



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:20 AM UTC

PDB ID : 8TRH / pdb_00008trh
EMDB ID : EMD-41580
Title : The IDRc bound human core 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 : 2023-08-09
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

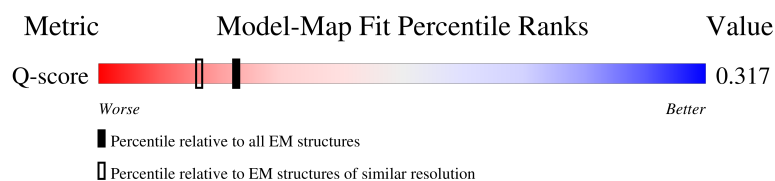
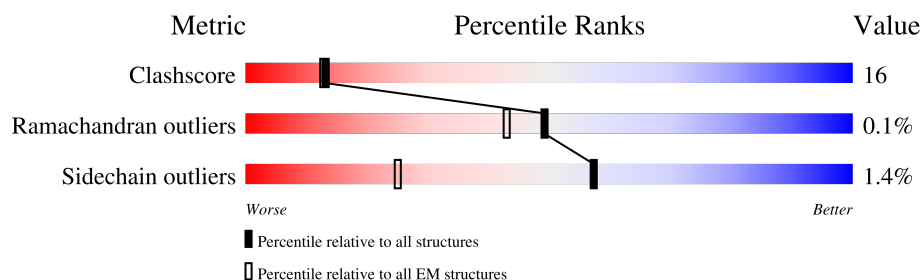
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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	
6	A	1581	
7	B	20	
8	D	270	
9	F	246	
10	G	233	
11	H	268	
12	I	146	
13	J	135	
14	K	117	
15	N	1454	
16	O	788	
17	P	877	
18	Q	651	
19	R	208	
20	T	212	
21	V	200	
22	W	1368	
23	X	989	
24	d	2174	
25	S	244	
26	U	144	

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 59957 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	106	Total	C	N	O	S	0	0
			932	610	161	156	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
			1266	790	228	242	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	167	Total	C	N	O	S	0	0
			1374	888	238	243	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	159	Total	C	N	O	S	0	0
			1284	812	227	235	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
			834	521	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
			7768	4955	1364	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	556	Total	C	N	O	S	0	0
			4387	2774	782	812	19		

- 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 20.

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

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

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

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

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

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

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

- Molecule 24 is a protein called Mediator of RNA polymerase II transcription subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	d	37	Total	C	N	O	S	0	0
			295	194	46	52	3		

- Molecule 25 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	74	Total	C	N	O	S	0	0
			435	264	81	89	1		

- Molecule 26 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	116	Total	C	N	O	S	0	0
			869	537	144	183	5		

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

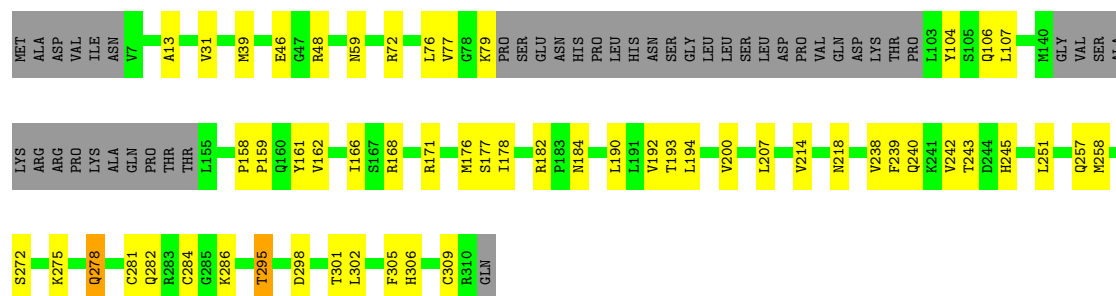
Mol	Chain	Residues	Atoms		AltConf
27	0	1	Total	Zn	0
			1	1	
27	P	1	Total	Zn	0
			1	1	

3 Residue-property plots [i](#)

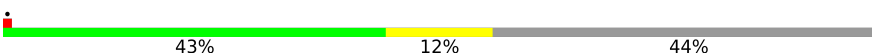
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

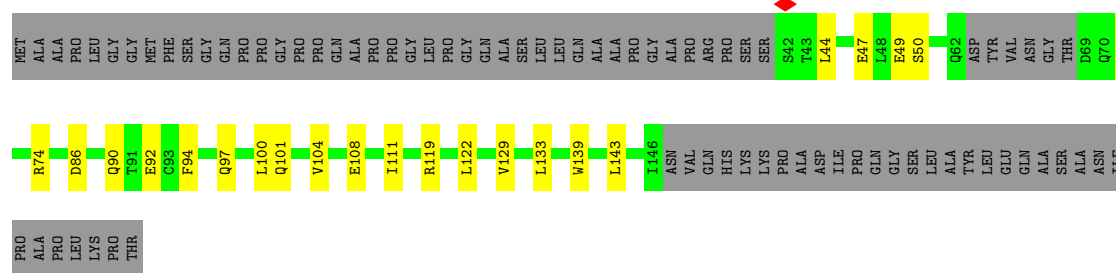
- Molecule 1: Mediator of RNA polymerase II transcription subunit 27

Chain 0: 



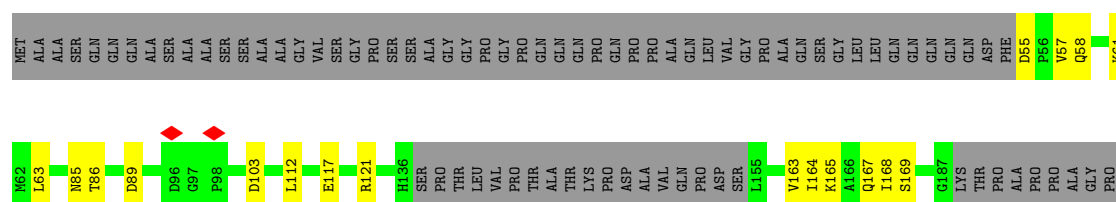
- Molecule 2: Mediator of RNA polymerase II transcription subunit 28

Chain 1: 



- Molecule 3: Mediator of RNA polymerase II transcription subunit 29

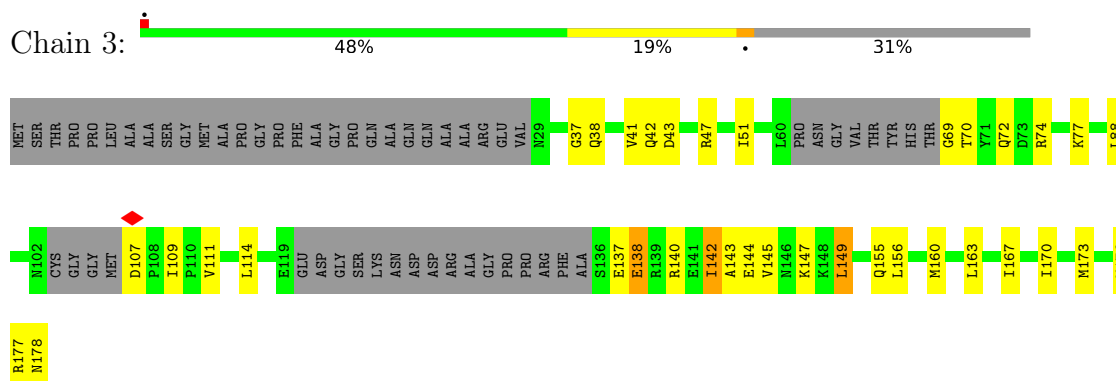
Chain 2: 



GLY
THR
LEU

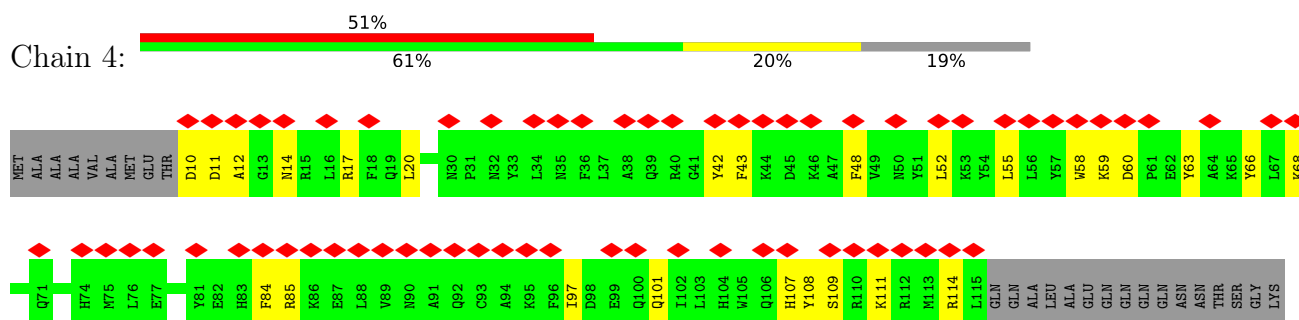
• Molecule 4: Mediator of RNA polymerase II transcription subunit 30

Chain 3:



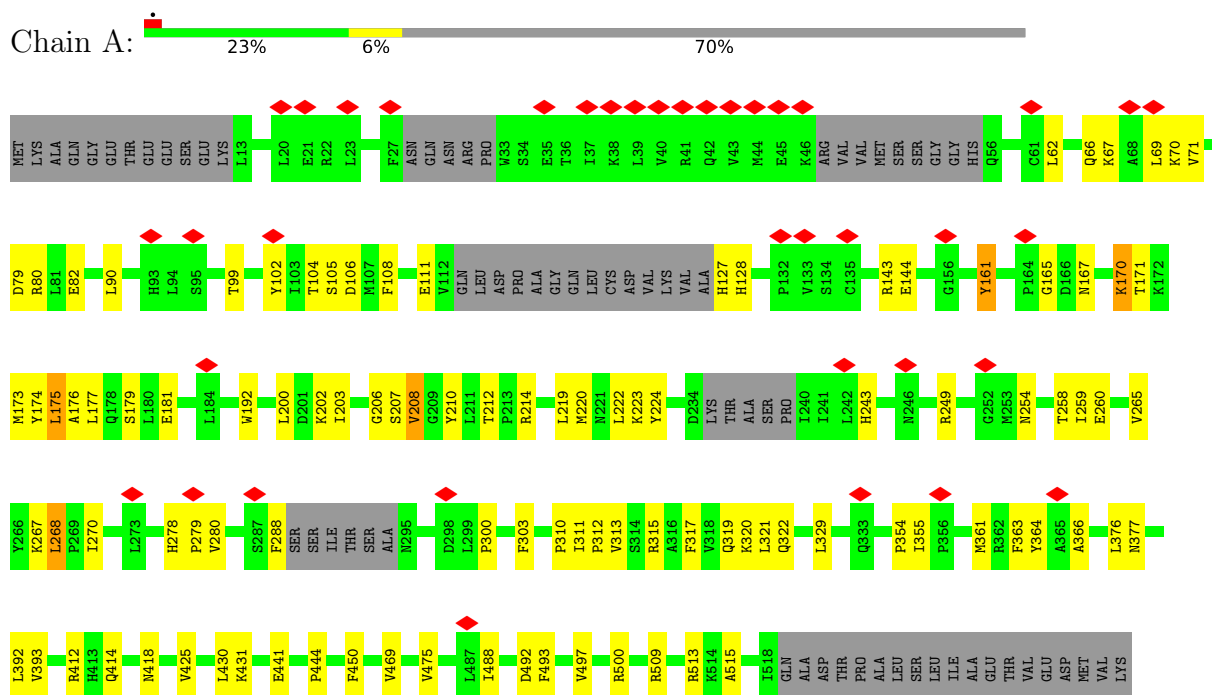
• Molecule 5: Mediator of RNA polymerase II transcription subunit 31

Chain 4:



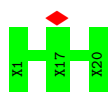
• Molecule 6: Mediator of RNA polymerase II transcription subunit 1

Chain A:

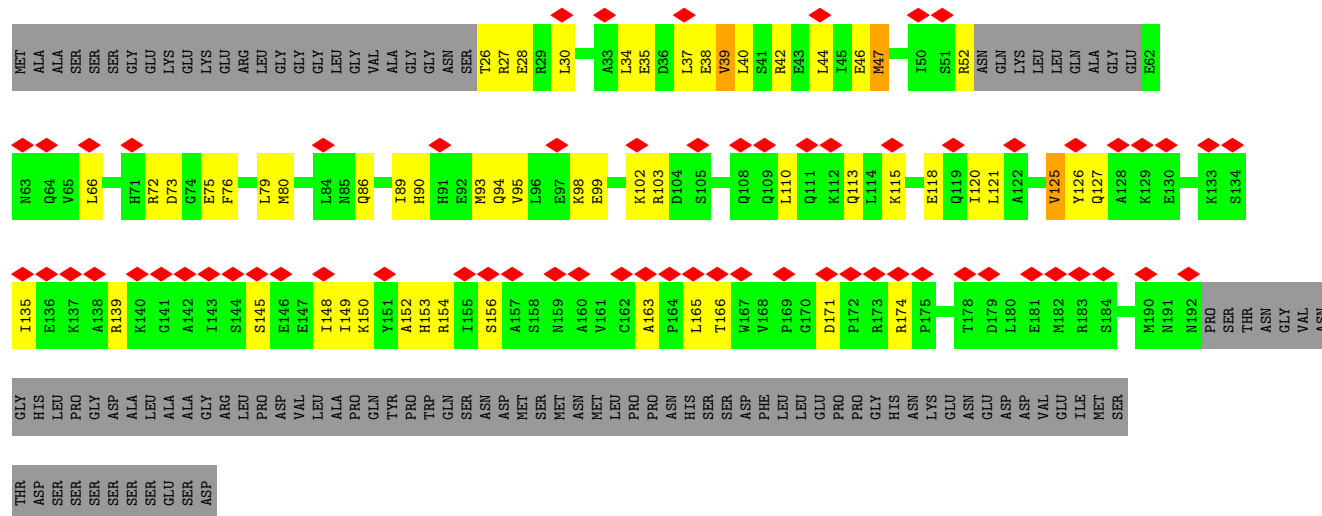


- Molecule 7: Unknown Chain

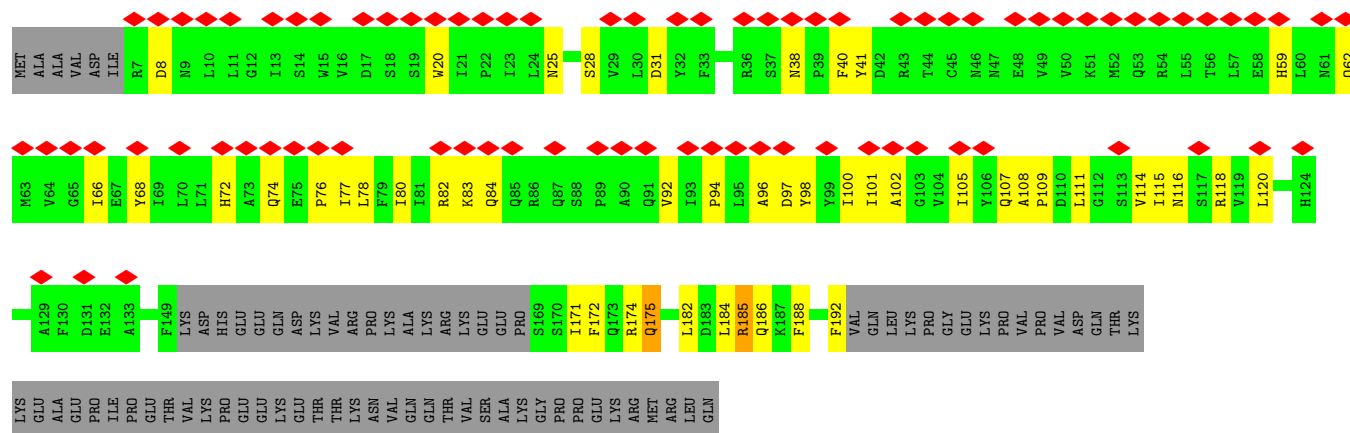




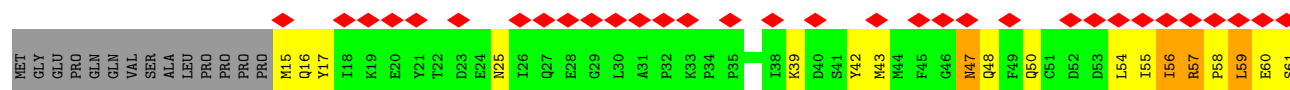
• Molecule 8: Mediator of RNA polymerase II transcription subunit 4

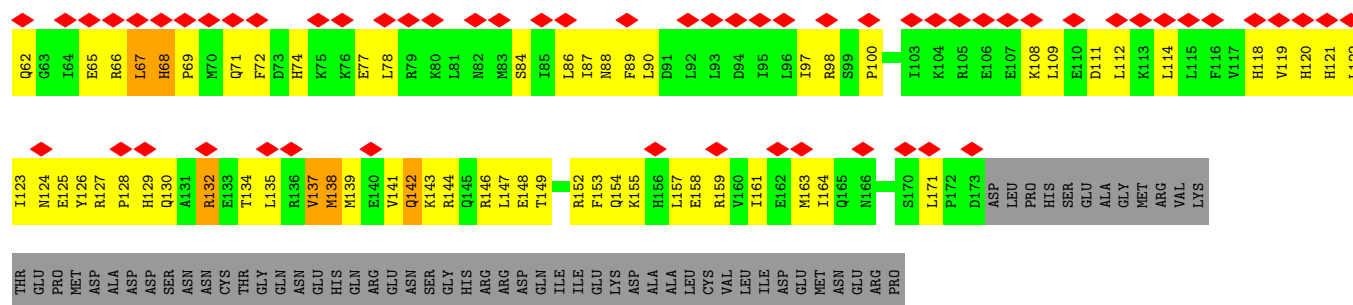


• Molecule 9: Mediator of RNA polymerase II transcription subunit 6

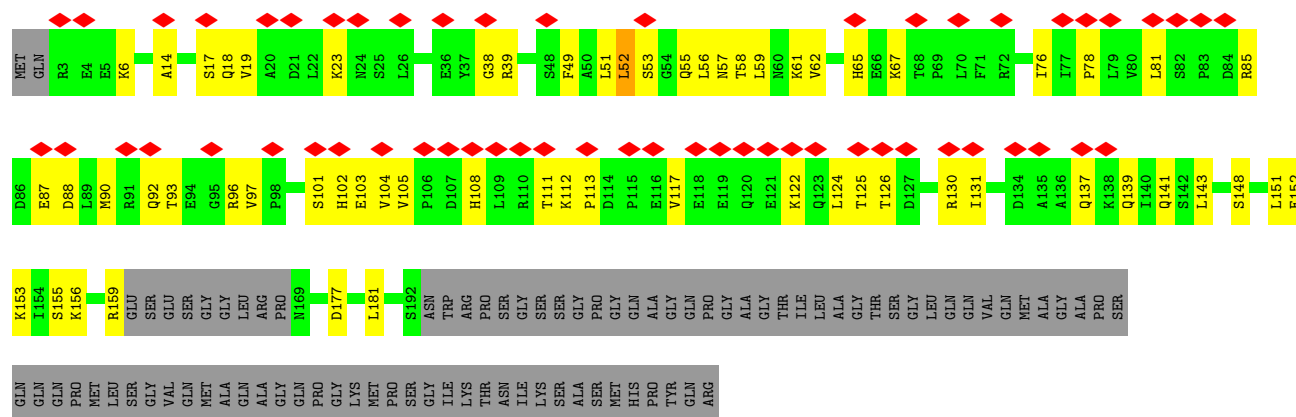


• Molecule 10: Mediator of RNA polymerase II transcription subunit 7

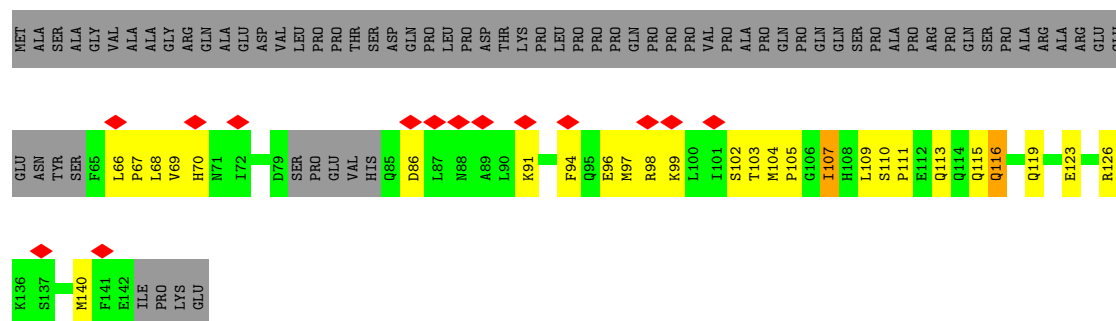
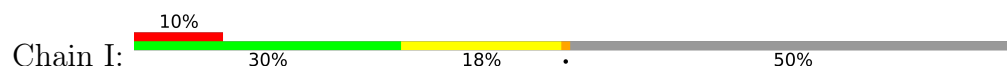




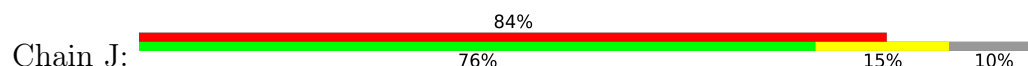
• Molecule 11: Mediator of RNA polymerase II transcription subunit 8



• Molecule 12: Mediator of RNA polymerase II transcription subunit 9

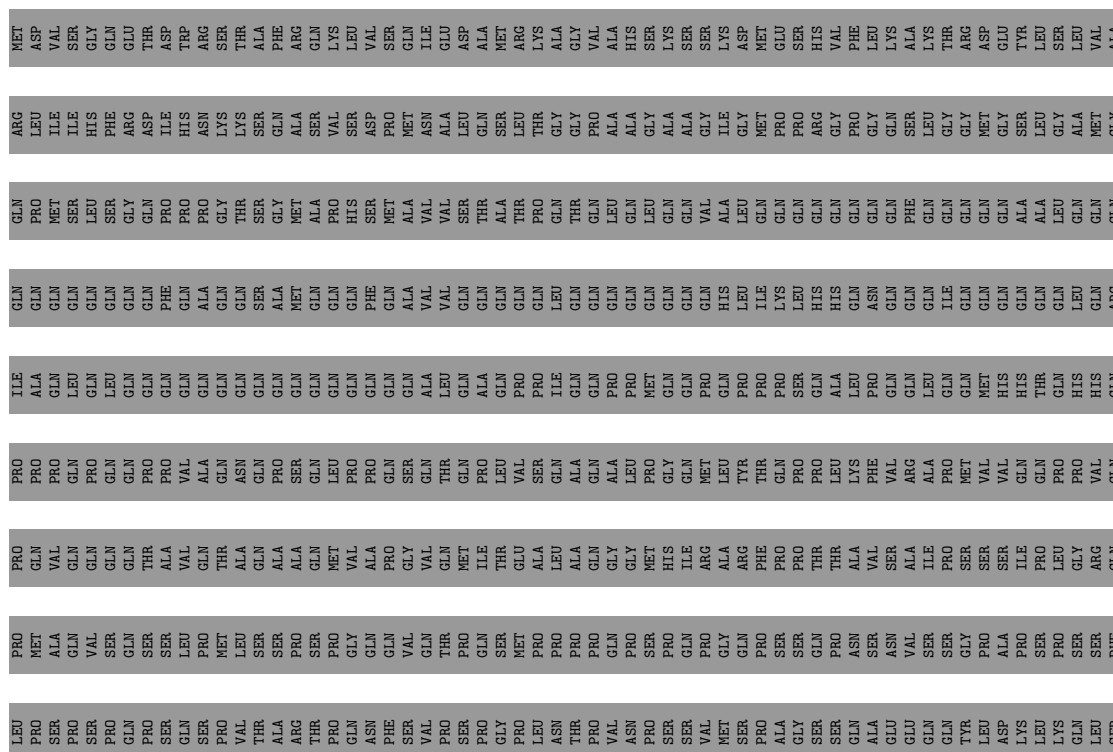


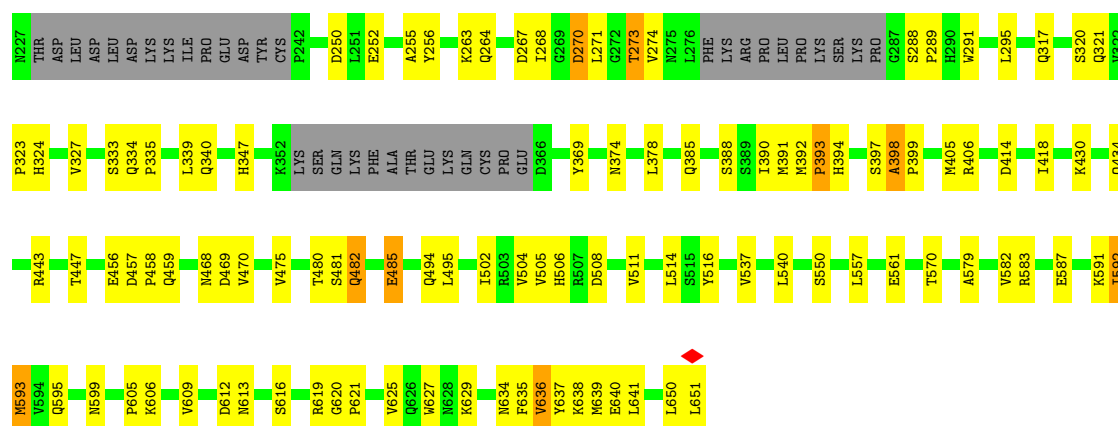
• Molecule 13: Mediator of RNA polymerase II transcription subunit 10



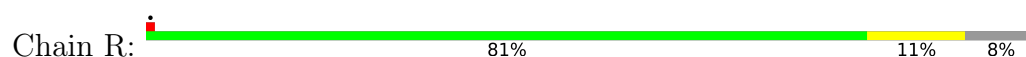


Chain 0: 16% . 80%

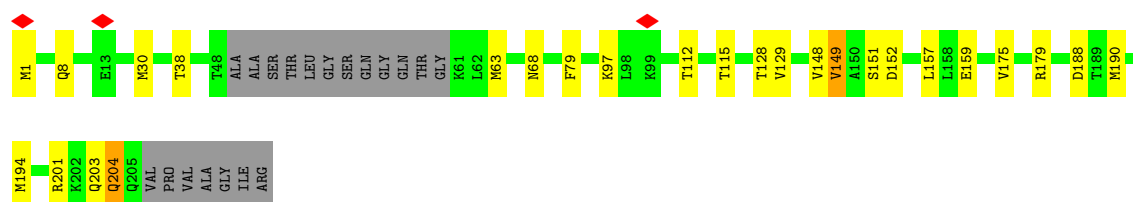
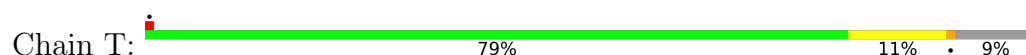




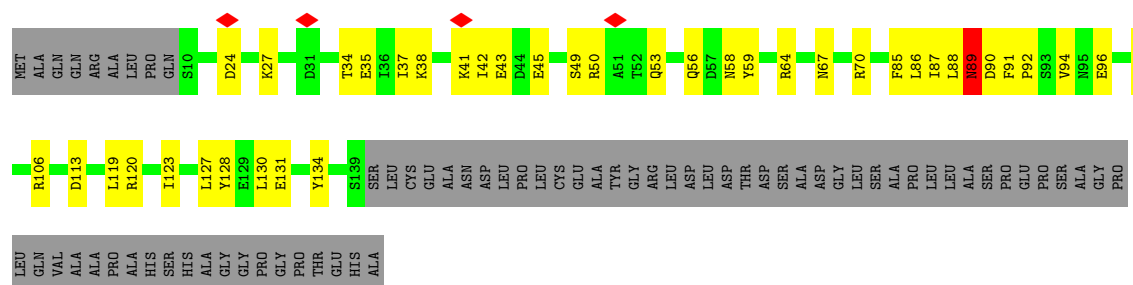
- Molecule 19: Mediator of RNA polymerase II transcription subunit 18



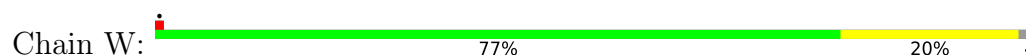
- Molecule 20: Mediator of RNA polymerase II transcription subunit 20

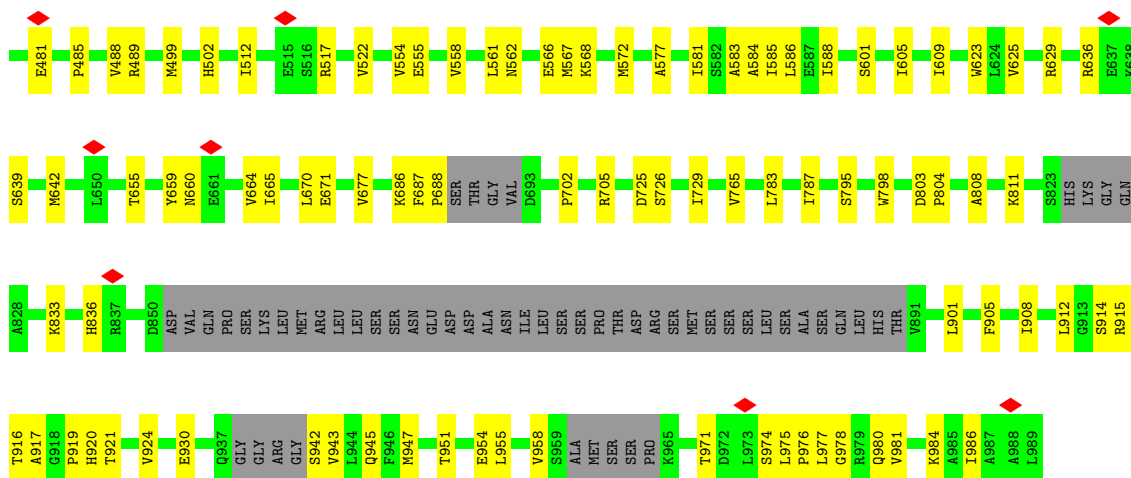


- Molecule 21: Mediator of RNA polymerase II transcription subunit 22

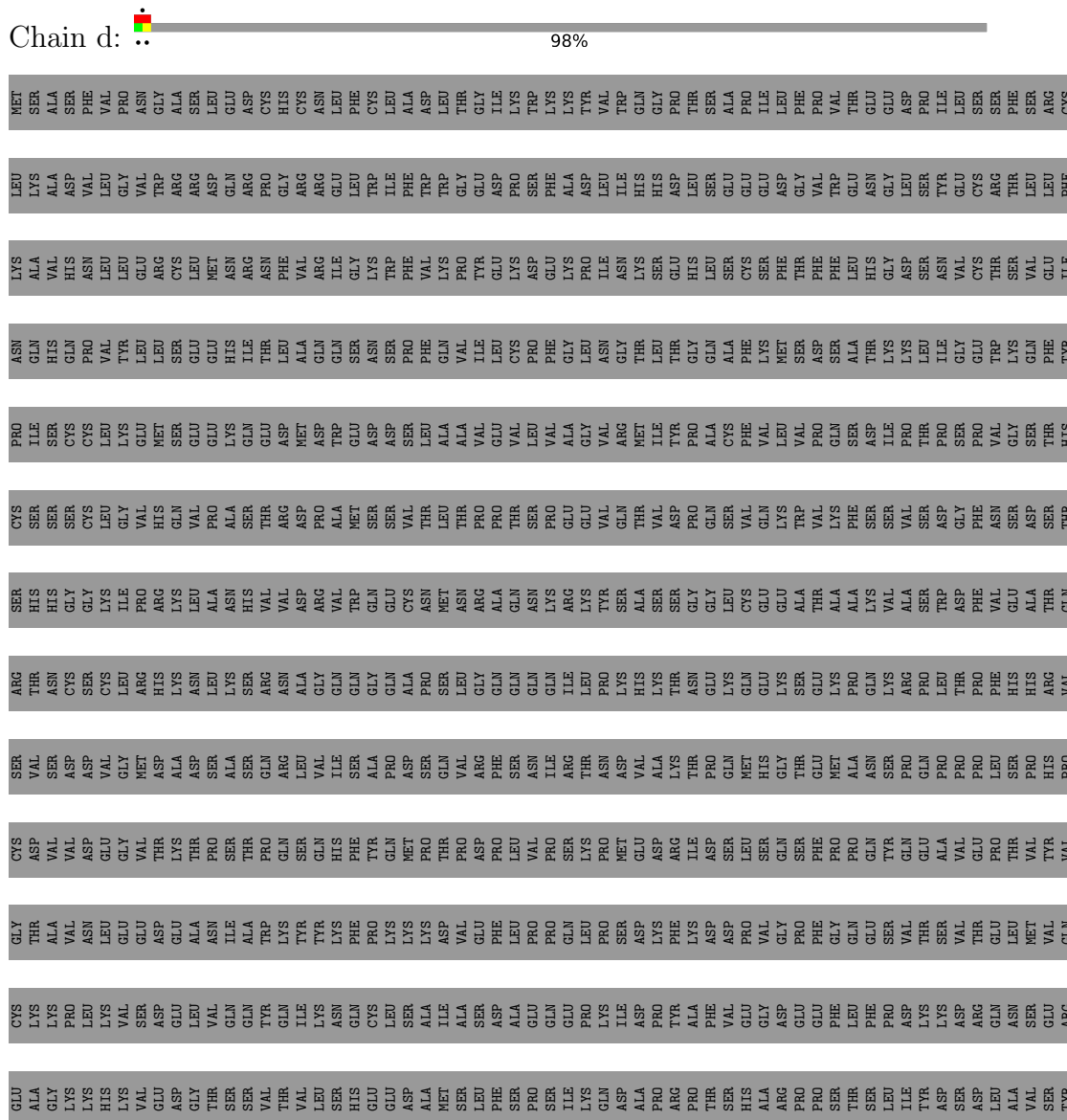


- Molecule 22: Mediator of RNA polymerase II transcription subunit 23

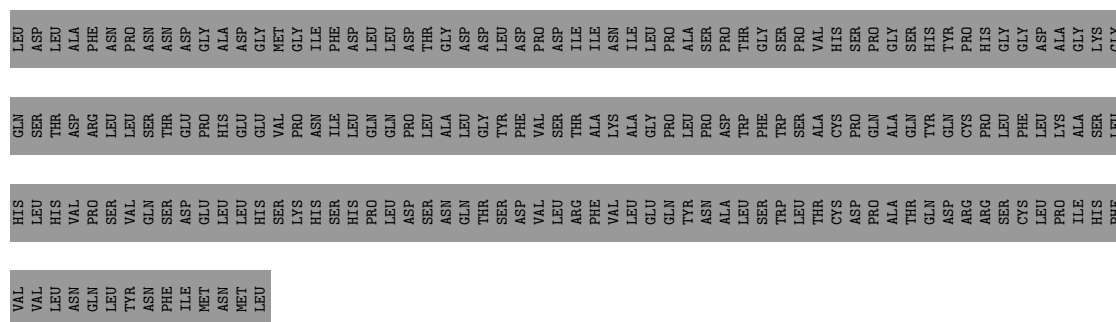




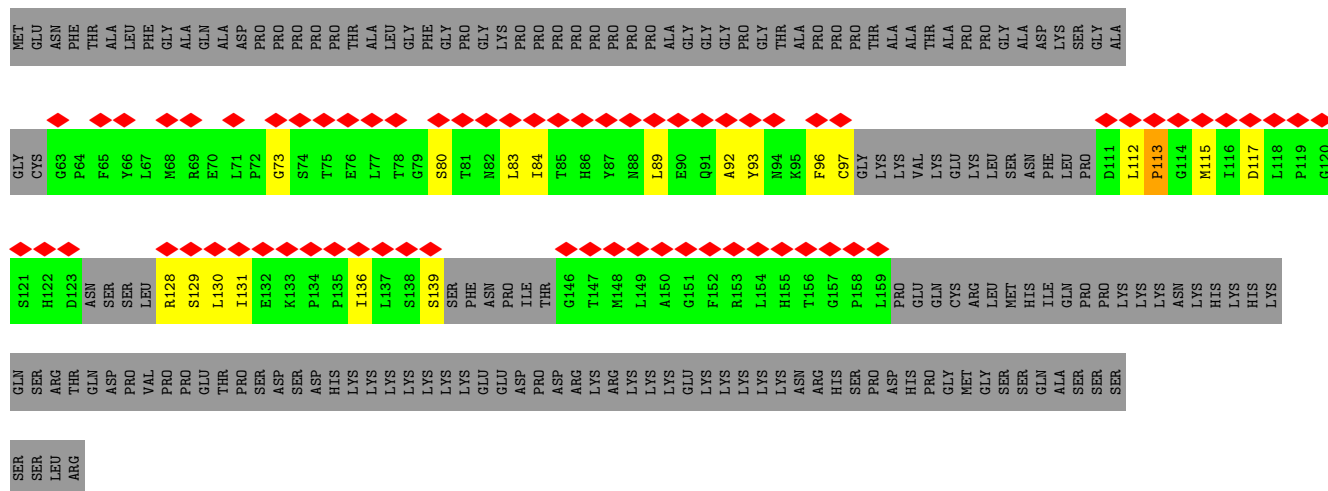
- Molecule 24: Mediator of RNA polymerase II transcription subunit 13



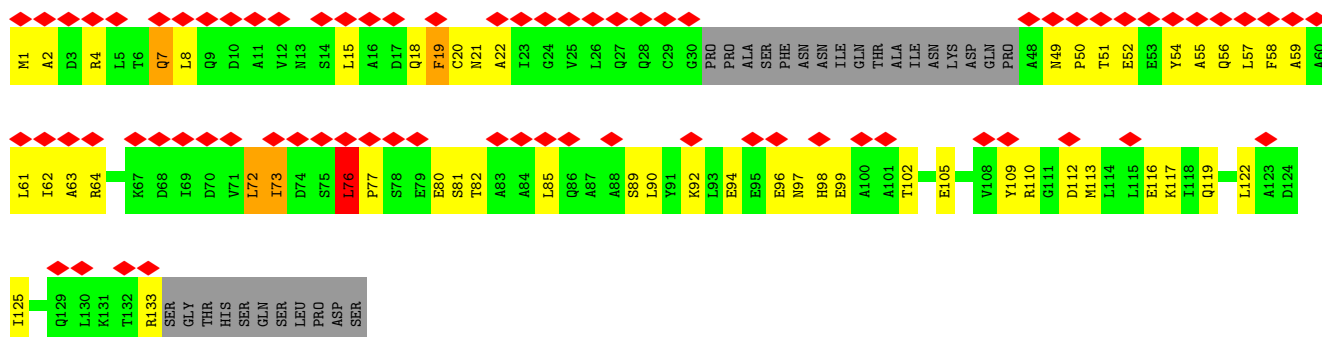




- Molecule 25: Mediator of RNA polymerase II transcription subunit 19



- Molecule 26: Mediator of RNA polymerase II transcription subunit 21



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97904	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	0.187	Depositor
Minimum map value	-0.103	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	549.3488, 549.3488, 549.3488	wwPDB
Map dimensions	392, 392, 392	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4014001, 1.4014001, 1.4014001	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	0.20	0/2201	0.41	0/2972
2	1	0.28	0/825	0.55	0/1107
3	2	0.18	0/911	0.37	0/1229
4	3	0.21	0/1029	0.45	0/1378
5	4	0.19	0/959	0.44	0/1291
6	A	0.21	0/3653	0.53	2/4961 (0.0%)
8	D	0.24	0/1279	0.60	0/1715
9	F	0.22	0/1411	0.51	0/1916
10	G	0.29	0/1310	0.83	4/1769 (0.2%)
11	H	0.24	0/1441	0.63	0/1946
12	I	0.28	0/612	0.78	1/815 (0.1%)
13	J	0.16	0/842	0.34	0/1141
14	K	0.34	0/885	0.71	0/1190
15	N	0.28	0/7919	0.75	31/10757 (0.3%)
16	O	0.18	0/1261	0.40	0/1731
17	P	0.15	0/6001	0.36	0/8151
18	Q	0.33	0/4469	0.76	3/6038 (0.0%)
19	R	0.19	0/1562	0.41	0/2101
20	T	0.20	0/1530	0.45	1/2066 (0.0%)
21	V	0.27	0/1072	0.57	2/1440 (0.1%)
22	W	0.27	0/11056	0.55	4/15023 (0.0%)
23	X	0.17	0/7191	0.39	0/9728
24	d	0.29	0/304	1.47	8/413 (1.9%)
25	S	0.49	1/436 (0.2%)	1.21	7/594 (1.2%)
26	U	0.32	0/875	0.81	4/1186 (0.3%)
All	All	0.24	1/61034 (0.0%)	0.58	67/82658 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	129	SER	CA-C	5.75	1.60	1.52

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	204	VAL	N-CA-C	11.60	121.44	110.53
25	S	129	SER	N-CA-C	-11.08	98.96	111.71
24	d	929	PRO	CA-C-N	10.54	130.87	119.28
24	d	929	PRO	C-N-CA	10.54	130.87	119.28
10	G	68	HIS	CA-C-N	9.14	129.07	120.03
10	G	68	HIS	C-N-CA	9.14	129.07	120.03
24	d	923	LEU	CA-C-N	8.78	128.94	119.28
24	d	923	LEU	C-N-CA	8.78	128.94	119.28
24	d	933	LEU	CA-C-N	8.60	130.59	119.84
24	d	933	LEU	C-N-CA	8.60	130.59	119.84
15	N	678	PHE	N-CA-C	8.30	120.32	111.28
15	N	247	LEU	N-CA-C	8.19	121.59	108.41
15	N	545	LEU	CA-C-N	7.99	127.88	120.21
15	N	545	LEU	C-N-CA	7.99	127.88	120.21
15	N	229	GLU	N-CA-C	7.84	123.42	113.55
15	N	543	THR	N-CA-C	7.82	119.88	111.36
15	N	468	TYR	N-CA-C	7.66	119.63	111.28
24	d	928	LEU	CA-C-N	7.63	128.24	120.38
24	d	928	LEU	C-N-CA	7.63	128.24	120.38
26	U	76	LEU	CA-C-N	7.57	128.02	119.92
26	U	76	LEU	C-N-CA	7.57	128.02	119.92
18	Q	398	ALA	CA-C-N	7.35	127.27	120.21
18	Q	398	ALA	C-N-CA	7.35	127.27	120.21
15	N	378	LEU	CA-C-N	7.01	127.18	120.31
15	N	378	LEU	C-N-CA	7.01	127.18	120.31
15	N	230	PHE	N-CA-C	6.86	119.18	108.96
25	S	113	PRO	N-CA-C	-6.84	104.24	113.40
15	N	222	VAL	N-CA-C	6.65	116.81	110.42
25	S	129	SER	CA-C-N	6.58	130.31	120.31
25	S	129	SER	C-N-CA	6.58	130.31	120.31
22	W	610	TYR	N-CA-C	6.50	120.52	112.59
25	S	115	MET	N-CA-C	-6.40	104.30	111.28
15	N	151	SER	N-CA-C	6.33	117.85	108.60
15	N	679	SER	N-CA-C	6.13	118.94	109.07
15	N	692	GLY	N-CA-C	6.07	123.69	115.32
20	T	204	GLN	CB-CA-C	-6.00	109.64	116.54
26	U	73	ILE	N-CA-C	5.91	116.65	110.62
15	N	150	PRO	N-CA-C	5.90	121.30	113.40
15	N	688	PRO	CA-C-N	5.74	125.42	119.05
15	N	688	PRO	C-N-CA	5.74	125.42	119.05
15	N	178	ILE	N-CA-C	5.70	114.39	107.61
25	S	73	GLY	CA-C-N	5.63	128.14	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	S	73	GLY	C-N-CA	5.63	128.14	120.54
15	N	381	SER	N-CA-C	5.50	117.98	107.75
21	V	88	LEU	N-CA-C	5.50	117.35	111.36
15	N	414	GLN	CA-C-N	-5.39	112.03	122.06
15	N	414	GLN	C-N-CA	-5.39	112.03	122.06
15	N	181	ASP	CA-C-N	5.35	125.33	120.03
15	N	181	ASP	C-N-CA	5.35	125.33	120.03
10	G	118	HIS	N-CA-C	5.35	116.92	111.14
12	I	130	GLU	N-CA-CB	5.35	118.57	110.28
15	N	177	ILE	N-CA-C	5.35	116.12	110.72
10	G	111	ASP	N-CA-C	-5.33	105.47	111.28
6	A	280	VAL	CA-C-N	5.27	133.42	122.41
6	A	280	VAL	C-N-CA	5.27	133.42	122.41
15	N	685	LEU	N-CA-C	5.26	117.01	111.28
15	N	376	PRO	CA-C-N	5.25	124.58	118.85
15	N	376	PRO	C-N-CA	5.25	124.58	118.85
22	W	892	LYS	CA-C-N	5.24	126.39	119.84
22	W	892	LYS	C-N-CA	5.24	126.39	119.84
15	N	375	ASP	CA-C-N	-5.14	115.08	120.38
15	N	375	ASP	C-N-CA	-5.14	115.08	120.38
22	W	387	ASN	N-CA-C	5.13	117.66	109.81
18	Q	482	GLN	N-CA-C	5.13	116.87	111.28
26	U	72	LEU	N-CA-C	5.07	116.80	111.28
21	V	89	ASN	N-CA-C	5.06	119.41	112.88
15	N	272	SER	N-CA-C	-5.02	105.89	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	2159	0	2176	49	0
2	1	817	0	818	30	0
3	2	899	0	908	14	0
4	3	1022	0	1054	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	4	932	0	914	35	0
6	A	3578	0	3522	94	0
7	B	100	0	23	0	0
8	D	1266	0	1300	94	0
9	F	1374	0	1357	77	0
10	G	1284	0	1248	174	0
11	H	1422	0	1440	67	0
12	I	605	0	628	68	0
13	J	834	0	711	80	0
14	K	879	0	886	63	0
15	N	7768	0	7546	385	0
16	O	1226	0	1217	27	0
17	P	5875	0	5969	73	0
18	Q	4387	0	4461	236	0
19	R	1532	0	1542	19	0
20	T	1499	0	1484	26	0
21	V	1063	0	1051	84	0
22	W	10774	0	10838	232	0
23	X	7061	0	7223	179	0
24	d	295	0	302	102	0
25	S	435	0	293	49	0
26	U	869	0	846	140	0
27	0	1	0	0	0	0
27	P	1	0	0	0	0
All	All	59957	0	59757	1956	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 16.

All (1956) 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)
13:J:108:LEU:HD21	26:U:55:ALA:CB	1.37	1.52
14:K:70:LEU:HD21	21:V:86:LEU:CD1	1.40	1.51
24:d:923:LEU:HG	24:d:924:PRO:CD	1.52	1.40
24:d:923:LEU:CG	24:d:924:PRO:HD3	1.52	1.39
10:G:68:HIS:ND1	10:G:69:PRO:HD2	1.41	1.35
24:d:928:LEU:CG	24:d:929:PRO:HD3	1.56	1.34
13:J:76:ASN:HB3	25:S:112:LEU:CB	1.56	1.33
10:G:89:PHE:HE2	26:U:19:PHE:CD1	1.47	1.31
24:d:928:LEU:HG	24:d:929:PRO:CD	1.62	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:188:LYS:CD	18:Q:47:ILE:HD11	1.62	1.28
15:N:187:GLU:OE2	18:Q:43:LEU:HD11	1.28	1.28
15:N:181:ASP:OD1	15:N:182:PRO:HD2	1.25	1.26
13:J:82:LYS:HD3	25:S:96:PHE:O	1.35	1.24
15:N:111:LYS:HE2	25:S:92:ALA:CB	1.67	1.23
18:Q:140:ASN:HA	18:Q:143:THR:CG2	1.68	1.23
15:N:442:ILE:HG21	15:N:496:LEU:CD1	1.67	1.22
14:K:70:LEU:CD2	21:V:86:LEU:HD11	1.70	1.21
22:W:396:MET:HE2	22:W:396:MET:HA	1.24	1.19
6:A:66:GLN:NE2	12:I:69:VAL:HG11	1.54	1.19
10:G:89:PHE:CE2	26:U:19:PHE:CD1	2.30	1.18
24:d:928:LEU:HB3	24:d:929:PRO:HD2	1.23	1.18
9:F:101:ILE:CD1	11:H:105:VAL:HG11	1.72	1.17
24:d:928:LEU:CG	24:d:929:PRO:CD	2.21	1.17
14:K:70:LEU:HD11	21:V:86:LEU:CD2	1.72	1.17
22:W:27:MET:HA	22:W:27:MET:HE2	1.24	1.17
23:X:4:VAL:HG11	23:X:31:PHE:CG	1.80	1.17
13:J:76:ASN:CB	25:S:112:LEU:CB	2.21	1.16
15:N:376:PRO:HG2	15:N:377:PRO:CD	1.75	1.16
10:G:97:ILE:HD11	13:J:102:MET:HE3	1.28	1.16
15:N:666:ILE:HG21	15:N:684:LEU:HD11	1.18	1.16
23:X:4:VAL:HG11	23:X:31:PHE:CB	1.75	1.15
14:K:70:LEU:CD2	21:V:86:LEU:CD1	2.22	1.15
10:G:74:HIS:CD2	10:G:126:TYR:HE2	1.64	1.15
12:I:140:MET:HG3	26:U:117:LYS:HE3	1.23	1.15
10:G:57:ARG:HD3	10:G:58:PRO:HD2	1.21	1.14
13:J:85:LEU:CD1	25:S:93:TYR:HA	1.75	1.14
10:G:74:HIS:CE1	10:G:122:LEU:CD1	2.31	1.14
9:F:118:ARG:HD2	18:Q:112:LEU:HD22	1.28	1.13
10:G:143:LYS:HG3	26:U:96:GLU:OE1	1.47	1.13
18:Q:139:GLN:O	18:Q:143:THR:HG22	1.46	1.13
13:J:85:LEU:HD13	25:S:93:TYR:HA	1.23	1.12
23:X:4:VAL:HG21	23:X:31:PHE:CD2	1.83	1.12
24:d:920:LEU:CA	24:d:923:LEU:HD21	1.79	1.12
6:A:66:GLN:HE22	12:I:69:VAL:HG11	1.04	1.12
24:d:920:LEU:HB3	24:d:923:LEU:HD11	1.13	1.12
13:J:76:ASN:HB3	25:S:112:LEU:CA	1.79	1.12
14:K:70:LEU:HD11	21:V:86:LEU:HD21	1.17	1.12
6:A:71:VAL:CG2	12:I:67:PRO:HD3	1.78	1.12
13:J:108:LEU:HD11	26:U:55:ALA:C	1.75	1.12
18:Q:394:HIS:CD2	19:R:78:ARG:HG3	1.85	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:30:LEU:HD23	8:D:34:LEU:HD23	1.29	1.11
6:A:71:VAL:HG21	12:I:67:PRO:HD3	1.27	1.11
15:N:216:THR:CB	15:N:223:LYS:HB3	1.79	1.10
23:X:4:VAL:HG11	23:X:31:PHE:CD1	1.86	1.10
15:N:666:ILE:HG21	15:N:684:LEU:CD1	1.82	1.10
24:d:928:LEU:CB	24:d:929:PRO:CD	2.28	1.10
13:J:76:ASN:N	25:S:112:LEU:H	1.50	1.09
15:N:216:THR:HB	15:N:223:LYS:HB3	1.10	1.09
13:J:108:LEU:CD2	26:U:55:ALA:CB	2.32	1.08
10:G:142:GLN:O	10:G:146:ARG:HG2	1.53	1.07
10:G:108:LYS:O	10:G:112:LEU:HG	1.55	1.07
13:J:108:LEU:HD21	26:U:55:ALA:HB1	1.31	1.07
14:K:70:LEU:HD21	21:V:86:LEU:HD11	1.16	1.07
24:d:946:GLY:HA3	26:U:61:LEU:HD22	1.20	1.07
15:N:376:PRO:HG2	15:N:377:PRO:HD3	1.10	1.07
24:d:920:LEU:CB	24:d:923:LEU:HD11	1.85	1.07
24:d:928:LEU:CB	24:d:929:PRO:HD2	1.84	1.07
15:N:442:ILE:HG21	15:N:496:LEU:HD11	1.09	1.06
9:F:101:ILE:HD13	11:H:105:VAL:HG11	1.35	1.06
10:G:138:MET:HE2	10:G:138:MET:HA	1.33	1.06
2:1:100:LEU:HD12	18:Q:641:LEU:HB3	1.29	1.06
23:X:4:VAL:CG1	23:X:31:PHE:CB	2.34	1.05
15:N:687:ILE:HG22	15:N:688:PRO:HD2	1.34	1.05
13:J:108:LEU:CD2	26:U:55:ALA:HB3	1.86	1.05
15:N:225:ARG:HB3	15:N:231:GLU:HG3	1.34	1.05
22:W:399:PHE:CE2	22:W:425:MET:HB2	1.92	1.05
15:N:213:ALA:HB1	15:N:224:PHE:CE1	1.91	1.05
18:Q:188:LEU:HD22	21:V:87:ILE:CD1	1.86	1.05
8:D:34:LEU:HD13	8:D:37:LEU:HD21	1.05	1.04
15:N:111:LYS:HE2	25:S:92:ALA:HB1	1.33	1.04
22:W:37:LEU:CD1	22:W:85:MET:HE1	1.85	1.04
13:J:76:ASN:CA	25:S:112:LEU:CB	2.36	1.04
15:N:188:LYS:HD3	18:Q:47:ILE:CD1	1.87	1.04
10:G:74:HIS:HE1	10:G:122:LEU:HD12	1.17	1.03
10:G:124:ASN:ND2	15:N:149:LEU:HD21	1.72	1.03
8:D:30:LEU:CD2	8:D:34:LEU:HD23	1.88	1.03
24:d:929:PRO:HB2	24:d:930:PRO:HD2	1.40	1.02
14:K:70:LEU:CD1	21:V:86:LEU:HD21	1.90	1.02
18:Q:142:GLN:HG3	21:V:43:GLU:O	1.58	1.02
23:X:4:VAL:HG11	23:X:31:PHE:CA	1.90	1.02
23:X:4:VAL:HG21	23:X:31:PHE:CG	1.94	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:442:ILE:CG2	15:N:496:LEU:HD11	1.90	1.02
26:U:49:ASN:OD1	26:U:50:PRO:HD3	1.59	1.02
17:P:12:MET:N	17:P:458:SER:HG	1.56	1.01
24:d:920:LEU:HD22	24:d:923:LEU:HD13	1.41	1.01
14:K:70:LEU:HD21	21:V:86:LEU:HD13	1.37	1.01
14:K:79:HIS:CE1	21:V:94:VAL:HG11	1.96	1.01
15:N:111:LYS:HE2	25:S:92:ALA:HB2	1.42	1.01
18:Q:141:PRO:HB3	21:V:45:GLU:HB3	1.39	1.01
8:D:27:ARG:HA	12:I:103:THR:OG1	1.60	1.00
23:X:31:PHE:HD1	23:X:32:PRO:HD2	1.20	1.00
15:N:315:LEU:HD13	15:N:320:TRP:HB2	1.44	0.99
8:D:35:GLU:O	8:D:39:VAL:HG12	1.62	0.99
10:G:74:HIS:CE1	10:G:122:LEU:HD12	1.93	0.99
10:G:74:HIS:HE1	10:G:122:LEU:CD1	1.70	0.99
8:D:34:LEU:HD13	8:D:37:LEU:CD2	1.93	0.99
8:D:52:ARG:HA	8:D:52:ARG:HE	1.26	0.99
24:d:920:LEU:HA	24:d:923:LEU:HD21	1.01	0.98
10:G:74:HIS:CE1	10:G:122:LEU:HD13	1.97	0.98
13:J:76:ASN:HA	25:S:112:LEU:CB	1.92	0.98
24:d:920:LEU:HD22	24:d:923:LEU:CD1	1.93	0.98
15:N:676:ASP:OD1	18:Q:593:MET:HE3	1.62	0.97
15:N:111:LYS:HA	25:S:89:LEU:HD21	1.47	0.97
18:Q:140:ASN:HA	18:Q:143:THR:HG23	1.41	0.96
8:D:90:HIS:CE1	12:I:105:PRO:HA	2.00	0.96
15:N:376:PRO:CG	15:N:377:PRO:CD	2.43	0.96
23:X:6:LEU:HD11	23:X:40:LEU:O	1.66	0.96
24:d:923:LEU:HD23	24:d:923:LEU:H	1.28	0.96
13:J:108:LEU:HD21	26:U:55:ALA:HB3	0.99	0.95
15:N:680:HIS:NE2	18:Q:557:LEU:HD11	1.81	0.95
18:Q:385:GLN:O	18:Q:391:MET:HE3	1.66	0.95
15:N:376:PRO:CG	15:N:377:PRO:HD3	1.95	0.95
18:Q:582:VAL:HG22	18:Q:592:ILE:HG23	1.46	0.95
6:A:165:GLY:HA3	6:A:170:LYS:HG3	1.49	0.95
22:W:601:LEU:HD21	22:W:630:LEU:HD11	1.46	0.95
8:D:34:LEU:HA	8:D:37:LEU:CD2	1.96	0.95
8:D:34:LEU:CD1	8:D:37:LEU:HD21	1.96	0.94
23:X:4:VAL:HG11	23:X:31:PHE:HA	1.47	0.94
13:J:76:ASN:H	25:S:112:LEU:H	0.94	0.94
15:N:188:LYS:HD3	18:Q:47:ILE:HD11	0.96	0.94
10:G:97:ILE:HD11	13:J:102:MET:CE	1.98	0.93
22:W:154:SER:H	23:X:915:ARG:NH2	1.65	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:136:LEU:HB3	26:U:20:CYS:HB2	1.47	0.93
15:N:693:ILE:HD12	15:N:697:THR:HB	1.47	0.93
10:G:74:HIS:CD2	10:G:126:TYR:CE2	2.56	0.93
14:K:12:ARG:HA	14:K:12:ARG:NH2	1.84	0.92
23:X:4:VAL:HG21	23:X:31:PHE:CE2	2.05	0.92
12:I:135:TYR:CE2	26:U:125:ILE:HG12	2.05	0.92
8:D:121:LEU:O	8:D:125:VAL:HG12	1.69	0.92
15:N:111:LYS:CE	25:S:92:ALA:HB1	1.98	0.92
24:d:932:LYS:NZ	24:d:935:GLU:HG2	1.84	0.92
10:G:68:HIS:HD1	10:G:69:PRO:HD2	1.32	0.92
10:G:89:PHE:CE2	26:U:19:PHE:CE1	2.57	0.92
4:3:107:ASP:CB	18:Q:651:LEU:HD13	1.98	0.92
10:G:127:ARG:HD3	15:N:152:PHE:CE1	2.05	0.92
15:N:376:PRO:CD	15:N:377:PRO:HD2	1.99	0.92
4:3:107:ASP:HB2	18:Q:651:LEU:HD13	1.49	0.92
15:N:693:ILE:HD12	15:N:697:THR:CB	1.99	0.92
23:X:4:VAL:CG1	23:X:31:PHE:HB2	1.99	0.92
24:d:920:LEU:HA	24:d:923:LEU:CD2	1.96	0.92
10:G:78:LEU:CD2	26:U:73:ILE:HG21	2.00	0.92
24:d:929:PRO:HB2	24:d:930:PRO:CD	1.99	0.92
23:X:12:GLN:HE22	23:X:30:PHE:HZ	1.12	0.91
9:F:120:LEU:HD21	11:H:117:VAL:HG11	1.51	0.91
18:Q:188:LEU:CD2	21:V:87:ILE:HD12	2.01	0.91
24:d:920:LEU:O	24:d:924:PRO:HG2	1.68	0.91
15:N:666:ILE:CG2	15:N:684:LEU:HD11	2.00	0.91
14:K:8:ASN:O	14:K:12:ARG:HG2	1.70	0.91
10:G:68:HIS:ND1	10:G:69:PRO:CD	2.31	0.91
18:Q:540:LEU:HD11	18:Q:640:GLU:OE1	1.71	0.91
26:U:49:ASN:OD1	26:U:50:PRO:CD	2.18	0.90
10:G:57:ARG:CD	10:G:58:PRO:HD2	1.99	0.90
22:W:37:LEU:HD12	22:W:85:MET:HE1	1.49	0.90
9:F:118:ARG:CD	18:Q:112:LEU:HD22	2.00	0.90
10:G:157:LEU:CD2	26:U:110:ARG:HH12	1.85	0.90
24:d:928:LEU:HB3	24:d:929:PRO:CD	1.97	0.90
13:J:82:LYS:HE3	25:S:97:CYS:HA	1.52	0.90
10:G:127:ARG:HD3	15:N:152:PHE:HE1	1.38	0.89
10:G:142:GLN:HE21	10:G:146:ARG:HH21	1.15	0.89
15:N:54:LEU:HA	25:S:139:SER:CB	2.02	0.89
15:N:292:MET:O	15:N:296:LEU:HD23	1.73	0.89
23:X:4:VAL:HB	23:X:31:PHE:HB2	1.53	0.89
24:d:920:LEU:HB3	24:d:923:LEU:CD1	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:102:SER:O	12:I:105:PRO:HD2	1.71	0.89
23:X:4:VAL:CG1	23:X:31:PHE:CA	2.50	0.89
23:X:4:VAL:CG1	23:X:31:PHE:CG	2.56	0.89
8:D:99:GLU:O	8:D:103:ARG:HD3	1.73	0.88
8:D:90:HIS:CE1	12:I:105:PRO:CA	2.56	0.88
15:N:213:ALA:CB	15:N:224:PHE:CE1	2.56	0.88
18:Q:141:PRO:HA	21:V:50:ARG:HD3	1.54	0.88
18:Q:394:HIS:CD2	19:R:78:ARG:CG	2.56	0.88
10:G:57:ARG:HG2	10:G:57:ARG:HH11	1.36	0.88
13:J:85:LEU:HD13	25:S:93:TYR:CA	2.05	0.87
1:O:272:SER:HB3	1:O:302:LEU:HD23	1.56	0.87
9:F:118:ARG:NH1	18:Q:112:LEU:HB3	1.88	0.87
15:N:216:THR:HB	15:N:223:LYS:CB	2.02	0.87
10:G:89:PHE:HE2	26:U:19:PHE:CE1	1.92	0.86
12:I:110:SER:HB3	12:I:111:PRO:HD2	1.57	0.86
10:G:78:LEU:HD22	26:U:73:ILE:HG21	1.56	0.86
23:X:31:PHE:CD1	23:X:32:PRO:HD2	2.09	0.86
15:N:691:LYS:O	15:N:691:LYS:NZ	2.08	0.86
4:3:142:ILE:O	4:3:145:VAL:HG12	1.76	0.85
13:J:82:LYS:CD	25:S:97:CYS:HA	2.06	0.85
13:J:108:LEU:CD2	26:U:55:ALA:HB1	2.03	0.85
24:d:945:VAL:HG21	26:U:64:ARG:HG3	1.59	0.85
9:F:185:ARG:O	9:F:185:ARG:HD3	1.77	0.85
14:K:12:ARG:HA	14:K:12:ARG:HH21	1.36	0.85
18:Q:46:ARG:HH11	18:Q:46:ARG:HG3	1.42	0.84
22:W:27:MET:HA	22:W:27:MET:CE	2.05	0.84
23:X:4:VAL:CG1	23:X:31:PHE:HA	2.06	0.84
15:N:181:ASP:OD1	15:N:182:PRO:CD	2.20	0.84
12:I:135:TYR:HE2	26:U:125:ILE:HG12	1.41	0.84
15:N:693:ILE:CD1	15:N:697:THR:CG2	2.55	0.84
15:N:693:ILE:HD12	15:N:697:THR:CG2	2.08	0.84
22:W:37:LEU:HD13	22:W:85:MET:HE1	1.59	0.84
23:X:12:GLN:NE2	23:X:30:PHE:HZ	1.76	0.84
15:N:296:LEU:O	15:N:300:CYS:SG	2.36	0.84
18:Q:9:ILE:HG13	26:U:94:GLU:OE2	1.77	0.83
14:K:70:LEU:HD21	21:V:86:LEU:CG	2.08	0.83
15:N:687:ILE:HG22	15:N:688:PRO:CD	2.07	0.83
8:D:34:LEU:HA	8:D:37:LEU:HD21	1.59	0.83
23:X:4:VAL:CB	23:X:31:PHE:HB2	2.07	0.83
15:N:315:LEU:CD1	15:N:320:TRP:HB2	2.08	0.83
13:J:76:ASN:CB	25:S:112:LEU:N	2.41	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:84:PHE:CZ	15:N:177:ILE:HD13	2.14	0.83
6:A:71:VAL:HG21	12:I:67:PRO:CD	2.09	0.82
23:X:4:VAL:CG2	23:X:31:PHE:CD2	2.62	0.82
24:d:935:GLU:OE2	26:U:2:ALA:CB	2.27	0.82
9:F:101:ILE:HD12	11:H:105:VAL:HG11	1.59	0.82
10:G:68:HIS:CE1	10:G:69:PRO:HD2	2.14	0.82
10:G:124:ASN:HD21	15:N:149:LEU:HD21	1.44	0.82
12:I:140:MET:CG	26:U:117:LYS:HE3	2.07	0.82
15:N:399:LYS:NZ	18:Q:271:LEU:HB3	1.94	0.82
17:P:640:ARG:HE	17:P:641:PRO:HD2	1.42	0.82
13:J:76:ASN:HB3	25:S:112:LEU:N	1.94	0.82
18:Q:140:ASN:HA	18:Q:143:THR:HG21	1.58	0.82
14:K:70:LEU:HD21	21:V:86:LEU:CD2	2.08	0.82
13:J:82:LYS:CE	25:S:97:CYS:HA	2.10	0.82
18:Q:9:ILE:CG1	26:U:94:GLU:OE2	2.28	0.82
24:d:933:LEU:CD1	26:U:7:GLN:HB2	2.10	0.82
24:d:943:TRP:HB3	26:U:64:ARG:HH12	1.44	0.82
22:W:399:PHE:HE2	22:W:425:MET:HB2	1.40	0.81
6:A:66:GLN:HE22	12:I:69:VAL:CG1	1.90	0.81
13:J:101:THR:HG22	26:U:51:THR:HG21	1.62	0.81
15:N:187:GLU:OE2	18:Q:43:LEU:CD1	2.21	0.81
9:F:171:ILE:HG22	15:N:263:ARG:NH1	1.95	0.81
15:N:135:ARG:NE	15:N:135:ARG:HA	1.96	0.80
5:4:84:PHE:CE2	15:N:177:ILE:HG21	2.16	0.80
18:Q:152:SER:HB2	21:V:58:ASN:OD1	1.80	0.80
10:G:153:PHE:HD1	24:d:914:CYS:HG	1.26	0.80
24:d:923:LEU:O	24:d:927:TYR:CE2	2.35	0.80
5:4:84:PHE:CD2	15:N:177:ILE:HG21	2.17	0.80
13:J:108:LEU:HD11	26:U:55:ALA:O	1.81	0.80
22:W:396:MET:HA	22:W:396:MET:CE	2.08	0.80
8:D:30:LEU:CD2	8:D:34:LEU:CD2	2.59	0.79
10:G:142:GLN:HE21	10:G:146:ARG:NH2	1.79	0.79
15:N:691:LYS:NZ	15:N:691:LYS:HB2	1.97	0.79
15:N:225:ARG:HB3	15:N:231:GLU:CG	2.12	0.79
10:G:55:ILE:HB	10:G:59:LEU:HD11	1.64	0.79
9:F:185:ARG:HD3	9:F:185:ARG:C	2.07	0.79
13:J:76:ASN:H	25:S:112:LEU:N	1.78	0.79
18:Q:144:LEU:HA	18:Q:147:ILE:HG23	1.63	0.79
9:F:174:ARG:HD2	15:N:270:GLN:NE2	1.98	0.79
10:G:100:PRO:HB2	15:N:125:GLN:HE22	1.47	0.79
10:G:68:HIS:CG	10:G:69:PRO:HD2	2.18	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:151:LEU:HD12	21:V:37:ILE:HG23	1.65	0.79
23:X:4:VAL:CG2	23:X:31:PHE:CG	2.66	0.79
9:F:74:GLN:HE21	9:F:78:LEU:H	1.30	0.79
9:F:38:ASN:HB3	9:F:41:TYR:HB3	1.64	0.78
18:Q:188:LEU:HD22	21:V:87:ILE:HD12	1.58	0.78
22:W:642:HIS:HA	22:W:645:VAL:HG12	1.65	0.78
6:A:69:LEU:HG	12:I:66:LEU:HD12	1.64	0.78
15:N:315:LEU:CD1	15:N:320:TRP:CB	2.61	0.78
18:Q:141:PRO:HG3	21:V:45:GLU:HG2	1.65	0.78
6:A:315:ARG:HG2	6:A:319:GLN:HE22	1.49	0.78
15:N:399:LYS:HZ1	18:Q:271:LEU:HB3	1.47	0.78
4:3:156:LEU:HD11	21:V:130:LEU:HD12	1.65	0.78
13:J:104:LYS:NZ	26:U:52:GLU:HB2	1.99	0.78
22:W:646:GLU:OE1	22:W:864:ARG:HG2	1.84	0.78
8:D:52:ARG:HA	8:D:52:ARG:NE	1.98	0.78
14:K:70:LEU:HD23	21:V:86:LEU:HD11	1.66	0.78
13:J:113:LEU:HD22	26:U:63:ALA:CB	2.14	0.78
22:W:389:LEU:O	22:W:389:LEU:HD23	1.84	0.78
10:G:130:GLN:HG3	24:d:931:ILE:HG21	1.66	0.77
4:3:138:GLU:OE1	4:3:138:GLU:HA	1.84	0.77
13:J:85:LEU:HD11	25:S:93:TYR:HA	1.65	0.77
22:W:154:SER:H	23:X:915:ARG:HH21	1.29	0.77
10:G:89:PHE:HE2	26:U:19:PHE:CG	2.02	0.77
15:N:676:ASP:CG	18:Q:593:MET:HE3	2.10	0.77
18:Q:34:LEU:HD13	24:d:916:MET:SD	2.24	0.77
6:A:310:PRO:HA	6:A:393:VAL:O	1.85	0.77
18:Q:109:MET:HA	18:Q:112:LEU:HG	1.67	0.77
13:J:95:VAL:HG21	15:N:122:LEU:CD2	2.15	0.77
24:d:916:MET:HE3	24:d:917:PHE:H	1.49	0.77
26:U:81:SER:HA	26:U:85:LEU:HD23	1.67	0.77
15:N:589:GLN:HG2	22:W:26:PHE:CD1	2.21	0.76
15:N:111:LYS:CE	25:S:92:ALA:CB	2.55	0.76
15:N:589:GLN:HG2	22:W:26:PHE:HD1	1.49	0.76
15:N:212:LEU:HD12	15:N:293:TYR:OH	1.85	0.76
15:N:189:GLN:HA	15:N:189:GLN:HE21	1.49	0.76
15:N:545:LEU:N	15:N:545:LEU:HD23	2.01	0.76
24:d:929:PRO:CB	24:d:930:PRO:CD	2.60	0.76
10:G:129:HIS:CD2	26:U:82:THR:OG1	2.38	0.76
15:N:693:ILE:CD1	15:N:697:THR:HB	2.15	0.76
2:1:111:ILE:HG21	4:3:138:GLU:HG3	1.66	0.76
6:A:165:GLY:HA3	6:A:170:LYS:CG	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:666:ILE:CG2	15:N:684:LEU:CD1	2.62	0.76
15:N:247:LEU:O	15:N:275:HIS:CE1	2.39	0.75
11:H:96:ARG:HG3	11:H:97:VAL:HG23	1.68	0.75
13:J:95:VAL:HG21	15:N:122:LEU:HD22	1.68	0.75
6:A:167:ASN:O	6:A:171:THR:CG2	2.34	0.75
10:G:98:ARG:HH12	13:J:128:ARG:HH12	1.34	0.75
15:N:149:LEU:HD22	15:N:149:LEU:N	2.01	0.75
6:A:71:VAL:HG23	12:I:67:PRO:HD3	1.69	0.75
10:G:135:LEU:HD23	10:G:135:LEU:O	1.86	0.75
22:W:889:LEU:O	22:W:893:PRO:HG2	1.87	0.75
18:Q:18:GLN:O	18:Q:30:TYR:CE2	2.39	0.75
18:Q:146:LEU:HD21	21:V:42:ILE:HD13	1.68	0.75
8:D:35:GLU:O	8:D:39:VAL:CG1	2.34	0.75
13:J:82:LYS:CD	25:S:96:PHE:O	2.27	0.75
15:N:376:PRO:CG	15:N:377:PRO:HD2	2.13	0.75
23:X:12:GLN:HA	23:X:15:LYS:HE2	1.66	0.75
23:X:4:VAL:CB	23:X:31:PHE:CG	2.70	0.75
15:N:188:LYS:CE	18:Q:47:ILE:HD11	2.16	0.74
18:Q:97:SER:O	18:Q:101:ASN:ND2	2.20	0.74
23:X:4:VAL:HG21	23:X:31:PHE:CD1	2.21	0.74
23:X:947:MET:HE1	23:X:971:THR:HB	1.68	0.74
14:K:79:HIS:HE1	21:V:94:VAL:HG11	1.50	0.74
15:N:315:LEU:C	15:N:315:LEU:HD12	2.12	0.74
17:P:282:HIS:HB2	17:P:297:CYS:HB3	1.69	0.74
15:N:301:LEU:HD23	15:N:361:ILE:HG12	1.69	0.74
24:d:946:GLY:HA3	26:U:61:LEU:CD2	2.10	0.74
10:G:138:MET:HA	10:G:138:MET:CE	2.15	0.74
26:U:57:LEU:O	26:U:57:LEU:HD23	1.87	0.74
15:N:247:LEU:O	15:N:275:HIS:NE2	2.20	0.74
23:X:37:TRP:CD1	23:X:72:MET:HE1	2.22	0.74
22:W:941:VAL:HG12	22:W:943:PRO:HD2	1.70	0.74
11:H:93:THR:HB	11:H:96:ARG:HE	1.52	0.74
15:N:136:LEU:HB3	26:U:20:CYS:CB	2.18	0.74
15:N:189:GLN:HA	15:N:189:GLN:NE2	2.03	0.74
15:N:245:TRP:HB2	15:N:282:LEU:HG	1.69	0.74
22:W:862:LEU:HD23	22:W:896:PHE:HE2	1.53	0.74
9:F:182:LEU:O	9:F:186:GLN:HG2	1.87	0.73
15:N:676:ASP:CG	18:Q:593:MET:CE	2.61	0.73
22:W:27:MET:HE2	22:W:27:MET:CA	2.14	0.73
15:N:250:LEU:HD23	15:N:250:LEU:C	2.13	0.73
23:X:21:TYR:O	23:X:25:ILE:HG13	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:30:LEU:HD23	8:D:34:LEU:CD2	2.12	0.73
10:G:143:LYS:HD2	10:G:143:LYS:C	2.13	0.73
12:I:102:SER:C	12:I:105:PRO:HD2	2.12	0.73
15:N:111:LYS:CD	25:S:92:ALA:HB1	2.19	0.73
15:N:442:ILE:HG21	15:N:496:LEU:HD12	1.67	0.73
9:F:115:ILE:HG12	9:F:118:ARG:HH21	1.52	0.73
18:Q:152:SER:CB	21:V:58:ASN:OD1	2.36	0.73
18:Q:582:VAL:HG22	18:Q:592:ILE:CG2	2.18	0.73
22:W:631:ALA:HB2	22:W:645:VAL:HG21	1.68	0.73
23:X:42:LEU:HD23	23:X:42:LEU:C	2.14	0.73
9:F:94:PRO:HG2	18:Q:130:VAL:HG11	1.69	0.72
10:G:120:HIS:HB3	15:N:147:ALA:HB1	1.70	0.72
18:Q:12:GLU:OE1	18:Q:12:GLU:N	2.17	0.72
3:2:86:THR:HG21	16:O:628:ASN:HD21	1.55	0.72
23:X:4:VAL:CG1	23:X:31:PHE:CD1	2.70	0.72
2:1:111:ILE:HG23	4:3:142:ILE:HD11	1.72	0.72
14:K:70:LEU:CD2	21:V:86:LEU:HD13	2.04	0.72
9:F:118:ARG:HH11	18:Q:112:LEU:HB3	1.54	0.72
11:H:52:LEU:HD23	11:H:52:LEU:C	2.15	0.72
14:K:70:LEU:CG	21:V:86:LEU:HD21	2.19	0.72
9:F:101:ILE:CD1	11:H:105:VAL:CG1	2.62	0.72
10:G:114:LEU:HD23	10:G:114:LEU:C	2.14	0.72
18:Q:140:ASN:CA	18:Q:143:THR:CG2	2.59	0.72
1:0:238:VAL:HG23	1:0:295:THR:HG21	1.71	0.72
6:A:69:LEU:HG	12:I:66:LEU:CD1	2.20	0.72
8:D:28:GLU:OE1	8:D:28:GLU:N	2.17	0.72
10:G:78:LEU:HD23	10:G:78:LEU:C	2.14	0.72
15:N:211:GLN:HA	26:U:133:ARG:HH21	1.53	0.72
15:N:718:ARG:NH2	15:N:752:LEU:O	2.22	0.72
14:K:79:HIS:CE1	21:V:94:VAL:CG1	2.73	0.72
15:N:208:LEU:HD12	15:N:208:LEU:C	2.14	0.72
24:d:932:LYS:HZ1	24:d:935:GLU:HG2	1.55	0.72
15:N:593:GLU:H	15:N:593:GLU:CD	1.95	0.72
18:Q:271:LEU:HD13	18:Q:271:LEU:C	2.15	0.72
10:G:59:LEU:HD22	10:G:59:LEU:N	2.06	0.71
15:N:181:ASP:CG	15:N:182:PRO:HD2	2.13	0.71
10:G:62:GLN:OE1	10:G:62:GLN:N	2.23	0.71
10:G:86:LEU:O	10:G:86:LEU:HD13	1.90	0.71
15:N:227:GLU:OE1	15:N:227:GLU:N	2.19	0.71
17:P:244:VAL:HG22	17:P:257:THR:HG22	1.72	0.71
21:V:38:LYS:HA	21:V:41:LYS:HZ2	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:53:SER:O	11:H:57:ASN:HB3	1.90	0.71
15:N:213:ALA:CB	15:N:224:PHE:CZ	2.73	0.71
15:N:277:LEU:HD23	15:N:277:LEU:C	2.15	0.71
15:N:693:ILE:CD1	15:N:697:THR:HG21	2.20	0.71
22:W:389:LEU:HD23	22:W:389:LEU:C	2.15	0.71
8:D:90:HIS:CE1	12:I:105:PRO:CB	2.74	0.71
22:W:630:LEU:C	22:W:630:LEU:HD23	2.15	0.71
6:A:313:VAL:HG12	6:A:414:GLN:HG2	1.70	0.71
10:G:100:PRO:HB2	15:N:125:GLN:NE2	2.05	0.71
11:H:126:THR:O	11:H:130:ARG:NH1	2.24	0.71
23:X:414:GLU:HG3	23:X:415:PRO:HD3	1.71	0.71
15:N:238:GLY:HA3	15:N:243:VAL:HG21	1.72	0.71
17:P:182:VAL:HG22	17:P:188:VAL:HG12	1.73	0.70
24:d:924:PRO:HA	24:d:927:TYR:CE2	2.26	0.70
9:F:25:ASN:H	9:F:28:SER:HB3	1.56	0.70
15:N:136:LEU:CB	26:U:20:CYS:HB2	2.21	0.70
4:3:155:GLN:OE1	4:3:155:GLN:HA	1.90	0.70
10:G:127:ARG:HG2	15:N:152:PHE:CZ	2.26	0.70
23:X:37:TRP:CD1	23:X:72:MET:CE	2.75	0.70
15:N:213:ALA:HB2	15:N:224:PHE:CZ	2.26	0.70
14:K:12:ARG:N	14:K:12:ARG:HD2	2.07	0.70
24:d:935:GLU:OE2	26:U:2:ALA:HB1	1.92	0.70
8:D:44:LEU:C	8:D:44:LEU:HD23	2.16	0.70
18:Q:144:LEU:HD22	18:Q:147:ILE:HD13	1.74	0.70
22:W:396:MET:HE2	22:W:396:MET:CA	2.15	0.70
15:N:545:LEU:HD23	15:N:545:LEU:H	1.57	0.70
24:d:928:LEU:CG	24:d:929:PRO:HD2	2.07	0.70
17:P:243:LYS:HG2	17:P:258:GLU:HG2	1.72	0.70
18:Q:43:LEU:O	18:Q:43:LEU:HD13	1.92	0.70
22:W:373:MET:HE2	22:W:402:LEU:HD23	1.73	0.70
6:A:70:LYS:HG2	12:I:70:HIS:NE2	2.07	0.70
18:Q:139:GLN:O	18:Q:143:THR:CG2	2.34	0.70
24:d:923:LEU:O	24:d:927:TYR:HE2	1.75	0.70
24:d:931:ILE:HD11	26:U:77:PRO:HG3	1.74	0.70
24:d:943:TRP:HB3	26:U:64:ARG:NH1	2.07	0.70
9:F:171:ILE:CG2	15:N:263:ARG:NH1	2.55	0.69
14:K:70:LEU:CD1	21:V:86:LEU:CD2	2.57	0.69
22:W:528:LEU:O	22:W:536:LYS:NZ	2.25	0.69
6:A:70:LYS:HG2	12:I:70:HIS:CE1	2.27	0.69
24:d:924:PRO:O	24:d:927:TYR:HD2	1.73	0.69
11:H:143:LEU:HD22	18:Q:146:LEU:HD22	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:149:VAL:HG22	20:T:152:ASP:HB2	1.74	0.69
8:D:120:ILE:HG21	10:G:159:ARG:NH2	2.07	0.69
14:K:8:ASN:HA	14:K:11:LEU:HD12	1.73	0.69
10:G:68:HIS:CG	10:G:69:PRO:CD	2.74	0.69
12:I:116:GLN:O	12:I:119:GLN:HG2	1.91	0.69
15:N:261:ASP:HB2	18:Q:250:ASP:OD2	1.93	0.69
4:3:143:ALA:O	4:3:147:LYS:HG2	1.93	0.69
15:N:592:LYS:HB3	22:W:27:MET:SD	2.33	0.69
15:N:693:ILE:HD12	15:N:697:THR:HG21	1.75	0.69
17:P:314:GLU:HB3	17:P:340:ARG:HH12	1.56	0.69
18:Q:38:GLN:OE1	18:Q:38:GLN:N	2.26	0.69
18:Q:629:LYS:HG3	18:Q:629:LYS:O	1.92	0.69
22:W:234:SER:HB2	22:W:660:GLU:HB3	1.73	0.69
22:W:399:PHE:CZ	22:W:425:MET:HB2	2.28	0.69
24:d:948:LEU:HD21	26:U:21:ASN:HB3	1.75	0.69
1:0:168:ARG:HA	1:0:171:ARG:HE	1.58	0.69
8:D:26:THR:HA	12:I:107:ILE:HG22	1.73	0.69
15:N:399:LYS:HE3	18:Q:271:LEU:H	1.58	0.69
22:W:509:LEU:HB2	22:W:514:CYS:HB3	1.74	0.69
23:X:40:LEU:N	23:X:40:LEU:HD23	2.07	0.69
9:F:72:HIS:HB3	9:F:80:ILE:HD12	1.75	0.69
11:H:143:LEU:HD22	18:Q:146:LEU:CD2	2.23	0.68
16:O:718:VAL:HG21	16:O:776:TRP:HE1	1.58	0.68
18:Q:599:ASN:ND2	18:Q:616:SER:O	2.26	0.68
10:G:137:VAL:HG12	10:G:138:MET:HE3	1.73	0.68
23:X:37:TRP:NE1	23:X:72:MET:HE1	2.09	0.68
23:X:577:ALA:O	23:X:581:ILE:HD12	1.94	0.68
8:D:30:LEU:HD23	8:D:30:LEU:O	1.94	0.68
15:N:199:LEU:HD21	15:N:222:VAL:CG2	2.22	0.68
18:Q:149:LYS:O	18:Q:153:LEU:HB3	1.94	0.68
22:W:153:SER:OG	23:X:915:ARG:NH2	2.26	0.68
10:G:86:LEU:HD13	10:G:86:LEU:C	2.19	0.68
22:W:707:ILE:HG23	22:W:738:PRO:HB2	1.76	0.68
17:P:536:LEU:HD21	17:P:739:VAL:HG12	1.74	0.68
22:W:399:PHE:HZ	22:W:425:MET:CG	2.06	0.68
8:D:30:LEU:CD2	12:I:99:LYS:HD3	2.24	0.68
10:G:74:HIS:CG	10:G:126:TYR:HE2	2.11	0.68
22:W:855:TRP:CZ3	22:W:896:PHE:HA	2.28	0.68
8:D:90:HIS:CE1	12:I:105:PRO:HB3	2.29	0.68
22:W:399:PHE:HZ	22:W:425:MET:HG3	1.59	0.68
15:N:277:LEU:HD23	15:N:277:LEU:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:152:ALA:O	8:D:156:SER:CB	2.42	0.67
8:D:152:ALA:O	8:D:156:SER:HB3	1.95	0.67
15:N:210:PRO:HG2	26:U:133:ARG:HG3	1.76	0.67
22:W:855:TRP:CH2	22:W:896:PHE:CD2	2.83	0.67
8:D:86:GLN:OE1	12:I:107:ILE:HB	1.93	0.67
9:F:188:PHE:HD1	15:N:281:ARG:HH22	1.42	0.67
22:W:608:PHE:HA	22:W:612:MET:HE1	1.77	0.67
6:A:161:TYR:CD1	6:A:170:LYS:NZ	2.58	0.67
10:G:60:GLU:HG2	10:G:121:HIS:NE2	2.09	0.67
13:J:82:LYS:HE3	25:S:97:CYS:CA	2.24	0.67
16:O:759:ARG:NH2	16:O:782:GLN:OE1	2.27	0.67
18:Q:457:ASP:HB2	18:Q:458:PRO:HD3	1.76	0.67
10:G:71:GLN:OE1	10:G:71:GLN:N	2.22	0.67
12:I:68:LEU:HB2	12:I:91:LYS:HZ1	1.59	0.67
2:1:143:LEU:HD11	14:K:97:VAL:HG13	1.76	0.67
8:D:34:LEU:O	8:D:37:LEU:HG	1.95	0.67
10:G:127:ARG:CD	15:N:152:PHE:HE1	2.07	0.67
15:N:376:PRO:HD2	15:N:377:PRO:HD2	1.77	0.67
26:U:99:GLU:OE2	26:U:99:GLU:HA	1.94	0.67
15:N:288:PRO:HB2	15:N:289:LEU:HD22	1.77	0.67
8:D:149:ILE:CD1	10:G:132:ARG:NH1	2.58	0.67
22:W:931:LYS:HD3	22:W:935:GLU:HB3	1.75	0.67
9:F:118:ARG:CG	18:Q:112:LEU:HD22	2.24	0.66
15:N:687:ILE:HD11	15:N:705:LEU:HD11	1.77	0.66
23:X:12:GLN:NE2	23:X:30:PHE:CZ	2.62	0.66
24:d:920:LEU:HD22	24:d:923:LEU:HD11	1.75	0.66
14:K:98:ASP:HA	14:K:101:ARG:HG2	1.77	0.66
24:d:920:LEU:O	24:d:924:PRO:CG	2.40	0.66
15:N:918:PHE:HB3	15:N:922:TYR:HB2	1.76	0.66
22:W:646:GLU:OE1	22:W:864:ARG:CG	2.44	0.66
24:d:933:LEU:HD11	26:U:7:GLN:HG2	1.78	0.66
18:Q:289:PRO:HB2	18:Q:291:TRP:CE2	2.30	0.66
8:D:30:LEU:HD22	12:I:99:LYS:HD3	1.78	0.66
15:N:281:ARG:HD2	15:N:291:ASP:OD2	1.95	0.66
11:H:112:LYS:NZ	11:H:113:PRO:O	2.28	0.66
22:W:630:LEU:HD23	22:W:630:LEU:O	1.94	0.66
1:0:184:ASN:OD1	21:V:120:ARG:NH2	2.29	0.66
13:J:108:LEU:CD1	26:U:55:ALA:C	2.62	0.66
24:d:924:PRO:HA	24:d:927:TYR:CD2	2.30	0.66
8:D:30:LEU:HD23	8:D:30:LEU:C	2.21	0.66
15:N:691:LYS:HZ1	15:N:691:LYS:C	2.03	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:19:VAL:HG23	18:Q:28:GLU:HB3	1.78	0.66
26:U:49:ASN:N	26:U:50:PRO:HD2	2.11	0.66
15:N:223:LYS:HD2	15:N:231:GLU:OE2	1.95	0.66
24:d:920:LEU:CG	24:d:923:LEU:HD11	2.24	0.66
13:J:76:ASN:N	25:S:112:LEU:N	2.35	0.66
13:J:104:LYS:HZ2	26:U:52:GLU:HB2	1.59	0.66
15:N:1187:LEU:HD12	15:N:1188:PRO:HD2	1.76	0.65
26:U:94:GLU:O	26:U:98:HIS:ND1	2.28	0.65
17:P:56:GLN:NE2	17:P:59:THR:OG1	2.29	0.65
22:W:427:CYS:O	22:W:431:HIS:ND1	2.29	0.65
6:A:212:THR:O	6:A:220:MET:HA	1.97	0.65
8:D:90:HIS:NE2	12:I:105:PRO:HA	2.11	0.65
15:N:706:LEU:HB2	15:N:725:VAL:HG13	1.78	0.65
15:N:802:VAL:HB	15:N:809:ILE:HB	1.77	0.65
23:X:655:THR:HG21	23:X:659:TYR:HB3	1.77	0.65
10:G:60:GLU:HG2	10:G:121:HIS:CE1	2.32	0.65
15:N:212:LEU:HD11	15:N:367:SER:CA	2.27	0.65
17:P:596:MET:HE3	17:P:664:ILE:HG12	1.76	0.65
22:W:37:LEU:HD13	22:W:85:MET:CE	2.27	0.65
23:X:39:ILE:HD12	23:X:39:ILE:N	2.11	0.65
23:X:975:LEU:HG	23:X:976:PRO:HD2	1.79	0.65
6:A:206:GLY:O	6:A:412:ARG:NH1	2.23	0.65
6:A:322:GLN:HE21	6:A:329:LEU:H	1.43	0.65
15:N:443:LEU:HD12	15:N:500:LEU:HD23	1.77	0.65
21:V:85:PHE:HD1	21:V:86:LEU:HD22	1.61	0.65
23:X:4:VAL:HG12	23:X:30:PHE:C	2.20	0.65
24:d:933:LEU:CD1	26:U:7:GLN:CB	2.73	0.65
8:D:52:ARG:HE	8:D:52:ARG:CA	2.06	0.65
15:N:545:LEU:HD11	15:N:652:MET:HB2	1.79	0.65
26:U:57:LEU:HD23	26:U:57:LEU:C	2.22	0.65
5:4:84:PHE:CZ	15:N:177:ILE:CD1	2.80	0.65
11:H:51:LEU:O	11:H:55:GLN:HG3	1.97	0.65
23:X:4:VAL:HG21	23:X:31:PHE:CZ	2.32	0.65
6:A:165:GLY:CA	6:A:170:LYS:HG3	2.25	0.65
10:G:143:LYS:O	10:G:147:LEU:HG	1.97	0.65
13:J:76:ASN:CG	25:S:112:LEU:N	2.55	0.65
18:Q:18:GLN:OE1	18:Q:18:GLN:HA	1.96	0.65
18:Q:152:SER:HB2	21:V:58:ASN:CG	2.21	0.65
8:D:98:LYS:O	8:D:102:LYS:HD3	1.97	0.64
10:G:74:HIS:ND1	10:G:122:LEU:HD13	2.12	0.64
10:G:97:ILE:CD1	13:J:102:MET:HE3	2.18	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:208:VAL:O	6:A:412:ARG:NH2	2.31	0.64
15:N:196:ASN:HB3	15:N:217:VAL:CG2	2.28	0.64
22:W:1322:LYS:HD3	22:W:1324:ALA:H	1.62	0.64
24:d:932:LYS:C	24:d:932:LYS:HD3	2.22	0.64
8:D:27:ARG:CA	12:I:103:THR:OG1	2.40	0.64
15:N:234:LEU:HD13	15:N:247:LEU:HA	1.80	0.64
18:Q:146:LEU:O	18:Q:150:LYS:HG2	1.97	0.64
14:K:79:HIS:HE1	21:V:94:VAL:CG1	2.09	0.64
10:G:138:MET:HE2	10:G:138:MET:CA	2.20	0.64
18:Q:140:ASN:CA	18:Q:143:THR:HG23	2.22	0.64
6:A:104:THR:HG22	6:A:105:SER:H	1.61	0.64
12:I:107:ILE:HD11	12:I:110:SER:HA	1.79	0.64
11:H:87:GLU:HA	11:H:90:MET:HG2	1.78	0.64
1:O:178:ILE:HG12	1:O:192:VAL:HG22	1.79	0.64
10:G:78:LEU:HD21	26:U:73:ILE:HG21	1.76	0.64
15:N:687:ILE:CG2	15:N:688:PRO:HD2	2.21	0.64
23:X:4:VAL:CB	23:X:31:PHE:CB	2.73	0.64
1:O:218:ASN:ND2	20:T:1:MET:CG	2.61	0.64
15:N:125:GLN:HA	15:N:125:GLN:OE1	1.98	0.64
24:d:920:LEU:CD2	24:d:923:LEU:CD1	2.73	0.64
15:N:376:PRO:N	15:N:377:PRO:HD2	2.13	0.64
15:N:677:GLY:O	18:Q:557:LEU:HD22	1.98	0.64
25:S:113:PRO:O	25:S:117:ASP:N	2.30	0.64
15:N:183:ILE:HD11	15:N:188:LYS:HD3	1.80	0.63
8:D:28:GLU:H	8:D:28:GLU:CD	2.04	0.63
23:X:4:VAL:HG12	23:X:30:PHE:O	1.98	0.63
10:G:48:GLN:CD	10:G:48:GLN:H	2.06	0.63
23:X:803:ASP:HB2	23:X:804:PRO:HD3	1.80	0.63
6:A:173:MET:HE3	6:A:173:MET:HA	1.80	0.63
9:F:78:LEU:HA	9:F:100:ILE:O	1.99	0.63
10:G:43:MET:HE3	10:G:50:GLN:HG3	1.81	0.63
12:I:107:ILE:HD11	12:I:111:PRO:HD3	1.81	0.63
18:Q:188:LEU:HD21	21:V:87:ILE:HD12	1.81	0.63
22:W:627:LEU:HD21	22:W:648:THR:HG21	1.80	0.63
24:d:920:LEU:CD2	24:d:923:LEU:HD11	2.28	0.63
4:3:177:ARG:NH1	4:3:178:ASN:OD1	2.32	0.63
10:G:143:LYS:CG	26:U:96:GLU:OE1	2.37	0.63
24:d:932:LYS:HZ3	24:d:935:GLU:HG2	1.64	0.63
15:N:339:VAL:O	15:N:355:HIS:HB2	1.98	0.63
15:N:835:LEU:HD12	15:N:852:LEU:HD12	1.80	0.63
14:K:33:LEU:HD23	14:K:45:LEU:HD13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:691:LYS:HB2	15:N:691:LYS:HZ2	1.63	0.63
17:P:55:ASP:HB3	17:P:58:LEU:HD13	1.81	0.63
18:Q:459:GLN:HB2	18:Q:480:THR:O	1.98	0.63
24:d:933:LEU:CD1	26:U:7:GLN:HG2	2.27	0.63
15:N:371:GLN:HA	15:N:371:GLN:OE1	1.98	0.63
18:Q:46:ARG:HH11	18:Q:46:ARG:CG	2.11	0.63
4:3:137:GLU:OE1	4:3:137:GLU:HA	1.98	0.63
10:G:127:ARG:CD	15:N:152:PHE:CE1	2.79	0.63
11:H:52:LEU:HA	11:H:56:LEU:HD12	1.79	0.63
22:W:559:LEU:HD21	22:W:563:LEU:HD22	1.81	0.63
24:d:923:LEU:N	24:d:924:PRO:CD	2.62	0.63
9:F:118:ARG:HB3	18:Q:112:LEU:CD2	2.28	0.62
15:N:1337:GLN:HA	15:N:1355:PRO:CB	2.29	0.62
22:W:892:LYS:N	22:W:893:PRO:CD	2.62	0.62
24:d:928:LEU:HG	24:d:929:PRO:HD3	0.73	0.62
8:D:149:ILE:HD13	10:G:132:ARG:NH1	2.14	0.62
10:G:142:GLN:NE2	10:G:146:ARG:HH21	1.93	0.62
15:N:713:GLN:HE21	15:N:721:VAL:CG2	2.12	0.62
18:Q:31:LEU:HG	18:Q:31:LEU:O	1.99	0.62
22:W:855:TRP:HZ3	22:W:896:PHE:HA	1.63	0.62
23:X:142:LEU:HD13	23:X:155:GLU:HB2	1.80	0.62
9:F:114:VAL:HG12	11:H:111:THR:HG22	1.81	0.62
15:N:676:ASP:OD1	18:Q:593:MET:CE	2.41	0.62
15:N:713:GLN:NE2	15:N:721:VAL:HG21	2.14	0.62
24:d:924:PRO:C	24:d:927:TYR:HD2	2.08	0.62
9:F:118:ARG:HB3	18:Q:112:LEU:CD1	2.29	0.62
11:H:92:GLN:NE2	18:Q:121:ASP:OD2	2.33	0.62
22:W:154:SER:HB2	23:X:917:ALA:HB3	1.81	0.62
24:d:923:LEU:N	24:d:924:PRO:HD2	2.14	0.62
10:G:142:GLN:NE2	10:G:146:ARG:NH2	2.47	0.62
16:O:675:PRO:HG2	16:O:678:LEU:HD23	1.79	0.62
21:V:53:GLN:HA	21:V:56:GLN:HG2	1.81	0.62
18:Q:505:VAL:HG22	18:Q:511:VAL:HG12	1.82	0.62
2:1:129:VAL:HG11	14:K:114:MET:HE1	1.81	0.62
3:2:165:LYS:NZ	3:2:169:SER:HB3	2.14	0.62
4:3:156:LEU:HD11	21:V:130:LEU:CD1	2.30	0.62
15:N:399:LYS:NZ	18:Q:271:LEU:CB	2.62	0.62
10:G:153:PHE:HD1	24:d:914:CYS:SG	2.22	0.61
14:K:70:LEU:HD13	21:V:85:PHE:CD1	2.33	0.61
23:X:175:ARG:HD3	23:X:221:LEU:HD21	1.81	0.61
15:N:212:LEU:HD11	15:N:367:SER:HA	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:592:LYS:CB	22:W:27:MET:SD	2.88	0.61
22:W:640:GLN:HG3	22:W:933:TYR:HE1	1.64	0.61
15:N:392:ILE:O	15:N:392:ILE:HG22	2.00	0.61
15:N:111:LYS:HD3	25:S:92:ALA:HB1	1.82	0.61
23:X:4:VAL:HG12	23:X:31:PHE:CA	2.30	0.61
8:D:30:LEU:CD2	12:I:99:LYS:HB2	2.30	0.61
15:N:496:LEU:HD12	15:N:496:LEU:C	2.26	0.61
24:d:923:LEU:CB	24:d:924:PRO:HD3	2.27	0.61
26:U:102:THR:O	26:U:105:GLU:HG2	1.99	0.61
23:X:259:GLU:HG3	23:X:261:GLN:H	1.65	0.61
2:1:139:TRP:CD1	21:V:119:LEU:HD13	2.35	0.61
6:A:177:LEU:HD12	6:A:259:ILE:HG12	1.80	0.61
9:F:77:ILE:HB	9:F:102:ALA:H	1.65	0.61
10:G:67:LEU:C	10:G:67:LEU:HD12	2.25	0.61
10:G:157:LEU:HD21	26:U:110:ARG:HH12	1.63	0.61
17:P:266:ARG:NH2	17:P:269:THR:OG1	2.34	0.61
23:X:36:THR:HG23	23:X:36:THR:O	2.00	0.61
15:N:234:LEU:CD1	15:N:246:ARG:O	2.49	0.61
26:U:15:LEU:O	26:U:19:PHE:HD2	1.84	0.61
13:J:113:LEU:HD13	26:U:63:ALA:HB1	1.83	0.61
23:X:833:LYS:HA	23:X:836:HIS:CE1	2.36	0.61
8:D:113:GLN:NE2	10:G:163:MET:SD	2.72	0.61
15:N:214:ASN:O	15:N:224:PHE:HA	2.01	0.61
18:Q:468:ASN:OD1	18:Q:469:ASP:N	2.34	0.61
26:U:49:ASN:CG	26:U:50:PRO:HD3	2.25	0.61
9:F:184:LEU:HD11	15:N:295:CYS:SG	2.41	0.60
13:J:85:LEU:CD1	25:S:93:TYR:CA	2.65	0.60
18:Q:188:LEU:HD22	21:V:87:ILE:HD13	1.82	0.60
8:D:145:SER:HB2	10:G:135:LEU:HD11	1.84	0.60
11:H:151:LEU:HD13	21:V:41:LYS:NZ	2.16	0.60
6:A:66:GLN:CD	12:I:69:VAL:HG11	2.24	0.60
8:D:171:ASP:O	8:D:174:ARG:NH1	2.33	0.60
17:P:659:MET:HA	17:P:662:ILE:HG12	1.83	0.60
18:Q:485:GLU:OE1	18:Q:485:GLU:N	2.28	0.60
15:N:247:LEU:HB3	15:N:275:HIS:NE2	2.17	0.60
18:Q:394:HIS:NE2	19:R:78:ARG:HG3	2.16	0.60
6:A:210:TYR:O	6:A:222:LEU:HA	2.02	0.60
8:D:110:LEU:HD21	10:G:171:LEU:HD21	1.83	0.60
9:F:186:GLN:OE1	9:F:186:GLN:HA	2.00	0.60
15:N:713:GLN:HE21	15:N:721:VAL:HG21	1.66	0.60
9:F:82:ARG:NH2	9:F:96:ALA:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:171:ILE:HG23	15:N:263:ARG:CZ	2.31	0.60
10:G:57:ARG:HH11	10:G:57:ARG:CG	2.11	0.60
22:W:808:TYR:HE1	22:W:934:PHE:HB2	1.66	0.60
23:X:170:SER:O	23:X:175:ARG:NH2	2.35	0.60
9:F:77:ILE:HD12	9:F:101:ILE:HG23	1.82	0.60
13:J:108:LEU:CG	26:U:55:ALA:HB1	2.31	0.60
10:G:57:ARG:HG2	10:G:57:ARG:NH1	2.13	0.60
10:G:88:ASN:ND2	10:G:112:LEU:CD2	2.65	0.60
11:H:85:ARG:NH1	11:H:97:VAL:O	2.34	0.60
10:G:142:GLN:HG3	10:G:146:ARG:HE	1.66	0.60
15:N:729:CYS:SG	15:N:743:ARG:NH1	2.75	0.60
22:W:719:ILE:O	22:W:723:THR:OG1	2.20	0.60
10:G:129:HIS:NE2	26:U:82:THR:OG1	2.35	0.59
17:P:273:ARG:O	17:P:276:LYS:NZ	2.35	0.59
18:Q:141:PRO:CB	21:V:45:GLU:HB3	2.26	0.59
18:Q:335:PRO:HB2	18:Q:339:LEU:HD23	1.84	0.59
21:V:91:PHE:HB2	21:V:92:PRO:HD3	1.82	0.59
10:G:61:SER:HB3	10:G:66:ARG:HH21	1.67	0.59
18:Q:43:LEU:HD13	18:Q:43:LEU:C	2.26	0.59
22:W:765:ARG:HA	22:W:768:LYS:HG2	1.84	0.59
5:4:107:HIS:HE1	18:Q:26:GLY:HA2	1.67	0.59
13:J:105:PHE:HA	26:U:55:ALA:HB1	1.82	0.59
15:N:534:SER:OG	15:N:535:LYS:N	2.34	0.59
17:P:474:LEU:HD13	17:P:495:VAL:HG12	1.83	0.59
3:2:63:LEU:HD22	3:2:112:LEU:HD11	1.84	0.59
8:D:44:LEU:HD23	8:D:44:LEU:O	2.02	0.59
14:K:31:VAL:HG23	18:Q:157:ALA:HB2	1.85	0.59
15:N:658:ARG:NH1	22:W:20:GLU:OE1	2.35	0.59
16:O:723:LEU:HD21	16:O:772:LEU:HD23	1.84	0.59
2:1:108:GLU:OE2	4:3:138:GLU:HG2	2.03	0.59
8:D:30:LEU:HD21	12:I:99:LYS:HB2	1.83	0.59
14:K:12:ARG:HH21	14:K:12:ARG:CA	2.13	0.59
14:K:26:GLN:HE22	14:K:52:PHE:HD1	1.50	0.59
22:W:399:PHE:CZ	22:W:425:MET:CG	2.86	0.59
24:d:933:LEU:CD1	26:U:7:GLN:CG	2.80	0.59
22:W:627:LEU:CD2	22:W:648:THR:HG21	2.32	0.59
22:W:731:THR:HG21	22:W:973:ARG:HH22	1.68	0.59
15:N:114:LYS:CB	25:S:89:LEU:HD22	2.32	0.59
15:N:200:ARG:O	15:N:204:VAL:HG12	2.02	0.59
3:2:117:GLU:OE1	3:2:121:ARG:NH2	2.36	0.59
4:3:163:LEU:HD11	21:V:123:ILE:HG23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:809:SER:HB3	17:P:812:ARG:HD3	1.83	0.59
21:V:50:ARG:NH1	21:V:50:ARG:O	2.36	0.59
5:4:84:PHE:HB2	15:N:178:ILE:HD11	1.85	0.59
10:G:139:MET:HE1	26:U:90:LEU:CB	2.33	0.59
18:Q:207:LEU:HD21	18:Q:295:LEU:HD22	1.83	0.59
23:X:4:VAL:HB	23:X:31:PHE:CB	2.31	0.59
1:0:286:LYS:HB3	20:T:159:GLU:OE2	2.03	0.58
2:1:129:VAL:HG21	14:K:114:MET:HE3	1.84	0.58
10:G:61:SER:HA	10:G:66:ARG:HE	1.68	0.58
15:N:199:LEU:HD21	15:N:222:VAL:HG23	1.85	0.58
1:0:257:GLN:HE22	1:0:258:MET:HE2	1.68	0.58
11:H:88:ASP:O	11:H:92:GLN:HB3	2.03	0.58
13:J:82:LYS:HD2	25:S:97:CYS:HA	1.85	0.58
15:N:217:VAL:HG22	15:N:217:VAL:O	2.02	0.58
15:N:312:THR:OG1	15:N:397:ILE:HD13	2.03	0.58
22:W:67:ILE:HD12	22:W:79:LEU:HB3	1.86	0.58
13:J:76:ASN:CA	25:S:112:LEU:H	2.16	0.58
15:N:297:HIS:CE1	15:N:301:LEU:HD22	2.37	0.58
11:H:61:LYS:O	11:H:65:HIS:ND1	2.32	0.58
15:N:183:ILE:CD1	15:N:188:LYS:CD	2.80	0.58
15:N:315:LEU:CD1	15:N:320:TRP:HB3	2.33	0.58
13:J:76:ASN:CB	25:S:112:LEU:H	2.16	0.58
15:N:687:ILE:CG2	15:N:688:PRO:CD	2.80	0.58
2:1:94:PHE:HB2	18:Q:650:LEU:HD22	1.85	0.58
2:1:104:VAL:HG11	4:3:114:LEU:HG	1.84	0.58
20:T:151:SER:CB	20:T:179:ARG:HH22	2.17	0.58
24:d:935:GLU:OE1	24:d:935:GLU:HA	2.02	0.58
18:Q:188:LEU:CD2	21:V:87:ILE:CD1	2.62	0.58
22:W:818:ALA:O	22:W:822:HIS:ND1	2.30	0.58
22:W:1274:PHE:HD2	22:W:1301:MET:HE1	1.69	0.58
5:4:84:PHE:CD2	15:N:177:ILE:CG2	2.85	0.58
8:D:90:HIS:HE1	12:I:105:PRO:CA	2.12	0.58
12:I:107:ILE:O	12:I:107:ILE:HD13	2.02	0.58
12:I:140:MET:HG3	26:U:117:LYS:CE	2.16	0.58
22:W:898:ASN:O	22:W:928:TYR:OH	2.22	0.58
23:X:169:LEU:HD13	23:X:221:LEU:HD22	1.84	0.58
11:H:151:LEU:HD12	21:V:37:ILE:CG2	2.33	0.58
22:W:154:SER:N	23:X:915:ARG:NH2	2.46	0.58
22:W:827:ALA:HB1	22:W:869:LEU:HD23	1.85	0.58
1:0:218:ASN:ND2	20:T:1:MET:HG3	2.18	0.58
18:Q:469:ASP:OD1	18:Q:470:VAL:N	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:d:945:VAL:HG23	26:U:61:LEU:HD13	1.85	0.58
18:Q:31:LEU:HD23	18:Q:31:LEU:H	1.67	0.57
15:N:234:LEU:HD12	15:N:246:ARG:O	2.04	0.57
18:Q:152:SER:OG	21:V:58:ASN:HA	2.03	0.57
22:W:726:ASN:HD21	22:W:750:GLN:HG3	1.69	0.57
1:O:218:ASN:HD22	20:T:1:MET:HG3	1.68	0.57
10:G:57:ARG:HE	10:G:128:PRO:HG2	1.69	0.57
15:N:691:LYS:HE2	15:N:693:ILE:HG23	1.86	0.57
22:W:576:ILE:O	22:W:580:GLY:N	2.36	0.57
22:W:1203:MET:HG2	22:W:1204:SER:H	1.69	0.57
15:N:140:ALA:HA	15:N:144:LEU:HG	1.86	0.57
15:N:903:CYS:SG	15:N:904:PHE:N	2.77	0.57
1:O:298:ASP:OD2	1:O:301:THR:OG1	2.22	0.57
6:A:69:LEU:HD23	12:I:66:LEU:HD11	1.85	0.57
11:H:101:SER:H	11:H:104:VAL:HG12	1.69	0.57
23:X:566:GLU:HG2	23:X:567:MET:H	1.68	0.57
5:4:111:LYS:HD3	18:Q:17:LYS:NZ	2.20	0.57
10:G:100:PRO:CB	15:N:125:GLN:HE22	2.18	0.57
11:H:78:PRO:HA	18:Q:125:MET:HA	1.87	0.57
15:N:187:GLU:CD	18:Q:43:LEU:HD21	2.29	0.57
15:N:442:ILE:HG13	15:N:496:LEU:HD11	1.85	0.57
20:T:68:ASN:HB2	20:T:190:MET:HE1	1.86	0.57
22:W:293:HIS:NE2	22:W:295:GLN:OE1	2.31	0.57
22:W:312:MET:HE2	22:W:372:LEU:HD22	1.85	0.57
22:W:821:ALA:HA	22:W:824:ARG:HE	1.70	0.57
22:W:984:LEU:HD23	22:W:1022:LEU:HD11	1.86	0.57
23:X:86:ASP:HB2	23:X:133:ARG:HH21	1.69	0.57
1:O:39:MET:HE3	1:O:48:ARG:HG2	1.85	0.57
8:D:26:THR:HA	12:I:107:ILE:H	1.69	0.57
10:G:88:ASN:ND2	10:G:112:LEU:HD23	2.19	0.57
18:Q:612:ASP:OD1	18:Q:613:ASN:N	2.38	0.57
19:R:184:ASP:HA	19:R:187:LYS:HE3	1.86	0.57
22:W:526:ASN:O	22:W:530:SER:OG	2.20	0.57
2:1:129:VAL:HG22	14:K:111:CYS:SG	2.44	0.57
10:G:71:GLN:H	10:G:71:GLN:CD	2.10	0.57
17:P:20:GLU:HB3	17:P:451:LYS:HG3	1.86	0.57
18:Q:324:HIS:ND1	18:Q:333:SER:OG	2.37	0.57
19:R:164:SER:OG	19:R:165:LEU:N	2.38	0.57
1:O:166:ILE:HD13	1:O:190:LEU:HD21	1.85	0.57
2:1:129:VAL:HG21	14:K:114:MET:CE	2.35	0.57
3:2:89:ASP:OD1	16:O:640:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:85:ASN:HD22	16:O:641:THR:HB	1.70	0.56
13:J:101:THR:CG2	26:U:51:THR:HG21	2.32	0.56
15:N:312:THR:OG1	15:N:397:ILE:CD1	2.53	0.56
18:Q:144:LEU:HB2	21:V:50:ARG:HE	1.70	0.56
10:G:129:HIS:CD2	26:U:82:THR:HG1	2.21	0.56
11:H:155:SER:O	11:H:159:ARG:NH1	2.38	0.56
5:4:84:PHE:CD2	15:N:178:ILE:HD11	2.40	0.56
9:F:118:ARG:HH11	18:Q:112:LEU:CB	2.18	0.56
10:G:127:ARG:CG	15:N:152:PHE:CE1	2.88	0.56
10:G:161:ILE:HD12	10:G:164:ILE:CG2	2.35	0.56
15:N:183:ILE:HD12	15:N:188:LYS:CD	2.35	0.56
15:N:691:LYS:C	15:N:691:LYS:HE3	2.30	0.56
22:W:87:VAL:HG11	22:W:97:VAL:HG11	1.86	0.56
22:W:708:GLN:HA	22:W:713:LYS:HD2	1.87	0.56
23:X:478:GLY:HA3	23:X:489:ARG:HH11	1.70	0.56
23:X:702:PRO:HG2	23:X:705:ARG:HD3	1.86	0.56
6:A:167:ASN:O	6:A:171:THR:HG23	2.04	0.56
15:N:736:THR:O	15:N:737:ARG:NH1	2.34	0.56
18:Q:141:PRO:HA	21:V:50:ARG:CD	2.32	0.56
22:W:969:ILE:O	22:W:973:ARG:HG2	2.05	0.56
5:4:59:LYS:NZ	15:N:164:GLY:O	2.38	0.56
8:D:72:ARG:NE	8:D:75:GLU:OE2	2.39	0.56
15:N:183:ILE:HD12	15:N:188:LYS:HG2	1.86	0.56
5:4:84:PHE:CE2	15:N:177:ILE:CD1	2.88	0.56
8:D:76:PHE:O	8:D:80:MET:N	2.38	0.56
17:P:194:LYS:HD3	17:P:196:SER:H	1.69	0.56
26:U:49:ASN:OD1	26:U:50:PRO:HD2	2.04	0.56
13:J:104:LYS:HZ1	26:U:52:GLU:HB2	1.70	0.56
22:W:610:TYR:N	22:W:610:TYR:CD1	2.73	0.56
22:W:855:TRP:HH2	22:W:896:PHE:CG	2.24	0.56
23:X:4:VAL:HG21	23:X:31:PHE:CE1	2.40	0.56
15:N:450:GLU:OE2	15:N:504:ARG:NH2	2.36	0.56
22:W:208:PHE:O	22:W:211:THR:OG1	2.21	0.56
23:X:469:ILE:HD11	23:X:512:ILE:HG23	1.88	0.56
23:X:472:ASN:O	23:X:476:THR:HG23	2.06	0.56
3:2:57:VAL:O	3:2:61:LYS:HG2	2.05	0.56
9:F:77:ILE:HD11	11:H:81:LEU:HD13	1.87	0.56
12:I:135:TYR:CE2	26:U:125:ILE:CG1	2.84	0.56
18:Q:141:PRO:HG3	21:V:45:GLU:H	1.69	0.56
23:X:448:LEU:HD21	23:X:499:MET:HE2	1.87	0.56
4:3:144:GLU:HA	4:3:147:LYS:CG	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:62:LEU:CD2	8:D:66:LEU:HD13	2.37	0.55
9:F:77:ILE:HD13	11:H:102:HIS:NE2	2.21	0.55
18:Q:146:LEU:CD2	21:V:42:ILE:HD13	2.36	0.55
18:Q:627:TRP:NE1	18:Q:638:LYS:HD2	2.21	0.55
20:T:8:GLN:HE22	20:T:203:GLN:HE22	1.53	0.55
24:d:933:LEU:HD13	26:U:7:GLN:CG	2.36	0.55
11:H:148:SER:OG	11:H:152:GLU:OE2	2.24	0.55
14:K:70:LEU:CD2	21:V:86:LEU:CD2	2.82	0.55
15:N:306:GLU:OE1	15:N:306:GLU:HA	2.06	0.55
15:N:683:ARG:HD2	16:O:684:ARG:HG2	1.88	0.55
22:W:797:LEU:HA	22:W:801:ASP:H	1.71	0.55
5:4:52:LEU:HD23	5:4:55:LEU:HD12	1.89	0.55
15:N:261:ASP:HB2	18:Q:250:ASP:CG	2.31	0.55
22:W:399:PHE:O	22:W:403:TYR:HB2	2.07	0.55
23:X:912:LEU:HD11	23:X:958:VAL:HG21	1.88	0.55
2:1:47:GLU:HA	2:1:50:SER:HB3	1.89	0.55
6:A:79:ASP:OD1	6:A:82:GLU:OE2	2.23	0.55
15:N:273:PHE:CD1	15:N:273:PHE:C	2.85	0.55
15:N:691:LYS:HD3	15:N:693:ILE:HG12	1.87	0.55
18:Q:270:ASP:CG	18:Q:327:VAL:HG11	2.31	0.55
21:V:35:GLU:OE1	21:V:64:ARG:NH2	2.40	0.55
22:W:646:GLU:OE1	22:W:864:ARG:HD2	2.07	0.55
6:A:377:ASN:ND2	6:A:441:GLU:OE2	2.40	0.55
18:Q:537:VAL:CG2	18:Q:639:MET:HE3	2.37	0.55
4:3:144:GLU:HA	4:3:147:LYS:HD3	1.89	0.55
13:J:104:LYS:NZ	26:U:52:GLU:CB	2.68	0.55
13:J:113:LEU:HD22	26:U:63:ALA:HB2	1.89	0.55
15:N:199:LEU:HD21	15:N:222:VAL:HG22	1.88	0.55
17:P:362:SER:OG	17:P:367:ASP:OD2	2.25	0.55
23:X:53:GLY:O	23:X:90:ARG:NH2	2.40	0.55
8:D:135:ILE:CD1	10:G:146:ARG:NH1	2.70	0.55
9:F:174:ARG:HD2	15:N:270:GLN:HE22	1.68	0.55
14:K:98:ASP:O	14:K:101:ARG:HG2	2.06	0.55
15:N:800:VAL:HA	15:N:810:LEU:HD23	1.87	0.55
17:P:180:ILE:HG22	17:P:190:VAL:HG22	1.89	0.55
26:U:18:GLN:HE22	26:U:62:ILE:HG12	1.72	0.55
14:K:8:ASN:O	14:K:12:ARG:CG	2.51	0.55
15:N:235:THR:HG23	15:N:248:LEU:HD21	1.89	0.55
15:N:293:TYR:CD1	15:N:293:TYR:C	2.85	0.55
18:Q:641:LEU:N	18:Q:641:LEU:HD23	2.21	0.55
22:W:896:PHE:CD1	22:W:896:PHE:C	2.85	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:d:932:LYS:HE2	26:U:2:ALA:HB1	1.88	0.55
26:U:76:LEU:HD13	26:U:76:LEU:N	2.20	0.55
2:1:101:GLN:NE2	4:3:109:ILE:O	2.41	0.54
10:G:149:THR:HG22	24:d:915:SER:OG	2.06	0.54
1:0:239:PHE:HA	1:0:242:VAL:HG12	1.88	0.54
9:F:82:ARG:NH2	9:F:97:ASP:OD1	2.41	0.54
16:O:727:ALA:O	16:O:732:GLN:NE2	2.39	0.54
17:P:596:MET:HE1	17:P:667:LEU:HD12	1.88	0.54
18:Q:141:PRO:HB3	21:V:45:GLU:CB	2.27	0.54
22:W:154:SER:HA	22:W:157:VAL:HG13	1.90	0.54
22:W:369:ARG:NH1	22:W:403:TYR:OH	2.40	0.54
22:W:510:PRO:HB2	22:W:954:ILE:HD11	1.89	0.54
24:d:938:ILE:HA	24:d:941:GLN:HE21	1.71	0.54
2:1:129:VAL:HG13	14:K:115:LEU:HD21	1.89	0.54
10:G:100:PRO:CB	15:N:125:GLN:NE2	2.70	0.54
21:V:67:ASN:OD1	21:V:70:ARG:NH1	2.39	0.54
22:W:389:LEU:HD12	22:W:435:LYS:HG3	1.88	0.54
24:d:933:LEU:HD11	26:U:7:GLN:CB	2.36	0.54
6:A:62:LEU:HD22	8:D:66:LEU:HD13	1.90	0.54
8:D:115:LYS:O	8:D:118:GLU:HG3	2.08	0.54
17:P:177:GLU:HG2	17:P:193:LEU:HB2	1.88	0.54
18:Q:270:ASP:OD2	18:Q:327:VAL:HB	2.07	0.54
15:N:175:ASP:N	15:N:175:ASP:OD1	2.37	0.54
18:Q:99:ARG:HG2	18:Q:103:ARG:NE	2.22	0.54
24:d:933:LEU:HD12	26:U:4:ARG:HA	1.90	0.54
15:N:521:GLN:HG3	20:T:30:MET:SD	2.48	0.54
15:N:709:THR:HG21	16:O:684:ARG:HH12	1.72	0.54
16:O:704:VAL:HG12	16:O:725:VAL:HB	1.90	0.54
17:P:787:LEU:HD13	17:P:791:PRO:HB3	1.90	0.54
22:W:316:GLU:HG2	22:W:367:LYS:HB2	1.88	0.54
1:0:218:ASN:HD22	20:T:1:MET:CG	2.19	0.54
2:1:111:ILE:CG2	4:3:138:GLU:HG3	2.37	0.54
11:H:17:SER:OG	11:H:18:GLN:NE2	2.38	0.54
11:H:151:LEU:HD11	21:V:38:LYS:NZ	2.23	0.54
15:N:247:LEU:HD21	15:N:278:VAL:HG11	1.89	0.54
15:N:666:ILE:HG21	15:N:684:LEU:HD12	1.83	0.54
16:O:690:LEU:HD21	18:Q:605:PRO:HB2	1.90	0.54
18:Q:397:SER:HB2	19:R:84:HIS:ND1	2.23	0.54
22:W:155:ALA:N	23:X:915:ARG:HH22	2.06	0.54
12:I:94:PHE:HB3	12:I:98:ARG:NH1	2.22	0.54
18:Q:291:TRP:O	18:Q:295:LEU:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:30:LEU:HD21	8:D:34:LEU:HG	1.89	0.54
8:D:90:HIS:HE1	12:I:105:PRO:O	1.91	0.54
26:U:19:PHE:CD1	26:U:19:PHE:C	2.85	0.54
1:O:272:SER:CB	1:O:302:LEU:HD23	2.33	0.54
6:A:267:LYS:NZ	6:A:288:PHE:HB2	2.23	0.54
23:X:629:ARG:O	23:X:636:ARG:NH2	2.41	0.54
26:U:8:LEU:CD1	26:U:72:LEU:HD12	2.38	0.54
1:O:31:VAL:HG22	1:O:59:ASN:HB3	1.90	0.53
1:O:218:ASN:ND2	20:T:148:VAL:CG1	2.72	0.53
23:X:554:VAL:HG11	23:X:583:ALA:HB3	1.89	0.53
8:D:30:LEU:O	8:D:34:LEU:HD23	2.08	0.53
1:O:158:PRO:HG2	1:O:161:TYR:HB2	1.90	0.53
6:A:143:ARG:HG3	6:A:144:GLU:HG3	1.91	0.53
8:D:30:LEU:CG	8:D:34:LEU:HD23	2.39	0.53
10:G:74:HIS:CG	10:G:126:TYR:CE2	2.93	0.53
22:W:862:LEU:HD23	22:W:896:PHE:CE2	2.38	0.53
23:X:46:LEU:HD22	23:X:60:ILE:HG23	1.90	0.53
23:X:112:GLY:O	23:X:984:LYS:NZ	2.36	0.53
18:Q:495:LEU:HG	18:Q:504:VAL:HG22	1.90	0.53
11:H:122:LYS:O	11:H:125:THR:OG1	2.22	0.53
15:N:54:LEU:CA	25:S:139:SER:CB	2.81	0.53
15:N:183:ILE:CD1	15:N:188:LYS:HD3	2.38	0.53
15:N:211:GLN:HA	26:U:133:ARG:NH2	2.21	0.53
15:N:691:LYS:O	15:N:771:ASN:ND2	2.42	0.53
18:Q:9:ILE:HG12	26:U:94:GLU:OE2	2.06	0.53
23:X:783:LEU:HA	23:X:787:ILE:HD13	1.91	0.53
10:G:84:SER:HA	10:G:87:ILE:HG22	1.90	0.53
15:N:135:ARG:HA	15:N:135:ARG:HE	1.72	0.53
18:Q:45:GLN:OE1	18:Q:45:GLN:HA	2.09	0.53
23:X:811:LYS:HG2	23:X:930:GLU:HG2	1.91	0.53
6:A:69:LEU:CG	12:I:66:LEU:CD1	2.86	0.53
6:A:315:ARG:HG2	6:A:319:GLN:NE2	2.21	0.53
11:H:108:HIS:CD2	18:Q:118:ILE:HD12	2.43	0.53
18:Q:271:LEU:HD13	18:Q:271:LEU:O	2.07	0.53
21:V:96:GLU:OE1	21:V:96:GLU:HA	2.08	0.53
22:W:328:GLN:HG2	22:W:329:LEU:HD12	1.91	0.53
22:W:684:ASN:HD21	22:W:723:THR:HG21	1.73	0.53
23:X:14:TRP:O	23:X:17:ARG:NH2	2.42	0.53
24:d:923:LEU:H	24:d:923:LEU:CD2	2.06	0.53
26:U:7:GLN:HE21	26:U:7:GLN:H	1.56	0.53
10:G:155:LYS:HD2	10:G:155:LYS:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:104:LYS:NZ	26:U:52:GLU:HA	2.23	0.53
18:Q:506:HIS:ND1	18:Q:508:ASP:OD1	2.41	0.53
22:W:399:PHE:CZ	22:W:425:MET:SD	3.02	0.53
23:X:584:ALA:O	23:X:588:ILE:HD12	2.08	0.53
24:d:920:LEU:C	24:d:923:LEU:HD21	2.31	0.53
26:U:18:GLN:HE22	26:U:62:ILE:CG1	2.22	0.53
4:3:107:ASP:HB3	18:Q:651:LEU:HD13	1.87	0.53
15:N:203:LEU:HD23	15:N:289:LEU:HD21	1.90	0.53
15:N:297:HIS:CE1	15:N:366:VAL:O	2.62	0.53
15:N:449:SER:O	15:N:451:CYS:N	2.42	0.53
22:W:855:TRP:HZ3	22:W:896:PHE:CA	2.21	0.53
8:D:120:ILE:HG21	10:G:159:ARG:HH21	1.73	0.53
11:H:151:LEU:HD13	21:V:41:LYS:HZ1	1.74	0.53
15:N:250:LEU:O	15:N:271:ILE:HD11	2.09	0.53
18:Q:99:ARG:HG2	18:Q:103:ARG:HE	1.74	0.53
18:Q:634:ASN:O	18:Q:638:LYS:HG3	2.09	0.53
22:W:672:PRO:HB2	22:W:718:THR:HG21	1.91	0.53
22:W:866:ILE:HG23	22:W:886:ILE:HD12	1.91	0.53
23:X:502:HIS:HB2	23:X:665:ILE:HD11	1.89	0.53
10:G:56:ILE:HD12	10:G:56:ILE:O	2.09	0.52
11:H:108:HIS:CE1	18:Q:115:VAL:HG23	2.44	0.52
13:J:113:LEU:HD22	26:U:63:ALA:HA	1.89	0.52
15:N:678:PHE:CD1	18:Q:583:ARG:HD2	2.45	0.52
13:J:85:LEU:HD12	25:S:96:PHE:HB2	1.90	0.52
13:J:99:ILE:HD13	25:S:80:SER:HB2	1.89	0.52
15:N:820:ILE:HG22	15:N:835:LEU:HD23	1.90	0.52
22:W:1005:LEU:HD21	22:W:1030:ILE:HG13	1.90	0.52
6:A:265:VAL:HA	6:A:300:PRO:HA	1.91	0.52
6:A:267:LYS:C	6:A:268:LEU:HD23	2.35	0.52
10:G:142:GLN:HG3	10:G:146:ARG:NE	2.23	0.52
12:I:110:SER:HB3	12:I:111:PRO:CD	2.36	0.52
14:K:70:LEU:HD11	21:V:86:LEU:HD22	1.80	0.52
20:T:201:ARG:O	20:T:204:GLN:NE2	2.43	0.52
22:W:338:LEU:HD23	22:W:338:LEU:O	2.10	0.52
22:W:447:ILE:HD12	22:W:448:PRO:HD2	1.91	0.52
10:G:50:GLN:HG3	10:G:50:GLN:O	2.10	0.52
10:G:135:LEU:HD23	10:G:135:LEU:C	2.34	0.52
11:H:38:GLY:C	11:H:39:ARG:HD3	2.35	0.52
15:N:444:GLU:HG2	15:N:563:GLN:HE21	1.75	0.52
15:N:465:LEU:HD13	15:N:478:MET:HG3	1.91	0.52
16:O:735:LEU:HD21	22:W:73:PRO:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:d:924:PRO:O	24:d:927:TYR:CD2	2.61	0.52
6:A:224:TYR:HB2	6:A:412:ARG:HE	1.75	0.52
11:H:23:LYS:HA	18:Q:109:MET:HE1	1.91	0.52
18:Q:592:ILE:HG13	18:Q:627:TRP:CE3	2.44	0.52
23:X:31:PHE:HD1	23:X:32:PRO:CD	2.09	0.52
9:F:188:PHE:HD1	15:N:281:ARG:NH2	2.06	0.52
10:G:138:MET:CE	10:G:138:MET:CA	2.85	0.52
15:N:937:ARG:NH2	15:N:941:TYR:O	2.43	0.52
22:W:490:LEU:HB3	22:W:491:PRO:HD3	1.92	0.52
5:4:111:LYS:HD3	18:Q:17:LYS:HZ2	1.74	0.52
11:H:88:ASP:O	11:H:92:GLN:CB	2.58	0.52
23:X:39:ILE:N	23:X:39:ILE:CD1	2.73	0.52
6:A:363:PHE:HE2	6:A:425:VAL:HG13	1.74	0.52
10:G:143:LYS:HD2	10:G:143:LYS:O	2.09	0.52
15:N:362:ASP:O	15:N:368:LYS:NZ	2.42	0.52
15:N:208:LEU:HD12	15:N:208:LEU:O	2.10	0.52
18:Q:595:GLN:HE22	18:Q:619:ARG:HB2	1.75	0.52
22:W:1024:ARG:O	22:W:1028:HIS:ND1	2.29	0.52
10:G:78:LEU:CD1	26:U:73:ILE:HG22	2.40	0.52
10:G:120:HIS:CB	15:N:147:ALA:HB1	2.38	0.52
10:G:127:ARG:HG2	15:N:152:PHE:CE1	2.45	0.52
15:N:216:THR:OG1	15:N:223:LYS:HB3	2.09	0.52
15:N:410:HIS:ND1	15:N:410:HIS:O	2.43	0.52
15:N:740:GLY:O	15:N:742:SER:N	2.42	0.52
18:Q:267:ASP:OD1	18:Q:268:ILE:N	2.43	0.52
18:Q:289:PRO:HB2	18:Q:291:TRP:NE1	2.25	0.52
19:R:21:TYR:HD1	19:R:102:VAL:HG22	1.75	0.52
22:W:270:LEU:HD11	22:W:303:GLN:HG3	1.90	0.52
22:W:854:VAL:HG12	22:W:855:TRP:CD1	2.45	0.52
5:4:84:PHE:CE2	15:N:177:ILE:HD13	2.43	0.51
8:D:135:ILE:HD13	10:G:146:ARG:NH1	2.25	0.51
23:X:10:ILE:HG21	23:X:49:GLN:HG3	1.92	0.51
23:X:432:PRO:HB2	23:X:488:VAL:HG11	1.92	0.51
23:X:625:VAL:HG13	23:X:677:VAL:HG21	1.92	0.51
24:d:931:ILE:O	26:U:4:ARG:CB	2.58	0.51
14:K:63:LEU:O	14:K:67:ILE:HG12	2.10	0.51
18:Q:635:PHE:C	18:Q:635:PHE:CD1	2.88	0.51
22:W:155:ALA:H	23:X:915:ARG:HH22	1.56	0.51
22:W:366:ILE:HD11	22:W:369:ARG:HE	1.76	0.51
22:W:805:GLN:HB3	22:W:941:VAL:HG11	1.92	0.51
25:S:84:ILE:HG23	25:S:89:LEU:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:109:LEU:HB3	26:U:59:ALA:HB2	1.91	0.51
17:P:52:ARG:NH1	17:P:56:GLN:OE1	2.43	0.51
21:V:86:LEU:O	21:V:90:ASP:HB2	2.10	0.51
22:W:25:MET:SD	22:W:25:MET:C	2.94	0.51
4:3:149:LEU:C	4:3:149:LEU:HD12	2.36	0.51
15:N:216:THR:CB	15:N:223:LYS:CB	2.71	0.51
15:N:399:LYS:HD2	18:Q:271:LEU:HB2	1.93	0.51
17:P:547:TYR:O	17:P:550:LYS:HB3	2.11	0.51
5:4:43:PHE:HB3	5:4:85:ARG:HD3	1.92	0.51
13:J:95:VAL:CG2	15:N:122:LEU:HD22	2.40	0.51
11:H:58:THR:O	11:H:62:VAL:HG22	2.11	0.51
15:N:247:LEU:CB	15:N:275:HIS:NE2	2.73	0.51
15:N:593:GLU:N	15:N:593:GLU:OE1	2.43	0.51
18:Q:591:LYS:HG2	18:Q:591:LYS:O	2.09	0.51
8:D:47:MET:SD	8:D:47:MET:C	2.94	0.51
8:D:126:TYR:CD1	8:D:126:TYR:C	2.88	0.51
17:P:133:ALA:HB3	17:P:182:VAL:HB	1.92	0.51
18:Q:288:SER:HB2	18:Q:289:PRO:HD2	1.92	0.51
18:Q:289:PRO:CB	18:Q:291:TRP:CE2	2.93	0.51
22:W:819:LEU:O	22:W:822:HIS:HB2	2.11	0.51
23:X:978:GLY:HA2	23:X:981:VAL:HG12	1.92	0.51
24:d:935:GLU:OE2	26:U:2:ALA:HB2	2.08	0.51
9:F:115:ILE:HG12	9:F:118:ARG:NH2	2.25	0.51
5:4:84:PHE:HD2	15:N:178:ILE:HD11	1.76	0.51
8:D:38:GLU:OE2	8:D:42:ARG:HD2	2.11	0.51
9:F:84:GLN:HG3	9:F:92:VAL:HG13	1.92	0.51
10:G:60:GLU:HB3	10:G:121:HIS:CD2	2.46	0.51
11:H:131:ILE:H	11:H:131:ILE:HD12	1.76	0.51
12:I:94:PHE:HB3	12:I:98:ARG:HH12	1.76	0.51
15:N:189:GLN:HE21	15:N:189:GLN:CA	2.13	0.51
15:N:203:LEU:CD2	15:N:289:LEU:HD21	2.41	0.51
15:N:370:LEU:H	15:N:370:LEU:HD12	1.76	0.51
22:W:855:TRP:HH2	22:W:896:PHE:CD2	2.26	0.51
23:X:6:LEU:HD13	23:X:45:ALA:HB2	1.93	0.51
6:A:67:LYS:HA	6:A:70:LYS:HG3	1.93	0.51
6:A:312:PRO:O	6:A:418:ASN:ND2	2.36	0.51
10:G:152:ARG:O	10:G:152:ARG:HD3	2.11	0.51
15:N:399:LYS:HE3	18:Q:271:LEU:N	2.25	0.51
15:N:399:LYS:CE	18:Q:271:LEU:HB2	2.41	0.51
22:W:37:LEU:CD1	22:W:85:MET:CE	2.74	0.51
22:W:775:ASP:O	22:W:779:HIS:ND1	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:1079:MET:HE1	22:W:1147:ASN:HD22	1.76	0.50
23:X:975:LEU:HB3	23:X:978:GLY:H	1.76	0.50
10:G:124:ASN:CG	15:N:149:LEU:HD21	2.36	0.50
11:H:137:GLN:O	11:H:141:GLN:HG3	2.10	0.50
12:I:113:GLN:HA	12:I:116:GLN:HG3	1.92	0.50
15:N:554:MET:HB3	15:N:564:LEU:HD23	1.93	0.50
18:Q:39:ASN:O	18:Q:42:ARG:HG3	2.10	0.50
5:4:11:ASP:OD1	5:4:12:ALA:N	2.44	0.50
15:N:508:SER:OG	15:N:637:PHE:O	2.23	0.50
21:V:50:ARG:HA	21:V:53:GLN:NE2	2.26	0.50
5:4:66:TYR:HE2	10:G:39:LYS:HG2	1.77	0.50
9:F:175:GLN:N	9:F:175:GLN:HE21	2.10	0.50
14:K:70:LEU:HD13	21:V:85:PHE:CE1	2.47	0.50
18:Q:115:VAL:O	18:Q:119:VAL:HG23	2.12	0.50
22:W:102:ILE:HD11	22:W:122:VAL:HG21	1.94	0.50
23:X:118:ILE:HD11	23:X:980:GLN:HB3	1.92	0.50
6:A:174:TYR:C	6:A:174:TYR:CD1	2.90	0.50
6:A:310:PRO:HB2	6:A:392:LEU:HB2	1.93	0.50
8:D:27:ARG:HA	12:I:103:THR:HG1	1.72	0.50
14:K:98:ASP:O	14:K:101:ARG:CG	2.60	0.50
18:Q:145:GLN:OE1	21:V:42:ILE:HA	2.12	0.50
18:Q:394:HIS:CD2	19:R:78:ARG:HG2	2.46	0.50
22:W:281:ASP:OD1	22:W:281:ASP:N	2.43	0.50
22:W:481:TYR:O	22:W:488:PHE:HB2	2.12	0.50
23:X:86:ASP:OD1	23:X:87:ASP:N	2.45	0.50
23:X:172:THR:HA	23:X:175:ARG:HE	1.77	0.50
9:F:83:LYS:HZ1	9:F:98:TYR:HE1	1.58	0.50
9:F:175:GLN:N	9:F:175:GLN:NE2	2.60	0.50
15:N:573:VAL:HG23	15:N:584:MET:O	2.12	0.50
18:Q:502:ILE:HB	18:Q:514:LEU:HB2	1.94	0.50
22:W:821:ALA:O	22:W:825:THR:HG23	2.12	0.50
23:X:37:TRP:CE3	23:X:40:LEU:HD12	2.47	0.50
22:W:67:ILE:HG22	22:W:76:ILE:HG23	1.94	0.50
26:U:15:LEU:O	26:U:15:LEU:HD12	2.12	0.50
2:1:92:GLU:HG2	4:3:38:GLN:HE22	1.77	0.50
10:G:86:LEU:C	10:G:86:LEU:CD1	2.85	0.50
11:H:124:LEU:HD13	18:Q:144:LEU:HD11	1.93	0.50
14:K:28:ALA:O	14:K:32:ILE:HG12	2.11	0.50
16:O:703:THR:HA	16:O:725:VAL:O	2.12	0.50
17:P:14:ASP:OD1	17:P:15:LEU:N	2.40	0.50
19:R:111:SER:OG	19:R:112:GLU:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:d:923:LEU:C	24:d:927:TYR:HE2	2.19	0.50
26:U:7:GLN:HE21	26:U:7:GLN:N	2.09	0.50
14:K:55:SER:HA	14:K:58:HIS:CE1	2.47	0.49
15:N:328:ARG:NH1	15:N:334:CYS:SG	2.84	0.49
17:P:343:SER:HB2	17:P:399:LEU:HD23	1.94	0.49
18:Q:31:LEU:HD23	18:Q:31:LEU:N	2.26	0.49
18:Q:289:PRO:HG3	18:Q:291:TRP:CZ2	2.46	0.49
22:W:389:LEU:C	22:W:389:LEU:CD2	2.85	0.49
22:W:810:VAL:O	22:W:814:ILE:HG12	2.12	0.49
23:X:671:GLU:HG2	23:X:687:PHE:CD2	2.46	0.49
8:D:93:MET:SD	8:D:94:GLN:N	2.85	0.49
9:F:97:ASP:H	9:F:107:GLN:HE21	1.59	0.49
10:G:67:LEU:C	10:G:67:LEU:CD1	2.85	0.49
10:G:68:HIS:CE1	10:G:72:PHE:HA	2.47	0.49
13:J:113:LEU:HD22	26:U:63:ALA:CA	2.41	0.49
22:W:60:ILE:O	22:W:63:ILE:HG22	2.12	0.49
23:X:42:LEU:C	23:X:42:LEU:CD2	2.85	0.49
5:4:60:ASP:HB3	5:4:63:TYR:HD2	1.75	0.49
13:J:75:ARG:HD2	13:J:79:LEU:HD12	1.93	0.49
15:N:496:LEU:O	15:N:499:TRP:N	2.45	0.49
23:X:68:ILE:HD11	23:X:78:VAL:HG21	1.94	0.49
23:X:686:LYS:NZ	23:X:688:PRO:HB2	2.27	0.49
26:U:20:CYS:SG	26:U:21:ASN:N	2.85	0.49
26:U:57:LEU:C	26:U:57:LEU:CD2	2.85	0.49
1:0:159:PRO:HB3	1:0:182:ARG:HH12	1.77	0.49
5:4:42:TYR:HB3	5:4:48:PHE:CE2	2.48	0.49
8:D:149:ILE:HD11	10:G:132:ARG:NH1	2.27	0.49
10:G:42:TYR:CD1	10:G:42:TYR:C	2.90	0.49
1:0:13:ALA:HB1	1:0:77:VAL:HG12	1.94	0.49
8:D:44:LEU:C	8:D:44:LEU:CD2	2.86	0.49
10:G:127:ARG:HG2	15:N:152:PHE:HZ	1.75	0.49
11:H:52:LEU:C	11:H:52:LEU:CD2	2.85	0.49
13:J:101:THR:HG22	26:U:51:THR:CG2	2.35	0.49
18:Q:152:SER:HB3	21:V:58:ASN:OD1	2.12	0.49
23:X:670:LEU:HB3	23:X:687:PHE:HE2	1.77	0.49
26:U:54:TYR:HD1	26:U:58:PHE:CZ	2.30	0.49
5:4:108:TYR:HD1	5:4:111:LYS:HD2	1.77	0.49
10:G:123:ILE:CD1	26:U:8:LEU:HD23	2.41	0.49
15:N:376:PRO:CD	15:N:377:PRO:CD	2.78	0.49
20:T:151:SER:HB3	20:T:179:ARG:HH22	1.78	0.49
22:W:729:SER:N	22:W:875:GLU:OE2	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:843:LEU:HD21	22:W:884:PHE:HE2	1.76	0.49
23:X:183:LEU:HD22	23:X:974:SER:HB3	1.93	0.49
23:X:517:ARG:HG2	23:X:522:VAL:HG12	1.95	0.49
2:1:100:LEU:CD1	18:Q:641:LEU:HB3	2.21	0.49
12:I:96:GLU:O	12:I:99:LYS:HG3	2.13	0.49
19:R:110:THR:HG21	19:R:114:LEU:HD13	1.94	0.49
1:0:218:ASN:ND2	20:T:1:MET:HG2	2.27	0.49
6:A:364:TYR:HE2	6:A:431:LYS:HA	1.78	0.49
8:D:86:GLN:HA	8:D:89:ILE:HB	1.94	0.49
9:F:40:PHE:HB3	9:F:98:TYR:HE2	1.78	0.49
15:N:184:THR:HG23	15:N:187:GLU:HB3	1.93	0.49
15:N:297:HIS:CE1	15:N:301:LEU:CD2	2.96	0.49
15:N:961:THR:O	15:N:965:MET:HG3	2.13	0.49
17:P:582:GLU:HA	17:P:585:THR:HG22	1.94	0.49
18:Q:263:LYS:HA	18:Q:340:GLN:OE1	2.13	0.49
18:Q:485:GLU:H	18:Q:485:GLU:CD	2.14	0.49
20:T:112:THR:HG22	20:T:129:VAL:HG22	1.95	0.49
1:0:107:LEU:HD13	3:2:164:ILE:HG23	1.93	0.49
10:G:89:PHE:CZ	26:U:19:PHE:CD1	2.95	0.49
10:G:123:ILE:HD11	26:U:8:LEU:HD23	1.95	0.49
11:H:152:GLU:O	11:H:156:LYS:HB2	2.11	0.49
15:N:268:SER:HA	15:N:271:ILE:HG22	1.95	0.49
15:N:454:ILE:HG12	15:N:465:LEU:HD23	1.93	0.49
18:Q:146:LEU:HD21	21:V:42:ILE:CD1	2.39	0.49
22:W:399:PHE:CZ	22:W:425:MET:CB	2.94	0.49
23:X:166:GLU:HA	23:X:169:LEU:HG	1.95	0.49
24:d:931:ILE:HD12	24:d:931:ILE:N	2.28	0.49
26:U:18:GLN:NE2	26:U:62:ILE:HG12	2.27	0.49
13:J:85:LEU:HD22	25:S:93:TYR:CB	2.42	0.49
15:N:183:ILE:CD1	15:N:188:LYS:HG2	2.43	0.49
15:N:687:ILE:HD12	15:N:770:TRP:CZ2	2.48	0.49
16:O:682:VAL:HA	16:O:685:LEU:HD23	1.93	0.49
17:P:375:GLN:HB2	17:P:465:LEU:HD11	1.95	0.49
18:Q:131:SER:OG	18:Q:132:GLN:N	2.45	0.49
18:Q:561:GLU:OE1	18:Q:587:GLU:HB3	2.13	0.49
21:V:102:ASN:O	21:V:106:ARG:HG3	2.13	0.49
22:W:1023:LYS:HD2	22:W:1114:ALA:HA	1.95	0.49
26:U:7:GLN:N	26:U:7:GLN:NE2	2.60	0.49
1:0:200:VAL:HG13	1:0:214:VAL:HG12	1.94	0.48
14:K:70:LEU:CD2	21:V:86:LEU:HD21	2.43	0.48
15:N:442:ILE:CB	15:N:496:LEU:HD11	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:896:PHE:C	22:W:896:PHE:HD1	2.20	0.48
10:G:143:LYS:C	10:G:143:LYS:CD	2.85	0.48
10:G:161:ILE:HD12	10:G:164:ILE:HG22	1.95	0.48
13:J:95:VAL:HG21	15:N:122:LEU:HD21	1.95	0.48
13:J:104:LYS:NZ	26:U:52:GLU:CA	2.76	0.48
15:N:184:THR:CG2	15:N:187:GLU:HB3	2.44	0.48
15:N:691:LYS:NZ	15:N:691:LYS:CB	2.73	0.48
17:P:218:ILE:HG12	17:P:228:VAL:HG12	1.95	0.48
18:Q:43:LEU:CD1	18:Q:43:LEU:C	2.86	0.48
22:W:718:THR:O	22:W:721:SER:OG	2.23	0.48
2:1:92:GLU:HG2	4:3:38:GLN:OE1	2.13	0.48
10:G:120:HIS:HA	10:G:123:ILE:HG22	1.96	0.48
13:J:68:PHE:HE1	25:S:136:ILE:CB	2.27	0.48
15:N:296:LEU:HD22	15:N:296:LEU:N	2.29	0.48
15:N:683:ARG:CD	16:O:684:ARG:HG2	2.43	0.48
17:P:713:LEU:HA	17:P:716:GLU:HG2	1.95	0.48
22:W:63:ILE:O	22:W:67:ILE:HG12	2.13	0.48
22:W:790:LEU:HB3	22:W:826:PHE:CE2	2.48	0.48
22:W:855:TRP:CH2	22:W:896:PHE:CG	3.01	0.48
25:S:128:ARG:HA	25:S:131:ILE:H	1.78	0.48
9:F:114:VAL:O	9:F:118:ARG:HG3	2.14	0.48
9:F:118:ARG:HD2	18:Q:112:LEU:CD2	2.21	0.48
15:N:370:LEU:HD12	15:N:370:LEU:N	2.28	0.48
15:N:442:ILE:CG1	15:N:496:LEU:HD11	2.43	0.48
16:O:684:ARG:O	16:O:684:ARG:HG3	2.14	0.48
19:R:21:TYR:HA	19:R:101:LEU:O	2.13	0.48
21:V:85:PHE:CD1	21:V:85:PHE:C	2.90	0.48
23:X:311:LEU:O	23:X:314:PRO:HD2	2.13	0.48
4:3:144:GLU:HA	4:3:147:LYS:CD	2.43	0.48
8:D:30:LEU:CD2	8:D:30:LEU:C	2.85	0.48
8:D:34:LEU:HA	8:D:37:LEU:HD23	1.88	0.48
10:G:88:ASN:ND2	10:G:112:LEU:HD21	2.29	0.48
15:N:234:LEU:HD13	15:N:246:ARG:O	2.14	0.48
22:W:646:GLU:OE1	22:W:864:ARG:CD	2.61	0.48
24:d:931:ILE:CD1	26:U:77:PRO:HG3	2.43	0.48
4:3:167:ILE:HA	4:3:170:ILE:HG22	1.95	0.48
9:F:174:ARG:CD	15:N:270:GLN:HE22	2.27	0.48
10:G:127:ARG:CG	15:N:152:PHE:HE1	2.26	0.48
11:H:55:GLN:O	11:H:59:LEU:HG	2.13	0.48
18:Q:46:ARG:CG	18:Q:46:ARG:NH1	2.72	0.48
18:Q:606:LYS:HE2	18:Q:606:LYS:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:558:VAL:O	23:X:562:ASN:ND2	2.47	0.48
23:X:942:SER:O	23:X:945:GLN:NE2	2.44	0.48
24:d:923:LEU:O	24:d:926:GLN:HG2	2.14	0.48
26:U:8:LEU:HD13	26:U:72:LEU:HD12	1.96	0.48
9:F:171:ILE:HG21	15:N:263:ARG:HB2	1.96	0.48
10:G:57:ARG:HD3	10:G:58:PRO:CD	2.16	0.48
11:H:19:VAL:HG21	18:Q:116:LEU:HD13	1.95	0.48
15:N:204:VAL:C	15:N:206:THR:H	2.22	0.48
5:4:42:TYR:HB3	5:4:48:PHE:HE2	1.79	0.48
6:A:317:PHE:CE2	6:A:414:GLN:HB2	2.49	0.48
16:O:738:ASP:OD1	16:O:739:ARG:N	2.46	0.48
17:P:556:ILE:HD11	17:P:617:LEU:HB3	1.96	0.48
23:X:404:GLN:OE1	23:X:408:GLN:NE2	2.47	0.48
2:1:94:PHE:HB2	18:Q:650:LEU:CD2	2.44	0.48
6:A:108:PHE:HB2	6:A:127:HIS:CE1	2.49	0.48
6:A:192:TRP:HE3	6:A:202:LYS:HZ1	1.62	0.48
15:N:188:LYS:HE3	18:Q:47:ILE:CD1	2.43	0.48
17:P:65:LEU:HD11	17:P:70:PRO:HA	1.96	0.48
22:W:855:TRP:CZ3	22:W:896:PHE:CA	2.96	0.48
23:X:174:ASN:HA	23:X:177:LEU:HD12	1.95	0.48
24:d:932:LYS:HZ1	24:d:935:GLU:CG	2.24	0.48
26:U:15:LEU:O	26:U:19:PHE:CD2	2.66	0.48
15:N:592:LYS:HA	22:W:27:MET:SD	2.53	0.48
16:O:721:LEU:HG	16:O:736:TRP:NE1	2.29	0.48
20:T:151:SER:OG	20:T:179:ARG:NH2	2.47	0.48
22:W:627:LEU:HD22	22:W:648:THR:CG2	2.44	0.48
22:W:743:PHE:O	22:W:747:ASN:ND2	2.47	0.48
1:0:106:GLN:HG2	3:2:168:ILE:HD11	1.96	0.47
6:A:214:ARG:HD3	6:A:219:LEU:HD23	1.96	0.47
8:D:153:HIS:HA	8:D:156:SER:HB3	1.96	0.47
15:N:230:PHE:CE2	15:N:296:LEU:HB3	2.49	0.47
15:N:846:ASN:O	15:N:846:ASN:ND2	2.46	0.47
23:X:241:PHE:CE2	23:X:276:ILE:HG12	2.49	0.47
23:X:481:GLU:HB3	23:X:485:PRO:HG2	1.96	0.47
23:X:605:ILE:O	23:X:609:ILE:HG12	2.14	0.47
6:A:192:TRP:HA	6:A:202:LYS:HZ2	1.78	0.47
10:G:157:LEU:HD21	26:U:110:ARG:HH22	1.78	0.47
15:N:273:PHE:O	15:N:276:GLN:HG3	2.14	0.47
18:Q:252:GLU:OE1	18:Q:252:GLU:N	2.47	0.47
22:W:57:GLU:HA	22:W:96:LEU:HD21	1.96	0.47
22:W:396:MET:CE	22:W:396:MET:CA	2.85	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:73:ASP:HA	8:D:76:PHE:HE1	1.79	0.47
9:F:74:GLN:HE22	9:F:76:PRO:HG2	1.79	0.47
9:F:98:TYR:HD2	9:F:105:ILE:HD11	1.78	0.47
10:G:65:GLU:HA	10:G:65:GLU:OE2	2.13	0.47
15:N:683:ARG:NE	16:O:684:ARG:HG2	2.30	0.47
15:N:885:LEU:HD11	15:N:1186:LEU:HD22	1.95	0.47
17:P:12:MET:N	17:P:458:SER:OG	2.35	0.47
22:W:131:TYR:HE1	22:W:132:LYS:HE3	1.78	0.47
22:W:457:PHE:O	22:W:460:GLN:HG3	2.13	0.47
22:W:809:ARG:NH2	22:W:812:GLU:OE1	2.41	0.47
23:X:42:LEU:HD23	23:X:42:LEU:O	2.13	0.47
23:X:173:LYS:HG2	23:X:986:ILE:HG13	1.96	0.47
23:X:795:SER:HA	23:X:798:TRP:CZ3	2.49	0.47
26:U:22:ALA:HB1	26:U:58:PHE:CD2	2.49	0.47
4:3:43:ASP:HB2	4:3:88:LEU:HD21	1.95	0.47
10:G:141:VAL:HA	10:G:144:ARG:HD3	1.96	0.47
13:J:101:THR:HB	26:U:51:THR:OG1	2.14	0.47
15:N:153:ALA:HB1	15:N:156:TYR:HD2	1.78	0.47
15:N:473:ALA:O	15:N:476:ASP:OD1	2.32	0.47
18:Q:94:PRO:HB2	18:Q:95:TRP:CE3	2.49	0.47
22:W:376:LEU:HA	22:W:379:PHE:HD2	1.80	0.47
22:W:894:ASN:HA	22:W:897:ARG:HE	1.78	0.47
23:X:37:TRP:HD1	23:X:72:MET:CE	2.23	0.47
13:J:82:LYS:HD3	25:S:96:PHE:C	2.29	0.47
15:N:460:SER:O	15:N:460:SER:OG	2.28	0.47
22:W:605:LEU:HB3	22:W:644:CYS:SG	2.54	0.47
22:W:662:GLN:HG2	22:W:711:TRP:CE2	2.49	0.47
5:4:14:ASN:HA	5:4:17:ARG:HG2	1.97	0.47
10:G:47:ASN:N	10:G:47:ASN:ND2	2.60	0.47
16:O:723:LEU:HD22	16:O:769:VAL:HG23	1.97	0.47
22:W:409:ILE:HG12	22:W:450:SER:HB3	1.97	0.47
22:W:506:ARG:HD3	22:W:506:ARG:HA	1.65	0.47
23:X:88:PHE:HZ	23:X:134:CYS:HB2	1.79	0.47
23:X:585:ILE:HD11	23:X:642:MET:HE1	1.96	0.47
1:0:251:LEU:HD11	18:Q:494:GLN:HB2	1.97	0.47
6:A:268:LEU:HD13	6:A:303:PHE:CZ	2.50	0.47
6:A:317:PHE:HA	6:A:320:LYS:HG2	1.97	0.47
6:A:509:ARG:O	6:A:513:ARG:HG2	2.14	0.47
8:D:76:PHE:HA	8:D:79:LEU:HB2	1.97	0.47
8:D:95:VAL:HA	8:D:98:LYS:HD2	1.95	0.47
11:H:38:GLY:O	11:H:39:ARG:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:151:LEU:HD11	21:V:38:LYS:HZ2	1.78	0.47
14:K:93:ALA:O	14:K:97:VAL:HG23	2.15	0.47
16:O:685:LEU:HD13	16:O:689:PHE:HB2	1.97	0.47
20:T:112:THR:HA	20:T:128:THR:O	2.14	0.47
22:W:53:GLN:HA	22:W:56:HIS:CD2	2.49	0.47
22:W:154:SER:O	22:W:157:VAL:HG22	2.15	0.47
22:W:854:VAL:HG11	22:W:862:LEU:HD13	1.96	0.47
23:X:20:ASP:OD1	23:X:21:TYR:N	2.48	0.47
23:X:472:ASN:HA	23:X:475:THR:HG22	1.97	0.47
24:d:929:PRO:CB	24:d:930:PRO:HD3	2.44	0.47
1:O:245:HIS:CD2	1:O:295:THR:O	2.68	0.47
8:D:30:LEU:HD21	12:I:99:LYS:CB	2.45	0.47
8:D:30:LEU:HD21	8:D:34:LEU:CD2	2.43	0.47
10:G:59:LEU:HD22	10:G:59:LEU:H	1.76	0.47
11:H:181:LEU:HB3	19:R:168:LEU:HD12	1.95	0.47
17:P:244:VAL:HG13	17:P:255:ILE:HG23	1.95	0.47
22:W:509:LEU:HB2	22:W:514:CYS:CB	2.44	0.47
22:W:862:LEU:CD2	22:W:896:PHE:HE2	2.27	0.47
8:D:152:ALA:O	8:D:156:SER:HB2	2.13	0.47
9:F:20:TRP:HZ3	9:F:31:ASP:HB3	1.80	0.47
10:G:149:THR:CG2	24:d:915:SER:OG	2.63	0.47
10:G:158:GLU:HA	10:G:161:ILE:HG22	1.95	0.47
15:N:399:LYS:CD	18:Q:271:LEU:HB2	2.45	0.47
16:O:759:ARG:HD2	16:O:779:SER:HB2	1.96	0.47
18:Q:138:LYS:HG2	18:Q:139:GLN:H	1.80	0.47
18:Q:320:SER:OG	18:Q:321:GLN:N	2.48	0.47
22:W:296:ARG:NH1	22:W:301:GLU:OE2	2.48	0.47
2:1:92:GLU:HG2	4:3:38:GLN:NE2	2.29	0.47
6:A:249:ARG:O	6:A:254:ASN:ND2	2.45	0.47
9:F:171:ILE:CG2	15:N:263:ARG:CZ	2.93	0.47
15:N:165:SER:OG	15:N:166:TYR:N	2.48	0.47
15:N:301:LEU:HD23	15:N:361:ILE:CG1	2.42	0.47
15:N:716:ASN:C	15:N:716:ASN:ND2	2.73	0.47
19:R:85:LEU:HG	19:R:114:LEU:HD21	1.97	0.47
23:X:31:PHE:CD1	23:X:32:PRO:CD	2.92	0.47
23:X:37:TRP:HE3	23:X:40:LEU:HD12	1.80	0.47
3:2:103:ASP:N	3:2:103:ASP:OD1	2.45	0.46
6:A:366:ALA:HB2	6:A:430:LEU:HD11	1.98	0.46
15:N:529:PRO:HB2	15:N:588:LEU:HD12	1.97	0.46
17:P:180:ILE:HD13	17:P:226:ILE:HD13	1.97	0.46
22:W:1132:LYS:HE2	22:W:1132:LYS:HB3	1.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:1183:TRP:HE1	22:W:1186:TYR:C	2.23	0.46
23:X:951:THR:HA	23:X:954:GLU:HB2	1.96	0.46
24:d:923:LEU:CG	24:d:924:PRO:CD	2.41	0.46
24:d:933:LEU:HD11	26:U:7:GLN:CG	2.40	0.46
2:1:129:VAL:HG13	14:K:115:LEU:HD11	1.96	0.46
5:4:109:SER:HB3	8:D:163:ALA:HB3	1.98	0.46
14:K:70:LEU:HD21	21:V:86:LEU:HD21	1.92	0.46
15:N:184:THR:HG23	15:N:187:GLU:H	1.79	0.46
21:V:50:ARG:HA	21:V:53:GLN:HE22	1.81	0.46
22:W:155:ALA:H	23:X:915:ARG:NH2	2.13	0.46
22:W:693:ARG:HD3	22:W:1007:ASN:HD22	1.80	0.46
23:X:296:SER:O	23:X:354:ARG:NH2	2.48	0.46
23:X:977:LEU:HA	23:X:980:GLN:NE2	2.31	0.46
24:d:924:PRO:CA	24:d:927:TYR:CD2	2.98	0.46
15:N:242:ASP:N	15:N:242:ASP:OD1	2.47	0.46
15:N:252:ILE:HG22	15:N:254:VAL:HG22	1.97	0.46
15:N:277:LEU:C	15:N:277:LEU:CD2	2.85	0.46
18:Q:255:ALA:HB2	18:Q:347:HIS:CD2	2.50	0.46
22:W:145:ILE:HD11	22:W:163:ALA:HB1	1.97	0.46
23:X:37:TRP:HE1	23:X:72:MET:HE1	1.78	0.46
8:D:145:SER:HA	8:D:148:ILE:HD12	1.96	0.46
15:N:320:TRP:O	18:Q:317:GLN:NE2	2.48	0.46
15:N:669:GLN:NE2	15:N:683:ARG:HD3	2.31	0.46
22:W:787:PRO:HB3	22:W:822:HIS:CD2	2.50	0.46
1:0:176:MET:HG2	1:0:194:LEU:HD21	1.97	0.46
1:0:306:HIS:HB2	1:0:309:CYS:SG	2.55	0.46
6:A:173:MET:HA	6:A:173:MET:CE	2.45	0.46
8:D:90:HIS:HE1	12:I:105:PRO:C	2.24	0.46
10:G:89:PHE:CD1	10:G:89:PHE:C	2.93	0.46
15:N:398:GLU:O	15:N:402:ILE:HG12	2.16	0.46
1:0:281:CYS:HB2	1:0:306:HIS:ND1	2.31	0.46
4:3:173:MET:HE1	18:Q:369:TYR:HE2	1.80	0.46
6:A:67:LYS:HD2	6:A:80:ARG:HG3	1.97	0.46
15:N:223:LYS:CD	15:N:231:GLU:OE2	2.61	0.46
18:Q:537:VAL:HG22	18:Q:639:MET:HE3	1.98	0.46
22:W:895:ASP:HA	22:W:898:ASN:ND2	2.30	0.46
23:X:558:VAL:HG23	23:X:588:ILE:HD11	1.97	0.46
23:X:686:LYS:HZ3	23:X:688:PRO:HB2	1.81	0.46
6:A:175:LEU:N	6:A:175:LEU:HD23	2.30	0.46
6:A:363:PHE:HD2	6:A:425:VAL:HA	1.80	0.46
11:H:139:GLN:HE22	14:K:37:LYS:HD2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:240:ASP:N	15:N:241:PRO:CD	2.78	0.46
20:T:149:VAL:CG2	20:T:152:ASP:HB2	2.44	0.46
25:S:128:ARG:C	25:S:130:LEU:N	2.71	0.46
4:3:69:GLY:O	4:3:72:GLN:NE2	2.49	0.46
15:N:589:GLN:CB	22:W:25:MET:HE1	2.46	0.46
17:P:439:THR:OG1	17:P:490:ASP:OD2	2.33	0.46
23:X:639:SER:O	23:X:642:MET:HG3	2.16	0.46
11:H:14:ALA:O	11:H:18:GLN:HG2	2.16	0.46
15:N:212:LEU:CD1	15:N:367:SER:HA	2.43	0.46
15:N:377:PRO:HB2	15:N:408:ARG:NH2	2.31	0.46
16:O:681:GLU:OE2	16:O:768:SER:OG	2.34	0.46
18:Q:153:LEU:HD12	18:Q:156:ALA:HB3	1.97	0.46
18:Q:334:GLN:OE1	18:Q:340:GLN:HG3	2.16	0.46
19:R:99:HIS:CD2	19:R:187:LYS:HD3	2.51	0.46
22:W:642:HIS:CE1	22:W:817:ARG:HA	2.51	0.46
22:W:896:PHE:HD1	22:W:896:PHE:O	1.99	0.46
22:W:1009:LEU:HD23	22:W:1113:MET:HE3	1.97	0.46
24:d:928:LEU:CD2	24:d:929:PRO:CD	2.92	0.46
5:4:84:PHE:CB	15:N:178:ILE:HD11	2.46	0.46
10:G:142:GLN:O	10:G:146:ARG:CG	2.44	0.46
15:N:177:ILE:HG22	15:N:178:ILE:CD1	2.46	0.46
15:N:183:ILE:HD11	15:N:188:LYS:CD	2.45	0.46
18:Q:482:GLN:OE1	18:Q:482:GLN:HA	2.16	0.46
23:X:4:VAL:CG2	23:X:31:PHE:CE2	2.91	0.46
1:0:168:ARG:O	1:0:171:ARG:HG2	2.15	0.45
13:J:104:LYS:HZ1	26:U:52:GLU:CB	2.29	0.45
15:N:149:LEU:HD22	15:N:149:LEU:H	1.77	0.45
15:N:222:VAL:HB	15:N:234:LEU:HB2	1.97	0.45
17:P:373:ASP:OD1	17:P:374:THR:N	2.49	0.45
18:Q:394:HIS:NE2	19:R:78:ARG:CG	2.76	0.45
18:Q:430:LYS:O	18:Q:434:GLN:HG3	2.16	0.45
20:T:38:THR:HA	20:T:115:THR:HA	1.99	0.45
23:X:39:ILE:CD1	23:X:39:ILE:H	2.29	0.45
23:X:901:LEU:HD21	23:X:943:VAL:HB	1.98	0.45
24:d:933:LEU:HD23	24:d:935:GLU:H	1.81	0.45
1:0:238:VAL:HG23	1:0:295:THR:CG2	2.43	0.45
1:0:278:GLN:HE21	1:0:278:GLN:HB2	1.57	0.45
6:A:444:PRO:HA	6:A:450:PHE:HA	1.97	0.45
9:F:77:ILE:HG13	9:F:78:LEU:N	2.31	0.45
15:N:376:PRO:N	15:N:377:PRO:CD	2.79	0.45
15:N:691:LYS:C	15:N:691:LYS:CE	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:555:GLU:HA	23:X:558:VAL:HG12	1.97	0.45
6:A:259:ILE:HG22	6:A:303:PHE:HD1	1.82	0.45
10:G:47:ASN:N	10:G:47:ASN:HD22	2.14	0.45
10:G:57:ARG:CZ	10:G:125:GLU:HG3	2.47	0.45
14:K:62:GLU:O	14:K:66:GLN:HG2	2.16	0.45
15:N:676:ASP:CG	18:Q:593:MET:HE2	2.39	0.45
22:W:473:LYS:HA	22:W:476:LEU:HD12	1.97	0.45
23:X:765:VAL:HG21	23:X:808:ALA:HB1	1.98	0.45
9:F:109:PRO:O	11:H:76:ILE:HG22	2.16	0.45
11:H:52:LEU:HD23	11:H:52:LEU:O	2.15	0.45
15:N:183:ILE:HD12	15:N:188:LYS:CG	2.46	0.45
15:N:212:LEU:HD11	15:N:367:SER:OG	2.15	0.45
17:P:51:LEU:H	17:P:59:THR:HG22	1.81	0.45
22:W:904:VAL:HG12	22:W:997:PHE:HE2	1.81	0.45
24:d:946:GLY:HA2	26:U:57:LEU:CD2	2.47	0.45
26:U:1:MET:HG2	26:U:1:MET:O	2.16	0.45
14:K:55:SER:HA	14:K:58:HIS:HD1	1.82	0.45
15:N:114:LYS:CB	25:S:89:LEU:CD2	2.94	0.45
15:N:359:ILE:CG2	15:N:370:LEU:HD23	2.47	0.45
15:N:738:GLU:N	15:N:739:GLN:OE1	2.49	0.45
18:Q:150:LYS:O	18:Q:154:ALA:HB2	2.16	0.45
22:W:859:ILE:HG23	22:W:860:VAL:HG22	1.98	0.45
6:A:267:LYS:HZ3	6:A:288:PHE:HB2	1.81	0.45
9:F:98:TYR:HB3	9:F:105:ILE:HD11	1.99	0.45
15:N:312:THR:HG21	15:N:337:LEU:HD11	1.99	0.45
17:P:751:GLN:HG2	17:P:752:PHE:H	1.81	0.45
18:Q:144:LEU:HD23	18:Q:147:ILE:HG21	1.97	0.45
22:W:338:LEU:HD23	22:W:338:LEU:C	2.42	0.45
22:W:773:GLU:O	22:W:777:ILE:HG13	2.17	0.45
23:X:185:GLU:OE1	23:X:188:SER:OG	2.24	0.45
1:O:275:LYS:O	1:O:275:LYS:HD3	2.16	0.45
4:3:144:GLU:HA	4:3:147:LYS:HG2	1.98	0.45
6:A:174:TYR:CD1	6:A:174:TYR:O	2.70	0.45
8:D:95:VAL:HA	8:D:98:LYS:CD	2.47	0.45
8:D:95:VAL:HA	8:D:98:LYS:CE	2.47	0.45
9:F:77:ILE:HD11	11:H:81:LEU:CD1	2.46	0.45
13:J:99:ILE:HA	13:J:102:MET:HE2	1.99	0.45
20:T:194:MET:HE3	20:T:194:MET:HB3	1.83	0.45
22:W:642:HIS:HA	22:W:645:VAL:CG1	2.43	0.45
23:X:566:GLU:HG2	23:X:567:MET:N	2.30	0.45
4:3:163:LEU:HD11	21:V:123:ILE:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:108:PHE:HB2	6:A:127:HIS:ND1	2.32	0.45
10:G:60:GLU:CG	10:G:121:HIS:NE2	2.79	0.45
13:J:98:LYS:O	13:J:102:MET:HG2	2.16	0.45
15:N:736:THR:HG22	15:N:739:GLN:HE22	1.82	0.45
15:N:937:ARG:NH1	15:N:939:GLY:HA2	2.32	0.45
22:W:202:GLY:HA2	23:X:803:ASP:OD2	2.15	0.45
6:A:210:TYR:HB3	6:A:223:LYS:HB2	1.99	0.45
6:A:488:ILE:HG23	6:A:515:ALA:HB2	1.99	0.45
13:J:95:VAL:O	13:J:98:LYS:HG3	2.16	0.45
15:N:250:LEU:C	15:N:250:LEU:CD2	2.86	0.45
22:W:434:ARG:HD2	22:W:484:ASN:HD21	1.82	0.45
23:X:182:LYS:HA	23:X:189:TRP:NE1	2.32	0.45
24:d:916:MET:CE	24:d:917:PHE:H	2.26	0.45
24:d:932:LYS:NZ	24:d:935:GLU:CG	2.69	0.45
5:4:84:PHE:CE2	15:N:177:ILE:HD12	2.52	0.45
6:A:165:GLY:CA	6:A:170:LYS:CG	2.89	0.45
6:A:258:THR:HG23	6:A:260:GLU:OE2	2.17	0.45
6:A:278:HIS:CG	6:A:279:PRO:HD2	2.52	0.45
9:F:97:ASP:HB2	9:F:108:ALA:HB3	1.99	0.45
15:N:212:LEU:HD11	15:N:367:SER:O	2.16	0.45
15:N:219:ASN:O	15:N:221:ARG:HG3	2.17	0.45
17:P:207:CYS:HG	17:P:242:TYR:HE2	1.59	0.45
18:Q:620:GLY:H	18:Q:621:PRO:HD2	1.80	0.45
22:W:376:LEU:O	22:W:380:ILE:HG13	2.17	0.45
22:W:618:HIS:HA	22:W:621:VAL:HG12	1.98	0.45
23:X:915:ARG:NE	23:X:916:THR:H	2.14	0.45
26:U:109:TYR:HD1	26:U:112:ASP:HB3	1.82	0.45
6:A:69:LEU:CG	12:I:66:LEU:HD11	2.46	0.44
8:D:145:SER:H	18:Q:9:ILE:HD13	1.81	0.44
9:F:172:PHE:O	9:F:172:PHE:CG	2.71	0.44
15:N:669:GLN:HE22	15:N:683:ARG:HD3	1.82	0.44
18:Q:140:ASN:C	18:Q:143:THR:HG23	2.41	0.44
21:V:24:ASP:OD1	21:V:27:LYS:HE3	2.17	0.44
21:V:89:ASN:ND2	21:V:89:ASN:C	2.73	0.44
22:W:999:ASP:OD1	22:W:1000:ARG:N	2.50	0.44
23:X:601:SER:O	23:X:605:ILE:HG12	2.16	0.44
15:N:801:ARG:HG2	15:N:802:VAL:HG23	2.00	0.44
18:Q:256:TYR:CD1	18:Q:256:TYR:C	2.95	0.44
18:Q:537:VAL:HG21	18:Q:639:MET:HE3	1.98	0.44
18:Q:592:ILE:H	18:Q:592:ILE:HG12	1.63	0.44
24:d:933:LEU:HD12	26:U:7:GLN:HB2	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:135:LEU:C	10:G:135:LEU:CD2	2.91	0.44
15:N:170:PRO:HA	18:Q:20:HIS:O	2.17	0.44
15:N:399:LYS:CE	18:Q:271:LEU:CB	2.95	0.44
15:N:554:MET:HE3	15:N:554:MET:HB2	1.82	0.44
18:Q:42:ARG:HE	18:Q:42:ARG:C	2.25	0.44
23:X:137:ALA:O	23:X:140:GLU:HG2	2.17	0.44
10:G:154:GLN:OE1	10:G:154:GLN:HA	2.15	0.44
12:I:107:ILE:CD1	12:I:110:SER:HA	2.47	0.44
17:P:148:GLU:HB2	17:P:370:VAL:HG21	1.99	0.44
18:Q:105:ALA:O	18:Q:109:MET:HG3	2.18	0.44
22:W:630:LEU:C	22:W:630:LEU:CD2	2.85	0.44
23:X:568:LYS:NZ	23:X:572:MET:HG3	2.33	0.44
26:U:49:ASN:N	26:U:50:PRO:CD	2.79	0.44
6:A:70:LYS:HE2	6:A:79:ASP:HB3	2.00	0.44
8:D:27:ARG:HG3	12:I:103:THR:OG1	2.17	0.44
9:F:172:PHE:O	9:F:172:PHE:CD2	2.70	0.44
10:G:42:TYR:CD1	10:G:42:TYR:O	2.71	0.44
10:G:71:GLN:N	10:G:71:GLN:CD	2.73	0.44
10:G:86:LEU:HD13	10:G:90:LEU:HD23	1.99	0.44
10:G:148:GLU:C	10:G:148:GLU:CD	2.86	0.44
12:I:104:MET:N	12:I:105:PRO:CD	2.80	0.44
14:K:55:SER:HA	14:K:58:HIS:ND1	2.32	0.44
18:Q:156:ALA:O	18:Q:159:ILE:HG22	2.18	0.44
22:W:561:PRO:O	22:W:565:GLU:HG2	2.17	0.44
23:X:905:PHE:HA	23:X:908:ILE:HG22	1.98	0.44
8:D:73:ASP:HA	8:D:76:PHE:CE1	2.52	0.44
13:J:108:LEU:CD1	26:U:55:ALA:O	2.61	0.44
15:N:277:LEU:O	15:N:280:SER:HB2	2.18	0.44
17:P:21:TRP:HH2	17:P:452:LEU:HD12	1.82	0.44
22:W:12:VAL:HG22	22:W:40:CYS:SG	2.58	0.44
22:W:493:GLY:O	22:W:496:VAL:N	2.50	0.44
23:X:302:GLU:OE1	23:X:354:ARG:NH2	2.50	0.44
5:4:107:HIS:CE1	18:Q:26:GLY:HA2	2.51	0.44
6:A:361:MET:HE3	6:A:376:LEU:HD12	2.00	0.44
6:A:363:PHE:CD2	6:A:425:VAL:HA	2.53	0.44
9:F:94:PRO:CG	18:Q:130:VAL:HG11	2.45	0.44
10:G:114:LEU:HD23	10:G:114:LEU:O	2.18	0.44
15:N:660:GLU:OE1	15:N:760:ARG:HD2	2.17	0.44
18:Q:144:LEU:CD2	18:Q:147:ILE:HD13	2.45	0.44
22:W:862:LEU:CD2	22:W:896:PHE:CE2	3.01	0.44
1:0:240:GLN:O	1:0:243:THR:OG1	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:119:ARG:HA	2:1:122:LEU:HD12	1.98	0.44
4:3:70:THR:O	4:3:74:ARG:HG3	2.17	0.44
5:4:10:ASP:N	5:4:10:ASP:OD1	2.51	0.44
8:D:38:GLU:CD	8:D:38:GLU:C	2.86	0.44
15:N:545:LEU:CD1	15:N:652:MET:HB2	2.47	0.44
18:Q:264:GLN:OE1	18:Q:264:GLN:N	2.39	0.44
22:W:27:MET:CE	22:W:27:MET:CA	2.85	0.44
22:W:1279:LEU:HD22	22:W:1317:ILE:HG23	2.00	0.44
2:1:86:ASP:O	2:1:90:GLN:HG3	2.18	0.44
8:D:34:LEU:HA	8:D:37:LEU:CG	2.46	0.44
9:F:171:ILE:HD11	15:N:264:ALA:O	2.17	0.44
15:N:256:ASP:OD1	15:N:259:THR:HG22	2.17	0.44
15:N:517:SER:O	15:N:538:LEU:HD12	2.18	0.44
17:P:395:HIS:HB3	17:P:398:SER:O	2.18	0.44
18:Q:398:ALA:HA	18:Q:399:PRO:HD3	1.68	0.44
22:W:83:LEU:HD23	22:W:83:LEU:HA	1.84	0.44
22:W:627:LEU:CD2	22:W:648:THR:CG2	2.96	0.44
22:W:684:ASN:HB2	22:W:719:ILE:HG23	1.99	0.44
22:W:787:PRO:HG2	22:W:825:THR:HG21	2.00	0.44
22:W:892:LYS:HB3	22:W:893:PRO:HD3	2.00	0.44
22:W:1064:ASP:OD1	22:W:1064:ASP:N	2.48	0.44
23:X:198:LYS:O	23:X:201:GLU:HG3	2.18	0.44
24:d:938:ILE:O	24:d:941:GLN:NE2	2.51	0.44
10:G:57:ARG:CG	10:G:57:ARG:NH1	2.72	0.43
10:G:78:LEU:HD23	10:G:78:LEU:O	2.17	0.43
13:J:113:LEU:CD2	26:U:63:ALA:HA	2.48	0.43
15:N:230:PHE:N	15:N:230:PHE:CD1	2.86	0.43
15:N:687:ILE:CD1	15:N:705:LEU:HD11	2.45	0.43
17:P:823:TRP:HZ3	17:P:828:LEU:HG	1.83	0.43
18:Q:156:ALA:O	18:Q:160:LEU:HG	2.17	0.43
18:Q:550:SER:HB3	18:Q:570:THR:HG22	2.00	0.43
22:W:369:ARG:HD2	22:W:403:TYR:CZ	2.53	0.43
22:W:896:PHE:CD1	22:W:896:PHE:O	2.70	0.43
24:d:923:LEU:HD23	24:d:923:LEU:N	2.12	0.43
24:d:924:PRO:CA	24:d:927:TYR:CE2	2.99	0.43
2:1:143:LEU:HD11	14:K:97:VAL:CG1	2.45	0.43
9:F:188:PHE:CD2	15:N:295:CYS:SG	2.91	0.43
15:N:468:TYR:CD1	18:Q:516:TYR:HE2	2.36	0.43
15:N:545:LEU:HD11	15:N:652:MET:CB	2.46	0.43
17:P:710:ASP:OD1	17:P:710:ASP:N	2.51	0.43
18:Q:103:ARG:O	18:Q:107:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:414:ASP:O	18:Q:418:ILE:HG12	2.18	0.43
22:W:847:ILE:HG12	22:W:888:LEU:HB3	1.99	0.43
22:W:853:MET:O	22:W:859:ILE:HG22	2.18	0.43
22:W:1082:LYS:HD3	22:W:1082:LYS:HA	1.87	0.43
23:X:905:PHE:O	23:X:908:ILE:HG22	2.18	0.43
23:X:977:LEU:HD12	23:X:980:GLN:HE21	1.83	0.43
26:U:49:ASN:CG	26:U:50:PRO:CD	2.87	0.43
26:U:80:GLU:C	26:U:80:GLU:CD	2.86	0.43
10:G:134:THR:HA	24:d:928:LEU:HD21	2.00	0.43
12:I:123:GLU:HA	12:I:126:ARG:HG2	2.00	0.43
17:P:684:ASP:HB3	17:P:687:SER:HB3	1.99	0.43
20:T:63:MET:HG3	20:T:79:PHE:CE1	2.53	0.43
22:W:726:ASN:ND2	22:W:748:VAL:O	2.51	0.43
22:W:1068:TYR:O	22:W:1072:ILE:HG12	2.19	0.43
15:N:297:HIS:O	15:N:300:CYS:HB2	2.18	0.43
15:N:821:SER:O	15:N:833:ILE:HA	2.17	0.43
18:Q:443:ARG:O	18:Q:447:THR:HG23	2.18	0.43
22:W:369:ARG:HD2	22:W:403:TYR:CE2	2.53	0.43
22:W:662:GLN:HG2	22:W:711:TRP:CZ2	2.53	0.43
23:X:47:LEU:HD12	23:X:81:ALA:HB1	1.99	0.43
23:X:262:SER:HA	23:X:265:GLU:HG2	1.99	0.43
23:X:798:TRP:CD1	23:X:919:PRO:HD2	2.54	0.43
24:d:938:ILE:O	24:d:941:GLN:CD	2.62	0.43
11:H:103:GLU:N	11:H:103:GLU:OE2	2.51	0.43
13:J:65:LEU:O	13:J:68:PHE:N	2.52	0.43
15:N:336:SER:HB2	15:N:358:THR:HG22	2.00	0.43
18:Q:595:GLN:OE1	18:Q:619:ARG:HD2	2.18	0.43
22:W:892:LYS:N	22:W:893:PRO:HD3	2.33	0.43
23:X:167:LYS:HA	23:X:167:LYS:HD2	1.75	0.43
9:F:82:ARG:NH2	9:F:94:PRO:HB2	2.33	0.43
10:G:89:PHE:CE2	26:U:19:PHE:CG	2.91	0.43
15:N:155:PRO:HA	15:N:158:ILE:HG22	1.99	0.43
15:N:178:ILE:CG2	15:N:179:PRO:HD2	2.49	0.43
15:N:183:ILE:HB	15:N:187:GLU:CG	2.49	0.43
15:N:1217:ARG:O	15:N:1221:GLN:HG2	2.19	0.43
17:P:576:PRO:HA	17:P:579:ARG:HG2	2.00	0.43
23:X:4:VAL:CG2	23:X:31:PHE:CD1	2.95	0.43
23:X:196:LEU:HD11	23:X:223:ARG:HH11	1.84	0.43
6:A:69:LEU:CD2	12:I:66:LEU:HD11	2.48	0.43
10:G:57:ARG:NE	10:G:125:GLU:HA	2.33	0.43
11:H:139:GLN:NE2	14:K:37:LYS:HD2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:86:ASP:OD1	12:I:86:ASP:N	2.49	0.43
13:J:85:LEU:HD13	25:S:93:TYR:CB	2.47	0.43
17:P:593:ASP:OD1	17:P:594:LYS:N	2.51	0.43
17:P:732:LEU:HB3	17:P:733:PRO:HD3	1.99	0.43
18:Q:456:GLU:OE1	18:Q:456:GLU:N	2.52	0.43
23:X:65:LYS:HG2	23:X:103:MET:HE1	2.00	0.43
15:N:1202:TYR:HD2	15:N:1292:PRO:HG2	1.83	0.43
18:Q:162:LYS:HA	18:Q:165:GLU:HG3	2.00	0.43
22:W:51:LEU:HD12	22:W:51:LEU:HA	1.90	0.43
23:X:336:CYS:O	23:X:339:GLU:HG3	2.18	0.43
23:X:345:THR:OG1	23:X:346:PRO:HD3	2.19	0.43
23:X:660:ASN:O	23:X:664:VAL:HG23	2.19	0.43
2:1:97:GLN:HG2	4:3:111:VAL:HG11	2.01	0.43
15:N:245:TRP:HB2	15:N:282:LEU:CG	2.45	0.43
22:W:16:GLU:HB3	22:W:19:GLU:HG3	2.00	0.43
22:W:622:GLN:O	22:W:626:HIS:ND1	2.43	0.43
5:4:68:LYS:HB2	8:D:154:ARG:HH12	1.84	0.43
6:A:90:LEU:HD11	6:A:102:TYR:HB3	2.01	0.43
6:A:179:SER:OG	6:A:270:ILE:O	2.29	0.43
6:A:203:ILE:HG12	6:A:210:TYR:HB2	2.00	0.43
11:H:49:PHE:HD2	21:V:59:TYR:OH	2.02	0.43
15:N:208:LEU:C	15:N:208:LEU:CD1	2.85	0.43
15:N:376:PRO:CB	15:N:377:PRO:CD	2.92	0.43
15:N:464:GLN:OE1	18:Q:323:PRO:HD3	2.19	0.43
17:P:696:LEU:HD13	17:P:713:LEU:HD21	2.01	0.43
18:Q:16:GLU:HB3	24:d:921:LYS:HB3	2.01	0.43
22:W:850:LEU:HD21	22:W:889:LEU:HD22	2.01	0.43
23:X:140:GLU:HB2	23:X:143:ARG:HH22	1.84	0.43
6:A:69:LEU:HB3	12:I:66:LEU:CD1	2.49	0.42
9:F:101:ILE:HD12	11:H:105:VAL:CG1	2.39	0.42
11:H:51:LEU:C	11:H:51:LEU:HD12	2.44	0.42
17:P:149:LYS:HD2	17:P:157:GLU:HG3	2.00	0.42
22:W:894:ASN:HA	22:W:897:ARG:HH21	1.84	0.42
24:d:946:GLY:HA2	26:U:57:LEU:HD21	2.00	0.42
9:F:74:GLN:NE2	9:F:78:LEU:H	2.08	0.42
13:J:108:LEU:HD11	26:U:55:ALA:CB	2.50	0.42
15:N:188:LYS:CE	18:Q:47:ILE:CD1	2.90	0.42
15:N:222:VAL:CG1	15:N:224:PHE:HB2	2.49	0.42
18:Q:46:ARG:HG3	18:Q:46:ARG:NH1	2.21	0.42
22:W:401:LEU:O	22:W:401:LEU:HD12	2.19	0.42
22:W:712:CYS:O	22:W:716:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:d:938:ILE:HA	24:d:941:GLN:NE2	2.33	0.42
1:0:104:TYR:O	1:0:107:LEU:HB3	2.20	0.42
1:0:245:HIS:HD2	1:0:295:THR:O	2.01	0.42
6:A:62:LEU:CD2	8:D:66:LEU:CD1	2.97	0.42
9:F:174:ARG:HH21	15:N:267:HIS:N	2.17	0.42
10:G:74:HIS:ND1	10:G:122:LEU:CD1	2.73	0.42
13:J:63:VAL:HG12	15:N:105:TRP:HZ3	1.83	0.42
14:K:70:LEU:HD23	14:K:70:LEU:HA	1.84	0.42
23:X:586:LEU:HD12	23:X:623:TRP:CZ2	2.54	0.42
4:3:47:ARG:O	4:3:51:ILE:HG12	2.19	0.42
6:A:492:ASP:OD1	6:A:493:PHE:N	2.52	0.42
15:N:229:GLU:CG	15:N:300:CYS:HB3	2.49	0.42
15:N:328:ARG:HD2	15:N:330:HIS:CE1	2.55	0.42
15:N:376:PRO:HG2	15:N:377:PRO:HD2	1.72	0.42
15:N:861:LYS:HG2	15:N:862:THR:HG23	2.00	0.42
16:O:679:GLN:HG2	18:Q:609:VAL:HG12	2.01	0.42
17:P:49:MET:SD	17:P:450:GLY:HA2	2.60	0.42
18:Q:139:GLN:HB3	18:Q:142:GLN:OE1	2.20	0.42
22:W:547:VAL:HG12	22:W:559:LEU:HD11	2.01	0.42
22:W:977:LEU:HG	22:W:979:PRO:HD2	2.02	0.42
1:0:218:ASN:ND2	20:T:148:VAL:HG12	2.35	0.42
6:A:321:LEU:HD22	6:A:329:LEU:HD12	2.02	0.42
10:G:127:ARG:HG3	10:G:130:GLN:OE1	2.19	0.42
15:N:497:LYS:NZ	15:N:556:GLU:OE1	2.49	0.42
24:d:933:LEU:HA	24:d:934:PRO:HD2	1.70	0.42
26:U:89:SER:HA	26:U:92:LYS:CE	2.48	0.42
4:3:160:MET:HE1	21:V:134:TYR:HB3	2.00	0.42
5:4:114:ARG:HE	5:4:114:ARG:HB3	1.62	0.42
6:A:106:ASP:HB3	6:A:128:HIS:HD2	1.85	0.42
14:K:14:LEU:HA	14:K:17:ILE:HD12	2.00	0.42
18:Q:579:ALA:HB2	18:Q:619:ARG:NH1	2.33	0.42
5:4:58:TRP:CE3	5:4:63:TYR:HB3	2.54	0.42
10:G:78:LEU:HD11	26:U:73:ILE:HG22	2.01	0.42
11:H:153:LYS:HE3	11:H:153:LYS:HB3	1.77	0.42
13:J:99:ILE:HG12	13:J:102:MET:HE2	2.02	0.42
14:K:95:LYS:HE2	14:K:95:LYS:HB3	1.68	0.42
17:P:718:CYS:O	17:P:721:PRO:HD2	2.20	0.42
17:P:744:PRO:O	17:P:746:GLN:HG2	2.20	0.42
18:Q:140:ASN:N	18:Q:141:PRO:HD2	2.34	0.42
22:W:543:ILE:HD12	22:W:563:LEU:HD11	2.02	0.42
14:K:42:GLU:HB2	14:K:43:ARG:HH21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:469:LEU:O	17:P:473:HIS:ND1	2.36	0.42
17:P:579:ARG:O	17:P:582:GLU:HG3	2.19	0.42
18:Q:150:LYS:O	18:Q:154:ALA:CB	2.68	0.42
18:Q:374:ASN:O	18:Q:378:LEU:HD23	2.19	0.42
18:Q:405:MET:HE3	18:Q:405:MET:HB3	1.75	0.42
21:V:34:THR:O	21:V:38:LYS:HG2	2.20	0.42
23:X:96:ALA:O	23:X:100:ILE:HG12	2.20	0.42
12:I:104:MET:HB2	12:I:105:PRO:HD3	2.01	0.42
15:N:118:ILE:HD11	25:S:83:LEU:HB3	2.01	0.42
17:P:207:CYS:SG	17:P:242:TYR:CE2	3.11	0.42
18:Q:205:GLY:O	18:Q:221:THR:HA	2.18	0.42
22:W:869:LEU:HD23	22:W:869:LEU:HA	1.90	0.42
1:O:257:GLN:NE2	1:O:258:MET:HE2	2.34	0.42
2:1:44:LEU:HA	2:1:47:GLU:OE2	2.19	0.42
9:F:111:LEU:HD12	9:F:111:LEU:HA	1.94	0.42
10:G:114:LEU:C	10:G:114:LEU:CD2	2.86	0.42
11:H:67:LYS:O	11:H:67:LYS:HD3	2.20	0.42
12:I:109:LEU:HD21	12:I:113:GLN:NE2	2.34	0.42
15:N:82:LYS:HD3	15:N:82:LYS:HA	1.78	0.42
15:N:223:LYS:HG3	15:N:223:LYS:O	2.20	0.42
15:N:247:LEU:HD12	15:N:247:LEU:N	2.34	0.42
15:N:397:ILE:HG13	15:N:398:GLU:N	2.35	0.42
15:N:513:PRO:O	15:N:543:THR:HG22	2.20	0.42
22:W:5:LEU:HD23	22:W:5:LEU:HA	1.95	0.42
23:X:4:VAL:HG12	23:X:31:PHE:N	2.35	0.42
23:X:6:LEU:CD1	23:X:40:LEU:O	2.53	0.42
23:X:309:THR:HG23	23:X:310:PHE:HD1	1.85	0.42
23:X:561:LEU:HD13	23:X:609:ILE:HD11	2.01	0.42
24:d:928:LEU:CD2	24:d:929:PRO:HD2	2.49	0.42
6:A:99:THR:HA	6:A:111:GLU:O	2.20	0.41
6:A:167:ASN:O	6:A:171:THR:HG21	2.18	0.41
6:A:200:LEU:HD21	6:A:243:HIS:ND1	2.35	0.41
12:I:94:PHE:HA	12:I:97:MET:HG3	2.01	0.41
12:I:97:MET:SD	12:I:98:ARG:HD3	2.59	0.41
15:N:545:LEU:N	15:N:545:LEU:CD2	2.73	0.41
17:P:559:THR:O	17:P:563:LEU:HB2	2.20	0.41
18:Q:18:GLN:O	18:Q:30:TYR:HE2	1.98	0.41
19:R:145:VAL:HG22	19:R:169:VAL:HG22	2.01	0.41
22:W:4:GLN:HB3	22:W:47:PHE:HE2	1.85	0.41
22:W:775:ASP:OD1	22:W:776:ILE:N	2.52	0.41
22:W:1268:ILE:HG23	22:W:1310:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:113:LYS:N	23:X:116:GLU:OE1	2.52	0.41
2:1:133:LEU:HB2	14:K:111:CYS:SG	2.60	0.41
3:2:55:ASP:HA	3:2:58:GLN:HE21	1.85	0.41
8:D:150:LYS:HD2	10:G:56:ILE:HB	2.01	0.41
9:F:83:LYS:HE2	9:F:96:ALA:H	1.85	0.41
9:F:116:ASN:CG	21:V:49:SER:HB3	2.45	0.41
9:F:185:ARG:C	9:F:185:ARG:CD	2.86	0.41
15:N:248:LEU:HD12	15:N:248:LEU:N	2.35	0.41
17:P:357:PRO:HD3	17:P:382:LEU:HD23	2.02	0.41
19:R:188:ASN:O	19:R:192:GLN:HG2	2.21	0.41
22:W:517:SER:HB2	22:W:560:ALA:HB2	2.01	0.41
22:W:592:VAL:O	22:W:595:SER:OG	2.36	0.41
22:W:885:ILE:HD13	22:W:885:ILE:HA	1.82	0.41
1:0:79:LYS:HG2	3:2:57:VAL:HG21	2.02	0.41
15:N:157:ALA:O	15:N:161:LEU:HB2	2.19	0.41
15:N:197:GLN:OE1	15:N:197:GLN:HA	2.20	0.41
17:P:216:ALA:HA	17:P:229:ALA:O	2.20	0.41
18:Q:273:THR:HG22	18:Q:274:VAL:H	1.85	0.41
22:W:59:CYS:SG	22:W:60:ILE:N	2.94	0.41
23:X:160:MET:N	23:X:160:MET:SD	2.94	0.41
23:X:725:ASP:OD1	23:X:726:SER:N	2.50	0.41
23:X:921:THR:HA	23:X:924:VAL:HG22	2.01	0.41
1:0:200:VAL:HG22	1:0:214:VAL:HG12	2.02	0.41
2:1:71:GLU:O	2:1:74:ARG:HG2	2.20	0.41
6:A:497:VAL:HA	6:A:500:ARG:HG2	2.02	0.41
10:G:132:ARG:HD2	10:G:132:ARG:HA	1.74	0.41
15:N:198:ILE:HG21	15:N:239:ASP:HA	2.02	0.41
15:N:693:ILE:HD11	15:N:697:THR:CG2	2.47	0.41
18:Q:475:VAL:CG2	18:Q:495:LEU:HB2	2.50	0.41
20:T:157:LEU:HD23	20:T:157:LEU:HA	1.93	0.41
22:W:2:GLU:OE2	22:W:62:TRP:NE1	2.53	0.41
22:W:539:LEU:O	22:W:543:ILE:HG12	2.21	0.41
4:3:38:GLN:OE1	4:3:42:GLN:NE2	2.54	0.41
6:A:311:ILE:HD13	6:A:311:ILE:HA	1.96	0.41
10:G:109:LEU:HA	10:G:112:LEU:HD12	2.03	0.41
12:I:110:SER:CB	12:I:111:PRO:HD2	2.38	0.41
13:J:103:LYS:HB3	13:J:103:LYS:HE3	1.81	0.41
15:N:177:ILE:HG22	15:N:178:ILE:HD13	2.02	0.41
15:N:723:GLU:HG3	15:N:746:TYR:CD1	2.56	0.41
17:P:614:LEU:O	17:P:618:LEU:HG	2.21	0.41
17:P:618:LEU:HD22	17:P:662:ILE:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:388:SER:OG	18:Q:390:ILE:HG12	2.19	0.41
19:R:205:LYS:O	19:R:206:ARG:HD3	2.21	0.41
21:V:128:TYR:C	21:V:128:TYR:CD1	2.98	0.41
22:W:313:GLU:O	22:W:317:THR:HG23	2.21	0.41
26:U:15:LEU:HA	26:U:18:GLN:HG3	2.02	0.41
5:4:97:ILE:O	5:4:101:GLN:NE2	2.35	0.41
6:A:70:LYS:HA	12:I:70:HIS:NE2	2.35	0.41
6:A:354:PRO:HG2	6:A:355:ILE:HD12	2.02	0.41
8:D:135:ILE:O	8:D:139:ARG:HG2	2.20	0.41
10:G:15:MET:HE3	10:G:15:MET:HB3	1.97	0.41
10:G:129:HIS:HD2	26:U:82:THR:OG1	2.00	0.41
11:H:93:THR:HG21	11:H:97:VAL:HG21	2.02	0.41
12:I:109:LEU:HD21	12:I:113:GLN:HE21	1.86	0.41
15:N:254:VAL:HG21	15:N:303:LEU:HD23	2.03	0.41
17:P:207:CYS:SG	17:P:242:TYR:HE2	2.43	0.41
17:P:376:PHE:HD1	17:P:473:HIS:CD2	2.38	0.41
22:W:284:CYS:HB2	22:W:289:LEU:HB2	2.02	0.41
22:W:795:LYS:HA	22:W:798:LEU:HD22	2.02	0.41
23:X:46:LEU:HD22	23:X:60:ILE:HD12	2.02	0.41
23:X:214:GLN:HA	23:X:217:GLN:HG3	2.01	0.41
1:0:214:VAL:HG21	1:0:242:VAL:HG13	2.02	0.41
5:4:107:HIS:NE2	18:Q:28:GLU:OE2	2.43	0.41
6:A:79:ASP:O	6:A:82:GLU:HG2	2.21	0.41
10:G:78:LEU:CD2	26:U:73:ILE:CG2	2.86	0.41
11:H:177:ASP:OD2	19:R:166:SER:OG	2.31	0.41
15:N:188:LYS:HE3	18:Q:47:ILE:HD11	1.97	0.41
15:N:222:VAL:CG2	15:N:234:LEU:HB2	2.50	0.41
15:N:737:ARG:HD3	15:N:737:ARG:HA	1.81	0.41
15:N:882:ILE:HD12	15:N:916:LEU:HD11	2.02	0.41
17:P:24:TRP:CE3	17:P:51:LEU:HD21	2.55	0.41
20:T:175:VAL:HG11	20:T:188:ASP:HB3	2.02	0.41
22:W:598:TRP:HA	22:W:601:LEU:HB3	2.02	0.41
22:W:1189:ARG:HE	22:W:1189:ARG:HB2	1.59	0.41
23:X:343:LYS:HA	23:X:343:LYS:HD3	1.86	0.41
23:X:955:LEU:HA	23:X:958:VAL:HG22	2.03	0.41
1:0:177:SER:HB3	1:0:193:THR:CG2	2.50	0.41
1:0:284:CYS:SG	1:0:306:HIS:CE1	3.14	0.41
6:A:469:VAL:HA	6:A:475:VAL:HG22	2.01	0.41
10:G:16:GLN:NE2	10:G:17:TYR:O	2.54	0.41
11:H:6:LYS:HA	11:H:6:LYS:HD3	1.89	0.41
15:N:183:ILE:CD1	15:N:188:LYS:CG	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:375:ASP:N	15:N:376:PRO:HD2	2.35	0.41
17:P:393:ILE:HB	17:P:403:ALA:HB3	2.03	0.41
17:P:523:SER:O	17:P:526:ILE:HG22	2.21	0.41
18:Q:116:LEU:HA	18:Q:119:VAL:HB	2.01	0.41
18:Q:271:LEU:C	18:Q:271:LEU:CD1	2.86	0.41
20:T:8:GLN:HE22	20:T:203:GLN:NE2	2.18	0.41
24:d:933:LEU:HD13	26:U:7:GLN:HG2	2.02	0.41
26:U:8:LEU:HD12	26:U:72:LEU:HD12	2.02	0.41
1:0:194:LEU:HD23	1:0:194:LEU:HA	1.85	0.41
3:2:163:VAL:O	3:2:167:GLN:HG3	2.20	0.41
4:3:177:ARG:NE	21:V:113:ASP:OD2	2.53	0.41
5:4:17:ARG:HA	5:4:20:LEU:HG	2.03	0.41
8:D:165:LEU:HG	8:D:166:THR:HG23	2.03	0.41
9:F:41:TYR:CD1	9:F:68:TYR:HE2	2.39	0.41
10:G:57:ARG:NE	10:G:128:PRO:HG2	2.33	0.41
10:G:78:LEU:CD2	10:G:78:LEU:C	2.86	0.41
10:G:78:LEU:HD21	26:U:73:ILE:CG2	2.48	0.41
10:G:127:ARG:CG	15:N:152:PHE:CZ	3.01	0.41
15:N:149:LEU:N	15:N:149:LEU:CD2	2.73	0.41
15:N:229:GLU:H	15:N:229:GLU:HG2	1.65	0.41
15:N:315:LEU:HD11	15:N:320:TRP:CB	2.47	0.41
15:N:691:LYS:CE	15:N:693:ILE:HG12	2.51	0.41
15:N:693:ILE:CD1	15:N:697:THR:CB	2.75	0.41
15:N:1355:PRO:O	15:N:1364:LEU:CB	2.69	0.41
18:Q:15:CYS:O	18:Q:15:CYS:SG	2.79	0.41
18:Q:392:MET:HA	18:Q:393:PRO:HD3	1.95	0.41
22:W:911:HIS:HA	22:W:914:GLN:HE21	1.85	0.41
22:W:915:ASN:OD1	22:W:915:ASN:N	2.53	0.41
23:X:4:VAL:HG11	23:X:31:PHE:HD1	1.71	0.41
23:X:131:LEU:HD23	23:X:131:LEU:HA	1.95	0.41
23:X:208:ASN:HB3	23:X:211:LEU:HB3	2.03	0.41
23:X:250:LEU:HD12	23:X:729:ILE:HD12	2.02	0.41
26:U:113:MET:HA	26:U:116:GLU:HG2	2.03	0.41
26:U:119:GLN:HA	26:U:122:LEU:HG	2.03	0.41
4:3:176:MET:O	4:3:176:MET:HG2	2.21	0.41
6:A:173:MET:HE3	6:A:176:ALA:HB3	2.02	0.41
9:F:118:ARG:HB3	18:Q:112:LEU:HD22	2.02	0.41
14:K:11:LEU:O	14:K:14:LEU:HG	2.21	0.41
15:N:135:ARG:NE	15:N:135:ARG:CA	2.73	0.41
15:N:229:GLU:HG3	15:N:300:CYS:HB3	2.01	0.41
15:N:538:LEU:HB3	15:N:552:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:56:GLN:O	17:P:59:THR:OG1	2.36	0.41
18:Q:140:ASN:O	18:Q:143:THR:HG23	2.21	0.41
18:Q:481:SER:HB3	18:Q:636:VAL:HG11	2.03	0.41
23:X:82:ILE:HG23	23:X:97:LEU:HD13	2.02	0.41
23:X:447:SER:O	23:X:451:LEU:HG	2.21	0.41
2:1:129:VAL:HG22	14:K:115:LEU:HD21	2.03	0.40
10:G:62:GLN:HG2	10:G:62:GLN:O	2.21	0.40
14:K:90:CYS:O	14:K:94:LEU:HD23	2.20	0.40
15:N:252:ILE:CG2	15:N:254:VAL:HG22	2.51	0.40
17:P:751:GLN:HG2	17:P:752:PHE:N	2.37	0.40
18:Q:295:LEU:HD23	18:Q:295:LEU:HA	1.86	0.40
21:V:38:LYS:HA	21:V:41:LYS:NZ	2.29	0.40
22:W:863:ASP:OD1	22:W:864:ARG:N	2.54	0.40
22:W:1125:ALA:O	22:W:1129:VAL:HG23	2.21	0.40
23:X:914:SER:OG	23:X:915:ARG:N	2.54	0.40
1:0:72:ARG:HH12	1:0:76:LEU:HB2	1.87	0.40
1:0:282:GLN:HB2	1:0:305:PHE:CE1	2.55	0.40
3:2:86:THR:HG21	16:O:628:ASN:ND2	2.29	0.40
5:4:84:PHE:CE2	15:N:177:ILE:CG2	2.97	0.40
8:D:30:LEU:CD2	8:D:34:LEU:CG	2.99	0.40
9:F:8:ASP:N	9:F:8:ASP:OD1	2.53	0.40
9:F:59:HIS:ND1	9:F:62:GLN:OE1	2.54	0.40
9:F:66:ILE:HA	9:F:84:GLN:O	2.21	0.40
10:G:68:HIS:CG	10:G:69:PRO:HD3	2.56	0.40
10:G:157:LEU:HD21	26:U:110:ARG:NH1	2.32	0.40
13:J:108:LEU:HD13	26:U:56:GLN:HA	2.04	0.40
15:N:753:LEU:HA	15:N:753:LEU:HD23	1.83	0.40
18:Q:138:LYS:HG2	18:Q:139:GLN:N	2.36	0.40
22:W:161:LEU:O	22:W:165:GLU:HG2	2.20	0.40
22:W:305:VAL:HA	22:W:308:VAL:HG12	2.03	0.40
22:W:363:ARG:HG3	22:W:365:LEU:HG	2.04	0.40
23:X:320:LEU:HD23	23:X:320:LEU:HA	1.92	0.40
23:X:566:GLU:C	23:X:568:LYS:H	2.30	0.40
24:d:923:LEU:HG	24:d:924:PRO:HD3	0.60	0.40
26:U:58:PHE:N	26:U:58:PHE:CD1	2.89	0.40
1:0:46:GLU:OE1	1:0:46:GLU:HA	2.22	0.40
1:0:162:VAL:HG13	1:0:207:LEU:HD12	2.03	0.40
4:3:37:GLY:O	4:3:41:VAL:HG23	2.22	0.40
4:3:77:LYS:HB2	4:3:77:LYS:HE3	1.91	0.40
10:G:54:LEU:HD11	10:G:59:LEU:HD23	2.03	0.40
11:H:49:PHE:CD2	21:V:59:TYR:OH	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:53:SER:O	11:H:57:ASN:CB	2.65	0.40
14:K:80:GLU:HA	18:Q:195:LYS:HE2	2.03	0.40
15:N:723:GLU:HG3	15:N:746:TYR:CE1	2.56	0.40
17:P:26:LYS:HD2	17:P:26:LYS:HA	1.86	0.40
18:Q:399:PRO:O	18:Q:406:ARG:NH2	2.54	0.40
20:T:97:LYS:HA	20:T:97:LYS:HD3	1.86	0.40
22:W:914:GLN:HE22	22:W:917:TRP:HB2	1.86	0.40
23:X:920:HIS:O	23:X:924:VAL:HG13	2.21	0.40
8:D:139:ARG:HA	8:D:139:ARG:HD3	1.95	0.40
15:N:240:ASP:HB2	15:N:241:PRO:HD3	2.04	0.40
15:N:315:LEU:HD12	15:N:315:LEU:O	2.21	0.40
16:O:744:ASP:CG	16:O:745:ALA:H	2.29	0.40
21:V:127:LEU:O	21:V:131:GLU:HG3	2.20	0.40
23:X:385:ARG:HA	23:X:385:ARG:HD2	1.95	0.40
12:I:91:LYS:HA	12:I:94:PHE:HB2	2.03	0.40
15:N:780:VAL:HG11	15:N:803:TYR:CZ	2.56	0.40
17:P:270:ASP:O	17:P:271:LEU:HG	2.21	0.40
18:Q:414:ASP:OD1	18:Q:414:ASP:N	2.55	0.40
22:W:649:ALA:O	22:W:653:ILE:HG13	2.20	0.40
22:W:764:TYR:CD1	22:W:792:LEU:HD13	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	261/311 (84%)	254 (97%)	7 (3%)	0	100	100
2	1	95/178 (53%)	95 (100%)	0	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	4	104/131 (79%)	100 (96%)	4 (4%)	0	100	100
6	A	455/1581 (29%)	435 (96%)	19 (4%)	1 (0%)	43	72
8	D	154/270 (57%)	149 (97%)	5 (3%)	0	100	100
9	F	163/246 (66%)	145 (89%)	18 (11%)	0	100	100
10	G	157/233 (67%)	153 (98%)	4 (2%)	0	100	100
11	H	177/268 (66%)	160 (90%)	17 (10%)	0	100	100
12	I	69/146 (47%)	67 (97%)	2 (3%)	0	100	100
13	J	120/135 (89%)	116 (97%)	4 (3%)	0	100	100
14	K	110/117 (94%)	104 (94%)	6 (6%)	0	100	100
15	N	995/1454 (68%)	925 (93%)	66 (7%)	4 (0%)	30	60
16	O	153/788 (19%)	142 (93%)	11 (7%)	0	100	100
17	P	743/877 (85%)	695 (94%)	48 (6%)	0	100	100
18	Q	544/651 (84%)	496 (91%)	46 (8%)	2 (0%)	30	60
19	R	189/208 (91%)	181 (96%)	8 (4%)	0	100	100
20	T	189/212 (89%)	173 (92%)	16 (8%)	0	100	100
21	V	128/200 (64%)	126 (98%)	2 (2%)	0	100	100
22	W	1332/1368 (97%)	1277 (96%)	55 (4%)	0	100	100
23	X	877/989 (89%)	844 (96%)	33 (4%)	0	100	100
24	d	35/2174 (2%)	27 (77%)	6 (17%)	2 (6%)	1	15
25	S	66/244 (27%)	63 (96%)	3 (4%)	0	100	100
26	U	112/144 (78%)	107 (96%)	5 (4%)	0	100	100
All	All	7453/13303 (56%)	7053 (95%)	391 (5%)	9 (0%)	49	78

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	N	1355	PRO
18	Q	34	LEU
24	d	928	LEU
15	N	209	PRO
24	d	934	PRO
6	A	208	VAL
15	N	378	LEU
15	N	756	PRO
18	Q	393	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	241/280 (86%)	239 (99%)	2 (1%)	73	76
2	1	94/152 (62%)	93 (99%)	1 (1%)	65	73
3	2	102/163 (63%)	102 (100%)	0	100	100
4	3	116/155 (75%)	112 (97%)	4 (3%)	32	55
5	4	97/115 (84%)	97 (100%)	0	100	100
6	A	394/1391 (28%)	388 (98%)	6 (2%)	57	68
8	D	138/230 (60%)	132 (96%)	6 (4%)	26	50
9	F	151/223 (68%)	148 (98%)	3 (2%)	48	64
10	G	139/216 (64%)	127 (91%)	12 (9%)	10	34
11	H	161/225 (72%)	160 (99%)	1 (1%)	78	79
12	I	71/133 (53%)	68 (96%)	3 (4%)	26	51
13	J	65/124 (52%)	65 (100%)	0	100	100
14	K	94/98 (96%)	93 (99%)	1 (1%)	65	73
15	N	809/1271 (64%)	791 (98%)	18 (2%)	45	63
16	O	141/697 (20%)	141 (100%)	0	100	100
17	P	670/766 (88%)	669 (100%)	1 (0%)	88	88
18	Q	496/577 (86%)	481 (97%)	15 (3%)	36	57
19	R	169/183 (92%)	169 (100%)	0	100	100
20	T	166/178 (93%)	165 (99%)	1 (1%)	78	79
21	V	122/173 (70%)	121 (99%)	1 (1%)	73	76
22	W	1203/1232 (98%)	1192 (99%)	11 (1%)	70	75
23	X	789/864 (91%)	785 (100%)	4 (0%)	81	80
24	d	34/1918 (2%)	33 (97%)	1 (3%)	37	57
25	S	24/208 (12%)	24 (100%)	0	100	100
26	U	91/119 (76%)	87 (96%)	4 (4%)	25	50
All	All	6577/11691 (56%)	6482 (99%)	95 (1%)	57	70

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	278	GLN
1	0	295	THR
2	1	49	GLU
4	3	138	GLU
4	3	140	ARG
4	3	142	ILE
4	3	149	LEU
6	A	161	TYR
6	A	170	LYS
6	A	175	LEU
6	A	181	GLU
6	A	207	SER
6	A	268	LEU
8	D	39	VAL
8	D	40	LEU
8	D	46	GLU
8	D	47	MET
8	D	125	VAL
8	D	127	GLN
9	F	175	GLN
9	F	185	ARG
9	F	192	PHE
10	G	25	ASN
10	G	47	ASN
10	G	56	ILE
10	G	57	ARG
10	G	59	LEU
10	G	67	LEU
10	G	77	GLU
10	G	119	VAL
10	G	132	ARG
10	G	137	VAL
10	G	138	MET
10	G	142	GLN
11	H	52	LEU
12	I	107	ILE
12	I	115	GLN
12	I	116	GLN
14	K	102	LEU
15	N	149	LEU
15	N	187	GLU
15	N	211	GLN

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Mol	Chain	Res	Type
15	N	229	GLU
15	N	230	PHE
15	N	250	LEU
15	N	276	GLN
15	N	282	LEU
15	N	290	GLN
15	N	305	LEU
15	N	315	LEU
15	N	496	LEU
15	N	545	LEU
15	N	593	GLU
15	N	674	GLU
15	N	678	PHE
15	N	691	LYS
15	N	716	ASN
17	P	243	LYS
18	Q	42	ARG
18	Q	43	LEU
18	Q	45	GLN
18	Q	46	ARG
18	Q	47	ILE
18	Q	143	THR
18	Q	147	ILE
18	Q	270	ASP
18	Q	273	THR
18	Q	485	GLU
18	Q	592	ILE
18	Q	593	MET
18	Q	625	VAL
18	Q	636	VAL
18	Q	637	TYR
20	T	149	VAL
21	V	89	ASN
22	W	33	GLU
22	W	152	VAL
22	W	396	MET
22	W	471	ASP
22	W	610	TYR
22	W	650	LEU
22	W	669	LEU
22	W	830	LEU
22	W	935	GLU

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Mol	Chain	Res	Type
22	W	1074	ARG
22	W	1276	ASP
23	X	36	THR
23	X	39	ILE
23	X	40	LEU
23	X	217	GLN
24	d	923	LEU
26	U	7	GLN
26	U	19	PHE
26	U	76	LEU
26	U	97	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	218	ASN
1	0	245	HIS
1	0	254	GLN
1	0	257	GLN
1	0	278	GLN
1	0	289	GLN
2	1	132	HIS
2	1	140	GLN
3	2	58	GLN
4	3	59	GLN
5	4	19	GLN
5	4	32	ASN
5	4	74	HIS
6	A	66	GLN
6	A	309	GLN
6	A	345	GLN
6	A	360	ASN
8	D	63	ASN
8	D	90	HIS
8	D	153	HIS
9	F	72	HIS
9	F	74	GLN
9	F	107	GLN
9	F	175	GLN
10	G	25	ASN
10	G	47	ASN
10	G	48	GLN

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Mol	Chain	Res	Type
10	G	74	HIS
10	G	88	ASN
10	G	120	HIS
10	G	124	ASN
10	G	129	HIS
10	G	142	GLN
11	H	57	ASN
11	H	139	GLN
12	I	116	GLN
14	K	26	GLN
14	K	79	HIS
15	N	189	GLN
15	N	297	HIS
15	N	374	HIS
15	N	669	GLN
15	N	713	GLN
15	N	771	ASN
15	N	849	ASN
15	N	909	GLN
16	O	628	ASN
16	O	742	GLN
16	O	746	ASN
17	P	683	GLN
17	P	751	GLN
17	P	781	HIS
18	Q	184	ASN
18	Q	218	HIS
18	Q	486	GLN
19	R	37	HIS
19	R	99	HIS
20	T	8	GLN
20	T	36	GLN
20	T	47	HIS
20	T	67	HIS
22	W	61	GLN
22	W	351	HIS
22	W	552	HIS
22	W	726	ASN
22	W	783	GLN
22	W	844	ASN
22	W	914	GLN
22	W	1037	ASN

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Mol	Chain	Res	Type
22	W	1197	HIS
23	X	8	GLN
23	X	12	GLN
23	X	408	GLN
23	X	472	ASN
23	X	679	GLN
23	X	799	HIS
23	X	892	ASN
23	X	903	ASN
23	X	945	GLN
24	d	941	GLN
26	U	7	GLN
26	U	13	ASN
26	U	18	GLN

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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41580. These allow visual inspection of the internal detail of the map and identification of artifacts.

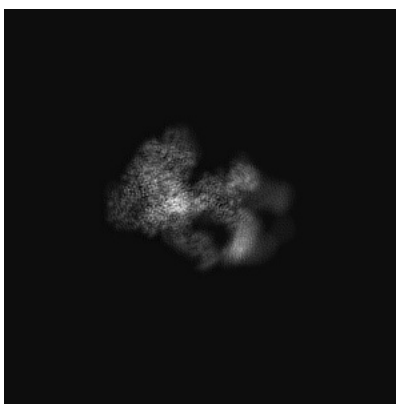
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

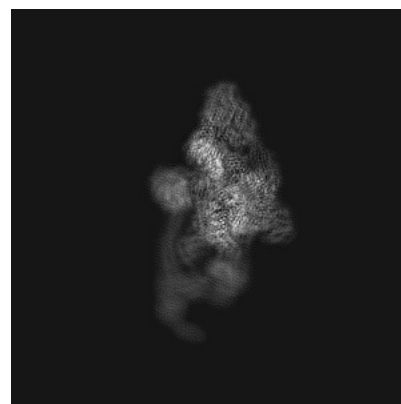
6.1.1 Primary map



X

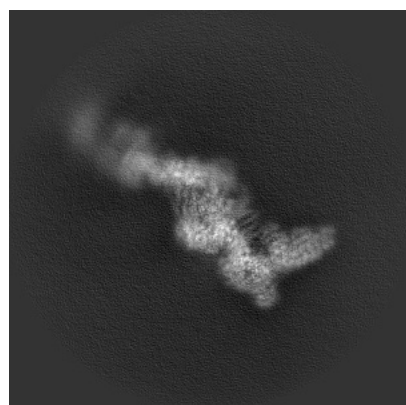


Y

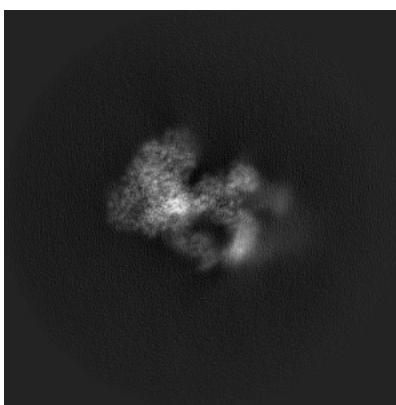


Z

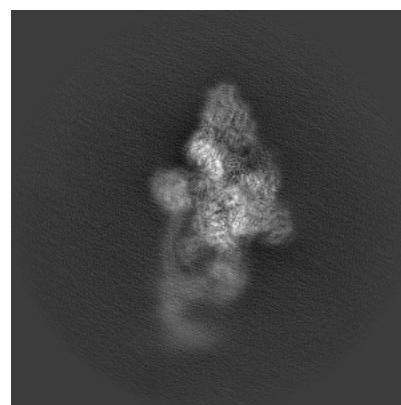
6.1.2 Raw map



X



Y

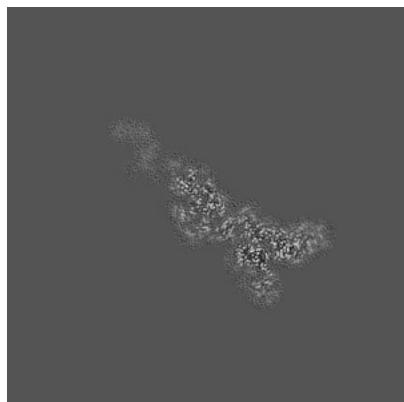


Z

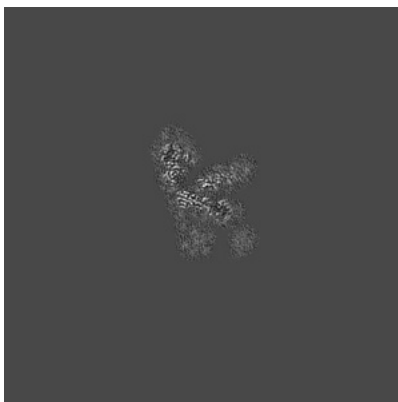
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

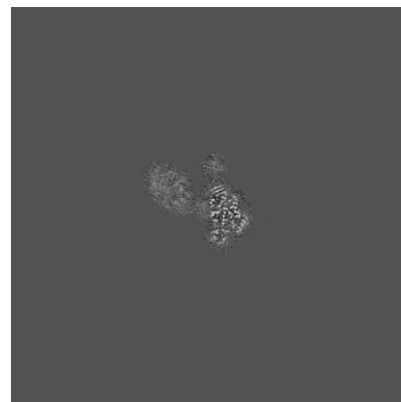
6.2.1 Primary map



X Index: 196

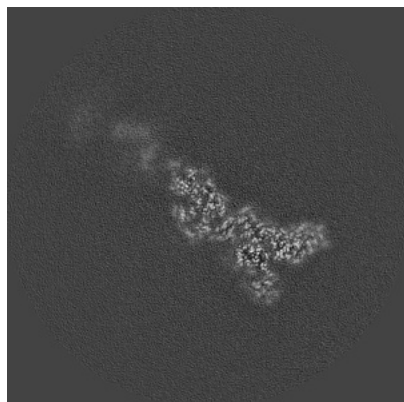


Y Index: 196

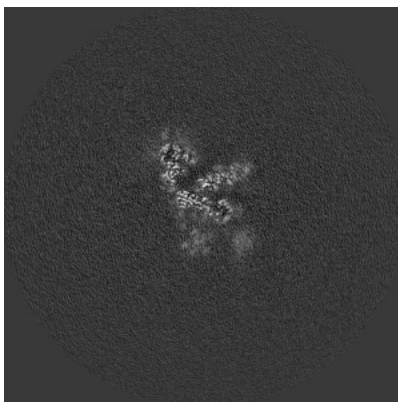


Z Index: 196

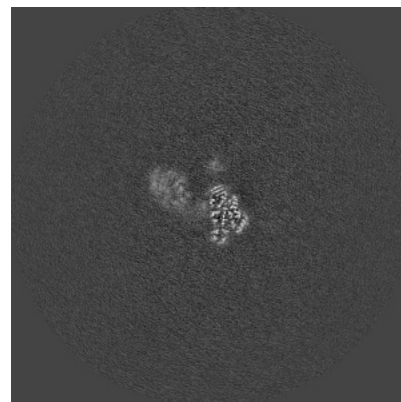
6.2.2 Raw map



X Index: 196



Y Index: 196

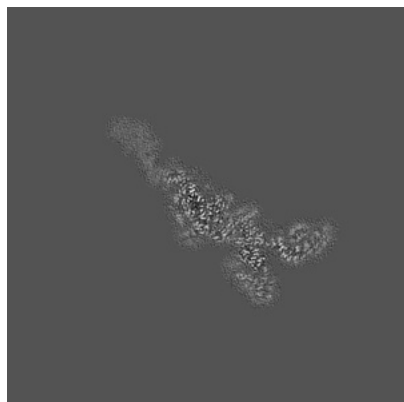


Z Index: 196

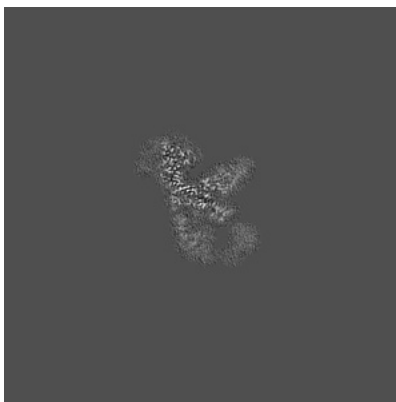
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

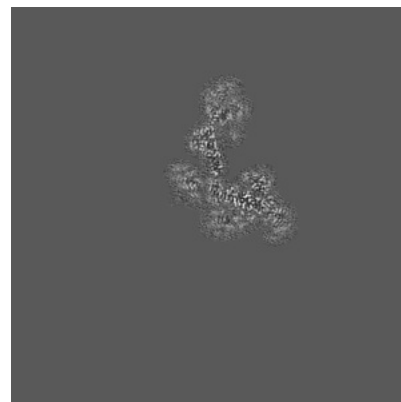
6.3.1 Primary map



X Index: 203

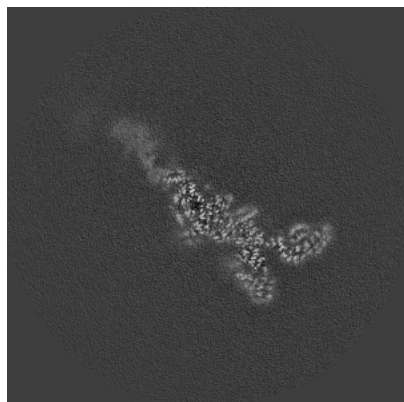


Y Index: 202

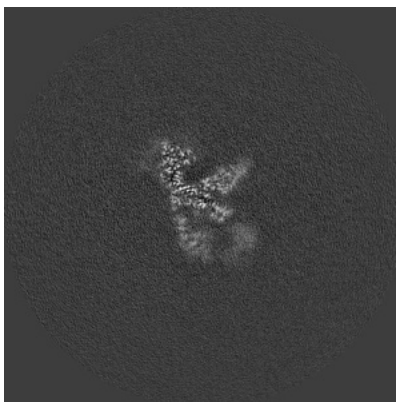


Z Index: 167

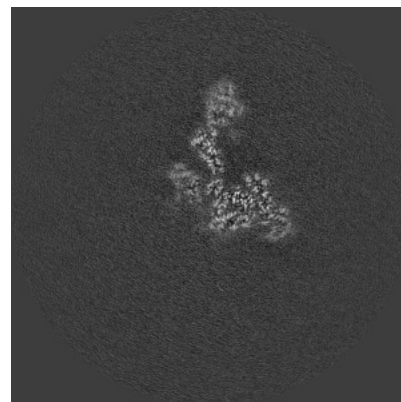
6.3.2 Raw map



X Index: 203



Y Index: 202

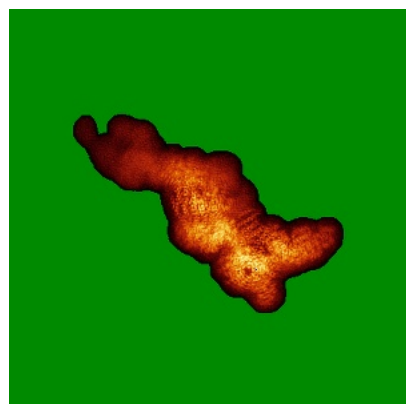


Z Index: 170

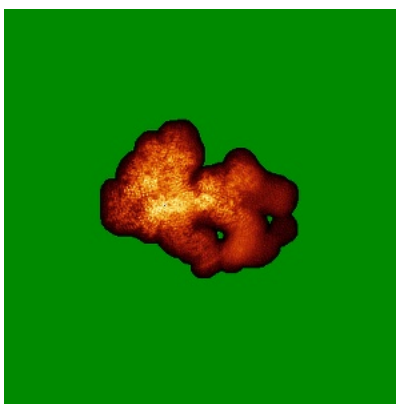
The images above show the largest variance slices of the map in three orthogonal directions.

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

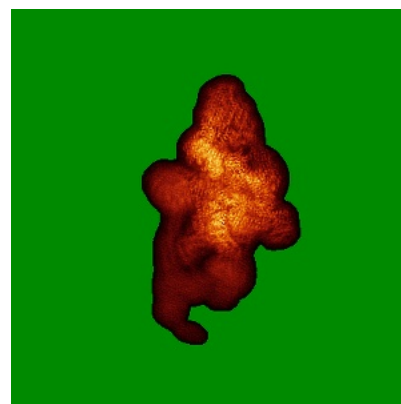
6.4.1 Primary map



X

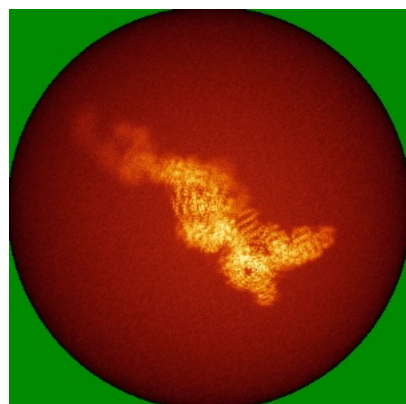


Y

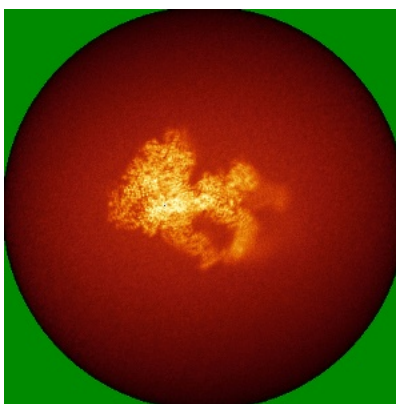


Z

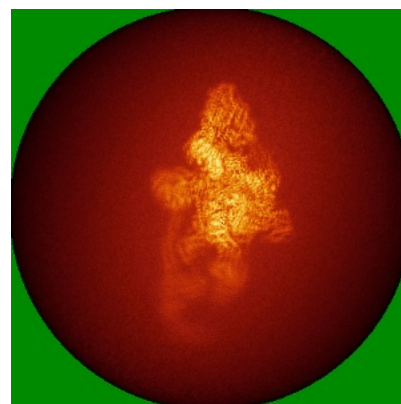
6.4.2 Raw map



X



Y

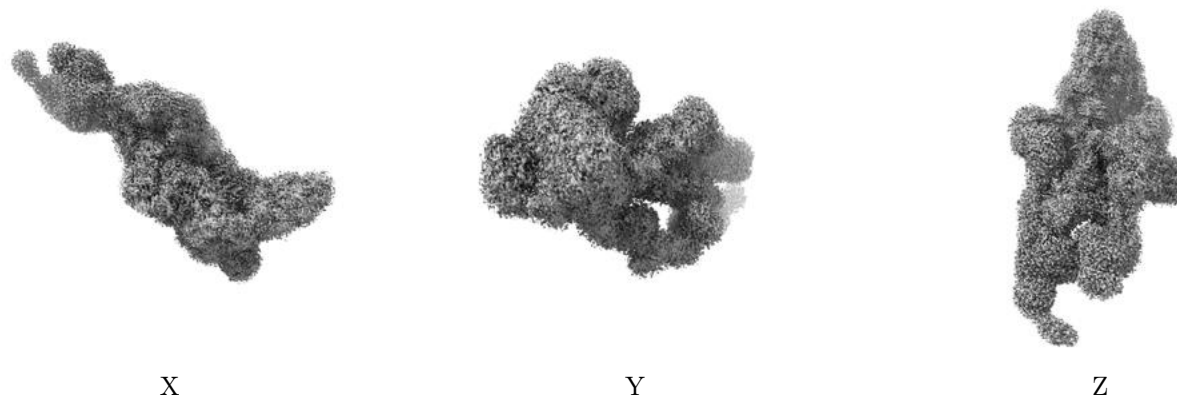


Z

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.

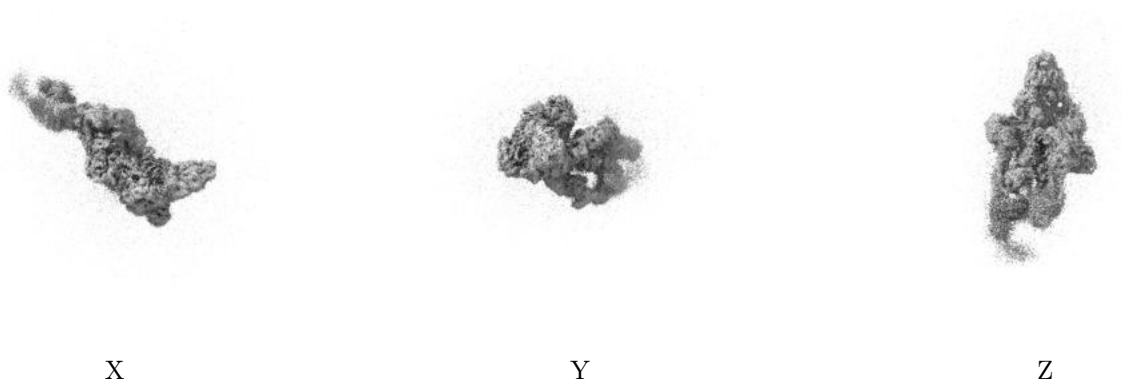
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

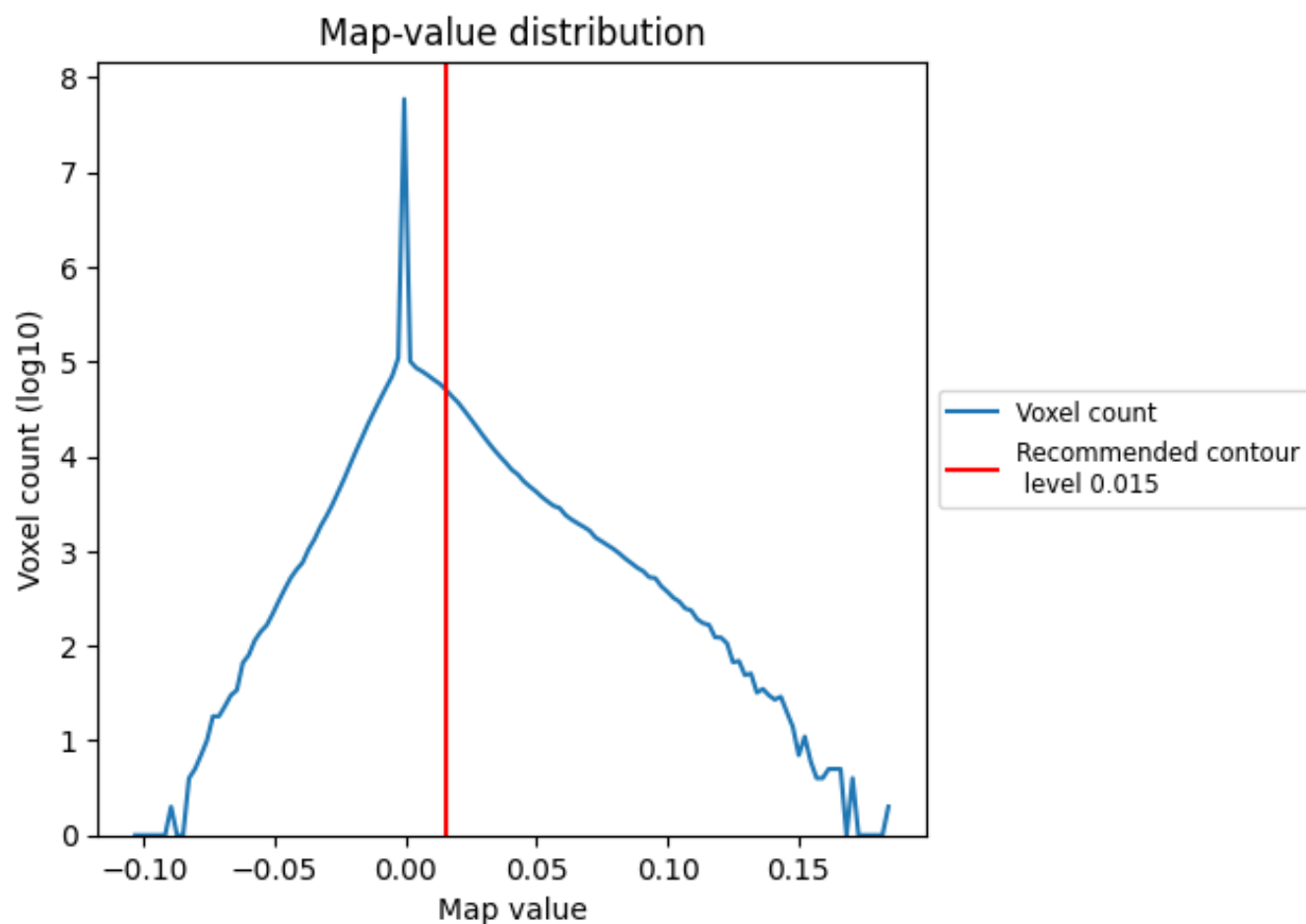
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

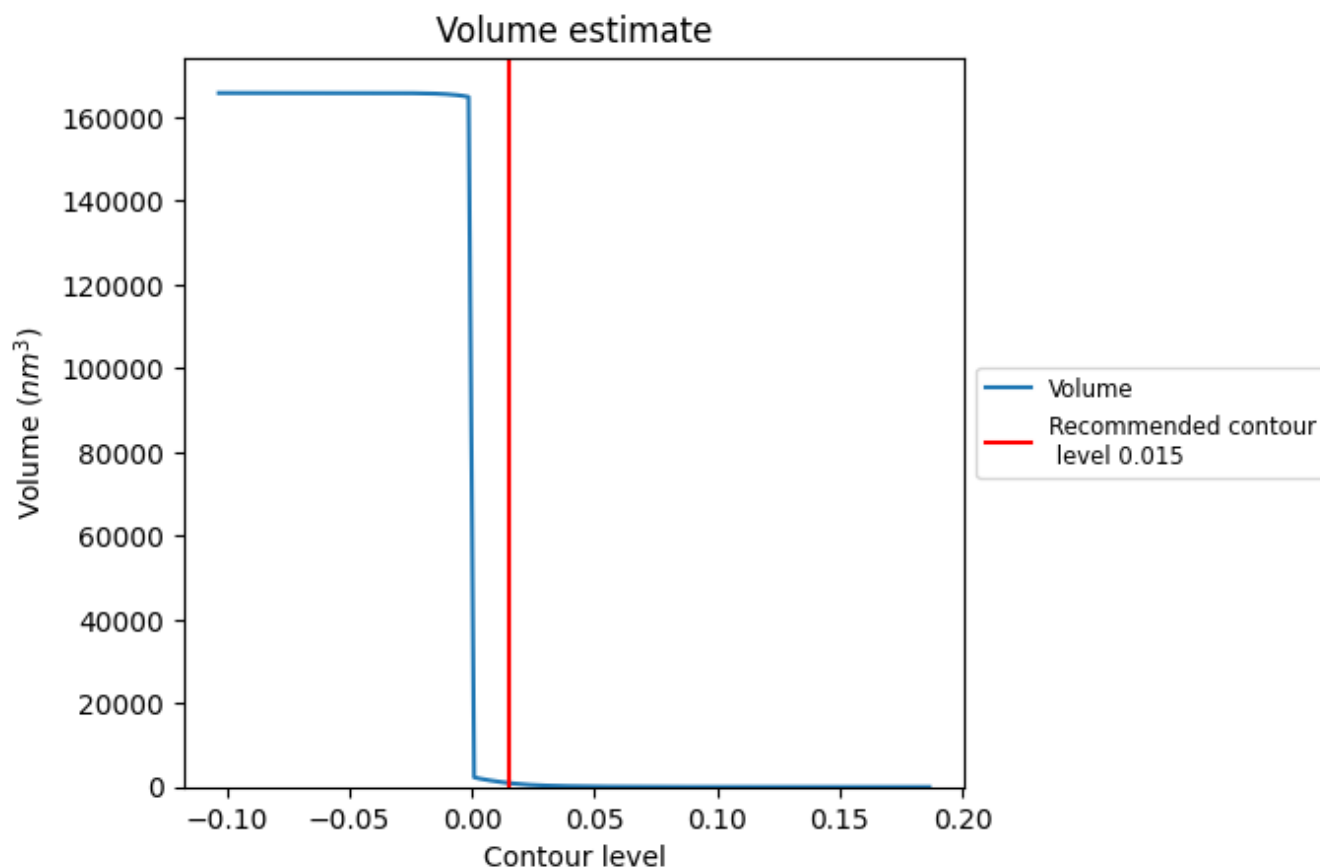
This section contains the results of statistical analysis of the map.

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.

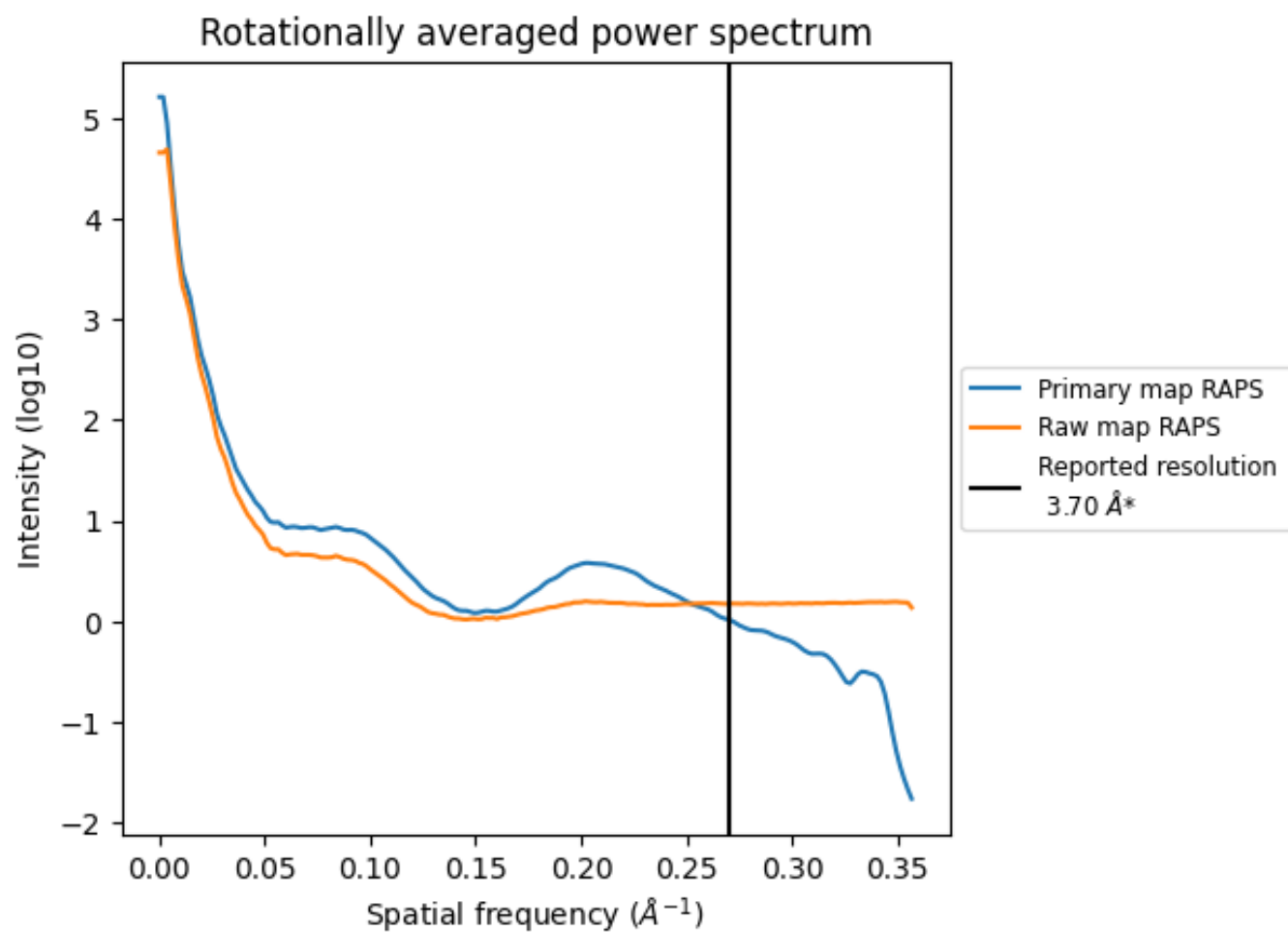
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 945 nm³; this corresponds to an approximate mass of 853 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 ⓘ

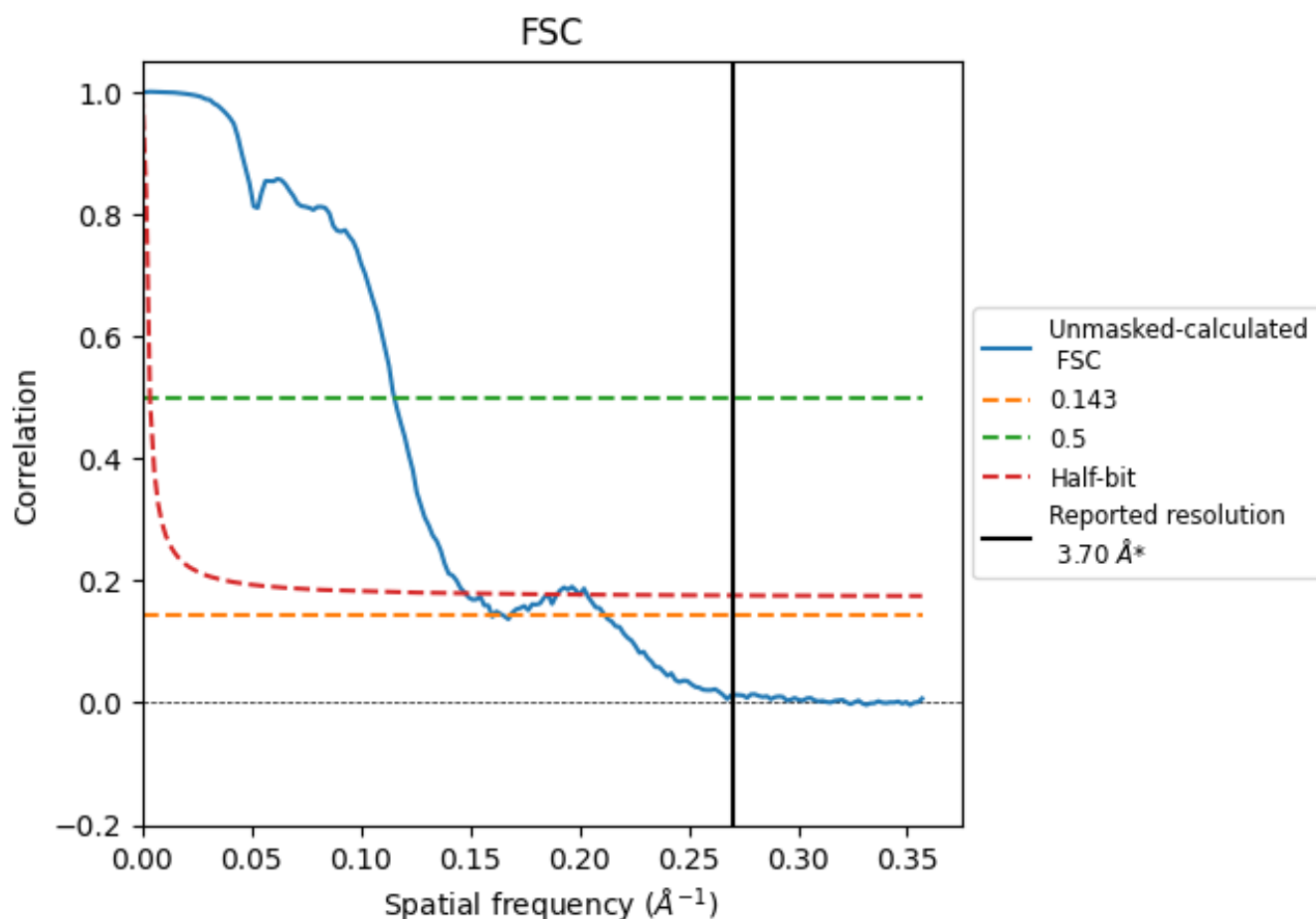


*Reported resolution corresponds to spatial frequency of $0.270 \text{ \AA}^{-1}$

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 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

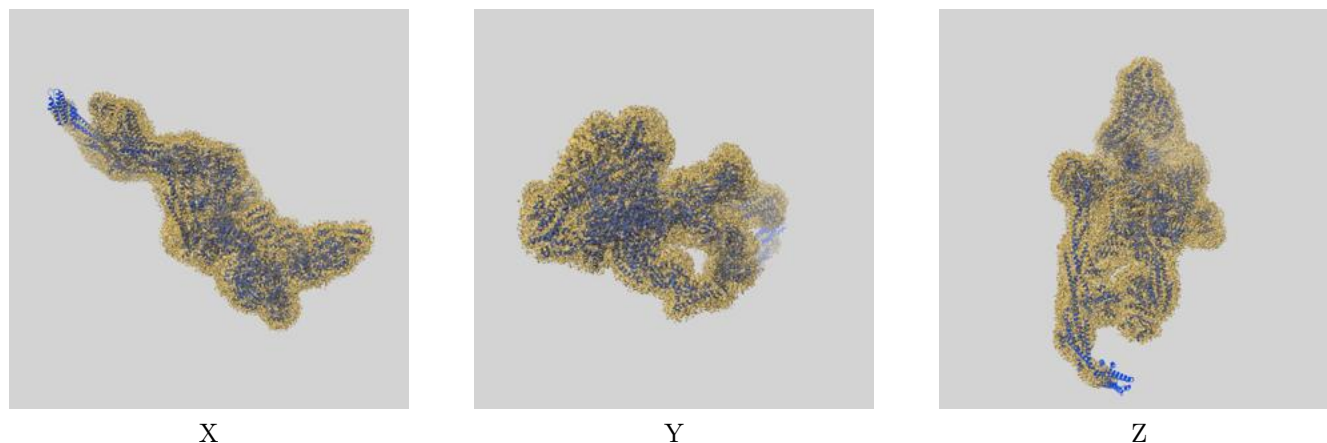
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.25	8.67	6.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.25 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

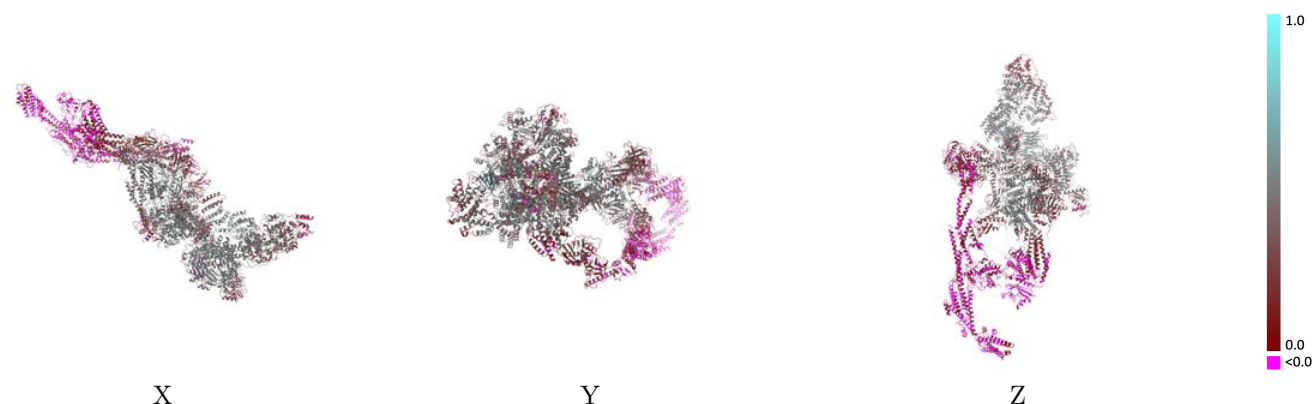
This section contains information regarding the fit between EMDB map EMD-41580 and PDB model 8TRH. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



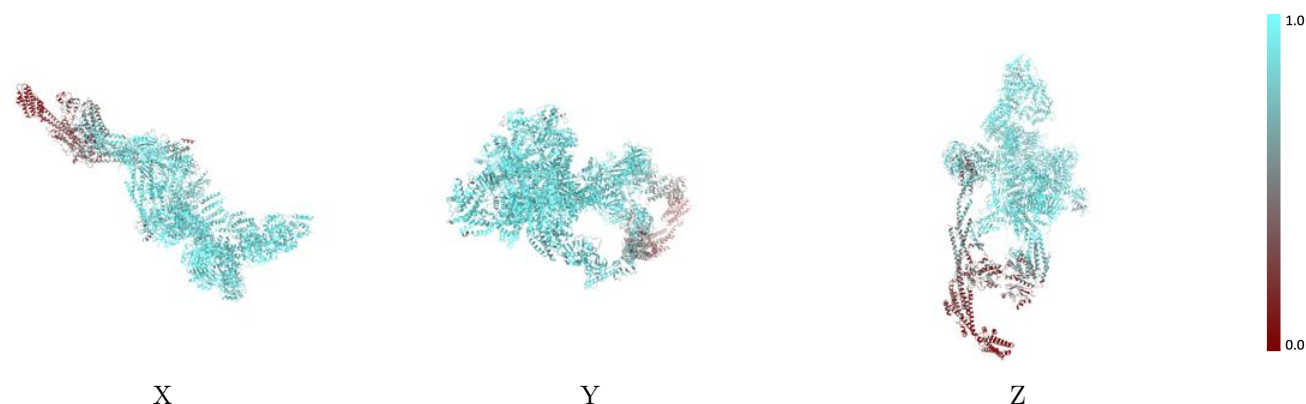
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



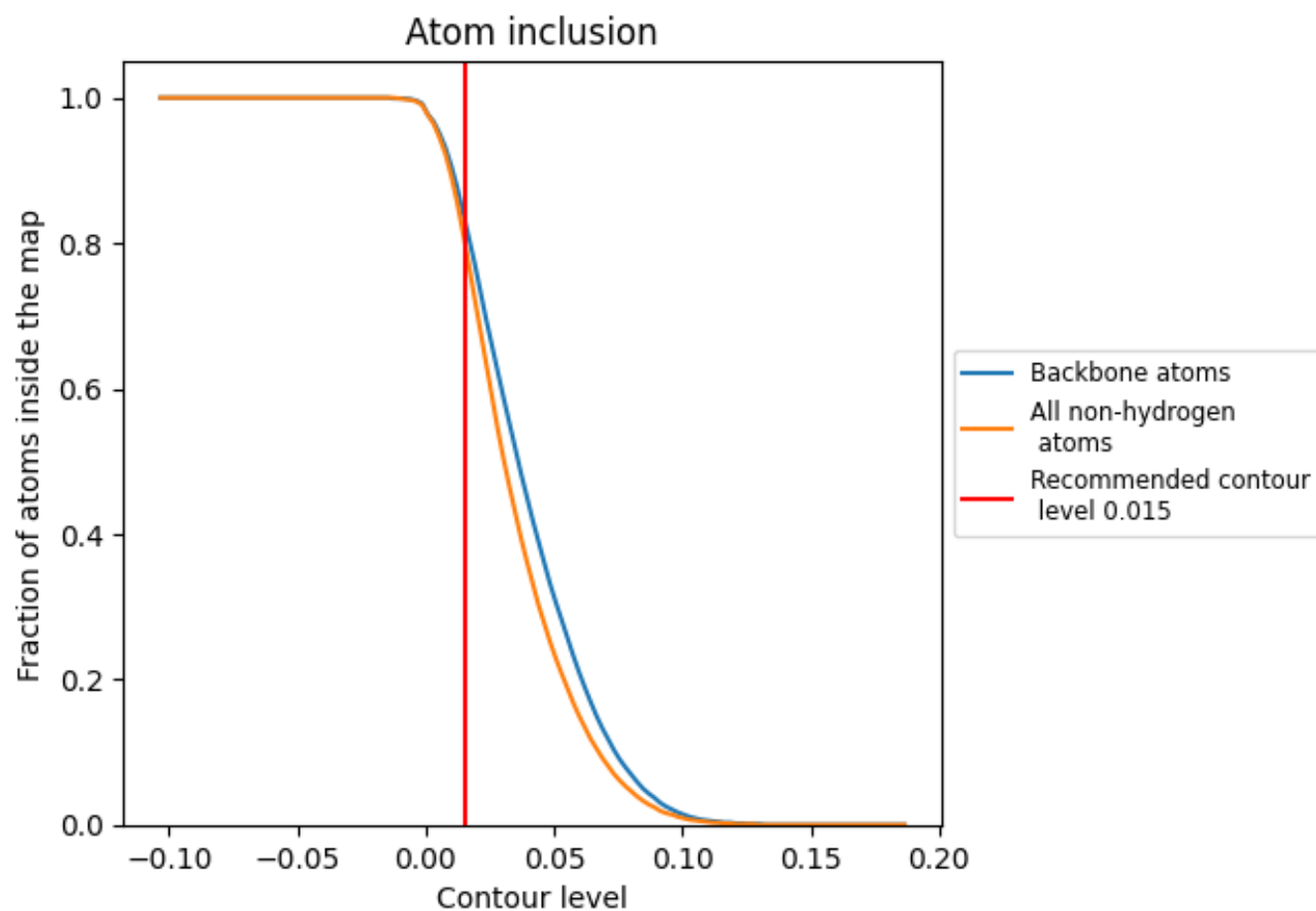
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 81% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8060	 0.3170
0	 0.9430	 0.4670
1	 0.9520	 0.4210
2	 0.9100	 0.4040
3	 0.9250	 0.4000
4	 0.3490	 0.0150
A	 0.7810	 0.2080
B	 0.8700	 0.2510
D	 0.4710	 0.0200
F	 0.4680	 0.0590
G	 0.3670	 0.0150
H	 0.5390	 0.0480
I	 0.5850	 0.0570
J	 0.1130	 0.0170
K	 0.8070	 0.2610
N	 0.8090	 0.3390
O	 0.9240	 0.4100
P	 0.9350	 0.4470
Q	 0.8410	 0.3620
R	 0.8850	 0.2980
S	 0.1010	 -0.0070
T	 0.8890	 0.3230
U	 0.3500	 0.0010
V	 0.8340	 0.2780
W	 0.9300	 0.4070
X	 0.9000	 0.3810
d	 0.1450	 -0.0340

