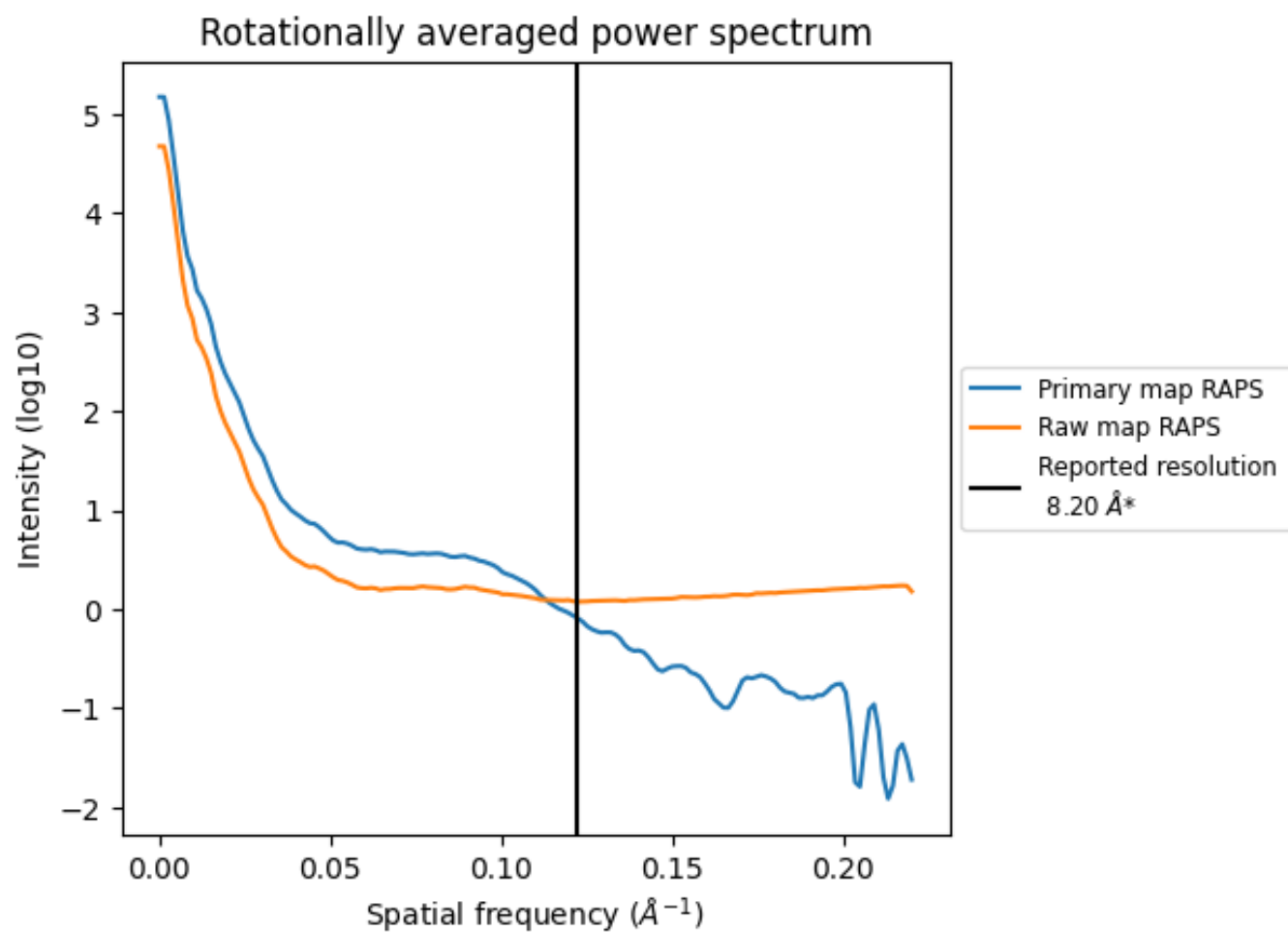
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4396 nm^3 ; this corresponds to an approximate mass of 3971 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 ⓘ

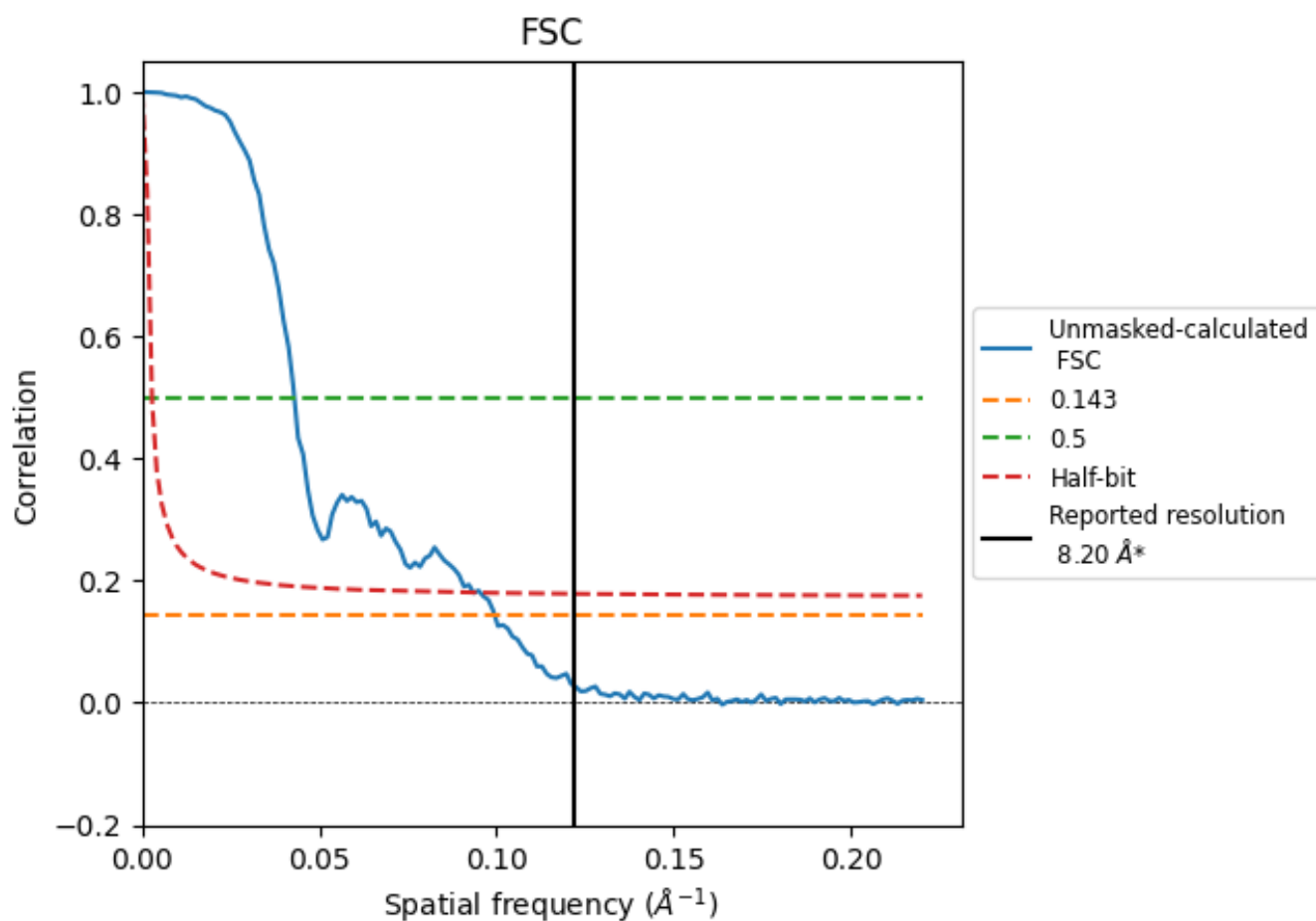


*Reported resolution corresponds to spatial frequency of 0.122 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.122 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

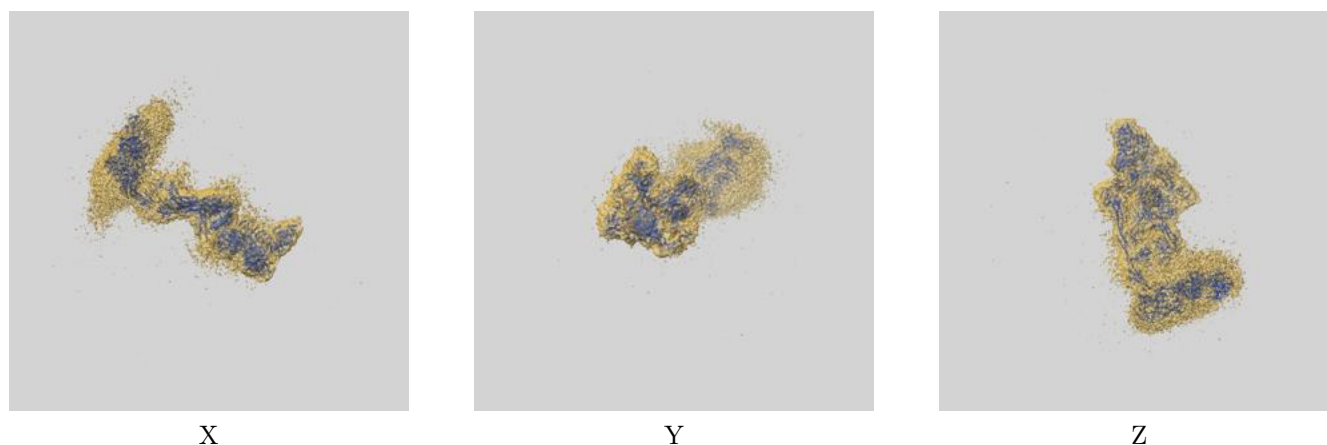
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	10.05	23.31	10.70

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 10.05 differs from the reported value 8.2 by more than 10 %

9 Map-model fit [i](#)

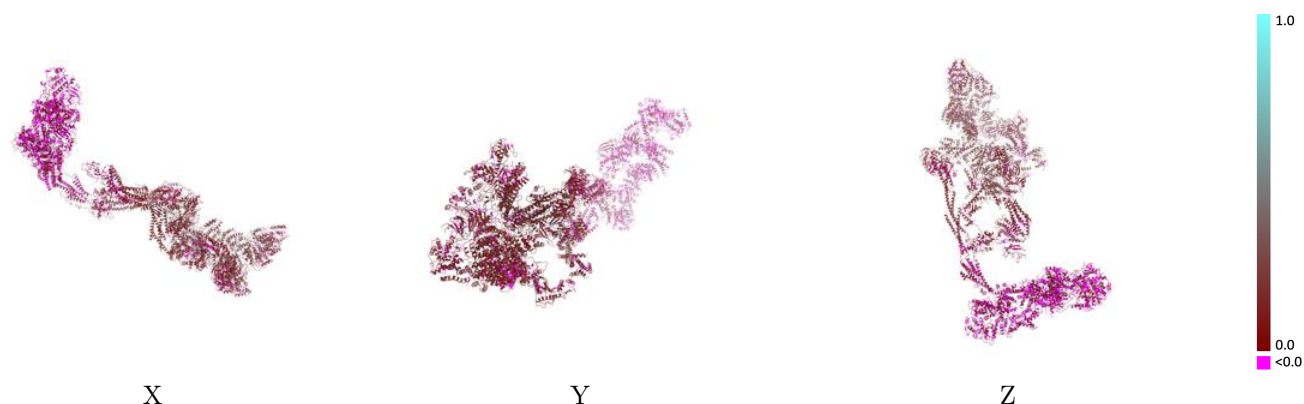
This section contains information regarding the fit between EMDB map EMD-41565 and PDB model 8TQW. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



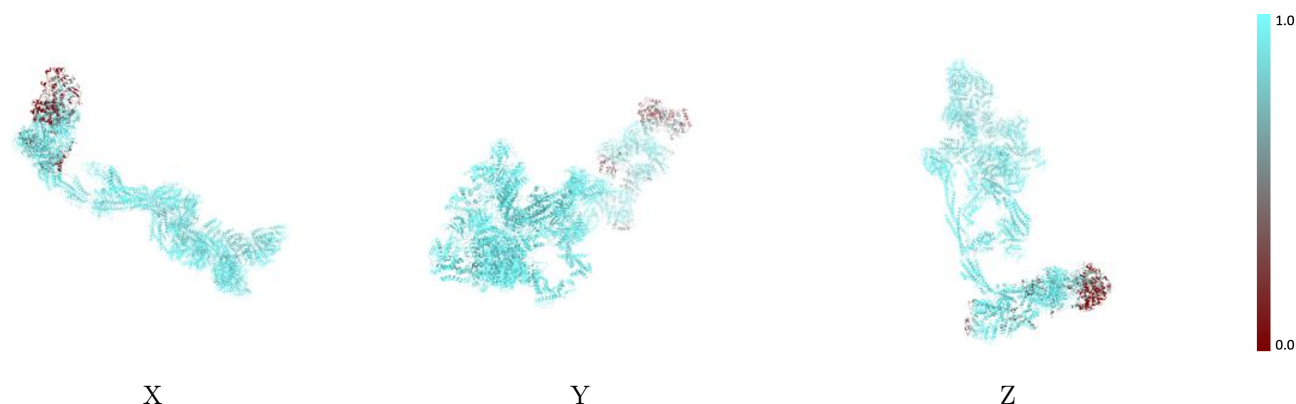
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



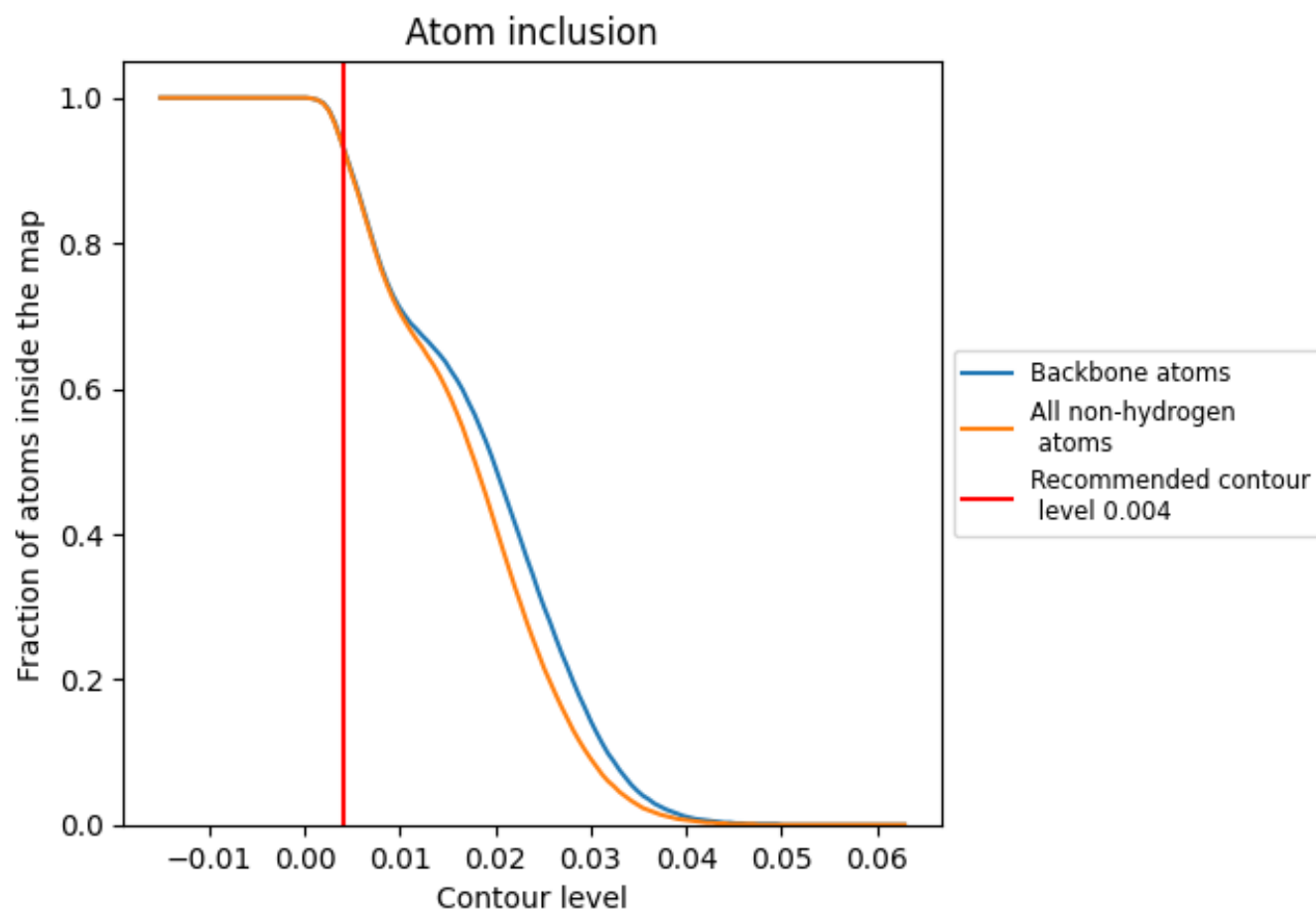
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.004).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 93% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9340	 0.1110
0	 0.9980	 0.1790
1	 1.0000	 0.1670
2	 1.0000	 0.1470
3	 1.0000	 0.1610
4	 1.0000	 0.0940
A	 1.0000	 0.1290
B	 1.0000	 0.2460
D	 1.0000	 0.1340
F	 1.0000	 0.0940
G	 0.9990	 0.0980
H	 0.9950	 0.1220
I	 1.0000	 0.1670
J	 0.9960	 0.0370
K	 1.0000	 0.1270
N	 1.0000	 0.1720
O	 1.0000	 0.2010
P	 0.9990	 0.1450
Q	 1.0000	 0.1780
R	 1.0000	 0.1390
S	 1.0000	 0.0690
T	 1.0000	 0.1490
U	 0.9960	 0.0850
V	 1.0000	 0.1440
W	 1.0000	 0.1550
X	 0.9990	 0.1660
a	 0.3260	 0.0050
b	 0.2570	 0.0040
c	 0.8820	 0.0110
d	 0.8920	 0.0170

