



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 02:08 PM UTC

PDB ID : 6TBM / pdb_00006tbm
EMDB ID : EMD-10446
Title : Structure of SAGA bound to TBP, including Spt8 and DUB
Authors : Papai, G.; Frechard, A.; Kolesnikova, O.; Crucifix, C.; Schultz, P.; Ben-Shem, A.
Deposited on : 2019-11-01
Resolution : 20.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

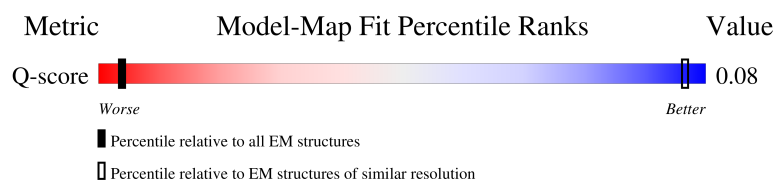
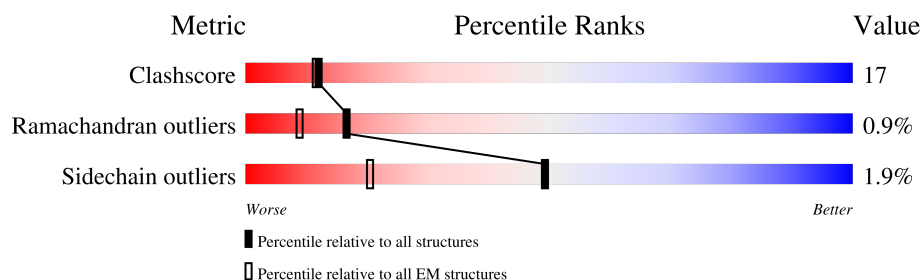
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 20.00 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	28 (19.50 - 20.50)

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	M	240	10% 34% 33% 8% 25%
2	A	448	9% 31% 7% 61%
3	C	698	5% 9% 86%
4	F	517	33% 7% 59%

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Mol	Chain	Length	Quality of chain
5	D	341	
6	E	1191	
7	J	217	
8	K	609	
9	G	722	
10	H	485	
11	I	153	
12	L	3825	
13	B	722	
14	N	400	
15	R	76	
16	Q	502	
17	O	123	
18	P	96	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 48800 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 TATA-box Binding Protein (TBP).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	180	Total	C	N	O	S	0	0
			1415	921	242	246	6		

- Molecule 2 is a protein called Transcriptional coactivator HFI1/ADA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	173	Total	C	N	O	S	0	0
			1300	816	228	250	6		

- Molecule 3 is a protein called Subunit of SAGA histone acetyltransferase complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	95	Total	C	N	O	S	0	0
			761	480	142	133	6		

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	645	LEU	-	expression tag	UNP C4QZ39
C	646	GLU	-	expression tag	UNP C4QZ39
C	647	GLY	-	expression tag	UNP C4QZ39
C	648	GLY	-	expression tag	UNP C4QZ39
C	649	GLY	-	expression tag	UNP C4QZ39
C	650	GLY	-	expression tag	UNP C4QZ39
C	651	SER	-	expression tag	UNP C4QZ39
C	652	MET	-	expression tag	UNP C4QZ39
C	653	ASP	-	expression tag	UNP C4QZ39
C	654	GLU	-	expression tag	UNP C4QZ39
C	655	LYS	-	expression tag	UNP C4QZ39
C	656	THR	-	expression tag	UNP C4QZ39
C	657	THR	-	expression tag	UNP C4QZ39
C	658	GLY	-	expression tag	UNP C4QZ39
C	659	TRP	-	expression tag	UNP C4QZ39

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Chain	Residue	Modelled	Actual	Comment	Reference
C	660	ARG	-	expression tag	UNP C4QZ39
C	661	GLY	-	expression tag	UNP C4QZ39
C	662	GLY	-	expression tag	UNP C4QZ39
C	663	HIS	-	expression tag	UNP C4QZ39
C	664	VAL	-	expression tag	UNP C4QZ39
C	665	VAL	-	expression tag	UNP C4QZ39
C	666	GLU	-	expression tag	UNP C4QZ39
C	667	GLY	-	expression tag	UNP C4QZ39
C	668	LEU	-	expression tag	UNP C4QZ39
C	669	ALA	-	expression tag	UNP C4QZ39
C	670	GLY	-	expression tag	UNP C4QZ39
C	671	GLU	-	expression tag	UNP C4QZ39
C	672	LEU	-	expression tag	UNP C4QZ39
C	673	GLU	-	expression tag	UNP C4QZ39
C	674	GLN	-	expression tag	UNP C4QZ39
C	675	LEU	-	expression tag	UNP C4QZ39
C	676	ARG	-	expression tag	UNP C4QZ39
C	677	ALA	-	expression tag	UNP C4QZ39
C	678	ARG	-	expression tag	UNP C4QZ39
C	679	LEU	-	expression tag	UNP C4QZ39
C	680	GLU	-	expression tag	UNP C4QZ39
C	681	HIS	-	expression tag	UNP C4QZ39
C	682	HIS	-	expression tag	UNP C4QZ39
C	683	PRO	-	expression tag	UNP C4QZ39
C	684	GLN	-	expression tag	UNP C4QZ39
C	685	GLY	-	expression tag	UNP C4QZ39
C	686	GLN	-	expression tag	UNP C4QZ39
C	687	ARG	-	expression tag	UNP C4QZ39
C	688	GLU	-	expression tag	UNP C4QZ39
C	689	PRO	-	expression tag	UNP C4QZ39
C	690	GLY	-	expression tag	UNP C4QZ39
C	691	GLY	-	expression tag	UNP C4QZ39
C	692	SER	-	expression tag	UNP C4QZ39
C	693	HIS	-	expression tag	UNP C4QZ39
C	694	HIS	-	expression tag	UNP C4QZ39
C	695	HIS	-	expression tag	UNP C4QZ39
C	696	HIS	-	expression tag	UNP C4QZ39
C	697	HIS	-	expression tag	UNP C4QZ39
C	698	HIS	-	expression tag	UNP C4QZ39

- Molecule 4 is a protein called Spt20.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	210	Total	C	N	O	S	0	0
			1682	1071	292	315	4		

- Molecule 5 is a protein called Subunit of the SAGA and SAGA-like transcriptional regulatory complexes, interacts with Spt15p to act.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	209	Total	C	N	O	S	0	0
			1616	1016	298	295	7		

- Molecule 6 is a protein called Subunit of the SAGA transcriptional regulatory complex, involved in proper assembly of the complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	154	Total	C	N	O	S	0	0
			1232	784	208	233	7		

- Molecule 7 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	96	Total	C	N	O	S	0	0
			768	489	120	156	3		

- Molecule 8 is a protein called Subunit (61/68 kDa) of TFIID and SAGA complexes.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	154	Total	C	N	O	S	0	0
			1192	747	216	226	3		

- Molecule 9 is a protein called Subunit (90 kDa) of TFIID and SAGA complexes.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	522	Total	C	N	O	S	0	0
			4075	2581	719	756	19		

- Molecule 10 is a protein called Subunit (60 kDa) of TFIID and SAGA complexes.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	421	Total	C	N	O	S	0	0
			3263	2084	556	617	6		

- Molecule 11 is a protein called Subunit (17 kDa) of TFIID and SAGA complexes, involved

in RNA polymerase II transcription initiation.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	123	Total	C	N	O	S	0	0
			981	632	169	178	2		

- Molecule 12 is a protein called Transcription-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	2968	Total	C	N	O	S	0	0
			22318	14296	3864	4071	87		

- Molecule 13 is a protein called Transcriptional regulator involved in glucose repression of Gal4p-regulated genes.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	B	76	Total	C	N	O	0	0
			373	221	76	76		

- Molecule 14 is a protein called Spt8.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	335	Total	C	N	O	0	0
			1648	978	335	335		

- Molecule 15 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	76	Total	C	N	O	S	2	0
			611	384	105	121	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	76	GLZ	-	expression tag	UNP J3QS39

- Molecule 16 is a protein called Ubiquitin carboxyl-terminal hydrolase.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	482	Total	C	N	O	S	0	0
			3817	2410	657	719	31		

- Molecule 17 is a protein called SAGA-associated factor 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	117	Total	C	N	O	S	0	0
			922	563	169	184	6		

- Molecule 18 is a protein called Transcription and mRNA export factor SUS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	90	Total	C	N	O	S	0	0
			735	470	122	142	1		

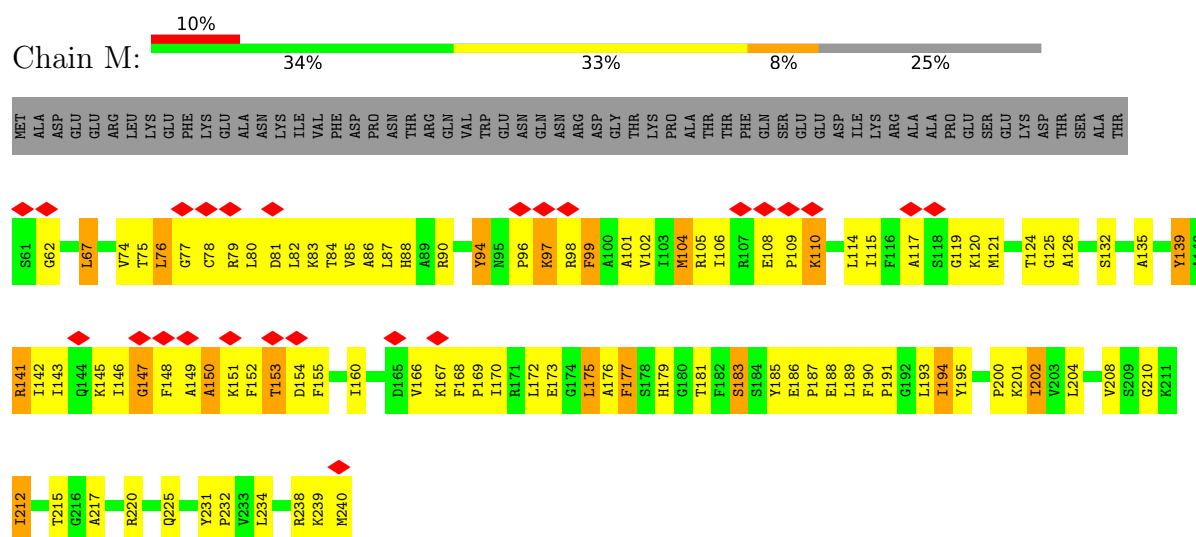
- Molecule 19 is water.

Mol	Chain	Residues	Atoms		AltConf
19	R	83	Total	O	0
			83	83	
19	Q	8	Total	O	0
			8	8	

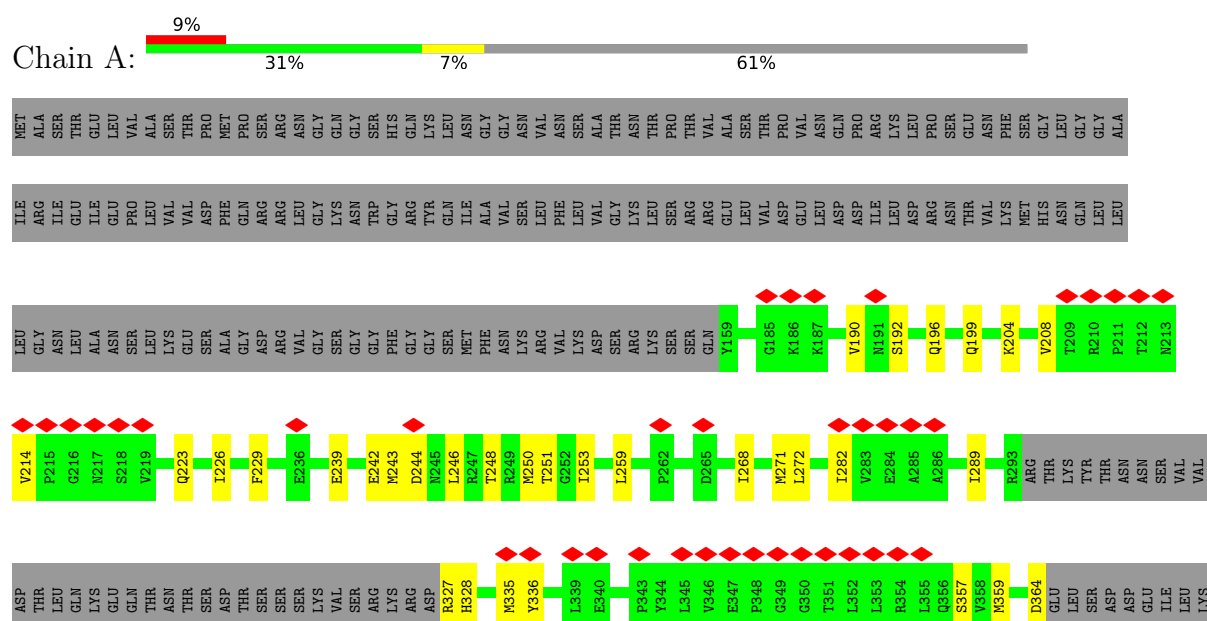
3 Residue-property plots

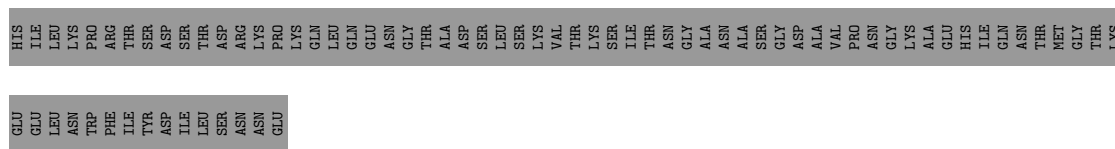
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: TATA-box Binding Protein (TBP)

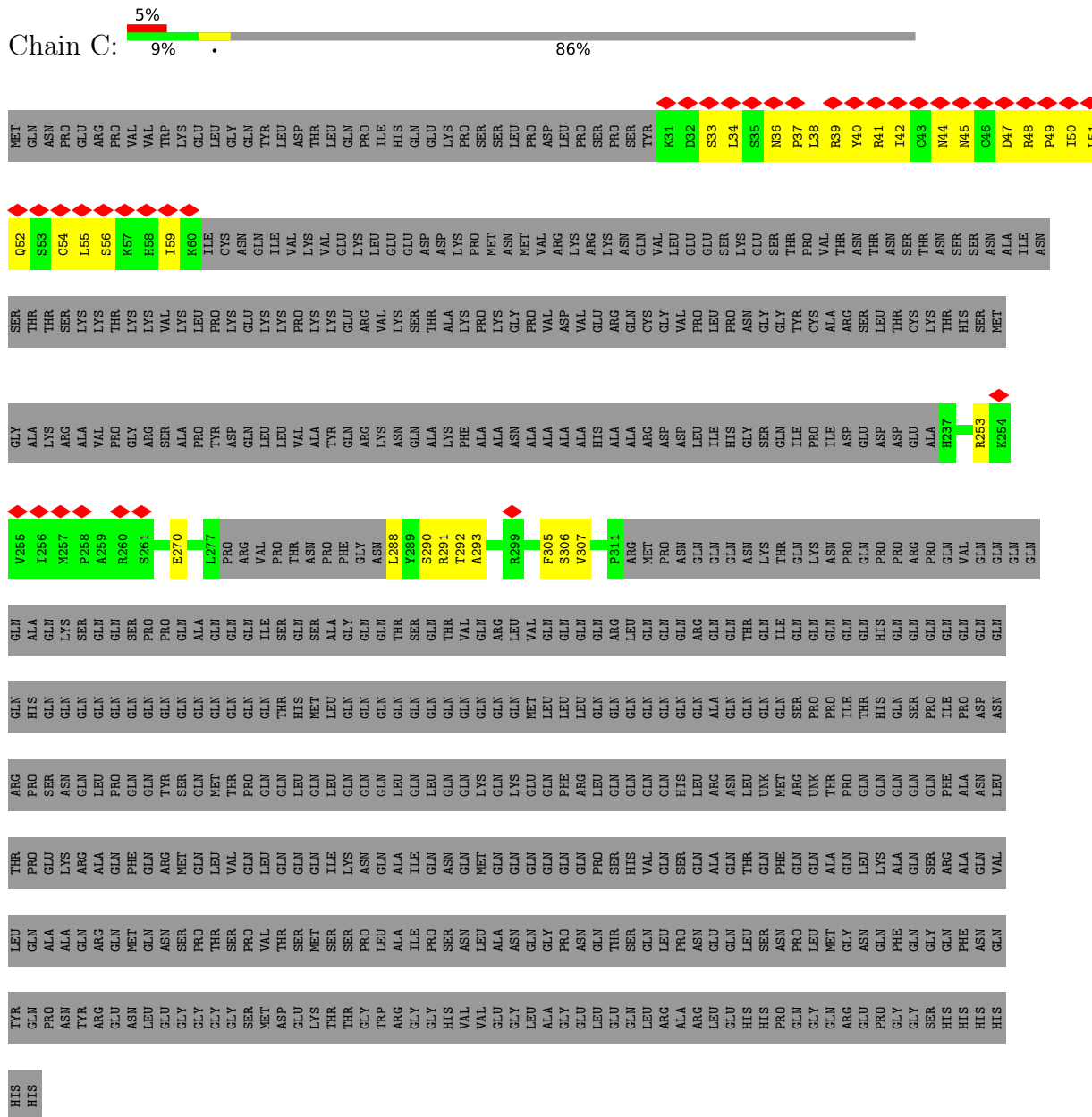


• Molecule 2: Transcriptional coactivator HFI1/ADA1

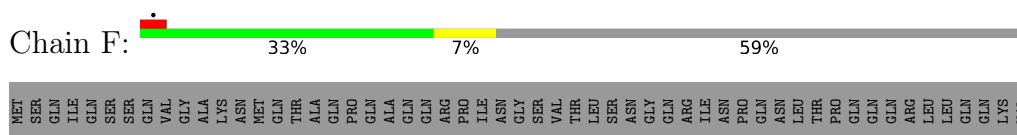




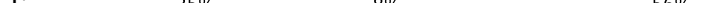
- Molecule 3: Subunit of SAGA histone acetyltransferase complex

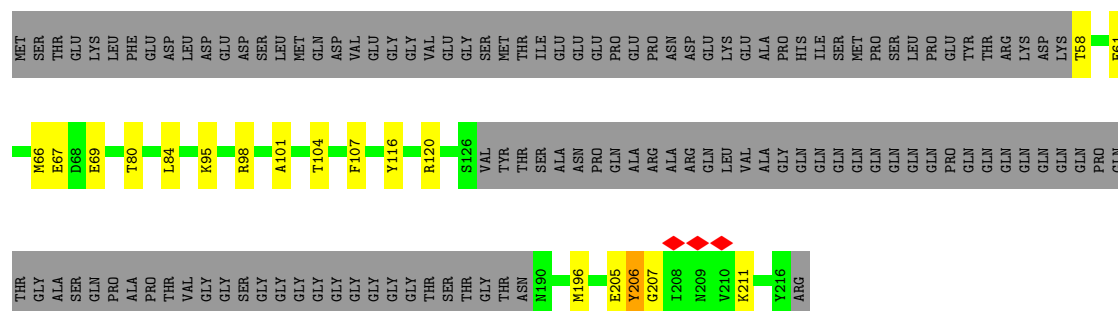


- Molecule 4: Spt20

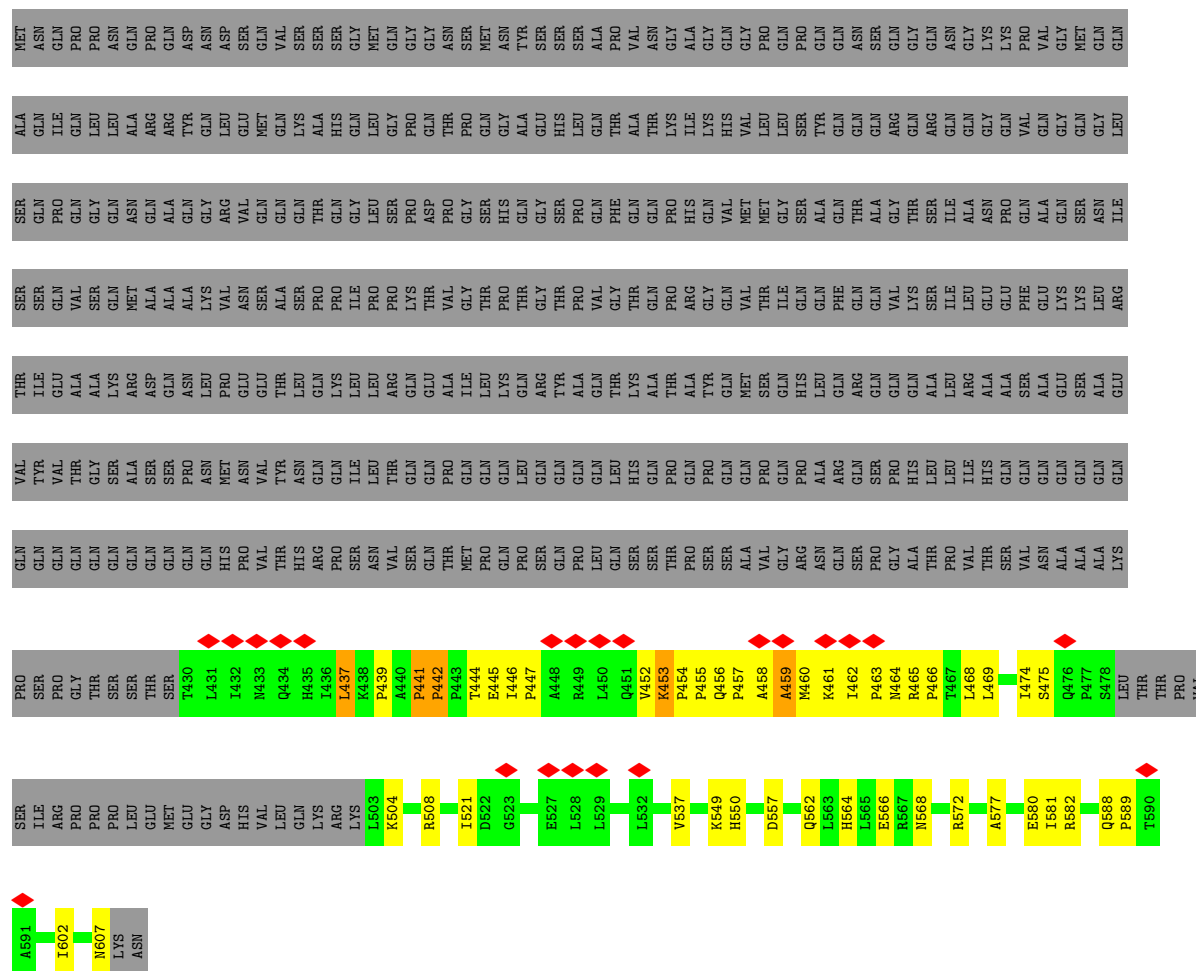


- Molecule 7: Transcription initiation factor TFIID subunit 10

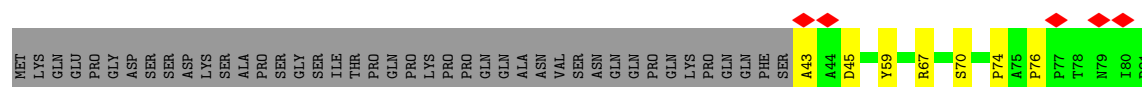
Chain J: 

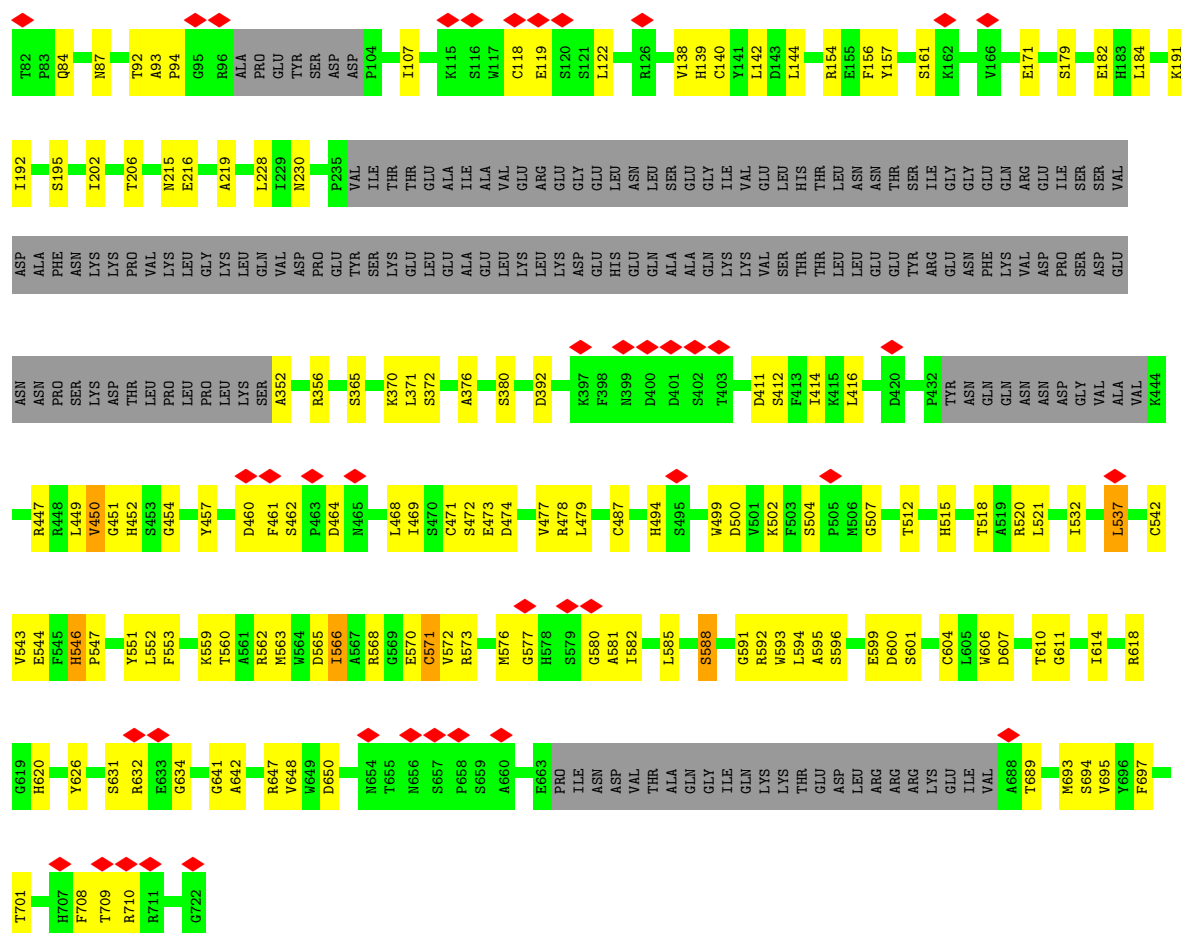


• Molecule 8: Subunit (61/68 kDa) of TFIID and SAGA complexes

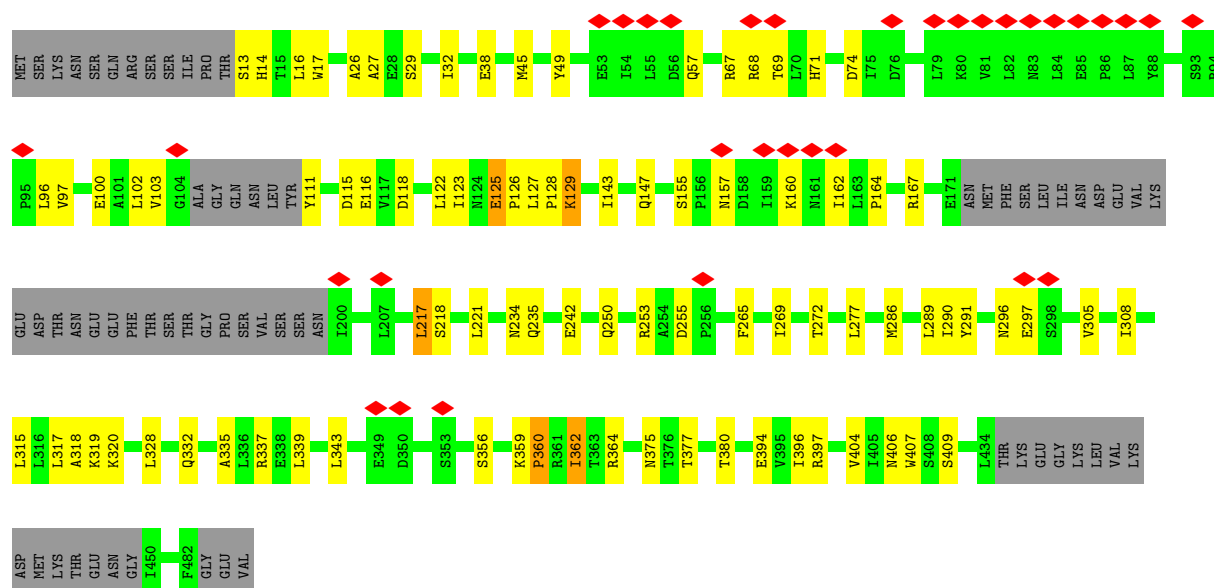


• Molecule 9: Subunit (90 kDa) of TFIID and SAGA complexes

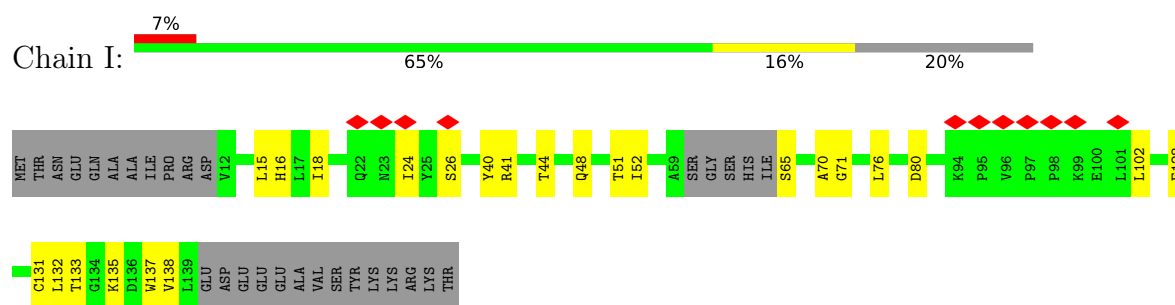




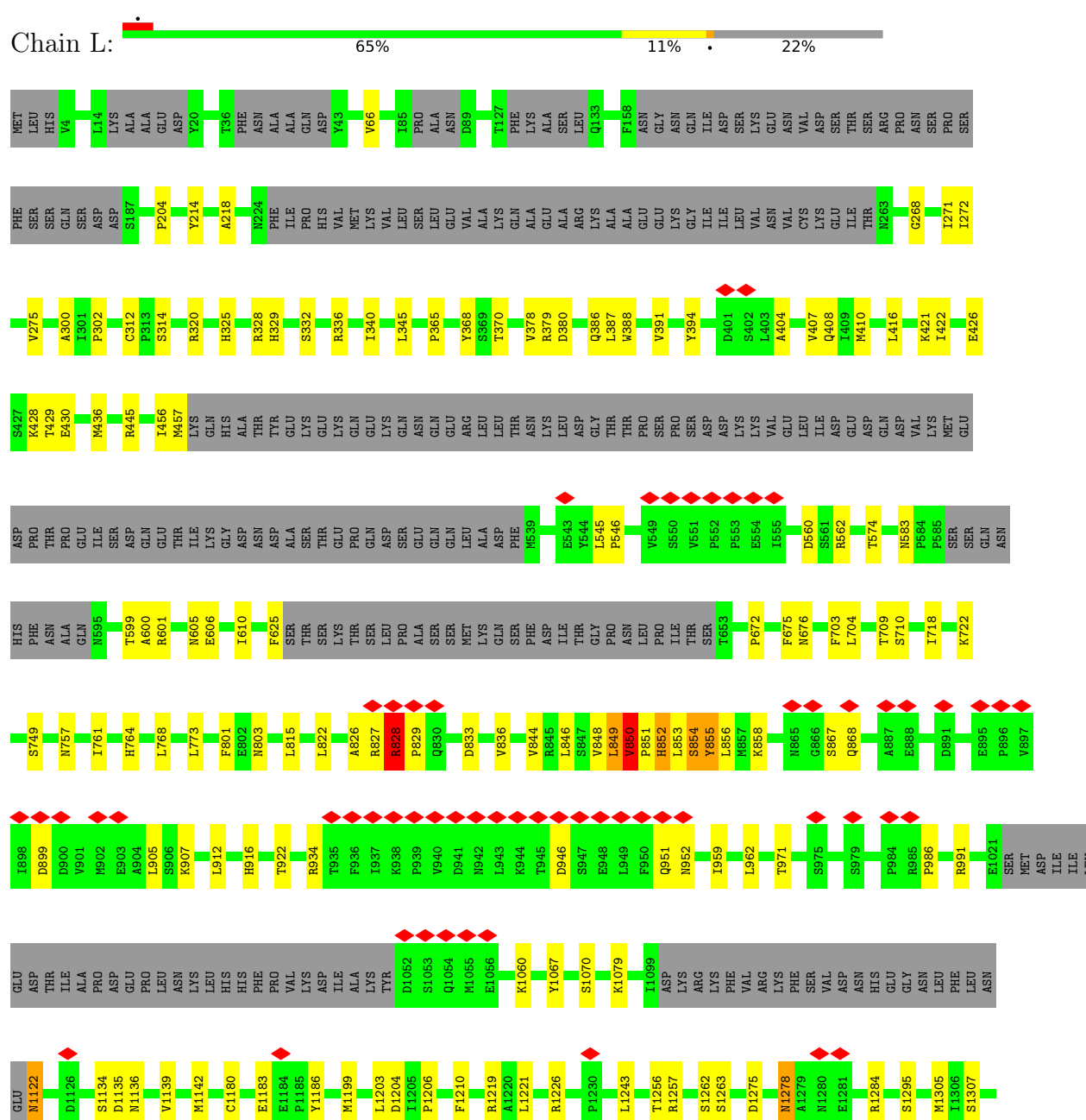
• Molecule 10: Subunit (60 kDa) of TFIID and SAGA complexes



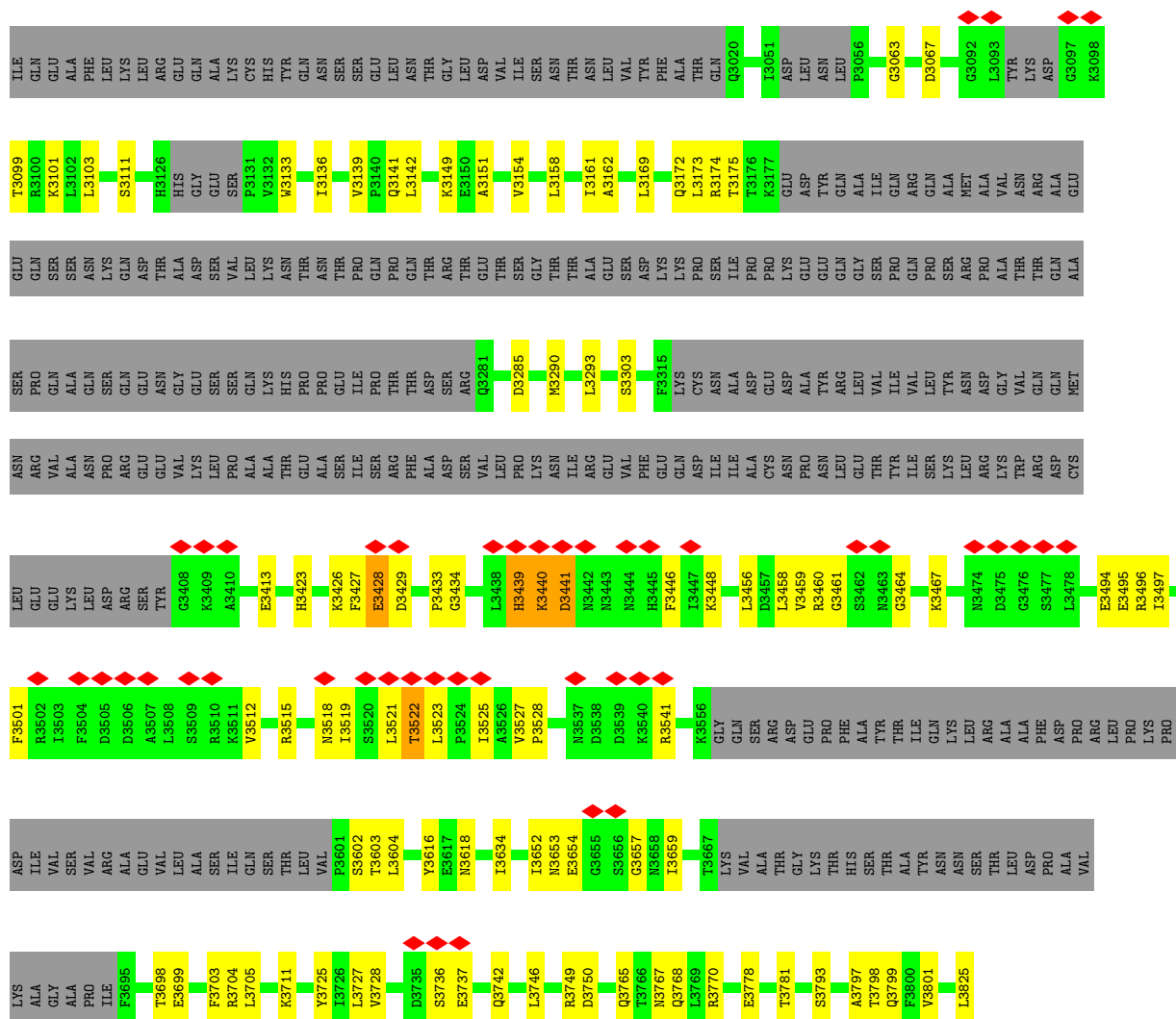
- Molecule 11: Subunit (17 kDa) of TFIID and SAGA complexes, involved in RNA polymerase II transcription initiation



- Molecule 12: Transcription-associated protein

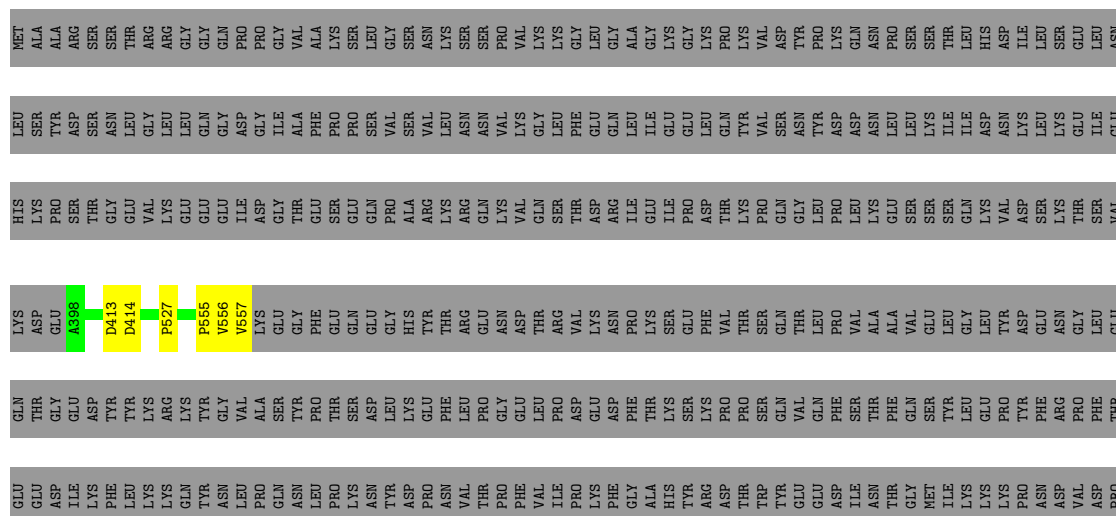


V2904	V2905	V2906	V2907	V2908	H2909	V2910	V2911	V2912	V2913	V2914	V2915	V2916	V2919	PRO	PHE	VAL	PRO	VAL	LEU	GLN	SER	ASN	GLY	THR	ASN	ASN	GLY	ASN	THR	TYR	A2938	E2944	F2952	H2959	E2960	M2961	P2962	E2963	V2964	C2965	I2966	N2967	Q2968	LEU	THR	THR	LYS	ILE	TYR	THR	LEU	PRO	ASN	ILE	GLU
V2815	S2816	G2817	L2818	G2822	V2829	Q2835	V2836	V2837	V2838	V2839	G2843	L2844	Q2849	L2854	S2858	Q2859	V2860	S2861	S2862	V2865	THR	THR	ASN	ALA	ASN	GLN	ASN	GLN	LEU	VAL	ASN	GLN	D2787	I2788	P2789	T2790	P2791	R2792	Q2793	Q2794	Q2797	T2798	L2802	Q2803	G2804	F2805	S2806	Q2807	K2808	K2809	D2810	T2811	L2812	Q2813	D2814
T2690	I2701	L2708	F2721	P2722	Y2737	E2740	K2741	W2745	T2749	E2750	L2751	T2758	L2762	R2767	GLY	ALA	ASP	W2771	L2778	K2783	T2784	D2787	I2788	P2789	T2790	P2791	R2792	Q2793	Q2794	Q2797	T2798	L2802	Q2803	G2804	F2805	S2806	Q2807	K2808	K2809	D2810	T2811	L2812	Q2813	D2814											
ALA	PRO	GLN	ASN	I2521	L2522	D2523	H2528	F2531	L2532	T2539	A2540	G2541	I2548	A2555	E2556	N2560	A2572	D2592	Y2593	H2594	R2595	Q2597	R2601	P2602	N2603	K2614	C2615	P2616	N2633	G2648	L2665	E2666	M2669	Q2672	E2673	D2674	F2677	T2680	Y2687																
T2415	A2416	R2417	M2418	F2422	G2425	L2428	L2433	L2437	T2440	L2441	E2446	L2447	D2448	L2449	R2452	L2465	S2466	D2467	L2475	Q2476	Y2479	S2491	PRO	GLU	GLU	ASN	THR	LEU	PRO	SER	PRO	LEU	GLN	ILE	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR					
MET	THR	V2248	A2286	ILE	SER	LEU	GLN	GLY	ASN	PRO	GLN	SER	GLY	PHE	ALA	ASN	ILE	E2303	A2322	ARG	ILE	SER	SER	LEU	ASP	D2329	F2353	THR	ARG	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR				
GLU	LYS	ASP	I1753	D1774	A1775	R1776	Y1780	I1783	P1786	I1789	R1800	LEU	SER	THR	GLN	THR	ASN	ASN	GLU	LEU	PRO	A1811	K1822	A1823	T1824	L1827	D1837	R1840	A1848	P1855	D1860	M1861	K1862	D1864	D1876	A1884	Y1885	Y1886	V1887	F1895	THR														
R1582	S1587	F1588	V1608	G1609	L1610	D1611	R1617	S1623	R1626	G1629	H1632	Q1633	GLU	GLY	SER	ALA	GLU	E1639	L1680	R1684	S1690	P1691	Y1692	L1693	F1694	Q1698	E1701	L1716	G1717	H1718	F1724	K1727	E1731	G1732	L1733	P1734	F1735	V1736	L1737	E1738	V1748	LYS													
K1310	L1314	I1317	H1333	C1340	L1343	F1347	E1352	E1353	L1354	N1355	R1356	L1357	V1358	Q1359	E1360	L1364	VAL	ASP	ALA	GLU	ASP	GLU	SER	LEU	VAL	SER	ALA	HIS	ARG	ILE	SER	GLU	HIS	K1382	R1391	C1394	R1417	V1418	K1419	I1420	V1421	V1423	F1424	F1425	S1427	K1428									

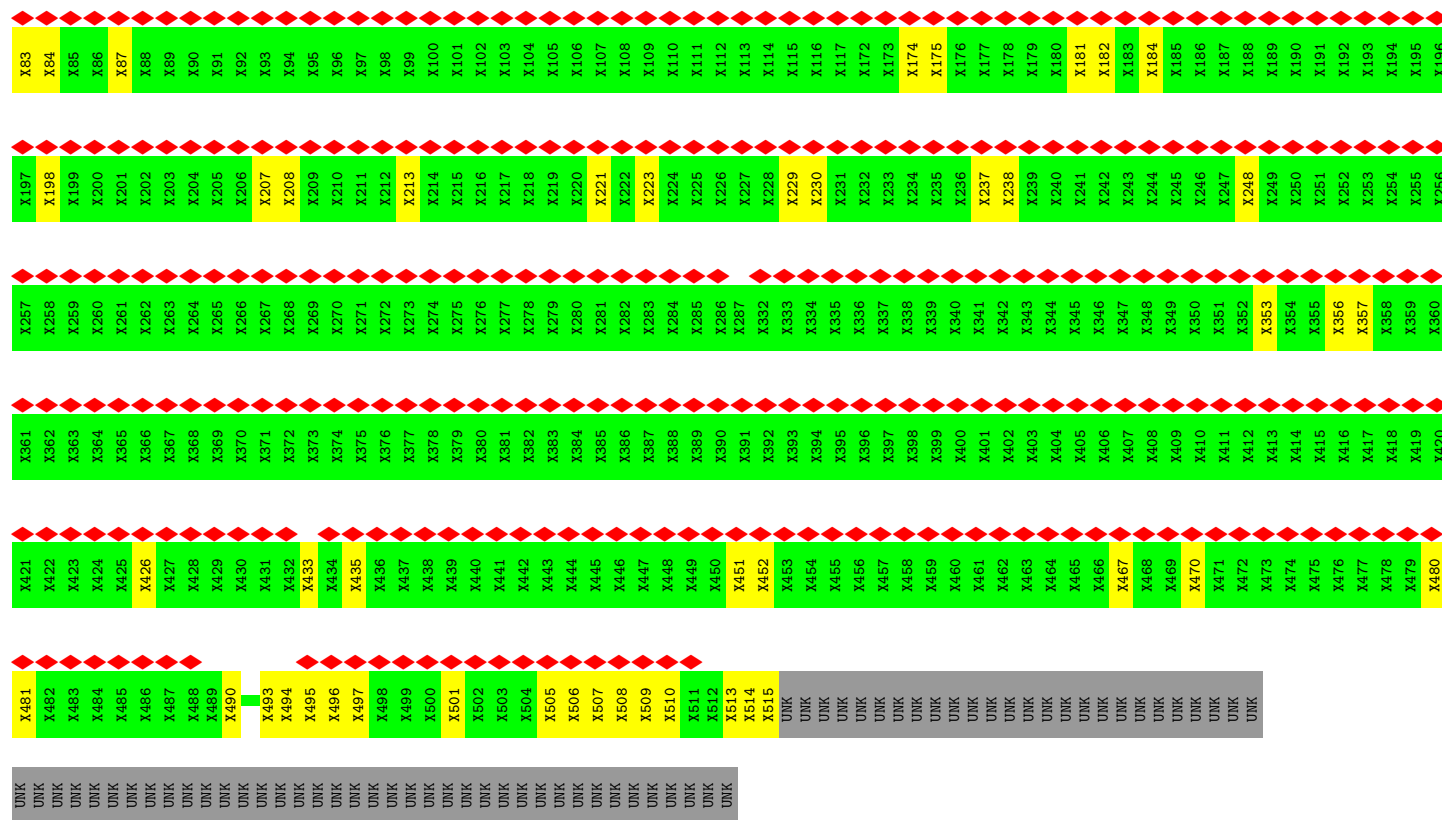
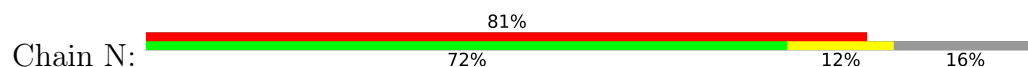


● Molecule 13: Transcriptional regulator involved in glucose repression of Gal4p-regulated genes

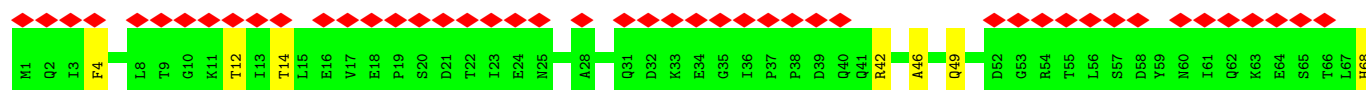
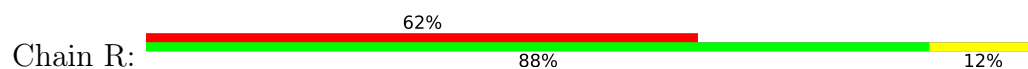
Chain B: 10% 89%

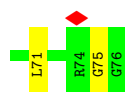


- Molecule 14: Spt8

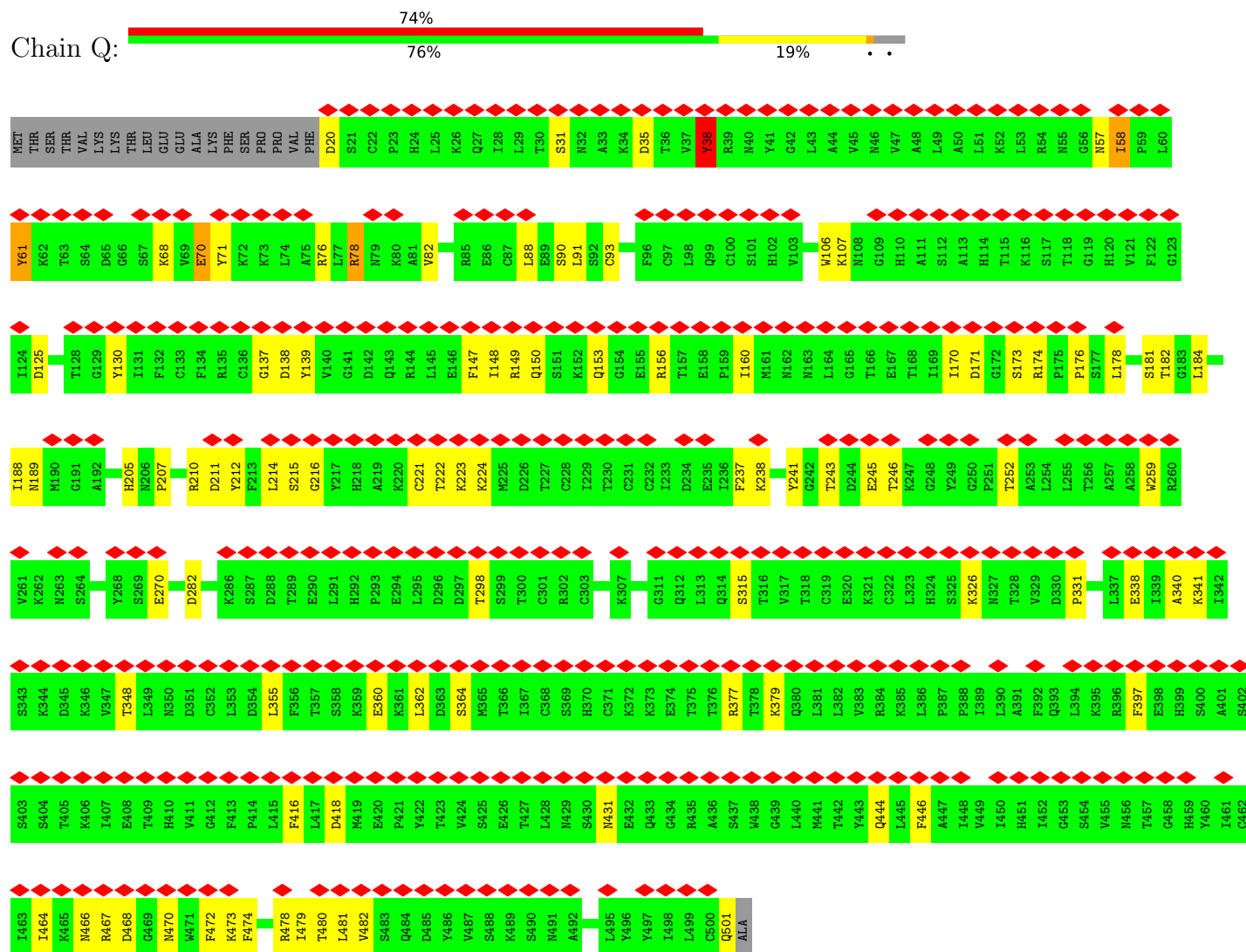


- Molecule 15: Polyubiquitin-B

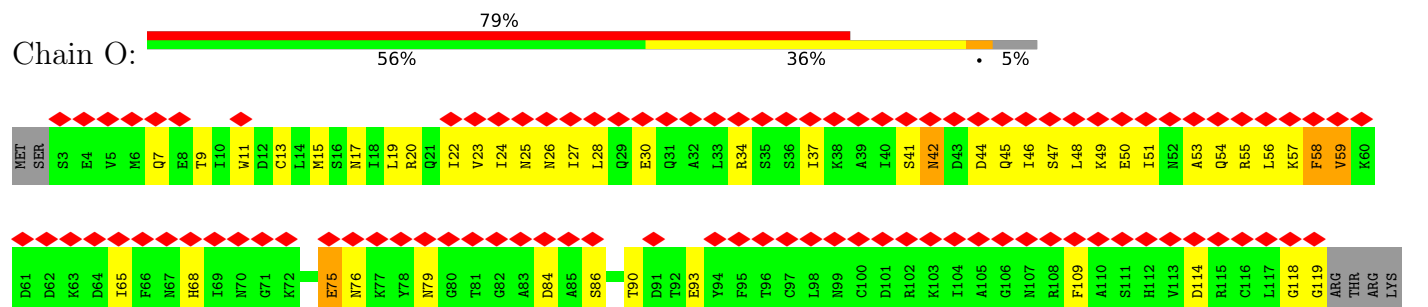




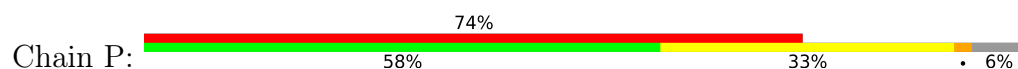
• Molecule 16: Ubiquitin carboxyl-terminal hydrolase



• Molecule 17: SAGA-associated factor 11



• Molecule 18: Transcription and mRNA export factor SUS1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	354104	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52.8	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	558.08, 558.08, 558.08	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.18, 2.18, 2.18	Depositor

5 Model quality

5.1 Standard geometry

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

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	M	1.50	2/1442 (0.1%)	1.11	11/1942 (0.6%)
2	A	0.49	0/1319	0.73	0/1794
3	C	0.63	0/774	0.93	0/1039
4	F	0.30	0/1718	0.57	0/2335
5	D	0.69	0/1641	1.01	3/2213 (0.1%)
6	E	0.50	0/1246	0.72	1/1667 (0.1%)
7	J	0.45	0/779	0.62	0/1051
8	K	0.46	0/1213	0.77	3/1647 (0.2%)
9	G	0.61	0/4177	0.76	5/5661 (0.1%)
10	H	0.35	0/3315	0.61	4/4500 (0.1%)
11	I	0.40	0/1006	0.61	0/1374
12	L	0.32	2/22712 (0.0%)	0.61	14/30825 (0.0%)
13	B	0.83	0/370	1.26	2/509 (0.4%)
15	R	0.99	0/619	0.88	0/833
16	Q	0.88	0/3897	1.49	13/5265 (0.2%)
17	O	1.05	1/931 (0.1%)	1.67	10/1250 (0.8%)
18	P	0.96	1/747 (0.1%)	1.67	3/1011 (0.3%)
All	All	0.57	6/47906 (0.0%)	0.84	69/64916 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	0	1
16	Q	2	5
All	All	2	6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	194	ILE	C-N	50.73	1.97	1.33
1	M	183	SER	C-N	12.09	1.48	1.33
18	P	60	SER	C-O	-6.40	1.16	1.24
17	O	58	PHE	C-O	-5.46	1.17	1.24
12	L	828	ARG	C-N	5.41	1.38	1.33
12	L	340	ILE	C-N	5.30	1.39	1.34

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	O	42	ASN	CA-CB-CG	9.24	121.84	112.60
13	B	527	PRO	N-CA-CB	7.56	111.18	103.25
1	M	62	GLY	N-CA-C	7.29	130.46	113.18
12	L	2595	ILE	N-CA-C	-7.25	105.46	111.91
8	K	453	LYS	CA-C-N	6.80	127.39	120.38
8	K	453	LYS	C-N-CA	6.80	127.39	120.38
17	O	41	SER	N-CA-C	-6.78	104.89	113.43
16	Q	221	CYS	N-CA-C	6.76	119.67	110.55
5	D	323	LYS	N-CA-C	-6.73	105.04	113.18
1	M	141	ARG	N-CA-C	-6.58	103.31	112.12
17	O	118	GLY	CA-C-N	6.31	133.06	121.70
17	O	118	GLY	C-N-CA	6.31	133.06	121.70
16	Q	418	ASP	CA-CB-CG	-6.15	106.45	112.60
16	Q	58	ILE	O-C-N	-6.11	114.14	121.10
17	O	84	ASP	CA-C-N	6.11	131.19	120.87
17	O	84	ASP	C-N-CA	6.11	131.19	120.87
1	M	86	ALA	N-CA-C	-6.06	104.23	111.69
10	H	125	GLU	CA-C-N	5.92	127.24	119.84
10	H	125	GLU	C-N-CA	5.92	127.24	119.84
1	M	194	ILE	O-C-N	-5.90	115.19	122.57
12	L	850	VAL	N-CA-CB	5.89	114.21	110.50
1	M	177	PHE	CB-CA-C	5.85	119.28	111.14
9	G	588	SER	CA-C-N	5.81	125.48	119.56
9	G	588	SER	C-N-CA	5.81	125.48	119.56
12	L	1425	PHE	CA-C-N	5.77	132.56	121.54
12	L	1425	PHE	C-N-CA	5.77	132.56	121.54
16	Q	57	ASN	CA-CB-CG	5.70	118.30	112.60
5	D	293	LEU	CA-C-N	5.68	132.39	121.54
5	D	293	LEU	C-N-CA	5.68	132.39	121.54
1	M	94	TYR	N-CA-C	-5.65	99.21	108.76
12	L	828	ARG	CA-C-N	5.65	127.38	120.94
12	L	828	ARG	C-N-CA	5.65	127.38	120.94
12	L	761	ILE	CA-C-N	5.63	128.02	120.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	761	ILE	C-N-CA	5.63	128.02	120.58
17	O	75	GLU	CB-CG-CD	5.62	122.16	112.60
18	P	41	ASP	CA-CB-CG	-5.61	106.99	112.60
12	L	300	ALA	CA-C-N	5.60	123.77	120.24
12	L	300	ALA	C-N-CA	5.60	123.77	120.24
12	L	3521	LEU	CA-C-N	5.55	130.28	122.46
12	L	3521	LEU	C-N-CA	5.55	130.28	122.46
17	O	53	ALA	N-CA-C	5.54	118.06	110.24
9	G	546	HIS	CA-C-N	5.44	125.11	119.56
9	G	546	HIS	C-N-CA	5.44	125.11	119.56
17	O	119	GLY	N-CA-C	5.44	129.07	113.30
1	M	139	TYR	N-CA-C	5.43	117.96	111.71
1	M	167	LYS	N-CA-C	5.42	119.06	111.74
16	Q	341	LYS	CA-C-N	5.41	127.87	120.46
16	Q	341	LYS	C-N-CA	5.41	127.87	120.46
12	L	3521	LEU	N-CA-C	5.36	119.30	112.87
8	K	441	PRO	N-CA-C	5.35	117.22	110.70
13	B	555	PRO	N-CA-CB	5.32	109.18	103.33
18	P	54	GLU	CA-C-N	5.30	129.67	122.19
18	P	54	GLU	C-N-CA	5.30	129.67	122.19
16	Q	38	TYR	CA-CB-CG	5.30	123.44	113.90
17	O	59	VAL	N-CA-C	5.26	120.28	109.34
6	E	930	LYS	CB-CA-C	5.24	119.75	110.85
16	Q	78	ARG	N-CA-C	5.24	116.99	111.28
9	G	611	GLY	N-CA-C	-5.23	108.40	115.36
12	L	3522	THR	N-CA-C	5.22	118.39	111.30
10	H	359	LYS	CA-C-N	5.19	126.33	119.84
10	H	359	LYS	C-N-CA	5.19	126.33	119.84
16	Q	298	THR	CA-C-N	5.11	130.90	121.70
16	Q	298	THR	C-N-CA	5.11	130.90	121.70
16	Q	68	LYS	CA-C-N	5.10	130.33	122.68
16	Q	68	LYS	C-N-CA	5.10	130.33	122.68
16	Q	224	LYS	N-CA-C	5.08	117.85	109.72
1	M	183	SER	CA-C-N	-5.04	113.07	121.64
1	M	183	SER	C-N-CA	-5.04	113.07	121.64
1	M	220	ARG	N-CA-C	5.02	117.14	111.02

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	Q	31	SER	CA
16	Q	222	THR	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	183	SER	Mainchain
16	Q	149	ARG	Sidechain
16	Q	212	TYR	Sidechain
16	Q	241	TYR	Sidechain
16	Q	38	TYR	Sidechain
16	Q	61	TYR	Sidechain

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	M	1415	0	1491	107	0
2	A	1300	0	1254	31	0
3	C	761	0	779	194	0
4	F	1682	0	1622	30	0
5	D	1616	0	1558	125	0
6	E	1232	0	1276	41	0
7	J	768	0	754	13	0
8	K	1192	0	1214	90	0
9	G	4075	0	3934	106	0
10	H	3263	0	3258	71	0
11	I	981	0	982	18	0
12	L	22318	0	20960	390	0
13	B	373	0	190	2	0
14	N	1648	0	382	60	0
15	R	611	0	636	19	0
16	Q	3817	0	3772	525	0
17	O	922	0	897	413	0
18	P	735	0	743	191	0
19	Q	8	0	0	10	0
19	R	83	0	0	6	0
All	All	48800	0	45702	1636	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 17.

All (1636) 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)
16:Q:472:PHE:CZ	17:O:45:GLN:HB3	1.29	1.65
17:O:11:TRP:CD1	18:P:83:LEU:HD23	1.14	1.61
16:Q:479:ILE:HG23	17:O:47:SER:CA	1.19	1.61
16:Q:479:ILE:CG2	17:O:47:SER:HA	1.14	1.60
17:O:34:ARG:HH11	18:P:57:PRO:CB	1.11	1.58
16:Q:464:ILE:CD1	17:O:46:ILE:CD1	1.74	1.57
17:O:9:THR:HG22	18:P:10:LYS:CE	1.29	1.56
17:O:22:ILE:CD1	18:P:43:ILE:HD11	1.14	1.55
3:C:38:LEU:HD22	16:Q:210:ARG:CD	1.33	1.55
16:Q:464:ILE:CG1	17:O:46:ILE:HD12	1.34	1.54
3:C:34:LEU:CD2	16:Q:446:PHE:HE1	0.95	1.54
3:C:38:LEU:HD13	16:Q:210:ARG:CZ	1.21	1.54
17:O:11:TRP:HD1	18:P:83:LEU:CD2	1.19	1.54
3:C:39:ARG:NH1	16:Q:148:ILE:CA	1.68	1.53
16:Q:178:LEU:HD13	17:O:37:ILE:CD1	1.34	1.53
17:O:22:ILE:HD13	18:P:43:ILE:CD1	1.13	1.53
3:C:34:LEU:HD22	16:Q:446:PHE:CE1	1.00	1.52
3:C:38:LEU:CD1	16:Q:210:ARG:NE	1.67	1.51
8:K:469:LEU:HD13	12:L:2788:ILE:CG2	1.31	1.51
16:Q:464:ILE:CD1	17:O:46:ILE:HD13	1.26	1.51
17:O:9:THR:CG2	18:P:10:LYS:HE3	1.08	1.50
14:N:207:UNK:C	14:N:208:UNK:H2	1.23	1.49
16:Q:472:PHE:CD2	17:O:46:ILE:HG12	1.45	1.49
3:C:49:PRO:HG2	16:Q:237:PHE:CE1	1.48	1.46
16:Q:178:LEU:CD1	17:O:37:ILE:HD13	1.42	1.45
17:O:11:TRP:NE1	18:P:83:LEU:HA	1.18	1.45
16:Q:182:THR:CG2	17:O:44:ASP:HB2	1.47	1.44
3:C:38:LEU:CD2	16:Q:210:ARG:HD2	1.46	1.44
17:O:56:LEU:CD1	18:P:52:THR:H	1.18	1.43
17:O:55:ARG:C	18:P:52:THR:HG21	1.01	1.42
3:C:39:ARG:HH11	16:Q:148:ILE:CG2	1.29	1.41
17:O:9:THR:CG2	18:P:10:LYS:CE	1.86	1.41
14:N:207:UNK:C	14:N:208:UNK:N	1.79	1.40
17:O:11:TRP:CE2	18:P:86:ILE:HD12	1.55	1.40
16:Q:182:THR:N	17:O:44:ASP:CB	1.70	1.40
16:Q:482:VAL:HG12	17:O:49:LYS:N	1.30	1.39
17:O:11:TRP:CD1	18:P:83:LEU:CD2	1.93	1.39
16:Q:78:ARG:NH2	18:P:23:TYR:HE2	1.15	1.39
17:O:55:ARG:C	18:P:52:THR:CG2	1.96	1.39
17:O:27:ILE:CD1	18:P:59:PHE:HA	1.53	1.38
16:Q:78:ARG:NH2	18:P:23:TYR:CE2	1.88	1.38
16:Q:479:ILE:HG23	17:O:47:SER:CB	1.53	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:472:PHE:CD2	17:O:46:ILE:CG1	2.06	1.38
1:M:88:HIS:O	14:N:515:UNK:C	1.71	1.36
15:R:4:PHE:CZ	16:Q:377:ARG:NH1	1.94	1.35
17:O:22:ILE:CD1	18:P:43:ILE:CD1	1.76	1.35
8:K:469:LEU:CD1	12:L:2788:ILE:HG21	1.57	1.34
3:C:47:ASP:CB	16:Q:243:THR:O	1.75	1.34
17:O:19:LEU:HD23	18:P:67:GLU:CG	1.57	1.34
16:Q:464:ILE:HD12	17:O:46:ILE:CD1	1.44	1.33
14:N:451:UNK:C	14:N:452:UNK:H2	1.42	1.32
17:O:19:LEU:CD2	18:P:67:GLU:HG3	1.57	1.32
16:Q:106:TRP:HD1	17:O:20:ARG:CZ	1.41	1.31
16:Q:472:PHE:CB	17:O:46:ILE:HG13	1.60	1.31
16:Q:416:PHE:HE1	18:P:35:TYR:CE2	0.98	1.31
16:Q:479:ILE:HB	17:O:68:HIS:CE1	1.59	1.31
1:M:147:GLY:O	14:N:435:UNK:CB	1.78	1.30
3:C:34:LEU:CD2	16:Q:446:PHE:CE1	1.74	1.30
16:Q:416:PHE:CE1	18:P:35:TYR:CE2	1.87	1.30
16:Q:139:TYR:CB	17:O:28:LEU:HD21	1.62	1.29
3:C:38:LEU:CD1	16:Q:210:ARG:CZ	2.01	1.29
3:C:51:LEU:N	16:Q:214:LEU:HG	1.47	1.29
3:C:39:ARG:NH1	16:Q:148:ILE:N	1.74	1.28
3:C:54:CYS:SG	16:Q:215:SER:HA	1.72	1.28
17:O:30:GLU:OE1	18:P:51:VAL:HG11	1.28	1.28
17:O:27:ILE:HG23	18:P:57:PRO:O	1.20	1.27
17:O:19:LEU:HD21	18:P:67:GLU:CA	1.64	1.27
3:C:52:GLN:NE2	16:Q:153:GLN:HG3	1.47	1.27
16:Q:189:ASN:ND2	19:Q:602:HOH:O	1.59	1.27
16:Q:178:LEU:CD1	17:O:37:ILE:CD1	2.02	1.26
17:O:11:TRP:HE1	18:P:83:LEU:CA	1.46	1.26
16:Q:71:TYR:HD1	18:P:24:ASP:OD2	1.12	1.25
16:Q:93:CYS:SG	17:O:20:ARG:HD2	1.75	1.25
16:Q:472:PHE:HD2	17:O:46:ILE:CG1	1.45	1.25
17:O:34:ARG:NH1	18:P:57:PRO:HB3	0.93	1.24
16:Q:91:LEU:HD21	17:O:13:CYS:SG	1.76	1.24
3:C:54:CYS:SG	16:Q:215:SER:CA	2.26	1.23
1:M:194:ILE:C	1:M:195:TYR:N	1.97	1.22
17:O:56:LEU:HD11	18:P:52:THR:N	1.22	1.21
14:N:451:UNK:C	14:N:452:UNK:N	1.99	1.21
16:Q:139:TYR:CE1	17:O:24:ILE:HG12	1.37	1.21
16:Q:182:THR:CA	17:O:44:ASP:HB3	1.70	1.21
16:Q:71:TYR:CD1	18:P:24:ASP:OD2	1.92	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:50:ILE:N	16:Q:214:LEU:HD11	1.53	1.20
17:O:56:LEU:N	18:P:52:THR:HG21	1.55	1.20
12:L:828:ARG:H	12:L:829:PRO:HD3	1.06	1.20
16:Q:479:ILE:CG2	17:O:47:SER:CA	1.91	1.20
16:Q:416:PHE:CE1	18:P:35:TYR:CD2	2.29	1.20
16:Q:472:PHE:CZ	17:O:45:GLN:CB	2.23	1.20
17:O:27:ILE:HD13	18:P:59:PHE:CA	1.71	1.20
16:Q:474:PHE:CG	17:O:47:SER:HB3	1.75	1.19
1:M:194:ILE:HG22	1:M:195:TYR:N	1.57	1.19
3:C:49:PRO:CG	16:Q:237:PHE:CE1	2.24	1.19
16:Q:182:THR:CB	17:O:44:ASP:CB	2.13	1.19
17:O:54:GLN:HE22	18:P:49:SER:N	1.37	1.18
17:O:55:ARG:O	18:P:52:THR:HG21	1.43	1.18
15:R:4:PHE:HZ	16:Q:377:ARG:CZ	1.57	1.18
16:Q:106:TRP:CD1	17:O:20:ARG:CZ	2.27	1.18
3:C:39:ARG:NH1	16:Q:148:ILE:HA	1.34	1.18
16:Q:259:TRP:CD1	17:O:114:ASP:OD1	1.97	1.17
17:O:11:TRP:NE1	18:P:83:LEU:CA	2.06	1.17
17:O:11:TRP:CD2	18:P:86:ILE:HD12	1.80	1.16
3:C:39:ARG:HD2	16:Q:147:PHE:CE1	1.80	1.16
16:Q:474:PHE:CD2	17:O:47:SER:HB3	1.79	1.16
17:O:19:LEU:CD2	18:P:67:GLU:HA	1.75	1.16
3:C:39:ARG:NH1	16:Q:147:PHE:C	2.03	1.16
3:C:51:LEU:HD23	16:Q:214:LEU:HD23	1.27	1.16
3:C:49:PRO:C	16:Q:214:LEU:CD1	2.19	1.15
16:Q:139:TYR:HB3	17:O:28:LEU:CD2	1.76	1.15
16:Q:479:ILE:HD12	17:O:47:SER:HB2	1.25	1.14
17:O:34:ARG:NH1	18:P:57:PRO:CB	1.82	1.14
3:C:40:TYR:CB	16:Q:214:LEU:HD21	1.78	1.13
19:R:153:HOH:O	16:Q:326:LYS:HB3	1.44	1.13
17:O:22:ILE:HD12	18:P:43:ILE:CD1	1.75	1.13
16:Q:184:LEU:HD12	17:O:44:ASP:O	1.49	1.13
3:C:47:ASP:HB2	16:Q:243:THR:O	1.29	1.13
16:Q:479:ILE:CB	17:O:68:HIS:CE1	2.26	1.12
3:C:51:LEU:HD11	16:Q:211:ASP:O	1.44	1.12
16:Q:182:THR:N	17:O:44:ASP:HB3	1.42	1.11
3:C:38:LEU:HD13	16:Q:210:ARG:NE	0.80	1.11
3:C:40:TYR:HB3	16:Q:214:LEU:HD21	1.33	1.11
16:Q:91:LEU:CD2	17:O:13:CYS:SG	2.37	1.11
16:Q:464:ILE:HD11	17:O:46:ILE:HD13	1.28	1.11
16:Q:474:PHE:CD2	17:O:47:SER:CB	2.33	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:11:TRP:CE2	18:P:86:ILE:CD1	2.32	1.11
5:D:212:GLN:HE21	5:D:212:GLN:HA	1.12	1.11
16:Q:93:CYS:SG	17:O:20:ARG:HB2	1.89	1.11
16:Q:139:TYR:CE1	17:O:24:ILE:CG1	2.34	1.11
16:Q:464:ILE:HD11	17:O:46:ILE:HG21	1.18	1.10
14:N:501:UNK:HA	14:N:505:UNK:HA	1.30	1.09
1:M:191:PRO:HA	5:D:211:ARG:HD2	1.25	1.09
16:Q:416:PHE:HE1	18:P:35:TYR:CD2	1.68	1.09
8:K:466:PRO:HA	12:L:2791:PRO:HG2	1.33	1.08
16:Q:130:TYR:CG	17:O:28:LEU:CD1	2.36	1.08
17:O:55:ARG:O	18:P:52:THR:CG2	1.95	1.08
5:D:21:MET:HE3	5:D:250:PHE:HA	1.36	1.08
17:O:27:ILE:CG2	18:P:57:PRO:O	2.00	1.08
3:C:39:ARG:NH1	16:Q:148:ILE:CG2	2.09	1.07
8:K:469:LEU:CD1	12:L:2788:ILE:CG2	2.22	1.07
8:K:468:LEU:HB3	12:L:2829:LYS:HZ1	1.05	1.07
8:K:469:LEU:HD13	12:L:2788:ILE:HG22	1.30	1.07
16:Q:482:VAL:CG2	17:O:49:LYS:HD2	1.61	1.07
3:C:34:LEU:CD2	16:Q:446:PHE:CD1	2.38	1.07
3:C:50:ILE:N	16:Q:214:LEU:CD1	2.17	1.07
17:O:11:TRP:CD2	18:P:86:ILE:CD1	2.38	1.06
16:Q:479:ILE:HG22	17:O:47:SER:HA	1.09	1.06
3:C:47:ASP:HB3	16:Q:243:THR:O	1.53	1.05
16:Q:182:THR:CA	17:O:44:ASP:CB	2.30	1.05
16:Q:472:PHE:HB3	17:O:47:SER:C	1.51	1.05
16:Q:464:ILE:HD11	17:O:46:ILE:CG2	1.86	1.05
16:Q:501:GLN:HB2	18:P:31:ARG:HH22	1.17	1.05
3:C:54:CYS:SG	16:Q:215:SER:O	2.13	1.05
5:D:78:LYS:HE3	5:D:78:LYS:HA	1.38	1.05
16:Q:482:VAL:HG23	17:O:49:LYS:HD2	1.29	1.05
17:O:11:TRP:NE1	18:P:83:LEU:HD23	1.71	1.05
8:K:468:LEU:HB3	12:L:2829:LYS:NZ	1.70	1.04
15:R:4:PHE:CE1	16:Q:377:ARG:NH1	2.25	1.04
16:Q:472:PHE:CG	17:O:46:ILE:HG13	1.90	1.04
16:Q:182:THR:HG23	17:O:44:ASP:CB	1.85	1.03
16:Q:472:PHE:CE2	17:O:50:GLU:HG2	1.93	1.03
16:Q:464:ILE:HG13	17:O:46:ILE:CD1	1.87	1.03
16:Q:482:VAL:CG1	17:O:49:LYS:H	1.70	1.03
3:C:34:LEU:CG	16:Q:446:PHE:HE1	1.70	1.03
17:O:34:ARG:HH12	18:P:57:PRO:HB3	1.23	1.02
16:Q:182:THR:CB	17:O:44:ASP:HB2	1.78	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:472:PHE:HB2	17:O:46:ILE:CG1	1.88	1.02
3:C:39:ARG:HH11	16:Q:148:ILE:HG23	1.22	1.02
16:Q:472:PHE:CE1	17:O:45:GLN:HB3	1.94	1.02
16:Q:479:ILE:O	17:O:68:HIS:CE1	2.12	1.02
17:O:54:GLN:NE2	18:P:49:SER:N	2.07	1.01
17:O:15:MET:HE3	18:P:74:VAL:HG21	1.39	1.01
3:C:38:LEU:CD2	16:Q:210:ARG:CD	2.18	1.01
3:C:52:GLN:HE21	16:Q:153:GLN:HG3	0.94	1.00
16:Q:93:CYS:SG	17:O:20:ARG:CD	2.49	1.00
3:C:39:ARG:NH2	16:Q:147:PHE:O	1.94	1.00
16:Q:472:PHE:CE2	17:O:50:GLU:CG	2.44	1.00
16:Q:479:ILE:HB	17:O:68:HIS:HE1	0.83	1.00
16:Q:482:VAL:HG12	17:O:49:LYS:CA	1.73	1.00
16:Q:464:ILE:HD11	17:O:46:ILE:CD1	1.72	1.00
3:C:51:LEU:HG	16:Q:214:LEU:CB	1.92	1.00
3:C:34:LEU:CG	16:Q:446:PHE:CE1	2.42	0.99
16:Q:473:LYS:HA	17:O:48:LEU:HD23	1.40	0.99
3:C:51:LEU:HG	16:Q:214:LEU:HB3	1.43	0.99
3:C:51:LEU:CD1	16:Q:211:ASP:O	2.09	0.99
5:D:66:VAL:HG12	5:D:67:PRO:HD2	1.44	0.99
1:M:88:HIS:C	14:N:515:UNK:C	2.35	0.99
17:O:51:ILE:HG21	18:P:45:ARG:HG3	1.43	0.99
16:Q:472:PHE:HZ	17:O:45:GLN:HB3	1.21	0.98
17:O:9:THR:HG21	18:P:10:LYS:HE3	1.44	0.98
16:Q:259:TRP:HD1	17:O:114:ASP:OD1	1.39	0.98
17:O:55:ARG:HD2	18:P:53:ASN:OD1	1.63	0.98
3:C:54:CYS:SG	16:Q:215:SER:C	2.47	0.98
16:Q:178:LEU:HD13	17:O:37:ILE:HD12	1.43	0.97
15:R:46:ALA:HA	16:Q:331:PRO:O	1.64	0.97
1:M:173:GLU:HG2	5:D:197:LYS:HA	1.44	0.97
16:Q:472:PHE:HB2	17:O:46:ILE:HG13	0.99	0.97
16:Q:474:PHE:CD1	17:O:47:SER:HB3	1.99	0.97
17:O:22:ILE:CD1	18:P:43:ILE:HD12	1.92	0.97
17:O:11:TRP:HD1	18:P:83:LEU:HD21	1.28	0.97
16:Q:479:ILE:HD12	17:O:47:SER:CB	1.94	0.96
3:C:50:ILE:CA	16:Q:214:LEU:HD11	1.95	0.96
3:C:34:LEU:HD22	16:Q:446:PHE:CD1	1.97	0.96
14:N:467:UNK:O	14:N:470:UNK:CB	2.14	0.96
3:C:39:ARG:HH11	16:Q:148:ILE:HG22	1.27	0.96
14:N:451:UNK:C	14:N:452:UNK:CA	2.43	0.96
8:K:465:ARG:HH21	12:L:2843:GLY:H	1.10	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:93:CYS:SG	17:O:17:ASN:HA	2.06	0.96
16:Q:178:LEU:CD1	17:O:37:ILE:HD12	1.94	0.95
19:R:165:HOH:O	16:Q:355:LEU:HD11	1.63	0.95
16:Q:182:THR:CB	17:O:44:ASP:HB3	1.77	0.95
17:O:34:ARG:HH11	18:P:57:PRO:CG	1.78	0.95
16:Q:474:PHE:CE2	17:O:47:SER:CB	2.50	0.95
12:L:849:LEU:HD12	12:L:849:LEU:H	1.31	0.95
16:Q:479:ILE:CB	17:O:68:HIS:HE1	1.70	0.95
16:Q:481:LEU:HD12	17:O:50:GLU:H	1.28	0.95
16:Q:482:VAL:CG1	17:O:49:LYS:N	2.26	0.94
16:Q:444:GLN:NE2	18:P:35:TYR:HE2	1.65	0.94
3:C:51:LEU:N	16:Q:214:LEU:CG	2.31	0.94
16:Q:464:ILE:CD1	17:O:46:ILE:HD12	1.59	0.94
17:O:54:GLN:NE2	18:P:49:SER:HA	1.83	0.94
3:C:39:ARG:NH1	16:Q:148:ILE:CB	2.31	0.93
17:O:56:LEU:CD1	18:P:52:THR:N	1.91	0.93
16:Q:130:TYR:CD2	17:O:28:LEU:HD12	2.04	0.93
5:D:66:VAL:CG1	5:D:67:PRO:HD2	1.99	0.93
14:N:182:UNK:HA	14:N:198:UNK:CB	1.97	0.93
17:O:54:GLN:NE2	18:P:49:SER:CA	2.31	0.93
3:C:34:LEU:CD1	16:Q:446:PHE:CE1	2.51	0.93
3:C:50:ILE:CA	16:Q:214:LEU:CD1	2.45	0.93
5:D:212:GLN:HA	5:D:212:GLN:NE2	1.81	0.93
16:Q:139:TYR:HE1	17:O:24:ILE:HG12	1.19	0.93
16:Q:474:PHE:CE2	17:O:47:SER:HB3	2.04	0.93
16:Q:88:LEU:CB	18:P:11:GLN:HG2	1.98	0.93
16:Q:106:TRP:HD1	17:O:20:ARG:NH2	1.66	0.93
16:Q:474:PHE:HA	17:O:47:SER:OG	1.69	0.93
17:O:54:GLN:HE22	18:P:48:GLN:C	1.76	0.93
3:C:51:LEU:HD12	16:Q:215:SER:OG	1.66	0.92
12:L:828:ARG:H	12:L:829:PRO:CD	1.82	0.92
8:K:441:PRO:HA	12:L:912:LEU:HD21	1.51	0.92
17:O:19:LEU:HD21	18:P:67:GLU:HA	0.93	0.92
16:Q:182:THR:CG2	17:O:44:ASP:CB	2.35	0.92
16:Q:472:PHE:HD2	17:O:46:ILE:HG12	0.79	0.92
3:C:34:LEU:HD21	16:Q:446:PHE:CD1	2.03	0.92
3:C:52:GLN:HE21	16:Q:153:GLN:CG	1.82	0.92
16:Q:78:ARG:CZ	18:P:23:TYR:CD2	2.53	0.92
1:M:99:PHE:CE2	1:M:101:ALA:HB3	2.05	0.91
1:M:172:LEU:HB3	1:M:193:LEU:HD13	1.50	0.91
12:L:828:ARG:N	12:L:829:PRO:HD3	1.83	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:464:ILE:HG13	17:O:46:ILE:HD12	0.92	0.91
3:C:39:ARG:CD	16:Q:147:PHE:CE1	2.52	0.91
12:L:2916:ARG:NH2	12:L:2916:ARG:HB2	1.84	0.91
3:C:50:ILE:C	16:Q:214:LEU:HD11	1.95	0.91
16:Q:473:LYS:N	17:O:47:SER:O	2.00	0.91
17:O:9:THR:HG23	18:P:10:LYS:HZ2	1.34	0.91
1:M:87:LEU:HD13	14:N:490:UNK:HA	1.52	0.91
16:Q:480:THR:O	17:O:47:SER:O	1.88	0.90
3:C:49:PRO:O	16:Q:214:LEU:HD12	1.71	0.90
16:Q:472:PHE:CB	17:O:46:ILE:C	2.43	0.90
9:G:546:HIS:CD2	9:G:547:PRO:HD2	2.06	0.90
3:C:38:LEU:CD1	16:Q:210:ARG:NH1	2.34	0.90
3:C:40:TYR:HB3	16:Q:214:LEU:CD2	2.01	0.90
16:Q:464:ILE:CG1	17:O:46:ILE:CD1	2.20	0.89
3:C:34:LEU:HD21	16:Q:446:PHE:CE1	2.03	0.89
16:Q:182:THR:HG23	17:O:44:ASP:HB2	0.91	0.89
3:C:51:LEU:H	16:Q:214:LEU:HG	1.26	0.89
3:C:39:ARG:NH1	16:Q:148:ILE:HG22	1.81	0.89
16:Q:181:SER:N	17:O:44:ASP:OD1	1.92	0.89
3:C:34:LEU:HD13	16:Q:446:PHE:CE1	2.08	0.89
3:C:40:TYR:HB2	16:Q:214:LEU:HD21	1.54	0.89
19:R:153:HOH:O	16:Q:326:LYS:CG	2.21	0.88
8:K:468:LEU:CB	12:L:2829:LYS:HZ1	1.87	0.88
9:G:543:VAL:HG22	9:G:552:LEU:HD11	1.55	0.88
3:C:39:ARG:HD2	16:Q:147:PHE:HE1	1.36	0.88
1:M:88:HIS:HB3	14:N:515:UNK:O	1.74	0.88
1:M:194:ILE:CG2	1:M:195:TYR:N	2.36	0.88
16:Q:93:CYS:SG	17:O:20:ARG:CB	2.62	0.88
17:O:27:ILE:HD11	18:P:62:VAL:HB	1.54	0.88
16:Q:444:GLN:NE2	18:P:35:TYR:CE2	2.38	0.88
16:Q:464:ILE:CD1	17:O:46:ILE:HG21	2.01	0.88
1:M:188:GLU:OE1	5:D:85:ARG:NH2	2.07	0.87
3:C:38:LEU:HD13	16:Q:210:ARG:NH1	1.88	0.87
6:E:938:ILE:HD12	6:E:938:ILE:H	1.38	0.87
16:Q:472:PHE:CG	17:O:46:ILE:CG1	2.54	0.87
17:O:9:THR:CG2	18:P:10:LYS:NZ	2.38	0.87
17:O:11:TRP:NE1	18:P:86:ILE:HD12	1.90	0.87
16:Q:178:LEU:CG	17:O:37:ILE:HD13	2.04	0.86
16:Q:501:GLN:HB2	18:P:31:ARG:NH2	1.90	0.86
17:O:19:LEU:CD2	18:P:67:GLU:CB	2.53	0.86
5:D:216:THR:CG2	5:D:246:GLY:HA3	2.06	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:462:ILE:HB	12:L:2737:TYR:HE1	1.38	0.86
16:Q:178:LEU:HD12	17:O:37:ILE:CD1	2.04	0.86
17:O:30:GLU:OE1	18:P:51:VAL:CG1	2.20	0.86
16:Q:78:ARG:HH21	18:P:23:TYR:HE2	0.86	0.86
5:D:78:LYS:HE3	5:D:78:LYS:CA	2.06	0.86
12:L:2854:LEU:HD13	12:L:2906:TRP:CH2	2.11	0.85
16:Q:78:ARG:NH2	18:P:23:TYR:CD2	2.42	0.85
16:Q:125:ASP:OD1	17:O:24:ILE:HD13	1.75	0.85
16:Q:474:PHE:CD2	17:O:47:SER:HB2	2.11	0.85
16:Q:466:ASN:ND2	17:O:46:ILE:HG23	1.90	0.85
3:C:39:ARG:HH11	16:Q:148:ILE:CB	1.89	0.85
8:K:474:ILE:HD13	12:L:2592:ASP:HB3	1.59	0.85
8:K:469:LEU:HD13	12:L:2788:ILE:HG21	0.88	0.85
15:R:4:PHE:CZ	16:Q:377:ARG:CZ	2.44	0.85
16:Q:474:PHE:CE1	17:O:48:LEU:HG	2.11	0.85
17:O:19:LEU:CD2	18:P:67:GLU:CA	2.45	0.85
17:O:19:LEU:CD2	18:P:67:GLU:CG	2.31	0.85
8:K:442:PRO:HD2	12:L:912:LEU:HD22	1.58	0.85
16:Q:130:TYR:CD1	17:O:28:LEU:HD13	2.11	0.85
16:Q:139:TYR:CB	17:O:28:LEU:CD2	2.42	0.85
14:N:353:UNK:O	14:N:357:UNK:HA	1.76	0.85
9:G:650:ASP:HB3	9:G:693:MET:HE3	1.57	0.84
17:O:19:LEU:HD21	18:P:67:GLU:CB	2.07	0.84
16:Q:282:ASP:CG	19:Q:603:HOH:O	2.19	0.84
17:O:22:ILE:CD1	18:P:43:ILE:HD13	2.08	0.84
14:N:480:UNK:N	14:N:496:UNK:HA	1.93	0.84
16:Q:479:ILE:O	17:O:68:HIS:CD2	2.30	0.84
16:Q:78:ARG:CZ	18:P:23:TYR:HD2	1.91	0.83
3:C:38:LEU:CD1	16:Q:210:ARG:HE	1.52	0.83
16:Q:464:ILE:HD12	17:O:46:ILE:HD13	0.84	0.83
16:Q:472:PHE:CD2	17:O:46:ILE:HG13	1.92	0.83
16:Q:472:PHE:CB	17:O:47:SER:C	2.36	0.83
3:C:38:LEU:HD22	16:Q:210:ARG:CG	2.08	0.83
12:L:1425:PHE:O	12:L:1428:LEU:N	2.10	0.83
17:O:9:THR:HG21	18:P:10:LYS:CE	1.97	0.83
16:Q:106:TRP:CD1	17:O:20:ARG:NH2	2.43	0.83
16:Q:464:ILE:O	17:O:46:ILE:HD11	1.77	0.83
16:Q:472:PHE:HB3	17:O:47:SER:CA	2.07	0.83
16:Q:481:LEU:HA	17:O:49:LYS:HA	1.58	0.83
3:C:38:LEU:HD11	16:Q:211:ASP:OD1	1.78	0.83
16:Q:479:ILE:HA	17:O:47:SER:OG	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:546:HIS:CD2	9:G:547:PRO:CD	2.62	0.82
16:Q:474:PHE:CG	17:O:47:SER:CB	2.56	0.82
10:H:27:ALA:HB1	10:H:32:ILE:HD11	1.62	0.82
3:C:49:PRO:O	16:Q:214:LEU:CD1	2.27	0.82
14:N:84:UNK:HA	14:N:506:UNK:O	1.80	0.82
16:Q:481:LEU:O	17:O:49:LYS:CE	2.23	0.82
16:Q:481:LEU:O	17:O:49:LYS:HE2	1.80	0.82
1:M:189:LEU:HA	5:D:85:ARG:HG2	1.61	0.81
14:N:353:UNK:HA	14:N:356:UNK:O	1.80	0.81
16:Q:252:THR:HG23	17:O:109:PHE:CE1	2.15	0.81
8:K:454:PRO:N	8:K:455:PRO:HD2	1.95	0.81
1:M:82:LEU:HD13	1:M:101:ALA:HA	1.61	0.81
9:G:537:LEU:HD12	9:G:537:LEU:H	1.46	0.81
15:R:4:PHE:HZ	16:Q:377:ARG:NH1	1.47	0.81
2:A:246:LEU:HD11	8:K:537:VAL:HG21	1.62	0.81
3:C:51:LEU:CD2	16:Q:214:LEU:HD23	2.10	0.81
16:Q:474:PHE:CE1	17:O:47:SER:HB3	2.16	0.81
12:L:1203:LEU:O	12:L:1203:LEU:HD23	1.81	0.80
16:Q:178:LEU:HD13	17:O:37:ILE:HD13	0.82	0.80
16:Q:479:ILE:O	17:O:68:HIS:CG	2.34	0.80
3:C:45:ASN:HD21	16:Q:171:ASP:HA	1.44	0.80
16:Q:472:PHE:CD2	17:O:46:ILE:N	2.49	0.80
16:Q:479:ILE:HG23	17:O:47:SER:HB2	1.62	0.80
3:C:45:ASN:HD21	16:Q:171:ASP:CA	1.91	0.80
14:N:221:UNK:CA	14:N:230:UNK:HA	2.11	0.80
1:M:81:ASP:HB2	14:N:433:UNK:O	1.80	0.80
17:O:55:ARG:CA	18:P:52:THR:HG21	2.12	0.80
17:O:24:ILE:HG13	18:P:59:PHE:CE1	2.17	0.80
3:C:49:PRO:C	16:Q:214:LEU:HD12	2.07	0.80
3:C:50:ILE:C	16:Q:214:LEU:CD1	2.54	0.80
3:C:55:LEU:HD23	16:Q:160:ILE:HG12	1.63	0.80
9:G:478:ARG:NH1	9:G:487:CYS:SG	2.55	0.80
3:C:38:LEU:HD13	16:Q:210:ARG:HE	0.98	0.80
16:Q:91:LEU:HD23	17:O:13:CYS:HB3	1.62	0.80
16:Q:470:ASN:HA	17:O:51:ILE:N	1.97	0.79
3:C:51:LEU:CD1	16:Q:215:SER:OG	2.31	0.79
16:Q:130:TYR:HB3	17:O:28:LEU:HD11	1.64	0.79
1:M:173:GLU:CG	5:D:197:LYS:HA	2.13	0.79
14:N:221:UNK:HA	14:N:230:UNK:HA	1.63	0.79
17:O:9:THR:HG23	18:P:10:LYS:NZ	1.97	0.79
16:Q:474:PHE:CZ	17:O:47:SER:N	2.49	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:51:ILE:CG2	18:P:45:ARG:HG3	2.12	0.79
17:O:54:GLN:NE2	18:P:48:GLN:C	2.40	0.79
3:C:51:LEU:CG	16:Q:214:LEU:HB3	2.13	0.79
16:Q:182:THR:HG21	17:O:45:GLN:H	1.47	0.79
16:Q:315:SER:CB	19:Q:605:HOH:O	2.31	0.79
8:K:453:LYS:C	8:K:455:PRO:HD2	2.08	0.79
16:Q:464:ILE:HD11	17:O:46:ILE:CB	2.13	0.79
17:O:9:THR:HG21	18:P:10:LYS:CD	2.13	0.79
16:Q:88:LEU:HB3	18:P:11:GLN:HG2	1.65	0.79
17:O:56:LEU:HD11	18:P:51:VAL:C	2.07	0.78
3:C:51:LEU:HD12	16:Q:215:SER:N	1.97	0.78
3:C:39:ARG:CZ	16:Q:148:ILE:HA	2.12	0.78
5:D:303:PRO:HB2	5:D:304:ILE:HG12	1.66	0.78
1:M:176:ALA:HB2	1:M:193:LEU:HD11	1.65	0.78
1:M:191:PRO:CA	5:D:211:ARG:HD2	2.09	0.78
8:K:465:ARG:HH21	12:L:2843:GLY:N	1.82	0.78
1:M:191:PRO:HA	5:D:211:ARG:CD	2.12	0.78
16:Q:472:PHE:CE2	17:O:46:ILE:N	2.51	0.78
6:E:938:ILE:HD12	6:E:938:ILE:N	1.99	0.78
16:Q:474:PHE:CD1	17:O:48:LEU:HG	2.18	0.78
3:C:39:ARG:CZ	16:Q:147:PHE:O	2.30	0.78
10:H:127:LEU:O	10:H:127:LEU:HD12	1.84	0.77
17:O:9:THR:HG23	18:P:10:LYS:CE	2.13	0.77
1:M:108:GLU:HA	1:M:110:LYS:N	1.99	0.77
17:O:27:ILE:HD12	18:P:59:PHE:CD1	2.18	0.77
16:Q:470:ASN:HA	17:O:51:ILE:H	1.50	0.77
16:Q:482:VAL:CG1	17:O:49:LYS:CA	2.48	0.77
3:C:38:LEU:CG	16:Q:210:ARG:NE	2.47	0.77
16:Q:107:LYS:CG	17:O:20:ARG:NH2	2.47	0.77
16:Q:178:LEU:HD22	17:O:37:ILE:HG21	1.64	0.77
16:Q:139:TYR:HB3	17:O:28:LEU:HD21	0.84	0.77
16:Q:474:PHE:CE1	17:O:48:LEU:N	2.52	0.77
17:O:27:ILE:HD13	18:P:59:PHE:HA	0.79	0.77
3:C:39:ARG:NH1	16:Q:147:PHE:O	2.16	0.77
3:C:51:LEU:HD11	16:Q:211:ASP:C	2.09	0.77
3:C:45:ASN:ND2	16:Q:171:ASP:CA	2.48	0.77
12:L:2593:TYR:H	12:L:2596:ARG:HG2	1.48	0.77
16:Q:479:ILE:O	17:O:68:HIS:NE2	2.16	0.77
3:C:44:ASN:OD1	16:Q:174:ARG:HG3	1.85	0.76
5:D:317:GLN:C	5:D:319:ARG:H	1.93	0.76
12:L:1122:ASN:HD22	12:L:1122:ASN:N	1.82	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:130:TYR:CG	17:O:28:LEU:HD13	2.20	0.76
16:Q:474:PHE:CE2	17:O:47:SER:HB2	2.18	0.76
17:O:11:TRP:CD1	18:P:83:LEU:CG	2.68	0.76
16:Q:479:ILE:CG2	17:O:47:SER:CB	2.49	0.76
12:L:1354:LEU:HA	12:L:1357:LEU:HD22	1.68	0.76
17:O:11:TRP:CZ2	18:P:86:ILE:HG13	2.20	0.76
16:Q:282:ASP:OD1	19:Q:603:HOH:O	2.02	0.76
1:M:101:ALA:HB1	1:M:115:ILE:O	1.85	0.76
12:L:2854:LEU:HD13	12:L:2906:TRP:HH2	1.49	0.76
2:A:239:GLU:N	2:A:239:GLU:OE1	2.18	0.76
3:C:37:PRO:O	16:Q:467:ARG:NH2	2.18	0.76
5:D:323:LYS:HE2	7:J:107:PHE:HD1	1.51	0.76
12:L:2916:ARG:HB2	12:L:2916:ARG:CZ	2.16	0.76
16:Q:130:TYR:CB	17:O:28:LEU:HD11	2.15	0.76
3:C:44:ASN:HD21	16:Q:174:ARG:HG3	1.51	0.76
12:L:2907:ARG:HH11	12:L:2907:ARG:HG2	1.51	0.76
16:Q:130:TYR:CD2	17:O:28:LEU:CD1	2.67	0.76
12:L:2884:GLN:HA	12:L:2884:GLN:NE2	2.00	0.75
16:Q:107:LYS:NZ	17:O:13:CYS:HA	2.00	0.75
17:O:11:TRP:CD2	18:P:86:ILE:HD11	2.20	0.75
3:C:52:GLN:NE2	16:Q:153:GLN:CG	2.40	0.75
12:L:844:VAL:HB	12:L:849:LEU:HD22	1.68	0.75
3:C:45:ASN:ND2	16:Q:171:ASP:HA	2.01	0.75
3:C:49:PRO:C	16:Q:214:LEU:HD13	2.11	0.75
3:C:51:LEU:CA	16:Q:214:LEU:HG	2.16	0.75
12:L:2601:ARG:HB3	12:L:2602:PRO:HD2	1.68	0.75
16:Q:466:ASN:HD22	17:O:46:ILE:HG23	1.50	0.75
16:Q:478:ARG:HG3	17:O:68:HIS:HD2	1.51	0.75
17:O:34:ARG:HH22	18:P:51:VAL:HG11	1.52	0.75
16:Q:474:PHE:CZ	17:O:47:SER:HB3	2.20	0.75
8:K:462:ILE:HB	12:L:2737:TYR:CE1	2.20	0.75
1:M:104:MET:HE1	1:M:143:ILE:HG23	1.69	0.74
2:A:327:ARG:NH1	2:A:328:HIS:O	2.20	0.74
10:H:129:LYS:HZ2	10:H:129:LYS:HA	1.52	0.74
16:Q:472:PHE:HB3	17:O:46:ILE:C	2.10	0.74
17:O:9:THR:HG21	18:P:10:LYS:HD2	1.69	0.74
5:D:322:GLU:OE2	5:D:322:GLU:HA	1.87	0.74
14:N:223:UNK:H	14:N:230:UNK:CB	2.00	0.74
16:Q:78:ARG:HH12	18:P:27:SER:CB	1.99	0.74
16:Q:474:PHE:HZ	17:O:46:ILE:HB	1.50	0.74
17:O:55:ARG:O	18:P:52:THR:HG23	1.84	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:428:LYS:HE2	12:L:430:GLU:HG3	1.68	0.74
16:Q:259:TRP:NE1	17:O:114:ASP:HA	2.02	0.74
3:C:38:LEU:CD1	16:Q:211:ASP:OD1	2.36	0.74
5:D:72:PHE:O	5:D:75:ARG:HB2	1.87	0.74
17:O:11:TRP:CE2	18:P:83:LEU:HA	2.20	0.74
3:C:55:LEU:HD11	16:Q:173:SER:OG	1.88	0.74
16:Q:478:ARG:HA	17:O:68:HIS:CD2	2.22	0.74
3:C:51:LEU:HD23	16:Q:214:LEU:CD2	2.15	0.74
8:K:441:PRO:HA	12:L:912:LEU:CD2	2.17	0.74
17:O:56:LEU:N	18:P:52:THR:CG2	2.33	0.74
16:Q:130:TYR:HE2	17:O:25:ASN:OD1	1.70	0.73
3:C:49:PRO:CG	16:Q:237:PHE:HE1	1.85	0.73
9:G:414:ILE:HB	9:G:449:LEU:HB2	1.68	0.73
16:Q:78:ARG:NE	18:P:23:TYR:HD2	1.86	0.73
17:O:11:TRP:CG	18:P:86:ILE:HD12	2.23	0.73
17:O:19:LEU:HD23	18:P:67:GLU:HG3	0.78	0.73
16:Q:479:ILE:C	17:O:68:HIS:CE1	2.52	0.73
16:Q:501:GLN:CB	18:P:31:ARG:HH22	2.00	0.73
16:Q:107:LYS:HG3	17:O:20:ARG:NH2	2.03	0.73
3:C:49:PRO:HG2	16:Q:237:PHE:HE1	0.98	0.73
12:L:1417:ARG:HA	12:L:1420:ILE:HD12	1.70	0.73
3:C:38:LEU:HB2	16:Q:210:ARG:NH2	2.03	0.73
14:N:207:UNK:C	14:N:208:UNK:CB	2.67	0.73
14:N:451:UNK:C	14:N:452:UNK:HA	2.19	0.73
9:G:537:LEU:HD12	9:G:537:LEU:N	2.04	0.73
9:G:568:ARG:HG2	9:G:570:GLU:HG2	1.69	0.73
9:G:546:HIS:HB2	9:G:553:PHE:HE1	1.54	0.72
14:N:221:UNK:C	14:N:230:UNK:HA	2.19	0.72
5:D:78:LYS:HA	5:D:78:LYS:CE	2.17	0.72
9:G:67:ARG:O	9:G:70:SER:OG	2.07	0.72
3:C:44:ASN:ND2	16:Q:174:ARG:HG3	2.05	0.72
3:C:54:CYS:SG	16:Q:215:SER:CB	2.77	0.72
4:F:115:VAL:HG22	4:F:190:LEU:HD21	1.71	0.72
12:L:849:LEU:HD12	12:L:849:LEU:N	2.03	0.72
17:O:54:GLN:HE21	18:P:49:SER:HA	1.53	0.72
16:Q:481:LEU:CD1	17:O:50:GLU:H	2.01	0.72
3:C:50:ILE:CA	16:Q:214:LEU:HD12	2.18	0.72
8:K:453:LYS:HG2	8:K:455:PRO:HD2	1.71	0.72
17:O:19:LEU:HD13	18:P:70:ALA:CB	2.20	0.72
3:C:38:LEU:HD12	16:Q:210:ARG:NH1	2.03	0.72
5:D:73:LEU:HD23	5:D:73:LEU:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:12:THR:N	16:Q:360:GLU:OE1	2.22	0.72
1:M:188:GLU:CG	5:D:247:PHE:HA	2.20	0.72
16:Q:472:PHE:HB3	17:O:47:SER:N	2.05	0.72
5:D:216:THR:HB	5:D:243:ASP:HA	1.70	0.71
7:J:66:MET:O	7:J:98:ARG:NH1	2.24	0.71
16:Q:107:LYS:CG	17:O:20:ARG:HH22	2.03	0.71
17:O:7:GLN:HG3	18:P:86:ILE:HB	1.72	0.71
16:Q:91:LEU:HD21	17:O:13:CYS:HG	1.50	0.71
5:D:320:ASN:C	5:D:322:GLU:H	1.95	0.71
16:Q:130:TYR:CG	17:O:28:LEU:HD11	2.24	0.71
3:C:54:CYS:HG	16:Q:215:SER:C	1.86	0.71
16:Q:482:VAL:O	17:O:50:GLU:O	2.09	0.71
14:N:451:UNK:O	14:N:452:UNK:N	2.21	0.71
1:M:87:LEU:CD1	14:N:490:UNK:CA	2.66	0.70
1:M:90:ARG:HH11	14:N:513:UNK:CB	2.04	0.70
8:K:468:LEU:O	12:L:2829:LYS:NZ	2.18	0.70
9:G:457:TYR:HE2	9:G:473:GLU:HB3	1.57	0.70
17:O:7:GLN:HG2	18:P:83:LEU:CD2	2.21	0.70
3:C:39:ARG:CD	16:Q:147:PHE:HE1	1.96	0.70
16:Q:472:PHE:HE2	17:O:50:GLU:OE2	1.74	0.70
16:Q:76:ARG:HH22	18:P:19:GLU:N	1.89	0.70
1:M:188:GLU:HG2	5:D:247:PHE:HA	1.72	0.70
8:K:474:ILE:CD1	12:L:2592:ASP:HB3	2.21	0.70
14:N:207:UNK:C	14:N:208:UNK:CA	2.68	0.70
16:Q:482:VAL:HG12	17:O:49:LYS:H	0.87	0.70
3:C:55:LEU:CD2	16:Q:160:ILE:HG23	2.22	0.70
16:Q:464:ILE:HD11	17:O:46:ILE:CG1	2.20	0.70
12:L:846:LEU:HG	12:L:850:VAL:HG11	1.74	0.70
16:Q:88:LEU:HB2	18:P:11:GLN:HG2	1.73	0.70
17:O:19:LEU:HD23	18:P:67:GLU:CB	2.19	0.70
16:Q:125:ASP:OD1	17:O:24:ILE:CD1	2.40	0.69
16:Q:326:LYS:O	19:Q:604:HOH:O	2.08	0.69
3:C:39:ARG:HH22	16:Q:150:GLN:HE21	1.40	0.69
3:C:49:PRO:HG2	16:Q:237:PHE:CD1	2.21	0.69
8:K:466:PRO:CA	12:L:2791:PRO:HG2	2.19	0.69
8:K:550:HIS:NE2	11:I:80:ASP:OD1	2.25	0.69
16:Q:76:ARG:HH22	18:P:18:VAL:C	1.99	0.69
16:Q:178:LEU:CB	17:O:37:ILE:HD13	2.22	0.69
16:Q:482:VAL:O	17:O:49:LYS:C	2.35	0.69
8:K:580:GLU:O	11:I:65:SER:N	2.25	0.69
3:C:47:ASP:HB3	16:Q:243:THR:HB	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:948:GLN:HA	6:E:948:GLN:OE1	1.93	0.69
16:Q:472:PHE:CE2	17:O:50:GLU:OE2	2.45	0.69
4:F:202:LEU:O	4:F:205:THR:OG1	2.08	0.69
16:Q:107:LYS:HZ3	17:O:13:CYS:HA	1.58	0.69
17:O:11:TRP:CD2	18:P:82:ILE:HG23	2.28	0.69
17:O:11:TRP:CE3	18:P:86:ILE:HD11	2.27	0.69
17:O:11:TRP:CD1	18:P:86:ILE:HD12	2.27	0.69
3:C:39:ARG:CZ	16:Q:148:ILE:HG22	2.23	0.68
16:Q:473:LYS:O	17:O:47:SER:OG	2.11	0.68
5:D:20:MET:SD	5:D:213:ALA:HB3	2.34	0.68
3:C:39:ARG:NE	16:Q:147:PHE:CD1	2.62	0.68
8:K:456:GLN:HA	12:L:2669:MET:HG3	1.74	0.68
9:G:581:ALA:HB3	9:G:599:GLU:HG2	1.75	0.68
5:D:20:MET:SD	5:D:210:CYS:HA	2.34	0.68
9:G:118:CYS:SG	9:G:119:GLU:N	2.67	0.68
16:Q:78:ARG:CZ	18:P:23:TYR:CE2	2.71	0.68
17:O:55:ARG:HB3	18:P:52:THR:HG22	1.74	0.68
16:Q:188:ILE:HD13	17:O:93:GLU:OE1	1.93	0.68
3:C:38:LEU:HD11	16:Q:210:ARG:HE	1.51	0.68
8:K:468:LEU:C	12:L:2829:LYS:HZ3	2.01	0.68
9:G:620:HIS:CE1	9:G:641:GLY:HA3	2.29	0.68
17:O:19:LEU:HD11	18:P:66:ILE:HG22	1.76	0.68
9:G:376:ALA:HB1	9:G:693:MET:HE1	1.74	0.67
16:Q:464:ILE:O	17:O:48:LEU:HB2	1.93	0.67
16:Q:479:ILE:O	17:O:68:HIS:ND1	2.27	0.67
3:C:38:LEU:CD2	16:Q:210:ARG:CG	2.71	0.67
12:L:846:LEU:HA	12:L:850:VAL:HB	1.77	0.67
3:C:51:LEU:HG	16:Q:214:LEU:CG	2.24	0.67
5:D:73:LEU:HD23	5:D:73:LEU:C	2.19	0.67
6:E:817:GLY:N	7:J:69:GLU:OE2	2.26	0.67
12:L:849:LEU:H	12:L:849:LEU:CD1	2.06	0.67
14:N:175:UNK:HA	14:N:213:UNK:C	2.24	0.67
16:Q:416:PHE:CE1	18:P:35:TYR:CG	2.67	0.67
16:Q:479:ILE:CG2	17:O:47:SER:N	2.57	0.67
3:C:51:LEU:HD12	16:Q:215:SER:CB	2.25	0.67
9:G:594:LEU:HG	9:G:606:TRP:HB2	1.75	0.67
5:D:66:VAL:HG12	5:D:67:PRO:CD	2.22	0.67
8:K:447:PRO:HG3	12:L:2788:ILE:HG23	1.77	0.67
11:I:48:GLN:O	11:I:51:THR:OG1	2.11	0.67
9:G:376:ALA:CB	9:G:693:MET:HE1	2.25	0.66
16:Q:91:LEU:HD23	17:O:13:CYS:CB	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:338:GLU:OE2	19:Q:601:HOH:O	0.66	0.66
3:C:34:LEU:HD21	16:Q:446:PHE:HD1	1.60	0.66
8:K:453:LYS:HG2	8:K:455:PRO:CD	2.26	0.66
9:G:157:TYR:O	9:G:161:SER:N	2.28	0.66
5:D:241:VAL:HA	5:D:244:ILE:HD12	1.78	0.66
17:O:11:TRP:CE2	18:P:82:ILE:HG23	2.31	0.66
3:C:50:ILE:HA	16:Q:214:LEU:HD12	1.77	0.66
6:E:938:ILE:H	6:E:938:ILE:CD1	2.08	0.66
9:G:520:ARG:HG3	9:G:532:ILE:HG12	1.78	0.66
14:N:426:UNK:CB	14:N:481:UNK:HA	2.26	0.66
10:H:129:LYS:HA	10:H:129:LYS:NZ	2.11	0.66
10:H:404:VAL:HG12	10:H:407:TRP:CZ2	2.31	0.66
6:E:946:LYS:HE2	6:E:946:LYS:HA	1.78	0.66
14:N:83:UNK:N	14:N:506:UNK:HA	2.10	0.66
9:G:43:ALA:N	9:G:45:ASP:OD1	2.28	0.65
16:Q:479:ILE:CD1	17:O:47:SER:HB2	2.16	0.65
12:L:2802:LEU:HD12	12:L:2815:VAL:HG11	1.77	0.65
12:L:2849:GLN:NE2	12:L:2889:ARG:O	2.29	0.65
5:D:320:ASN:C	5:D:322:GLU:N	2.53	0.65
16:Q:78:ARG:HD3	18:P:23:TYR:CD2	2.32	0.65
16:Q:182:THR:HG21	17:O:45:GLN:N	2.12	0.65
17:O:51:ILE:HD12	18:P:48:GLN:OE1	1.96	0.65
16:Q:107:LYS:HG2	17:O:20:ARG:NH2	2.11	0.65
5:D:76:HIS:C	5:D:78:LYS:H	2.04	0.65
14:N:84:UNK:HA	14:N:506:UNK:C	2.26	0.65
8:K:454:PRO:N	8:K:455:PRO:CD	2.59	0.65
3:C:39:ARG:CZ	16:Q:147:PHE:C	2.70	0.65
16:Q:91:LEU:CD2	17:O:13:CYS:CB	2.75	0.65
4:F:278:ALA:HB3	8:K:521:ILE:HG12	1.79	0.65
11:I:128:GLU:N	11:I:128:GLU:OE1	2.28	0.64
1:M:82:LEU:HB3	1:M:94:TYR:HE2	1.60	0.64
5:D:71:ILE:O	5:D:74:ILE:HG12	1.97	0.64
6:E:952:ASN:ND2	11:I:138:VAL:O	2.30	0.64
8:K:469:LEU:HD12	12:L:2788:ILE:HG21	1.72	0.64
16:Q:472:PHE:HZ	17:O:45:GLN:CB	1.89	0.64
17:O:34:ARG:HE	18:P:57:PRO:HG3	1.62	0.64
5:D:326:ILE:O	5:D:328:ASN:N	2.30	0.64
8:K:582:ARG:NH2	11:I:70:ALA:O	2.30	0.64
15:R:42:ARG:NH1	15:R:49:GLN:OE1	2.28	0.64
3:C:55:LEU:HD21	16:Q:160:ILE:HG23	1.80	0.64
5:D:76:HIS:C	5:D:78:LYS:N	2.53	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:154:ARG:NH2	9:G:179:SER:OG	2.31	0.64
12:L:848:VAL:C	12:L:851:PRO:HD2	2.23	0.64
12:L:1425:PHE:O	12:L:1427:SER:N	2.31	0.64
12:L:3303:SER:HB3	12:L:3427:PHE:HD2	1.61	0.64
3:C:34:LEU:HD13	16:Q:446:PHE:CZ	2.33	0.64
9:G:553:PHE:CZ	9:G:563:MET:HE3	2.33	0.64
14:N:467:UNK:C	14:N:470:UNK:CB	2.76	0.64
16:Q:474:PHE:HE1	17:O:48:LEU:HG	1.61	0.64
16:Q:481:LEU:HD11	17:O:50:GLU:HB2	1.78	0.64
17:O:7:GLN:HG2	18:P:83:LEU:HD22	1.79	0.64
17:O:56:LEU:HD13	18:P:51:VAL:HB	1.80	0.64
3:C:51:LEU:HD12	16:Q:215:SER:CA	2.27	0.64
17:O:55:ARG:CB	18:P:52:THR:HG22	2.27	0.64
5:D:259:GLU:HG3	5:D:316:LEU:HD21	1.80	0.64
7:J:67:GLU:OE1	7:J:95:LYS:NZ	2.30	0.64
12:L:328:ARG:HD3	12:L:370:THR:HG22	1.79	0.64
1:M:169:PRO:HA	1:M:208:VAL:O	1.99	0.63
3:C:44:ASN:CG	16:Q:174:ARG:HG3	2.23	0.63
5:D:21:MET:CE	5:D:250:PHE:HA	2.21	0.63
14:N:184:UNK:CB	14:N:237:UNK:HA	2.27	0.63
16:Q:315:SER:HB2	19:Q:605:HOH:O	1.97	0.63
17:O:11:TRP:CZ2	18:P:86:ILE:CD1	2.81	0.63
5:D:248:LEU:O	5:D:251:GLU:HG2	1.98	0.63
9:G:494:HIS:NE2	9:G:520:ARG:HD3	2.14	0.63
10:H:375:ASN:ND2	10:H:377:THR:O	2.31	0.63
16:Q:478:ARG:CD	17:O:76:ASN:HD21	2.11	0.63
14:N:221:UNK:HA	14:N:229:UNK:O	1.97	0.63
3:C:52:GLN:CD	16:Q:153:GLN:HG3	2.21	0.63
17:O:55:ARG:CB	18:P:52:THR:CG2	2.77	0.63
12:L:2878:GLU:HA	12:L:2881:ARG:HD3	1.79	0.63
14:N:83:UNK:HA	14:N:505:UNK:O	1.99	0.63
16:Q:106:TRP:CD1	17:O:20:ARG:NE	2.67	0.63
3:C:38:LEU:CG	16:Q:210:ARG:CD	2.77	0.63
3:C:51:LEU:HG	16:Q:214:LEU:C	2.24	0.63
12:L:365:PRO:HB3	12:L:407:VAL:HG11	1.81	0.63
12:L:2854:LEU:HD13	12:L:2906:TRP:CZ2	2.33	0.62
5:D:87:TYR:CD1	5:D:87:TYR:C	2.77	0.62
9:G:647:ARG:NH2	10:H:167:ARG:O	2.32	0.62
1:M:177:PHE:HB2	5:D:194:GLU:HA	1.80	0.62
17:O:34:ARG:HH22	18:P:51:VAL:CG1	2.11	0.62
12:L:846:LEU:HA	12:L:850:VAL:CG2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:478:ARG:CA	17:O:68:HIS:CD2	2.81	0.62
16:Q:139:TYR:HB2	17:O:28:LEU:CD2	2.27	0.62
5:D:17:ILE:N	5:D:17:ILE:HD12	2.14	0.62
12:L:2880:LYS:H	12:L:2880:LYS:HD2	1.64	0.62
16:Q:464:ILE:O	17:O:46:ILE:CD1	2.46	0.62
9:G:462:SER:OG	9:G:464:ASP:OD1	2.04	0.62
8:K:439:PRO:HB3	12:L:916:HIS:CE1	2.34	0.62
10:H:217:LEU:HD12	10:H:218:SER:H	1.65	0.62
12:L:1122:ASN:N	12:L:1122:ASN:ND2	2.44	0.62
9:G:546:HIS:CD2	9:G:547:PRO:HD3	2.35	0.61
12:L:3501:PHE:HB2	12:L:3523:LEU:HD21	1.81	0.61
17:O:9:THR:CG2	18:P:10:LYS:CD	2.65	0.61
1:M:189:LEU:HB3	5:D:84:LEU:HD22	1.81	0.61
3:C:47:ASP:HB3	16:Q:243:THR:C	2.25	0.61
5:D:49:ILE:HG23	5:D:73:LEU:HD13	1.82	0.61
3:C:39:ARG:NH2	16:Q:150:GLN:HE21	1.97	0.61
3:C:51:LEU:HD11	16:Q:211:ASP:HA	1.82	0.61
16:Q:472:PHE:HZ	17:O:45:GLN:CG	2.13	0.61
3:C:38:LEU:CG	16:Q:210:ARG:HD2	2.26	0.61
10:H:317:LEU:O	10:H:380:THR:HG22	2.00	0.61
17:O:26:ASN:HD22	18:P:47:THR:CB	2.13	0.61
1:M:115:ILE:HD13	1:M:121:MET:SD	2.40	0.61
10:H:265:PHE:CE2	10:H:289:LEU:HD11	2.36	0.61
12:L:1611:ASP:HA	12:L:1617:ARG:HH12	1.65	0.61
5:D:317:GLN:C	5:D:319:ARG:N	2.55	0.61
9:G:87:ASN:ND2	9:G:219:ALA:O	2.33	0.61
9:G:450:VAL:HG22	9:G:451:GLY:H	1.65	0.61
12:L:2812:LEU:O	12:L:2815:VAL:HG22	1.99	0.61
16:Q:474:PHE:HE1	17:O:48:LEU:H	1.46	0.61
1:M:204:LEU:HD23	1:M:212:ILE:HD12	1.83	0.61
5:D:78:LYS:O	5:D:78:LYS:HD3	2.01	0.61
15:R:12:THR:HG21	16:Q:379:LYS:HE3	1.83	0.61
8:K:461:LYS:HZ2	12:L:2792:ARG:NE	1.99	0.61
17:O:56:LEU:HD11	18:P:52:THR:H	0.45	0.60
2:A:289:ILE:O	6:E:958:LEU:HD21	2.01	0.60
5:D:320:ASN:CB	5:D:324:LYS:HB2	2.32	0.60
6:E:946:LYS:HA	6:E:946:LYS:CE	2.32	0.60
5:D:216:THR:HG23	5:D:246:GLY:HA3	1.83	0.60
12:L:428:LYS:HG3	12:L:430:GLU:HG2	1.84	0.60
3:C:39:ARG:CZ	16:Q:147:PHE:CD1	2.85	0.60
6:E:890:LEU:HD22	6:E:915:THR:HG23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:44:ASN:OD1	16:Q:174:ARG:CG	2.49	0.60
12:L:2907:ARG:HG2	12:L:2907:ARG:NH1	2.10	0.60
16:Q:478:ARG:CG	17:O:68:HIS:HD2	2.14	0.60
9:G:620:HIS:HA	9:G:647:ARG:HE	1.67	0.60
12:L:704:LEU:HD13	12:L:749:SER:HB2	1.82	0.60
14:N:221:UNK:HA	14:N:230:UNK:CA	2.32	0.60
17:O:27:ILE:CD1	18:P:59:PHE:CA	2.49	0.60
9:G:518:THR:HG21	11:I:102:LEU:HD22	1.82	0.60
12:L:3439:HIS:C	12:L:3440:LYS:HG2	2.27	0.60
10:H:277:LEU:O	10:H:320:LYS:NZ	2.34	0.60
12:L:853:LEU:O	12:L:855:TYR:N	2.35	0.60
12:L:1837:ASP:OD1	12:L:1840:ARG:NH1	2.35	0.60
12:L:3652:ILE:HG22	12:L:3659:ILE:HG12	1.82	0.60
16:Q:184:LEU:CD1	17:O:44:ASP:O	2.39	0.60
1:M:188:GLU:HA	1:M:188:GLU:OE2	2.02	0.60
5:D:88:LEU:C	5:D:88:LEU:HD13	2.27	0.60
1:M:185:TYR:OH	5:D:211:ARG:HD3	2.02	0.59
10:H:269:ILE:O	10:H:272:THR:OG1	2.16	0.59
12:L:3736:SER:OG	12:L:3737:GLU:N	2.35	0.59
16:Q:78:ARG:CD	18:P:23:TYR:CD2	2.85	0.59
16:Q:379:LYS:HE3	19:Q:607:HOH:O	2.02	0.59
1:M:202:ILE:HD11	1:M:217:ALA:HB2	1.84	0.59
3:C:38:LEU:CD1	16:Q:210:ARG:CD	2.75	0.59
3:C:38:LEU:HD12	16:Q:210:ARG:CZ	2.19	0.59
3:C:39:ARG:NE	16:Q:148:ILE:HG22	2.17	0.59
8:K:437:LEU:H	8:K:437:LEU:HD23	1.67	0.59
16:Q:91:LEU:HD23	17:O:13:CYS:SG	2.39	0.59
17:O:22:ILE:HD12	18:P:43:ILE:HD13	1.75	0.59
4:F:119:GLU:OE1	4:F:119:GLU:N	2.36	0.59
8:K:469:LEU:CD1	12:L:2788:ILE:HG22	2.14	0.59
16:Q:474:PHE:CZ	17:O:47:SER:CB	2.83	0.59
12:L:1352:GLU:HA	12:L:1355:ASN:HB2	1.83	0.59
2:A:226:ILE:HA	2:A:229:PHE:CE2	2.37	0.59
16:Q:468:ASP:O	17:O:51:ILE:HD11	2.03	0.59
1:M:104:MET:HE1	1:M:143:ILE:CG2	2.31	0.59
12:L:3440:LYS:HG3	12:L:3446:PHE:CE1	2.38	0.59
12:L:3704:ARG:NH2	12:L:3825:LEU:O	2.36	0.59
12:L:3767:ASN:OD1	12:L:3770:ARG:NH2	2.35	0.59
3:C:59:ILE:CG2	16:Q:170:ILE:HD11	2.32	0.59
16:Q:139:TYR:CZ	17:O:24:ILE:CG2	2.86	0.59
1:M:90:ARG:NH1	14:N:513:UNK:CB	2.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:55:LEU:CD2	16:Q:160:ILE:HG12	2.30	0.59
17:O:56:LEU:N	18:P:52:THR:CB	2.64	0.59
6:E:952:ASN:OD1	11:I:137:TRP:NE1	2.35	0.59
12:L:3169:LEU:HG	12:L:3173:LEU:HD23	1.85	0.59
12:L:2805:PHE:CZ	12:L:2812:LEU:HG	2.38	0.58
16:Q:478:ARG:HD2	17:O:76:ASN:HD21	1.67	0.58
17:O:22:ILE:HG21	18:P:43:ILE:HG13	1.85	0.58
17:O:22:ILE:HG21	18:P:43:ILE:CD1	2.33	0.58
6:E:921:TYR:HD1	7:J:104:THR:HG22	1.68	0.58
8:K:446:ILE:HG13	12:L:2595:ILE:HG12	1.84	0.58
10:H:100:GLU:OE2	10:H:111:TYR:N	2.35	0.58
12:L:2913:VAL:HG12	12:L:2914:ILE:HD13	1.84	0.58
16:Q:93:CYS:N	17:O:17:ASN:OD1	2.26	0.58
5:D:84:LEU:HD23	5:D:84:LEU:O	2.02	0.58
12:L:2593:TYR:HB2	12:L:2596:ARG:HA	1.86	0.58
1:M:190:PHE:HB3	5:D:88:LEU:HG	1.84	0.58
10:H:38:GLU:N	10:H:38:GLU:OE1	2.36	0.58
10:H:162:ILE:HG22	10:H:164:PRO:HD2	1.86	0.58
4:F:223:GLU:HG2	9:G:576:MET:HB2	1.85	0.58
10:H:296:ASN:OD1	10:H:297:GLU:N	2.36	0.58
1:M:168:PHE:CD1	1:M:238:ARG:HG3	2.39	0.58
4:F:83:LEU:O	4:F:142:LEU:HD13	2.03	0.58
6:E:946:LYS:HD2	6:E:946:LYS:N	2.17	0.58
14:N:493:UNK:HA	14:N:510:UNK:O	2.03	0.58
12:L:2601:ARG:N	12:L:2601:ARG:HE	2.02	0.58
15:R:14:THR:OG1	16:Q:364:SER:HB3	2.04	0.58
16:Q:138:ASP:OD2	18:P:58:THR:HA	2.03	0.58
3:C:51:LEU:HD11	16:Q:211:ASP:CA	2.32	0.58
8:K:468:LEU:C	12:L:2829:LYS:NZ	2.61	0.58
12:L:2428:LEU:HD11	12:L:2433:ILE:HD11	1.85	0.58
2:A:229:PHE:HZ	3:C:270:GLU:HG2	1.69	0.58
12:L:850:VAL:O	12:L:853:LEU:HB3	2.03	0.58
16:Q:472:PHE:CE2	17:O:50:GLU:HG3	2.37	0.58
1:M:82:LEU:CB	1:M:94:TYR:HE2	2.18	0.57
3:C:51:LEU:HG	16:Q:214:LEU:HG	1.84	0.57
15:R:4:PHE:HZ	16:Q:377:ARG:NH2	1.99	0.57
12:L:905:LEU:HD22	12:L:922:THR:HG23	1.85	0.57
12:L:1355:ASN:O	12:L:1358:VAL:HG13	2.04	0.57
12:L:2836:ARG:NH2	12:L:3618:ASN:OD1	2.37	0.57
10:H:125:GLU:N	10:H:126:PRO:HD3	2.18	0.57
6:E:921:TYR:CD1	7:J:104:THR:HG22	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:521:LEU:C	9:G:521:LEU:HD23	2.30	0.57
10:H:250:GLN:OE1	10:H:253:ARG:NE	2.33	0.57
11:I:41:ARG:O	11:I:44:THR:OG1	2.19	0.57
12:L:851:PRO:O	12:L:852:HIS:HB3	2.03	0.57
16:Q:472:PHE:CG	17:O:46:ILE:CA	2.82	0.57
10:H:129:LYS:HZ3	10:H:129:LYS:HB2	1.70	0.57
17:O:11:TRP:NE1	18:P:83:LEU:N	2.51	0.57
4:F:89:GLU:OE2	4:F:148:ARG:NH1	2.37	0.57
9:G:500:ASP:HB2	9:G:502:LYS:HE2	1.85	0.57
12:L:378:VAL:HG12	12:L:380:ASP:H	1.70	0.57
3:C:47:ASP:CB	16:Q:243:THR:HB	2.35	0.57
12:L:2860:VAL:HG13	12:L:2879:LEU:HD11	1.86	0.57
12:L:3458:LEU:H	12:L:3458:LEU:HD23	1.69	0.57
16:Q:473:LYS:O	17:O:47:SER:O	2.22	0.57
1:M:108:GLU:HA	1:M:110:LYS:H	1.70	0.57
5:D:84:LEU:HD23	5:D:84:LEU:C	2.29	0.57
9:G:620:HIS:NE2	9:G:641:GLY:HA3	2.20	0.57
12:L:3727:LEU:HD22	12:L:3798:THR:HG22	1.85	0.57
1:M:87:LEU:O	1:M:90:ARG:HG2	2.04	0.57
5:D:326:ILE:HD12	5:D:326:ILE:C	2.30	0.57
10:H:102:LEU:HD23	10:H:103:VAL:N	2.20	0.57
12:L:1355:ASN:HA	12:L:1358:VAL:CG1	2.35	0.57
16:Q:107:LYS:HG2	17:O:20:ARG:CZ	2.34	0.57
17:O:19:LEU:HD13	18:P:70:ALA:HB1	1.86	0.57
1:M:191:PRO:HB3	5:D:212:GLN:CG	2.34	0.56
3:C:51:LEU:CD1	16:Q:215:SER:N	2.68	0.56
9:G:572:VAL:HG12	9:G:573:ARG:HG2	1.87	0.56
10:H:157:ASN:HD22	10:H:160:LYS:HZ3	1.53	0.56
12:L:2880:LYS:N	12:L:2880:LYS:CD	2.67	0.56
16:Q:93:CYS:HG	17:O:17:ASN:HA	1.66	0.56
16:Q:178:LEU:CD2	17:O:37:ILE:HG21	2.33	0.56
17:O:11:TRP:CZ2	18:P:86:ILE:CG1	2.86	0.56
1:M:185:TYR:C	1:M:185:TYR:HD1	2.13	0.56
3:C:288:LEU:HD21	3:C:292:THR:HG21	1.87	0.56
5:D:218:ARG:C	5:D:220:ALA:H	2.12	0.56
9:G:546:HIS:HB2	9:G:553:PHE:CE1	2.35	0.56
12:L:853:LEU:O	12:L:856:LEU:N	2.37	0.56
12:L:2880:LYS:HD2	12:L:2880:LYS:N	2.20	0.56
12:L:2880:LYS:CA	12:L:2880:LYS:HE3	2.35	0.56
4:F:111:PHE:CE1	4:F:115:VAL:HG21	2.41	0.56
6:E:885:VAL:HA	10:H:128:PRO:CG	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:3433:PRO:HB2	12:L:3527:VAL:HG11	1.86	0.56
1:M:74:VAL:HG23	1:M:155:PHE:HA	1.87	0.56
8:K:456:GLN:HG3	12:L:2677:PHE:CE2	2.41	0.56
5:D:238:SER:OG	5:D:240:ASP:OD1	2.11	0.56
6:E:932:HIS:O	6:E:935:SER:HB2	2.04	0.56
8:K:460:MET:SD	8:K:460:MET:N	2.76	0.56
12:L:302:PRO:HD3	12:L:336:ARG:HH22	1.71	0.56
12:L:3174:ARG:NH1	12:L:3290:MET:SD	2.79	0.56
15:R:12:THR:OG1	16:Q:360:GLU:OE2	2.22	0.56
12:L:2896:ASP:HB3	12:L:2899:ILE:HG12	1.86	0.56
16:Q:464:ILE:O	17:O:48:LEU:CB	2.53	0.56
1:M:87:LEU:CD1	14:N:490:UNK:HA	2.28	0.56
10:H:356:SER:O	10:H:360:PRO:HG2	2.05	0.56
12:L:827:ARG:O	12:L:828:ARG:HB2	2.05	0.56
1:M:185:TYR:C	1:M:185:TYR:CD1	2.84	0.55
5:D:320:ASN:HB3	5:D:324:LYS:HB2	1.89	0.55
12:L:946:ASP:O	12:L:951:GLN:NE2	2.39	0.55
16:Q:184:LEU:HD12	17:O:44:ASP:C	2.12	0.55
16:Q:472:PHE:CE2	17:O:50:GLU:CD	2.83	0.55
12:L:583:ASN:ND2	12:L:600:ALA:O	2.39	0.55
3:C:42:ILE:HD12	16:Q:176:PRO:HA	1.87	0.55
3:C:54:CYS:SG	16:Q:215:SER:HB3	2.45	0.55
14:N:495:UNK:HA	14:N:508:UNK:O	2.07	0.55
16:Q:182:THR:CG2	17:O:45:GLN:N	2.69	0.55
16:Q:188:ILE:HG23	17:O:90:THR:HG22	1.88	0.55
3:C:40:TYR:CB	16:Q:214:LEU:CD2	2.64	0.55
8:K:455:PRO:HB2	8:K:457:PRO:HD2	1.88	0.55
9:G:551:TYR:CG	9:G:563:MET:HE2	2.41	0.55
12:L:2414:LEU:O	12:L:2417:ARG:NH1	2.40	0.55
16:Q:178:LEU:HD13	17:O:37:ILE:HG21	1.88	0.55
16:Q:479:ILE:HA	17:O:47:SER:HG	1.70	0.55
17:O:26:ASN:ND2	18:P:47:THR:HB	2.22	0.55
1:M:139:TYR:O	1:M:143:ILE:HG12	2.06	0.55
16:Q:501:GLN:OE1	18:P:31:ARG:NH2	2.28	0.55
5:D:78:LYS:HE3	5:D:78:LYS:C	2.31	0.55
5:D:326:ILE:HD12	5:D:327:ARG:N	2.21	0.55
10:H:265:PHE:HE2	10:H:289:LEU:HD11	1.70	0.55
9:G:546:HIS:CG	9:G:547:PRO:HD2	2.42	0.55
12:L:3698:THR:OG1	12:L:3699:GLU:N	2.39	0.55
16:Q:464:ILE:C	17:O:46:ILE:CD1	2.80	0.55
1:M:143:ILE:O	1:M:150:ALA:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:189:LEU:HD21	5:D:81:VAL:HG12	1.87	0.55
5:D:212:GLN:HE21	5:D:212:GLN:CA	2.02	0.55
1:M:83:LYS:O	1:M:87:LEU:HG	2.07	0.54
1:M:187:PRO:CB	5:D:211:ARG:HB2	2.37	0.54
3:C:39:ARG:HE	16:Q:148:ILE:HG22	1.71	0.54
5:D:317:GLN:O	5:D:319:ARG:N	2.35	0.54
10:H:218:SER:OG	10:H:221:LEU:N	2.38	0.54
12:L:3429:ASP:HB2	12:L:3448:LYS:HD2	1.89	0.54
16:Q:182:THR:HB	17:O:45:GLN:O	2.07	0.54
16:Q:444:GLN:HE21	18:P:35:TYR:HE2	0.80	0.54
16:Q:252:THR:HG23	17:O:109:PHE:HE1	1.68	0.54
1:M:99:PHE:CZ	1:M:114:LEU:HD12	2.43	0.54
2:A:208:VAL:HG21	2:A:214:VAL:HG11	1.88	0.54
17:O:7:GLN:HG2	18:P:83:LEU:HD23	1.88	0.54
1:M:115:ILE:CD1	1:M:121:MET:SD	2.95	0.54
1:M:189:LEU:HD13	5:D:84:LEU:HD13	1.89	0.54
5:D:22:PHE:CE2	5:D:30:PRO:HD3	2.43	0.54
12:L:822:LEU:HD22	12:L:1186:TYR:H	1.72	0.54
12:L:3458:LEU:HD23	12:L:3458:LEU:N	2.22	0.54
16:Q:205:HIS:CE1	17:O:46:ILE:HG22	2.43	0.54
3:C:47:ASP:CG	16:Q:243:THR:HB	2.32	0.54
5:D:259:GLU:HB2	5:D:312:ALA:HB1	1.88	0.54
9:G:593:TRP:HE1	9:G:614:ILE:HD12	1.72	0.54
9:G:631:SER:OG	9:G:634:GLY:N	2.39	0.54
12:L:1822:LYS:NZ	12:L:1864:ASP:OD2	2.41	0.54
17:O:54:GLN:H	17:O:57:LYS:HB2	1.73	0.54
1:M:173:GLU:HB2	5:D:204:TYR:CD1	2.43	0.54
4:F:212:PHE:HE2	4:F:218:LEU:HD21	1.72	0.54
5:D:199:MET:HA	5:D:203:GLU:CB	2.37	0.54
10:H:394:GLU:N	10:H:394:GLU:OE1	2.40	0.54
12:L:2916:ARG:HB2	12:L:2916:ARG:HH21	1.71	0.54
8:K:464:ASN:OD1	12:L:2669:MET:SD	2.65	0.54
10:H:115:ASP:OD1	10:H:116:GLU:N	2.41	0.54
11:I:40:TYR:O	11:I:44:THR:HG23	2.07	0.54
5:D:216:THR:CG2	5:D:243:ASP:HA	2.38	0.54
1:M:90:ARG:HD2	14:N:513:UNK:CB	2.38	0.54
3:C:51:LEU:CD2	16:Q:214:LEU:HB3	2.38	0.54
16:Q:93:CYS:SG	17:O:20:ARG:CG	2.95	0.54
16:Q:178:LEU:HB2	17:O:37:ILE:HD13	1.89	0.54
16:Q:468:ASP:O	17:O:51:ILE:CD1	2.56	0.54
5:D:17:ILE:HD12	5:D:17:ILE:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:184:LEU:O	9:G:191:LYS:NZ	2.41	0.54
12:L:3428:GLU:HG2	12:L:3429:ASP:H	1.73	0.54
13:B:556:VAL:O	13:B:557:VAL:C	2.50	0.54
16:Q:78:ARG:NH1	18:P:27:SER:CB	2.70	0.54
12:L:846:LEU:O	12:L:850:VAL:HB	2.08	0.53
17:O:11:TRP:CE3	18:P:82:ILE:CG2	2.91	0.53
17:O:27:ILE:HD12	18:P:59:PHE:HD1	1.70	0.53
5:D:216:THR:CB	5:D:243:ASP:HA	2.38	0.53
12:L:2911:PHE:CE2	12:L:2944:GLU:HG3	2.44	0.53
19:R:165:HOH:O	16:Q:355:LEU:CD1	2.39	0.53
17:O:23:VAL:HG21	18:P:63:ILE:HD12	1.90	0.53
12:L:1522:ASP:OD1	12:L:1522:ASP:N	2.41	0.53
16:Q:78:ARG:NE	18:P:23:TYR:CD2	2.70	0.53
5:D:66:VAL:HG13	5:D:67:PRO:HD2	1.87	0.53
5:D:317:GLN:HA	5:D:317:GLN:NE2	2.22	0.53
4:F:93:ARG:NH2	4:F:95:GLY:O	2.41	0.53
10:H:332:GLN:N	10:H:332:GLN:OE1	2.42	0.53
12:L:1727:LYS:HG3	12:L:1776:ARG:HH21	1.73	0.53
12:L:3136:ILE:HG22	12:L:3161:ILE:HD13	1.89	0.53
17:O:56:LEU:CD1	18:P:51:VAL:HB	2.38	0.53
4:F:277:ASN:OD1	4:F:278:ALA:N	2.42	0.53
9:G:411:ASP:N	9:G:411:ASP:OD1	2.42	0.53
9:G:537:LEU:H	9:G:537:LEU:CD1	2.20	0.53
12:L:1219:ARG:NH1	12:L:3413:GLU:OE2	2.41	0.53
16:Q:93:CYS:H	17:O:17:ASN:CG	2.14	0.53
16:Q:188:ILE:HG23	17:O:90:THR:CG2	2.38	0.53
3:C:34:LEU:C	16:Q:467:ARG:HG2	2.32	0.53
10:H:13:SER:OG	10:H:14:HIS:N	2.41	0.53
16:Q:106:TRP:HB3	17:O:20:ARG:HH21	1.72	0.53
16:Q:340:ALA:HB3	19:Q:601:HOH:O	2.09	0.53
3:C:48:ARG:HH12	16:Q:216:GLY:HA2	1.74	0.53
9:G:521:LEU:HD23	9:G:521:LEU:O	2.08	0.53
12:L:959:ILE:HG21	12:L:2449:ILE:HD12	1.91	0.53
16:Q:474:PHE:CD2	16:Q:479:ILE:HD12	2.44	0.53
10:H:406:ASN:O	10:H:409:SER:OG	2.15	0.53
12:L:345:LEU:O	12:L:386:GLN:NE2	2.42	0.53
12:L:1278:ASN:O	12:L:1284:ARG:NH2	2.42	0.53
16:Q:106:TRP:HB3	17:O:20:ARG:NH2	2.23	0.53
16:Q:472:PHE:CD2	17:O:46:ILE:CA	2.92	0.53
17:O:22:ILE:HG23	18:P:44:ASN:OD1	2.08	0.53
1:M:173:GLU:HG2	5:D:197:LYS:CA	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:188:GLU:OE1	5:D:85:ARG:CZ	2.57	0.53
3:C:39:ARG:HH22	16:Q:150:GLN:NE2	2.05	0.53
5:D:313:TRP:O	5:D:317:GLN:HG2	2.08	0.53
5:D:323:LYS:HG3	5:D:323:LYS:O	2.08	0.53
10:H:217:LEU:HD12	10:H:218:SER:O	2.08	0.53
12:L:416:LEU:HD11	12:L:574:THR:HB	1.91	0.53
12:L:3101:LYS:O	12:L:3742:GLN:NE2	2.42	0.53
16:Q:474:PHE:CA	17:O:47:SER:OG	2.50	0.53
1:M:84:THR:HA	1:M:87:LEU:HD12	1.90	0.52
9:G:76:PRO:O	9:G:592:ARG:NH1	2.42	0.52
9:G:546:HIS:CG	9:G:547:PRO:CD	2.92	0.52
8:K:469:LEU:HD23	12:L:2790:THR:CG2	2.39	0.52
12:L:1526:ASN:O	12:L:1530:GLN:NE2	2.43	0.52
12:L:2528:HIS:O	12:L:2531:PHE:N	2.42	0.52
7:J:80:THR:O	7:J:84:LEU:HD23	2.09	0.52
12:L:1886:VAL:HG22	12:L:1924:ALA:HB2	1.91	0.52
16:Q:259:TRP:HE1	17:O:114:ASP:HA	1.74	0.52
1:M:149:ALA:O	1:M:151:LYS:N	2.42	0.52
1:M:108:GLU:HA	1:M:109:PRO:C	2.31	0.52
3:C:50:ILE:C	16:Q:214:LEU:CG	2.83	0.52
9:G:544:GLU:O	9:G:552:LEU:HD12	2.09	0.52
16:Q:130:TYR:CB	17:O:28:LEU:CD1	2.81	0.52
16:Q:472:PHE:CD2	17:O:50:GLU:HG2	2.44	0.52
3:C:39:ARG:NH2	16:Q:150:GLN:NE2	2.57	0.52
3:C:42:ILE:CD1	16:Q:176:PRO:HA	2.40	0.52
9:G:562:ARG:HB3	9:G:571:CYS:SG	2.49	0.52
12:L:852:HIS:CG	12:L:852:HIS:O	2.62	0.52
12:L:1355:ASN:HA	12:L:1358:VAL:HG12	1.91	0.52
12:L:3515:ARG:NH1	12:L:3518:ASN:OD1	2.43	0.52
17:O:24:ILE:HG13	18:P:59:PHE:CZ	2.45	0.52
2:A:223:GLN:OE1	2:A:223:GLN:HA	2.09	0.52
2:A:226:ILE:HA	2:A:229:PHE:CD2	2.44	0.52
3:C:55:LEU:CD1	16:Q:173:SER:OG	2.57	0.52
5:D:73:LEU:C	5:D:73:LEU:CD2	2.82	0.52
8:K:442:PRO:CD	12:L:912:LEU:HD22	2.36	0.52
12:L:846:LEU:HA	12:L:850:VAL:CB	2.39	0.52
12:L:1307:SER:HA	12:L:1310:LYS:HD2	1.91	0.52
12:L:2884:GLN:NE2	12:L:2884:GLN:CA	2.72	0.52
6:E:947:PHE:CD1	6:E:947:PHE:C	2.88	0.52
8:K:468:LEU:CB	12:L:2829:LYS:NZ	2.58	0.52
8:K:602:ILE:O	8:K:607:ASN:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:12:THR:HG21	16:Q:379:LYS:CE	2.39	0.52
4:F:189:ILE:C	4:F:190:LEU:HD12	2.35	0.52
8:K:460:MET:HG3	12:L:2758:THR:HG22	1.92	0.52
12:L:710:SER:O	12:L:757:ASN:ND2	2.43	0.52
12:L:854:SER:C	12:L:856:LEU:H	2.18	0.52
16:Q:106:TRP:HD1	17:O:20:ARG:NH1	1.97	0.52
1:M:102:VAL:HG12	1:M:115:ILE:HB	1.92	0.51
9:G:84:GLN:OE1	9:G:215:ASN:O	2.28	0.51
9:G:202:ILE:HD11	9:G:206:THR:HG21	1.92	0.51
10:H:27:ALA:HB1	10:H:32:ILE:CD1	2.35	0.51
16:Q:178:LEU:HD22	17:O:37:ILE:CG2	2.38	0.51
16:Q:472:PHE:HZ	17:O:45:GLN:CD	2.18	0.51
9:G:607:ASP:HB2	9:G:614:ILE:HG13	1.92	0.51
12:L:672:PRO:HA	12:L:675:PHE:HB3	1.93	0.51
12:L:1419:LYS:O	12:L:1422:VAL:HG22	2.11	0.51
12:L:1947:ARG:NH2	12:L:1964:TYR:OH	2.43	0.51
12:L:3141:GLN:NE2	12:L:3750:ASP:OD2	2.42	0.51
12:L:3495:GLU:HG3	12:L:3496:ARG:HD2	1.91	0.51
14:N:221:UNK:C	14:N:230:UNK:CA	2.88	0.51
15:R:68:HIS:HE1	19:R:113:HOH:O	1.92	0.51
6:E:940:LYS:O	6:E:941:VAL:HB	2.09	0.51
12:L:1221:LEU:HD21	12:L:1243:LEU:HB3	1.92	0.51
19:R:153:HOH:O	16:Q:326:LYS:CB	2.11	0.51
16:Q:182:THR:CG2	17:O:45:GLN:H	2.19	0.51
16:Q:464:ILE:C	17:O:46:ILE:HD11	2.36	0.51
6:E:947:PHE:HD1	6:E:947:PHE:O	1.94	0.51
12:L:853:LEU:O	12:L:854:SER:C	2.54	0.51
12:L:2805:PHE:CE1	12:L:2812:LEU:HG	2.46	0.51
5:D:232:LEU:HD22	5:D:235:SER:OG	2.11	0.51
10:H:255:ASP:OD1	10:H:255:ASP:N	2.43	0.51
12:L:986:PRO:O	12:L:991:ARG:NH2	2.44	0.51
12:L:2601:ARG:O	12:L:2603:ASN:N	2.43	0.51
2:A:364:ASP:N	2:A:364:ASP:OD1	2.42	0.51
3:C:49:PRO:HG3	16:Q:237:PHE:CE1	2.36	0.51
3:C:51:LEU:N	16:Q:214:LEU:CD1	2.72	0.51
4:F:200:ASP:HA	4:F:203:TYR:HE2	1.75	0.51
6:E:935:SER:OG	6:E:940:LYS:HB2	2.11	0.51
10:H:362:ILE:N	10:H:362:ILE:HD13	2.24	0.51
12:L:3423:HIS:HA	12:L:3426:LYS:HB2	1.93	0.51
12:L:1203:LEU:O	12:L:1206:PRO:HD2	2.10	0.51
12:L:1203:LEU:HD23	12:L:1206:PRO:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:2601:ARG:O	12:L:2602:PRO:C	2.53	0.51
16:Q:70:GLU:OE1	18:P:24:ASP:HA	2.11	0.51
1:M:105:ARG:O	1:M:106:ILE:HG23	2.10	0.51
5:D:74:ILE:HG13	5:D:78:LYS:HB3	1.92	0.51
12:L:3456:LEU:HD12	12:L:3467:LYS:HB3	1.93	0.51
4:F:212:PHE:CE2	4:F:218:LEU:HD21	2.46	0.51
9:G:471:CYS:SG	9:G:499:TRP:O	2.69	0.51
10:H:328:LEU:O	10:H:332:GLN:NE2	2.43	0.51
12:L:562:ARG:NH1	12:L:625:PHE:O	2.44	0.51
12:L:2802:LEU:HD11	12:L:2858:SER:HB2	1.93	0.51
2:A:246:LEU:O	2:A:250:MET:HG3	2.11	0.51
9:G:472:SER:OG	9:G:474:ASP:OD1	2.28	0.51
9:G:494:HIS:CE1	9:G:520:ARG:HD3	2.45	0.51
17:O:22:ILE:HD12	18:P:43:ILE:HD12	1.68	0.51
2:A:192:SER:O	2:A:196:GLN:NE2	2.44	0.50
12:L:899:ASP:OD1	12:L:899:ASP:N	2.41	0.50
12:L:1314:LEU:O	12:L:1317:ILE:HG22	2.10	0.50
16:Q:474:PHE:CZ	17:O:46:ILE:HB	2.39	0.50
16:Q:479:ILE:HD12	17:O:47:SER:OG	2.12	0.50
4:F:326:ARG:HG2	12:L:2751:LEU:HD11	1.92	0.50
6:E:836:CYS:SG	6:E:993:LEU:HD13	2.51	0.50
12:L:1698:GLN:HA	12:L:1701:GLU:HG2	1.93	0.50
15:R:75:GLY:HA2	16:Q:270:GLU:OE2	2.11	0.50
1:M:170:ILE:HD13	1:M:234:LEU:HD22	1.93	0.50
9:G:565:ASP:HB3	9:G:568:ARG:HB3	1.93	0.50
12:L:703:PHE:O	12:L:709:THR:OG1	2.29	0.50
12:L:1860:ASP:OD1	12:L:1860:ASP:N	2.45	0.50
12:L:2556:GLU:O	12:L:2560:ASN:ND2	2.44	0.50
12:L:2802:LEU:HD22	12:L:2854:LEU:HD12	1.92	0.50
1:M:117:ALA:C	1:M:119:GLY:H	2.19	0.50
9:G:380:SER:OG	10:H:143:ILE:O	2.20	0.50
12:L:1314:LEU:HG	12:L:1347:PHE:CZ	2.47	0.50
12:L:1507:LEU:HA	12:L:1510:ALA:HB3	1.92	0.50
16:Q:90:SER:H	18:P:14:GLN:NE2	2.10	0.50
16:Q:472:PHE:CZ	17:O:50:GLU:HG2	2.44	0.50
12:L:2916:ARG:CZ	12:L:2916:ARG:CB	2.88	0.50
12:L:3746:LEU:HA	12:L:3749:ARG:HG2	1.93	0.50
1:M:67:LEU:HD13	1:M:160:ILE:HG23	1.94	0.50
3:C:38:LEU:HD22	16:Q:210:ARG:HD2	0.55	0.50
17:O:26:ASN:HB2	18:P:47:THR:HG21	1.94	0.50
1:M:142:ILE:HA	1:M:145:LYS:HE3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:122:PRO:HG3	4:F:195:LEU:HD23	1.93	0.50
8:K:562:GLN:CD	8:K:577:ALA:HB3	2.36	0.50
12:L:2880:LYS:HE3	12:L:2880:LYS:HA	1.94	0.50
12:L:3440:LYS:HG3	12:L:3446:PHE:HE1	1.75	0.50
10:H:290:ILE:HG22	10:H:343:LEU:HD11	1.93	0.50
12:L:854:SER:C	12:L:856:LEU:N	2.69	0.50
12:L:1516:GLN:NE2	12:L:1563:ASN:O	2.45	0.50
14:N:174:UNK:O	14:N:213:UNK:O	2.30	0.50
6:E:948:GLN:HG3	6:E:950:VAL:O	2.11	0.49
9:G:122:LEU:HD21	10:H:291:TYR:CD1	2.46	0.49
9:G:469:ILE:HD11	9:G:479:LEU:HD12	1.93	0.49
12:L:1947:ARG:NH1	12:L:1978:ARG:O	2.45	0.49
17:O:56:LEU:HD11	18:P:51:VAL:CA	2.42	0.49
4:F:219:ASN:O	4:F:222:THR:OG1	2.31	0.49
12:L:2880:LYS:H	12:L:2880:LYS:CD	2.23	0.49
17:O:56:LEU:CA	18:P:52:THR:CG2	2.90	0.49
1:M:80:LEU:HD21	1:M:143:ILE:HD12	1.93	0.49
12:L:2797:GLN:HG2	12:L:2818:LEU:HD21	1.93	0.49
16:Q:107:LYS:CA	17:O:20:ARG:HH22	2.26	0.49
10:H:96:LEU:HD23	10:H:97:VAL:N	2.27	0.49
16:Q:107:LYS:HG2	17:O:20:ARG:NH1	2.27	0.49
17:O:34:ARG:NH1	18:P:57:PRO:CA	2.69	0.49
4:F:200:ASP:HA	4:F:203:TYR:CE2	2.48	0.49
5:D:67:PRO:O	5:D:71:ILE:HG22	2.12	0.49
12:L:428:LYS:HG3	12:L:430:GLU:CG	2.42	0.49
12:L:2465:LEU:HB3	12:L:2593:TYR:HB3	1.95	0.49
12:L:3653:ASN:HB3	12:L:3657:GLY:H	1.78	0.49
16:Q:479:ILE:CD1	17:O:47:SER:OG	2.61	0.49
2:A:208:VAL:CG2	2:A:214:VAL:HG11	2.42	0.49
3:C:56:SER:HB2	16:Q:156:ARG:HD3	1.94	0.49
12:L:1425:PHE:C	12:L:1427:SER:N	2.70	0.49
12:L:1432:SER:OG	12:L:1433:ILE:N	2.45	0.49
12:L:2906:TRP:O	12:L:2910:VAL:HG23	2.12	0.49
4:F:279:ASP:O	8:K:521:ILE:HD11	2.12	0.49
5:D:329:PHE:N	5:D:329:PHE:CD1	2.80	0.49
1:M:82:LEU:CD1	1:M:101:ALA:HA	2.37	0.49
5:D:319:ARG:HG3	5:D:320:ASN:H	1.77	0.49
12:L:456:ILE:HG22	12:L:457:MET:HE2	1.94	0.49
12:L:3175:THR:HG21	12:L:3528:PRO:HB2	1.94	0.49
6:E:885:VAL:HA	10:H:128:PRO:HG3	1.95	0.49
12:L:1354:LEU:O	12:L:1358:VAL:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:1364:LEU:O	12:L:1391:ARG:NH1	2.45	0.49
16:Q:107:LYS:HZ2	17:O:13:CYS:HA	1.75	0.49
16:Q:472:PHE:CB	17:O:46:ILE:CG1	2.55	0.49
1:M:175:LEU:O	1:M:179:HIS:HB2	2.13	0.49
2:A:190:VAL:HG22	2:A:192:SER:H	1.77	0.49
6:E:946:LYS:CE	6:E:946:LYS:CA	2.91	0.49
8:K:460:MET:HE2	12:L:2758:THR:HG21	1.95	0.49
12:L:2475:LEU:O	12:L:2479:TYR:N	2.44	0.49
3:C:48:ARG:NH1	16:Q:216:GLY:HA2	2.27	0.48
4:F:223:GLU:OE1	4:F:223:GLU:N	2.46	0.48
5:D:78:LYS:O	5:D:78:LYS:CD	2.61	0.48
11:I:133:THR:O	11:I:135:LYS:N	2.44	0.48
12:L:1358:VAL:O	12:L:1359:GLN:C	2.56	0.48
12:L:2665:LEU:HD21	12:L:2680:THR:HB	1.95	0.48
4:F:129:LYS:HG2	4:F:203:TYR:CE1	2.47	0.48
8:K:454:PRO:CD	8:K:455:PRO:CD	2.92	0.48
12:L:1256:THR:OG1	12:L:1257:ARG:N	2.47	0.48
12:L:1358:VAL:HG23	12:L:1394:CYS:HB3	1.95	0.48
16:Q:130:TYR:HD2	17:O:24:ILE:HG22	1.76	0.48
17:O:15:MET:CE	18:P:74:VAL:HG21	2.28	0.48
8:K:564:HIS:ND1	8:K:568:ASN:OD1	2.44	0.48
9:G:139:HIS:ND1	9:G:228:LEU:HD22	2.29	0.48
12:L:545:LEU:HD12	12:L:546:PRO:HD2	1.94	0.48
3:C:38:LEU:CG	16:Q:210:ARG:CZ	2.89	0.48
6:E:880:LYS:C	6:E:881:LEU:HD12	2.38	0.48
8:K:439:PRO:HB3	12:L:916:HIS:HE1	1.75	0.48
14:N:87:UNK:HA	14:N:497:UNK:O	2.13	0.48
17:O:26:ASN:ND2	18:P:47:THR:CB	2.77	0.48
6:E:883:SER:O	6:E:886:SER:OG	2.28	0.48
6:E:885:VAL:HG22	10:H:128:PRO:HB2	1.95	0.48
10:H:26:ALA:O	10:H:29:SER:OG	2.22	0.48
12:L:599:THR:O	12:L:601:ARG:NH1	2.46	0.48
13:B:413:ASP:O	13:B:414:ASP:C	2.56	0.48
17:O:11:TRP:CE3	18:P:82:ILE:HG23	2.48	0.48
12:L:426:GLU:HG3	12:L:428:LYS:HD3	1.94	0.48
16:Q:139:TYR:CZ	17:O:24:ILE:HG23	2.48	0.48
16:Q:481:LEU:HD12	17:O:50:GLU:N	2.11	0.48
10:H:118:ASP:OD1	10:H:118:ASP:N	2.46	0.48
12:L:605:ASN:OD1	12:L:1568:GLN:NE2	2.46	0.48
3:C:306:SER:OG	3:C:307:VAL:N	2.45	0.48
12:L:387:LEU:HD21	12:L:422:ILE:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:7:GLN:HG3	18:P:86:ILE:CB	2.41	0.48
17:O:19:LEU:CD1	18:P:70:ALA:CB	2.91	0.48
6:E:909:PHE:O	6:E:913:VAL:HG23	2.14	0.48
9:G:171:GLU:OE1	9:G:171:GLU:N	2.45	0.48
10:H:317:LEU:HD12	10:H:319:LYS:H	1.78	0.48
12:L:2807:GLN:CB	12:L:2809:LYS:HE3	2.44	0.48
18:P:47:THR:HA	18:P:66:ILE:HD11	1.96	0.48
1:M:96:PRO:O	1:M:98:ARG:N	2.47	0.48
5:D:23:VAL:HA	5:D:27:THR:O	2.14	0.48
6:E:834:ARG:NH2	6:E:901:ASN:O	2.47	0.48
12:L:1514:THR:O	12:L:1517:GLN:NE2	2.44	0.48
12:L:1724:PHE:HB3	12:L:1776:ARG:HD2	1.96	0.48
12:L:2528:HIS:CD2	12:L:2532:LEU:HD23	2.49	0.48
16:Q:259:TRP:NE1	17:O:114:ASP:OD1	2.42	0.48
1:M:194:ILE:CA	1:M:195:TYR:N	2.76	0.47
4:F:115:VAL:HG13	4:F:190:LEU:HD11	1.96	0.47
8:K:458:ALA:O	8:K:459:ALA:HB2	2.14	0.47
9:G:94:PRO:HB3	9:G:566:ILE:HD11	1.96	0.47
11:I:131:CYS:SG	11:I:132:LEU:N	2.87	0.47
12:L:1180:CYS:HA	12:L:1183:GLU:HG2	1.96	0.47
12:L:2878:GLU:O	12:L:2882:VAL:HG13	2.14	0.47
12:L:2879:LEU:O	12:L:2882:VAL:HG22	2.14	0.47
16:Q:315:SER:HB3	19:Q:605:HOH:O	2.04	0.47
17:O:55:ARG:HB3	18:P:52:THR:CG2	2.41	0.47
2:A:229:PHE:CZ	3:C:270:GLU:HG2	2.50	0.47
3:C:39:ARG:NE	16:Q:147:PHE:CE1	2.82	0.47
5:D:84:LEU:HA	5:D:87:TYR:HD2	1.79	0.47
8:K:468:LEU:O	12:L:2790:THR:HG22	2.14	0.47
12:L:853:LEU:HD23	12:L:853:LEU:N	2.28	0.47
12:L:1855:PRO:HA	12:L:1862:ARG:HH22	1.79	0.47
5:D:207:TRP:CD1	5:D:207:TRP:C	2.91	0.47
5:D:319:ARG:HH12	5:D:335:ARG:HG2	1.79	0.47
8:K:469:LEU:HB3	12:L:2788:ILE:CG2	2.44	0.47
12:L:2904:VAL:HG21	12:L:2952:PHE:HB2	1.95	0.47
12:L:3519:ILE:O	12:L:3519:ILE:HG13	2.13	0.47
3:C:34:LEU:O	16:Q:467:ARG:HG2	2.15	0.47
5:D:17:ILE:H	5:D:17:ILE:CD1	2.26	0.47
5:D:208:SER:HB3	5:D:211:ARG:CZ	2.44	0.47
9:G:559:LYS:HG2	9:G:580:GLY:O	2.14	0.47
1:M:191:PRO:HB3	5:D:212:GLN:HG2	1.96	0.47
5:D:47:VAL:O	5:D:51:LEU:HD23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:328:ASN:ND2	6:E:963:ASN:OD1	2.48	0.47
10:H:305:VAL:HA	10:H:308:ILE:HG22	1.97	0.47
12:L:1469:LEU:O	12:L:1501:LYS:NZ	2.47	0.47
12:L:1824:THR:H	12:L:1827:LEU:HD21	1.79	0.47
12:L:2914:ILE:HD13	12:L:2914:ILE:N	2.28	0.47
12:L:3162:ALA:HB2	12:L:3169:LEU:HD23	1.95	0.47
2:A:246:LEU:HG	2:A:250:MET:HE2	1.95	0.47
2:A:246:LEU:HG	2:A:250:MET:CE	2.45	0.47
3:C:55:LEU:HD23	16:Q:160:ILE:CG1	2.41	0.47
4:F:118:GLU:O	4:F:191:ARG:N	2.45	0.47
4:F:304:LEU:CD2	8:K:475:SER:HB2	2.45	0.47
8:K:566:GLU:O	8:K:572:ARG:NH1	2.46	0.47
12:L:1417:ARG:HG2	12:L:1418:VAL:N	2.29	0.47
12:L:1684:ARG:HH12	12:L:1692:LEU:HD13	1.80	0.47
14:N:238:UNK:HA	14:N:248:UNK:O	2.14	0.47
16:Q:474:PHE:HD1	17:O:48:LEU:HG	1.76	0.47
17:O:27:ILE:HD12	18:P:59:PHE:HA	1.77	0.47
1:M:82:LEU:HG	1:M:117:ALA:HB2	1.97	0.47
6:E:909:PHE:CE2	7:J:196:MET:HE1	2.50	0.47
9:G:626:TYR:CE2	9:G:642:ALA:HB2	2.50	0.47
12:L:1716:LEU:HG	12:L:1718:HIS:H	1.79	0.47
16:Q:478:ARG:HD3	17:O:76:ASN:HD21	1.79	0.47
9:G:412:SER:OG	9:G:454:GLY:O	2.30	0.47
9:G:546:HIS:NE2	9:G:547:PRO:HD2	2.29	0.47
12:L:1134:SER:OG	12:L:1135:ASP:N	2.47	0.47
12:L:2808:GLN:HA	12:L:2808:GLN:OE1	2.14	0.47
16:Q:91:LEU:CD2	17:O:13:CYS:HB3	2.36	0.47
16:Q:479:ILE:CD1	17:O:47:SER:CB	2.79	0.47
2:A:244:ASP:O	2:A:248:THR:HG23	2.15	0.47
10:H:16:LEU:HD22	11:I:18:ILE:HG12	1.97	0.47
12:L:312:CYS:O	12:L:320:ARG:NH2	2.47	0.47
12:L:1203:LEU:HD22	12:L:1210:PHE:CE2	2.50	0.47
12:L:1554:MET:HE2	12:L:1554:MET:HB3	1.80	0.47
12:L:1848:ALA:HB2	12:L:1887:VAL:HG23	1.97	0.47
15:R:46:ALA:CA	16:Q:331:PRO:O	2.50	0.47
1:M:151:LYS:O	1:M:153:THR:HG22	2.15	0.46
2:A:271:MET:SD	8:K:537:VAL:HG23	2.55	0.46
3:C:33:SER:HB2	16:Q:207:PRO:HG3	1.96	0.46
8:K:441:PRO:CA	12:L:912:LEU:HD21	2.33	0.46
8:K:504:LYS:O	8:K:508:ARG:NH1	2.48	0.46
9:G:551:TYR:CD1	9:G:563:MET:HE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:22:ILE:HG21	18:P:43:ILE:CG1	2.44	0.46
17:O:56:LEU:HD23	18:P:52:THR:HG23	1.76	0.46
3:C:38:LEU:HB2	16:Q:210:ARG:HH21	1.76	0.46
9:G:576:MET:SD	9:G:577:GLY:N	2.88	0.46
12:L:952:ASN:OD1	12:L:952:ASN:N	2.48	0.46
15:R:71:LEU:HD12	16:Q:397:PHE:HB2	1.97	0.46
10:H:127:LEU:HD12	10:H:127:LEU:C	2.39	0.46
16:Q:130:TYR:CE2	17:O:25:ASN:OD1	2.59	0.46
16:Q:416:PHE:CE2	18:P:35:TYR:O	2.69	0.46
17:O:34:ARG:NH1	18:P:57:PRO:CG	2.55	0.46
4:F:137:GLU:O	9:G:59:TYR:N	2.45	0.46
5:D:75:ARG:O	5:D:75:ARG:HG2	2.16	0.46
8:K:444:THR:OG1	8:K:445:GLU:N	2.48	0.46
12:L:1441:GLY:HA2	12:L:1444:LYS:HG2	1.98	0.46
12:L:2959:HIS:HA	12:L:3512:VAL:HG11	1.96	0.46
1:M:75:THR:HB	1:M:120:LYS:HG2	1.97	0.46
1:M:88:HIS:HA	14:N:514:UNK:O	2.16	0.46
2:A:357:SER:O	2:A:357:SER:OG	2.34	0.46
7:J:196:MET:HE3	7:J:211:LYS:HB3	1.96	0.46
9:G:477:VAL:HG21	9:G:512:THR:HG21	1.97	0.46
12:L:1354:LEU:CA	12:L:1357:LEU:HD22	2.43	0.46
12:L:2425:GLY:HA2	12:L:2428:LEU:HD23	1.98	0.46
12:L:2812:LEU:HD11	12:L:2862:SER:HB2	1.97	0.46
16:Q:472:PHE:CB	17:O:47:SER:N	2.73	0.46
1:M:146:ILE:O	1:M:147:GLY:C	2.58	0.46
8:K:465:ARG:O	12:L:2829:LYS:HE2	2.16	0.46
8:K:588:GLN:NE2	8:K:589:PRO:O	2.45	0.46
12:L:853:LEU:HD23	12:L:853:LEU:H	1.80	0.46
12:L:934:ARG:H	12:L:934:ARG:HG2	1.55	0.46
17:O:55:ARG:CB	18:P:52:THR:HG21	2.43	0.46
12:L:606:GLU:HB2	12:L:1694:PHE:HB2	1.98	0.46
12:L:1262:SER:OG	12:L:1263:SER:N	2.47	0.46
5:D:78:LYS:CE	5:D:78:LYS:O	2.64	0.46
10:H:234:ASN:OD1	10:H:235:GLN:NE2	2.49	0.46
12:L:3434:GLY:HA3	12:L:3525:ILE:HD12	1.97	0.46
12:L:3602:SER:OG	12:L:3603:THR:N	2.48	0.46
9:G:642:ALA:O	10:H:68:ARG:NH2	2.49	0.46
10:H:69:THR:O	10:H:71:HIS:ND1	2.47	0.46
12:L:2901:ASN:O	12:L:2905:THR:HG22	2.16	0.46
15:R:4:PHE:CE1	16:Q:362:LEU:HD13	2.51	0.46
17:O:7:GLN:HG3	18:P:86:ILE:CG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:ARG:CG	16:Q:147:PHE:HE1	2.28	0.46
3:C:51:LEU:CG	16:Q:214:LEU:HG	2.46	0.46
5:D:66:VAL:CG1	5:D:67:PRO:CD	2.84	0.46
8:K:469:LEU:HB3	12:L:2788:ILE:HG22	1.97	0.46
12:L:2807:GLN:HB3	12:L:2809:LYS:HE3	1.98	0.46
16:Q:472:PHE:CZ	17:O:50:GLU:CG	2.98	0.46
1:M:172:LEU:HB2	5:D:204:TYR:CE2	2.52	0.45
2:A:242:GLU:O	2:A:243:MET:C	2.58	0.45
4:F:133:VAL:HG23	4:F:134:GLN:CD	2.41	0.45
5:D:17:ILE:N	5:D:17:ILE:CD1	2.79	0.45
7:J:58:THR:N	7:J:61:GLU:OE2	2.49	0.45
9:G:709:THR:HG22	9:G:710:ARG:H	1.80	0.45
12:L:329:HIS:O	12:L:332:SER:OG	2.33	0.45
12:L:828:ARG:N	12:L:829:PRO:CD	2.57	0.45
12:L:1608:VAL:O	12:L:1617:ARG:NH2	2.49	0.45
16:Q:472:PHE:CG	17:O:46:ILE:N	2.80	0.45
17:O:11:TRP:CG	18:P:86:ILE:CD1	2.94	0.45
3:C:290:SER:OG	3:C:291:ARG:N	2.49	0.45
12:L:2807:GLN:HB3	12:L:2809:LYS:HG3	1.97	0.45
12:L:3458:LEU:H	12:L:3458:LEU:CD2	2.28	0.45
5:D:18:GLN:CD	5:D:18:GLN:C	2.84	0.45
5:D:76:HIS:O	5:D:78:LYS:N	2.49	0.45
7:J:98:ARG:O	7:J:101:ALA:HB3	2.16	0.45
12:L:827:ARG:HH21	12:L:829:PRO:HB3	1.80	0.45
12:L:1136:ASN:HB3	12:L:1139:VAL:HG12	1.96	0.45
16:Q:130:TYR:CD2	17:O:24:ILE:HG22	2.51	0.45
16:Q:182:THR:CA	17:O:44:ASP:HB2	2.18	0.45
2:A:336:TYR:CG	2:A:359:MET:HE1	2.51	0.45
5:D:239:ASP:HA	5:D:242:ILE:HD12	1.97	0.45
8:K:462:ILE:HG23	8:K:463:PRO:HD3	1.98	0.45
16:Q:91:LEU:CD2	17:O:13:CYS:HG	2.19	0.45
16:Q:106:TRP:CD1	17:O:20:ARG:NH1	2.79	0.45
16:Q:107:LYS:N	17:O:20:ARG:HH22	2.14	0.45
16:Q:416:PHE:HZ	18:P:41:ASP:OD2	1.99	0.45
17:O:24:ILE:CG1	18:P:59:PHE:CE1	2.94	0.45
1:M:166:VAL:HG22	1:M:210:GLY:O	2.17	0.45
12:L:1916:ASP:OD1	12:L:1916:ASP:N	2.49	0.45
4:F:326:ARG:HD3	12:L:2751:LEU:HD21	1.97	0.45
10:H:17:TRP:HZ3	11:I:15:LEU:HD21	1.81	0.45
12:L:1418:VAL:O	12:L:1422:VAL:HG13	2.17	0.45
3:C:49:PRO:HB2	16:Q:214:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:460:ASP:O	9:G:468:LEU:HD12	2.17	0.45
9:G:546:HIS:NE2	9:G:591:GLY:HA2	2.32	0.45
9:G:594:LEU:CG	9:G:606:TRP:HB2	2.45	0.45
12:L:1199:MET:HE3	12:L:1199:MET:HB3	1.76	0.45
12:L:3461:GLY:N	12:L:3464:GLY:O	2.50	0.45
12:L:3798:THR:OG1	12:L:3799:GLN:N	2.44	0.45
14:N:221:UNK:HA	14:N:230:UNK:CB	2.47	0.45
1:M:124:THR:CG2	1:M:125:GLY:N	2.80	0.45
1:M:189:LEU:HD13	5:D:84:LEU:HD22	1.98	0.45
8:K:465:ARG:HG3	12:L:2844:LEU:CD1	2.47	0.45
9:G:697:PHE:O	10:H:147:GLN:NE2	2.50	0.45
12:L:962:LEU:HG	12:L:2572:ALA:HB2	1.98	0.45
12:L:1543:PRO:O	12:L:1547:HIS:NE2	2.49	0.45
12:L:3494:GLU:HA	12:L:3497:ILE:HG12	1.99	0.45
16:Q:35:ASP:HA	16:Q:38:TYR:CD2	2.52	0.45
1:M:135:ALA:O	1:M:139:TYR:CD2	2.70	0.45
5:D:27:THR:HG22	5:D:28:ASN:H	1.81	0.45
9:G:632:ARG:NH1	9:G:708:PHE:O	2.46	0.45
12:L:2708:LEU:HD21	12:L:3793:SER:HB2	1.98	0.45
12:L:2745:TRP:O	12:L:2749:THR:OG1	2.35	0.45
14:N:426:UNK:CB	14:N:481:UNK:CA	2.94	0.45
14:N:426:UNK:CB	14:N:481:UNK:CB	2.95	0.45
16:Q:130:TYR:CD1	17:O:28:LEU:CD1	2.77	0.45
16:Q:130:TYR:HB3	17:O:28:LEU:CD1	2.42	0.45
3:C:38:LEU:HB2	16:Q:210:ARG:CZ	2.46	0.45
8:K:437:LEU:H	8:K:437:LEU:CD2	2.28	0.45
9:G:107:ILE:HD11	9:G:140:CYS:HB2	1.99	0.45
14:N:83:UNK:C	14:N:506:UNK:C	2.95	0.45
1:M:98:ARG:O	1:M:99:PHE:C	2.60	0.44
3:C:39:ARG:NH1	16:Q:148:ILE:HG23	2.06	0.44
4:F:305:SER:O	8:K:452:VAL:HG21	2.16	0.44
6:E:946:LYS:N	6:E:946:LYS:CD	2.79	0.44
9:G:450:VAL:HG22	9:G:451:GLY:N	2.29	0.44
12:L:368:TYR:O	12:L:394:TYR:OH	2.31	0.44
12:L:2807:GLN:OE1	12:L:2807:GLN:HA	2.16	0.44
8:K:465:ARG:HD3	8:K:465:ARG:H	1.83	0.44
12:L:271:ILE:O	12:L:275:VAL:N	2.48	0.44
12:L:854:SER:O	12:L:856:LEU:N	2.50	0.44
12:L:1780:TYR:HA	12:L:1783:ILE:HG22	1.99	0.44
12:L:1876:ASP:OD1	12:L:1876:ASP:N	2.51	0.44
12:L:2539:THR:HG23	12:L:2541:GLY:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:371:LEU:HD12	9:G:372:SER:H	1.83	0.44
9:G:544:GLU:HG2	9:G:553:PHE:HB2	1.98	0.44
12:L:214:TYR:O	12:L:218:ALA:N	2.49	0.44
12:L:1340:CYS:HA	12:L:1343:LEU:HD13	1.98	0.44
12:L:2804:GLY:O	12:L:2809:LYS:N	2.50	0.44
12:L:3725:TYR:HA	12:L:3728:VAL:HG12	1.98	0.44
3:C:38:LEU:HD21	16:Q:210:ARG:HG2	1.99	0.44
5:D:218:ARG:C	5:D:220:ALA:N	2.76	0.44
9:G:192:ILE:O	9:G:195:SER:OG	2.31	0.44
12:L:3172:GLN:O	12:L:3175:THR:OG1	2.34	0.44
8:K:465:ARG:O	12:L:2791:PRO:HG3	2.18	0.44
9:G:215:ASN:OD1	9:G:216:GLU:N	2.50	0.44
9:G:352:ALA:O	9:G:356:ARG:N	2.46	0.44
9:G:504:SER:OG	9:G:507:GLY:N	2.44	0.44
12:L:1610:LEU:O	12:L:1617:ARG:NH2	2.51	0.44
5:D:20:MET:HE2	5:D:20:MET:HB3	1.89	0.44
6:E:946:LYS:HD2	6:E:946:LYS:H	1.82	0.44
9:G:618:ARG:HD3	9:G:689:THR:HG21	2.00	0.44
12:L:1623:SER:OG	12:L:1626:ARG:NE	2.51	0.44
12:L:2393:SER:HA	12:L:2396:PHE:HB3	1.99	0.44
12:L:2446:GLU:O	12:L:2452:ARG:NE	2.46	0.44
1:M:78:CYS:SG	1:M:80:LEU:HD11	2.57	0.44
2:A:250:MET:O	2:A:251:THR:C	2.60	0.44
3:C:38:LEU:CB	16:Q:210:ARG:CZ	2.95	0.44
5:D:24:SER:HB3	5:D:210:CYS:CB	2.48	0.44
12:L:379:ARG:O	12:L:421:LYS:NZ	2.50	0.44
12:L:410:MET:HE3	12:L:410:MET:HB3	1.84	0.44
12:L:1356:ARG:N	12:L:1356:ARG:NE	2.65	0.44
12:L:1727:LYS:HD2	12:L:1734:PRO:HG3	1.99	0.44
1:M:79:ARG:C	1:M:80:LEU:HD12	2.43	0.44
9:G:138:VAL:O	9:G:142:LEU:HD23	2.18	0.44
9:G:596:SER:OG	9:G:604:CYS:HB2	2.18	0.44
12:L:404:ALA:HB3	12:L:407:VAL:HG22	1.99	0.44
12:L:1358:VAL:O	12:L:1360:GLU:N	2.51	0.44
12:L:3522:THR:O	12:L:3522:THR:OG1	2.33	0.44
17:O:26:ASN:CB	18:P:47:THR:HG21	2.48	0.44
9:G:74:PRO:HB3	9:G:610:THR:CG2	2.47	0.44
10:H:269:ILE:HG22	10:H:286:MET:HE1	2.00	0.44
12:L:722:LYS:HG2	12:L:768:LEU:HD21	2.00	0.44
12:L:2437:LEU:HA	12:L:2440:ILE:HD12	2.00	0.44
12:L:2897:ILE:HD12	12:L:2897:ILE:HA	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:507:UNK:C	14:N:509:UNK:N	2.78	0.44
15:R:4:PHE:CE1	16:Q:362:LEU:CD1	3.01	0.44
1:M:76:LEU:O	1:M:78:CYS:N	2.51	0.43
8:K:461:LYS:HD2	12:L:2762:LEU:HD11	1.99	0.43
8:K:557:ASP:OD1	8:K:557:ASP:N	2.46	0.43
3:C:59:ILE:HG22	16:Q:170:ILE:HD11	1.99	0.43
1:M:126:ALA:HB3	1:M:132:SER:OG	2.19	0.43
5:D:259:GLU:HA	5:D:262:ILE:HD12	2.00	0.43
12:L:408:GLN:OE1	12:L:445:ARG:NH1	2.39	0.43
12:L:850:VAL:N	12:L:851:PRO:CD	2.82	0.43
12:L:2860:VAL:HG13	12:L:2879:LEU:CD1	2.49	0.43
12:L:3151:ALA:HA	12:L:3154:VAL:HG12	2.01	0.43
1:M:79:ARG:O	1:M:80:LEU:HD12	2.17	0.43
3:C:48:ARG:HG3	16:Q:238:LYS:HG2	2.00	0.43
5:D:215:PHE:HB3	5:D:223:PHE:HB2	2.01	0.43
8:K:452:VAL:O	12:L:2666:GLU:OE2	2.36	0.43
8:K:469:LEU:CD2	12:L:2790:THR:CG2	2.96	0.43
16:Q:130:TYR:CE2	17:O:28:LEU:HD12	2.51	0.43
10:H:318:ALA:HB3	10:H:337:ARG:NH1	2.32	0.43
12:L:801:PHE:HD1	12:L:803:ASN:H	1.66	0.43
12:L:850:VAL:HG13	12:L:853:LEU:HD13	1.99	0.43
12:L:3765:GLN:HB3	12:L:3768:GLN:HB3	2.00	0.43
14:N:207:UNK:CA	14:N:208:UNK:CB	2.96	0.43
1:M:200:PRO:HD3	1:M:225:GLN:OE1	2.18	0.43
5:D:321:VAL:HG12	5:D:321:VAL:O	2.17	0.43
8:K:469:LEU:HD23	8:K:469:LEU:N	2.33	0.43
12:L:773:LEU:HD13	12:L:815:LEU:HD13	2.00	0.43
12:L:3541:ARG:HB2	12:L:3654:GLU:HB2	2.01	0.43
17:O:11:TRP:CD1	18:P:83:LEU:HG	2.51	0.43
1:M:88:HIS:CB	14:N:515:UNK:O	2.56	0.43
2:A:282:ILE:CG2	2:A:335:MET:HE1	2.48	0.43
3:C:51:LEU:HG	16:Q:214:LEU:CA	2.48	0.43
5:D:71:ILE:HD12	5:D:74:ILE:HD11	2.01	0.43
12:L:1079:LYS:HG2	12:L:1142:MET:HE3	2.00	0.43
12:L:2741:LYS:NZ	12:L:2896:ASP:OD1	2.52	0.43
12:L:3099:THR:HG22	12:L:3103:LEU:HD13	2.00	0.43
12:L:3285:ASP:OD1	12:L:3285:ASP:N	2.48	0.43
12:L:2523:ASP:OD1	12:L:2523:ASP:N	2.42	0.43
1:M:153:THR:O	1:M:154:ASP:C	2.61	0.43
3:C:36:ASN:CB	16:Q:467:ARG:NH2	2.81	0.43
3:C:51:LEU:HD12	16:Q:215:SER:H	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:204:GLN:OE1	4:F:204:GLN:HA	2.19	0.43
5:D:17:ILE:HG22	5:D:21:MET:SD	2.59	0.43
7:J:206:TYR:HB3	7:J:207:GLY:H	1.71	0.43
9:G:92:THR:OG1	9:G:93:ALA:N	2.51	0.43
12:L:560:ASP:N	12:L:560:ASP:OD1	2.51	0.43
12:L:1204:ASP:OD1	12:L:1204:ASP:N	2.52	0.43
12:L:1690:SER:O	12:L:1690:SER:OG	2.32	0.43
12:L:2447:LEU:HD23	12:L:2447:LEU:HA	1.89	0.43
1:M:177:PHE:CB	5:D:194:GLU:HA	2.49	0.43
2:A:243:MET:CB	2:A:268:ILE:HD12	2.49	0.43
12:L:436:MET:HE3	12:L:610:ILE:HD11	2.00	0.43
12:L:1884:ALA:HA	12:L:1887:VAL:HG12	2.00	0.43
12:L:1967:ILE:HD12	12:L:1967:ILE:HA	1.91	0.43
12:L:2812:LEU:O	12:L:2813:GLN:C	2.62	0.43
14:N:181:UNK:O	14:N:198:UNK:CB	2.67	0.43
16:Q:470:ASN:HA	17:O:50:GLU:C	2.20	0.43
1:M:152:PHE:CD1	1:M:152:PHE:C	2.96	0.42
5:D:319:ARG:HD2	5:D:319:ARG:HA	1.65	0.42
6:E:885:VAL:HG13	10:H:128:PRO:HG2	2.01	0.42
6:E:929:LEU:CD1	6:E:955:ILE:HG22	2.49	0.42
6:E:950:VAL:O	6:E:950:VAL:HG23	2.19	0.42
12:L:867:SER:OG	12:L:868:GLN:N	2.48	0.42
12:L:1317:ILE:HD11	12:L:1333:ASN:HA	2.01	0.42
12:L:1357:LEU:N	12:L:1357:LEU:CD1	2.81	0.42
12:L:1736:VAL:HG13	12:L:1737:LEU:HD23	2.01	0.42
16:Q:78:ARG:HA	16:Q:82:VAL:HB	2.01	0.42
1:M:96:PRO:C	1:M:98:ARG:H	2.28	0.42
3:C:51:LEU:HD12	16:Q:211:ASP:O	2.08	0.42
12:L:1060:LYS:HD2	12:L:1060:LYS:HA	1.72	0.42
12:L:1786:PRO:HA	12:L:1789:ILE:HG12	2.01	0.42
12:L:2805:PHE:HA	12:L:2810:ASP:O	2.19	0.42
5:D:240:ASP:OD1	5:D:241:VAL:N	2.52	0.42
9:G:581:ALA:O	9:G:582:ILE:HD13	2.19	0.42
10:H:122:LEU:HD12	10:H:123:ILE:HB	2.00	0.42
10:H:129:LYS:NZ	10:H:129:LYS:CB	2.82	0.42
10:H:129:LYS:HZ3	10:H:129:LYS:CB	2.31	0.42
12:L:1226:ARG:NH2	12:L:1275:ASP:OD2	2.52	0.42
12:L:1354:LEU:O	12:L:1357:LEU:HB2	2.19	0.42
12:L:2601:ARG:NE	12:L:2601:ARG:CA	2.81	0.42
8:K:581:ILE:HD12	11:I:52:ILE:HD11	2.01	0.42
10:H:317:LEU:HD12	10:H:318:ALA:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:848:VAL:O	12:L:851:PRO:HD2	2.19	0.42
12:L:1541:LEU:HD12	12:L:1541:LEU:HA	1.93	0.42
12:L:3173:LEU:HD21	12:L:3293:LEU:HD22	2.02	0.42
16:Q:93:CYS:N	17:O:17:ASN:CG	2.76	0.42
5:D:22:PHE:HE2	5:D:30:PRO:HD3	1.85	0.42
6:E:817:GLY:O	6:E:820:LYS:N	2.52	0.42
8:K:437:LEU:HD23	8:K:437:LEU:N	2.32	0.42
9:G:392:ASP:CG	9:G:392:ASP:O	2.62	0.42
12:L:846:LEU:CA	12:L:850:VAL:HB	2.45	0.42
12:L:907:LYS:HE3	12:L:907:LYS:HB3	1.83	0.42
12:L:3111:SER:O	12:L:3111:SER:OG	2.33	0.42
12:L:3427:PHE:O	12:L:3428:GLU:C	2.62	0.42
17:O:34:ARG:NH2	18:P:51:VAL:CG1	2.79	0.42
3:C:47:ASP:HB3	16:Q:243:THR:CA	2.48	0.42
5:D:19:GLN:C	5:D:19:GLN:CD	2.86	0.42
9:G:416:LEU:N	9:G:447:ARG:O	2.52	0.42
10:H:242:GLU:OE1	10:H:242:GLU:N	2.52	0.42
12:L:1356:ARG:NE	12:L:1356:ARG:CA	2.82	0.42
12:L:1417:ARG:HH21	12:L:1417:ARG:HG3	1.85	0.42
12:L:2422:PHE:HE2	12:L:2441:LEU:HD22	1.85	0.42
12:L:2889:ARG:O	12:L:2889:ARG:HG2	2.20	0.42
16:Q:139:TYR:HE1	18:P:59:PHE:CD1	2.36	0.42
3:C:288:LEU:CD2	3:C:292:THR:HG21	2.48	0.42
5:D:72:PHE:HD1	5:D:72:PHE:HA	1.70	0.42
12:L:1727:LYS:O	12:L:1776:ARG:NH2	2.53	0.42
14:N:83:UNK:C	14:N:507:UNK:N	2.82	0.42
1:M:186:GLU:HB3	1:M:189:LEU:HB2	2.01	0.42
5:D:244:ILE:O	5:D:248:LEU:HG	2.20	0.42
6:E:947:PHE:HE1	6:E:949:LYS:HA	1.85	0.42
7:J:116:TYR:OH	7:J:120:ARG:NH2	2.53	0.42
8:K:582:ARG:NH1	11:I:71:GLY:O	2.52	0.42
10:H:315:LEU:O	10:H:318:ALA:HB2	2.20	0.42
12:L:2415:THR:HG22	12:L:2418:MET:HE3	2.01	0.42
12:L:2476:GLN:HG2	12:L:2548:ILE:HD12	2.02	0.42
12:L:2740:GLU:HB2	12:L:2745:TRP:CH2	2.55	0.42
16:Q:416:PHE:CZ	18:P:41:ASP:OD2	2.73	0.42
16:Q:478:ARG:HG3	17:O:68:HIS:CD2	2.41	0.42
1:M:187:PRO:HB3	5:D:211:ARG:HB2	2.02	0.42
2:A:204:LYS:HA	3:C:293:ALA:HB3	2.02	0.42
2:A:250:MET:O	2:A:253:ILE:N	2.52	0.42
3:C:253:ARG:NH2	10:H:49:TYR:OH	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:14:HIS:HB3	10:H:45:MET:HE1	2.01	0.42
10:H:67:ARG:NH2	10:H:74:ASP:OD1	2.53	0.42
12:L:1863:LYS:HA	12:L:1863:LYS:HD2	1.78	0.42
14:N:494:UNK:O	14:N:509:UNK:HA	2.20	0.42
17:O:26:ASN:HD22	18:P:47:THR:HG21	1.85	0.42
2:A:259:LEU:HD21	8:K:549:LYS:HB2	2.02	0.41
3:C:38:LEU:CD1	16:Q:210:ARG:HH11	2.27	0.41
9:G:600:ASP:OD1	9:G:601:SER:N	2.53	0.41
11:I:24:ILE:O	11:I:26:SER:N	2.51	0.41
12:L:328:ARG:HH11	12:L:370:THR:HG22	1.84	0.41
12:L:3149:LYS:HD3	12:L:3149:LYS:HA	1.89	0.41
6:E:930:LYS:O	6:E:934:GLU:HG2	2.21	0.41
9:G:144:LEU:HD22	9:G:156:PHE:CE2	2.56	0.41
9:G:450:VAL:HG13	9:G:451:GLY:N	2.35	0.41
10:H:155:SER:OG	10:H:157:ASN:OD1	2.36	0.41
12:L:718:ILE:HD12	12:L:718:ILE:HA	1.95	0.41
12:L:3634:ILE:HD12	12:L:3703:PHE:HB2	2.02	0.41
14:N:184:UNK:CB	14:N:238:UNK:N	2.82	0.41
14:N:496:UNK:N	14:N:508:UNK:CB	2.83	0.41
16:Q:178:LEU:HD12	17:O:37:ILE:HD12	1.81	0.41
1:M:74:VAL:HG23	1:M:155:PHE:CA	2.49	0.41
3:C:41:ARG:HB3	16:Q:173:SER:HB3	2.02	0.41
8:K:442:PRO:HB3	12:L:2817:ARG:NH1	2.35	0.41
8:K:469:LEU:CD2	12:L:2790:THR:HG23	2.50	0.41
9:G:515:HIS:NE2	10:H:57:GLN:OE1	2.53	0.41
9:G:585:LEU:HA	9:G:595:ALA:O	2.21	0.41
10:H:69:THR:HG23	10:H:71:HIS:HE1	1.84	0.41
12:L:764:HIS:NE2	12:L:1525:ASN:OD1	2.37	0.41
12:L:3603:THR:HG22	12:L:3711:LYS:HG2	2.01	0.41
16:Q:137:GLY:O	18:P:60:SER:OG	2.27	0.41
16:Q:472:PHE:HE2	17:O:50:GLU:CG	2.18	0.41
2:A:223:GLN:OE1	2:A:223:GLN:CA	2.68	0.41
12:L:1444:LYS:HE3	12:L:1444:LYS:HB2	1.80	0.41
12:L:2798:THR:HA	12:L:2818:LEU:HD23	2.02	0.41
12:L:3705:LEU:HD12	12:L:3705:LEU:HA	1.95	0.41
3:C:52:GLN:CG	16:Q:153:GLN:HG3	2.50	0.41
8:K:466:PRO:HA	12:L:2791:PRO:CG	2.23	0.41
9:G:709:THR:HG22	9:G:710:ARG:N	2.35	0.41
1:M:189:LEU:CD1	5:D:84:LEU:HD13	2.49	0.41
3:C:44:ASN:OD1	16:Q:174:ARG:CD	2.69	0.41
6:E:934:GLU:O	6:E:936:LYS:N	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:454:PRO:CD	8:K:455:PRO:HD2	2.50	0.41
9:G:460:ASP:OD1	9:G:461:PHE:N	2.54	0.41
12:L:388:TRP:HA	12:L:391:VAL:HG12	2.03	0.41
12:L:1587:SER:OG	12:L:1588:PHE:N	2.53	0.41
12:L:3133:TRP:CZ3	12:L:3441:ASP:HB3	2.56	0.41
17:O:11:TRP:CE2	18:P:86:ILE:CG1	2.97	0.41
1:M:84:THR:O	1:M:87:LEU:HB2	2.20	0.41
2:A:268:ILE:O	2:A:272:LEU:HD23	2.20	0.41
9:G:365:SER:O	9:G:370:LYS:N	2.49	0.41
10:H:129:LYS:NZ	10:H:129:LYS:CA	2.82	0.41
12:L:268:GLY:O	12:L:272:ILE:N	2.53	0.41
12:L:672:PRO:O	12:L:676:ASN:ND2	2.54	0.41
12:L:1629:GLY:HA2	12:L:1632:HIS:HD2	1.86	0.41
12:L:2794:GLN:HG2	12:L:2822:GLY:HA3	2.02	0.41
1:M:231:TYR:HB3	1:M:232:PRO:HD3	2.03	0.41
8:K:469:LEU:HD22	12:L:2790:THR:HG23	2.03	0.41
12:L:1295:SER:OG	12:L:1305:MET:SD	2.68	0.41
12:L:3136:ILE:HA	12:L:3139:VAL:HG23	2.03	0.41
3:C:51:LEU:CG	16:Q:214:LEU:CG	2.97	0.41
5:D:316:LEU:C	5:D:318:LYS:N	2.79	0.41
9:G:648:VAL:HG13	9:G:694:SER:H	1.86	0.41
9:G:701:THR:O	9:G:701:THR:OG1	2.39	0.41
10:H:396:ILE:HG23	10:H:397:ARG:N	2.36	0.41
11:I:51:THR:HG22	11:I:76:LEU:HD21	2.03	0.41
12:L:314:SER:O	12:L:314:SER:OG	2.33	0.41
12:L:853:LEU:H	12:L:853:LEU:CD2	2.34	0.41
12:L:858:LYS:HB2	12:L:858:LYS:HE3	1.87	0.41
12:L:1425:PHE:C	12:L:1427:SER:H	2.29	0.41
12:L:1540:HIS:O	12:L:1582:ARG:NH2	2.54	0.41
12:L:2465:LEU:H	12:L:2465:LEU:HG	1.71	0.41
12:L:2592:ASP:OD1	12:L:2592:ASP:N	2.53	0.41
12:L:2778:LEU:HD23	12:L:2778:LEU:HA	1.96	0.41
12:L:3142:LEU:HB3	12:L:3158:LEU:HD11	2.03	0.41
14:N:175:UNK:HA	14:N:213:UNK:O	2.21	0.41
16:Q:76:ARG:NH2	18:P:18:VAL:C	2.74	0.41
5:D:196:THR:O	5:D:197:LYS:C	2.63	0.41
10:H:335:ALA:O	10:H:339:LEU:HD23	2.20	0.41
1:M:105:ARG:O	1:M:106:ILE:CG2	2.69	0.40
1:M:115:ILE:HD13	1:M:121:MET:CG	2.51	0.40
2:A:199:GLN:NE2	3:C:305:PHE:O	2.54	0.40
8:K:460:MET:HG3	12:L:2758:THR:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:468:LEU:C	12:L:2790:THR:HG22	2.46	0.40
12:L:325:HIS:HA	12:L:328:ARG:HB3	2.03	0.40
12:L:1358:VAL:HG22	12:L:1359:GLN:N	2.36	0.40
12:L:1506:LEU:HA	12:L:1509:TRP:HD1	1.86	0.40
12:L:2231:ILE:O	12:L:2235:VAL:N	2.53	0.40
12:L:2721:PHE:HA	12:L:2722:PRO:HD3	1.90	0.40
12:L:3604:LEU:HD12	12:L:3604:LEU:HA	1.93	0.40
5:D:206:HIS:HA	5:D:209:GLU:CD	2.46	0.40
12:L:1067:TYR:O	12:L:1070:SER:OG	2.34	0.40
12:L:2687:TYR:HB2	12:L:2690:THR:HG22	2.02	0.40
12:L:2817:ARG:HA	12:L:2817:ARG:HD2	1.91	0.40
12:L:2907:ARG:HH11	12:L:2907:ARG:CG	2.25	0.40
12:L:2908:GLN:O	12:L:2909:HIS:C	2.65	0.40
12:L:3798:THR:HB	12:L:3801:VAL:HG22	2.04	0.40
17:O:9:THR:HG22	18:P:10:LYS:HE3	0.41	0.40
1:M:78:CYS:SG	1:M:80:LEU:CD1	3.10	0.40
3:C:49:PRO:CD	16:Q:238:LYS:HA	2.52	0.40
4:F:85:PHE:N	4:F:143:ARG:O	2.46	0.40
6:E:944:ASP:OD1	6:E:944:ASP:N	2.54	0.40
9:G:588:SER:HB3	9:G:593:TRP:HB2	2.04	0.40
10:H:217:LEU:HB2	10:H:221:LEU:HD22	2.02	0.40
12:L:833:ASP:HA	12:L:836:VAL:HG12	2.03	0.40
12:L:1611:ASP:OD1	12:L:1611:ASP:N	2.53	0.40
16:Q:20:ASP:N	16:Q:20:ASP:OD1	2.55	0.40
5:D:84:LEU:HA	5:D:87:TYR:CD2	2.56	0.40
8:K:461:LYS:HE2	8:K:463:PRO:HD2	2.03	0.40
9:G:45:ASP:OD1	9:G:45:ASP:N	2.55	0.40
12:L:2783:LYS:HA	12:L:2783:LYS:HD3	1.74	0.40
12:L:3063:GLY:O	12:L:3067:ASP:N	2.47	0.40
16:Q:182:THR:CB	17:O:45:GLN:O	2.69	0.40
17:O:22:ILE:CB	18:P:43:ILE:HD12	2.52	0.40
1:M:85:VAL:HG11	1:M:143:ILE:HG22	2.04	0.40
9:G:182:GLU:OE1	9:G:182:GLU:N	2.49	0.40
12:L:3778:GLU:HA	12:L:3781:THR:HG22	2.04	0.40
17:O:11:TRP:CZ2	18:P:82:ILE:HG23	2.55	0.40
17:O:22:ILE:CG2	18:P:44:ASN:OD1	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	178/240 (74%)	147 (83%)	24 (14%)	7 (4%)	2	19
2	A	122/448 (27%)	108 (88%)	14 (12%)	0	100	100
3	C	89/698 (13%)	83 (93%)	6 (7%)	0	100	100
4	F	191/517 (37%)	166 (87%)	24 (13%)	1 (0%)	24	63
5	D	164/341 (48%)	141 (86%)	16 (10%)	7 (4%)	2	17
6	E	150/1191 (13%)	135 (90%)	13 (9%)	2 (1%)	9	42
7	J	92/217 (42%)	82 (89%)	9 (10%)	1 (1%)	11	46
8	K	150/609 (25%)	125 (83%)	23 (15%)	2 (1%)	9	42
9	G	512/722 (71%)	448 (88%)	63 (12%)	1 (0%)	43	78
10	H	413/485 (85%)	365 (88%)	48 (12%)	0	100	100
11	I	119/153 (78%)	98 (82%)	21 (18%)	0	100	100
12	L	2874/3825 (75%)	2623 (91%)	233 (8%)	18 (1%)	21	59
13	B	70/722 (10%)	63 (90%)	7 (10%)	0	100	100
15	R	76/76 (100%)	75 (99%)	1 (1%)	0	100	100
16	Q	480/502 (96%)	444 (92%)	30 (6%)	6 (1%)	9	42
17	O	115/123 (94%)	103 (90%)	6 (5%)	6 (5%)	1	15
18	P	88/96 (92%)	85 (97%)	3 (3%)	0	100	100
All	All	5883/10965 (54%)	5291 (90%)	541 (9%)	51 (1%)	16	51

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	77	GLY
1	M	99	PHE
1	M	110	LYS
5	D	200	THR
5	D	327	ARG

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Mol	Chain	Res	Type
6	E	935	SER
8	K	459	ALA
12	L	66	VAL
12	L	204	PRO
12	L	828	ARG
12	L	854	SER
12	L	855	TYR
12	L	1425	PHE
12	L	1426	LYS
12	L	2602	PRO
12	L	3428	GLU
12	L	3797	ALA
16	Q	31	SER
16	Q	58	ILE
16	Q	223	LYS
17	O	59	VAL
17	O	75	GLU
17	O	79	ASN
1	M	97	LYS
1	M	147	GLY
1	M	150	ALA
5	D	219	LYS
5	D	330	GLN
7	J	206	TYR
9	G	450	VAL
12	L	826	ALA
12	L	2597	GLN
16	Q	70	GLU
17	O	65	ILE
1	M	201	LYS
5	D	77	ASP
6	E	941	VAL
12	L	1774	ASP
12	L	3460	ARG
16	Q	431	ASN
17	O	58	PHE
8	K	442	PRO
12	L	2594	HIS
12	L	3439	HIS
17	O	86	SER
4	F	80	PRO
5	D	218	ARG

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Mol	Chain	Res	Type
12	L	3616	TYR
16	Q	245	GLU
12	L	1359	GLN
5	D	321	VAL

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	M	152/205 (74%)	138 (91%)	14 (9%)	8	27
2	A	134/394 (34%)	134 (100%)	0	100	100
3	C	85/627 (14%)	85 (100%)	0	100	100
4	F	179/471 (38%)	179 (100%)	0	100	100
5	D	166/306 (54%)	153 (92%)	13 (8%)	11	32
6	E	142/1101 (13%)	135 (95%)	7 (5%)	22	43
7	J	85/183 (46%)	84 (99%)	1 (1%)	63	75
8	K	133/524 (25%)	132 (99%)	1 (1%)	73	80
9	G	439/635 (69%)	431 (98%)	8 (2%)	51	68
10	H	352/438 (80%)	347 (99%)	5 (1%)	59	72
11	I	104/130 (80%)	103 (99%)	1 (1%)	68	78
12	L	2156/3450 (62%)	2122 (98%)	34 (2%)	55	70
15	R	70/68 (103%)	70 (100%)	0	100	100
16	Q	431/449 (96%)	426 (99%)	5 (1%)	63	75
17	O	103/109 (94%)	102 (99%)	1 (1%)	68	78
18	P	85/91 (93%)	85 (100%)	0	100	100
All	All	4816/9181 (52%)	4726 (98%)	90 (2%)	49	67

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	67	LEU
1	M	76	LEU
1	M	97	LYS
1	M	104	MET
1	M	141	ARG
1	M	148	PHE
1	M	153	THR
1	M	175	LEU
1	M	181	THR
1	M	202	ILE
1	M	212	ILE
1	M	215	THR
1	M	239	LYS
1	M	240	MET
5	D	17	ILE
5	D	18	GLN
5	D	71	ILE
5	D	74	ILE
5	D	78	LYS
5	D	85	ARG
5	D	87	TYR
5	D	211	ARG
5	D	212	GLN
5	D	216	THR
5	D	322	GLU
5	D	329	PHE
5	D	338	VAL
6	E	933	ILE
6	E	938	ILE
6	E	941	VAL
6	E	942	MET
6	E	946	LYS
6	E	948	GLN
6	E	949	LYS
7	J	205	GLU
8	K	437	LEU
9	G	230	ASN
9	G	452	HIS
9	G	537	LEU
9	G	542	CYS
9	G	560	THR
9	G	566	ILE
9	G	571	CYS

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Mol	Chain	Res	Type
9	G	695	VAL
10	H	129	LYS
10	H	217	LEU
10	H	360	PRO
10	H	362	ILE
10	H	364	ARG
11	I	16	HIS
12	L	429	THR
12	L	849	LEU
12	L	850	VAL
12	L	852	HIS
12	L	971	THR
12	L	1122	ASN
12	L	1278	ASN
12	L	1314	LEU
12	L	1356	ARG
12	L	1358	VAL
12	L	1417	ARG
12	L	1419	LYS
12	L	1424	PHE
12	L	1680	LEU
12	L	2465	LEU
12	L	2595	ILE
12	L	2633	ASN
12	L	2701	ILE
12	L	2807	GLN
12	L	2879	LEU
12	L	2880	LYS
12	L	2881	ARG
12	L	2882	VAL
12	L	2883	LEU
12	L	2884	GLN
12	L	2887	ARG
12	L	2888	GLU
12	L	2907	ARG
12	L	2913	VAL
12	L	2914	ILE
12	L	2916	ARG
12	L	3440	LYS
12	L	3441	ASP
12	L	3459	VAL
16	Q	38	TYR

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Mol	Chain	Res	Type
16	Q	61	TYR
16	Q	222	THR
16	Q	246	THR
16	Q	348	THR
17	O	42	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	91	ASN
1	M	95	ASN
1	M	179	HIS
2	A	199	GLN
2	A	227	HIS
2	A	341	GLN
2	A	361	HIS
4	F	267	HIS
4	F	274	ASN
5	D	212	GLN
5	D	317	GLN
5	D	328	ASN
9	G	391	ASN
9	G	508	HIS
9	G	526	HIS
9	G	656	ASN
10	H	36	ASN
10	H	157	ASN
10	H	246	ASN
10	H	306	HIS
12	L	325	HIS
12	L	417	ASN
12	L	433	GLN
12	L	737	ASN
12	L	830	GLN
12	L	865	ASN
12	L	916	HIS
12	L	1072	GLN
12	L	1087	ASN
12	L	1095	ASN
12	L	1299	GLN
12	L	1516	GLN
12	L	1632	HIS

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Mol	Chain	Res	Type
12	L	1745	ASN
12	L	2553	GLN
12	L	2619	HIS
12	L	2623	HIS
12	L	2633	ASN
12	L	2698	GLN
12	L	2797	GLN
12	L	2884	GLN
12	L	2954	HIS
12	L	3312	ASN
12	L	3418	HIS
12	L	3423	HIS
12	L	3444	ASN
12	L	3765	GLN
12	L	3813	ASN
15	R	25	ASN
15	R	60	ASN
15	R	62	GLN
15	R	68	HIS
16	Q	55	ASN
16	Q	110	HIS
16	Q	150	GLN
16	Q	153	GLN
16	Q	205	HIS
16	Q	271	GLN
16	Q	312	GLN
16	Q	466	ASN
17	O	26	ASN
17	O	52	ASN
17	O	54	GLN
18	P	14	GLN
18	P	28	ASN
18	P	36	GLN
18	P	77	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	GLZ	R	76	16,15	3,3,3	0.68	0	1,2,2	0.09	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	GLZ	R	76	16,15	-	0/0/1/1	-

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.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
14	N	6
13	B	2
1	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	414:ASP	C	462:ALA	N	28.86
1	B	471:ASP	C	509:ASP	N	23.98
1	N	117:UNK	C	172:UNK	N	15.59
1	N	287:UNK	C	332:UNK	N	5.97
1	N	213:UNK	C	214:UNK	N	4.21
1	N	467:UNK	C	468:UNK	N	2.43
1	N	451:UNK	C	452:UNK	N	1.99
1	M	194:ILE	C	195:TYR	N	1.97
1	N	207:UNK	C	208:UNK	N	1.79

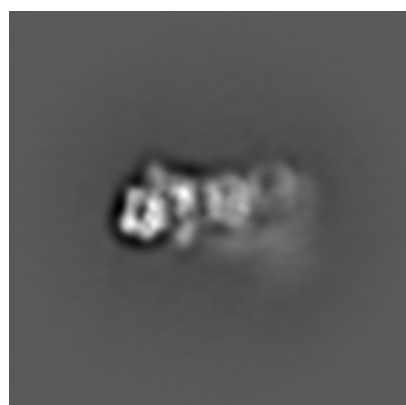
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10446. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y



Z

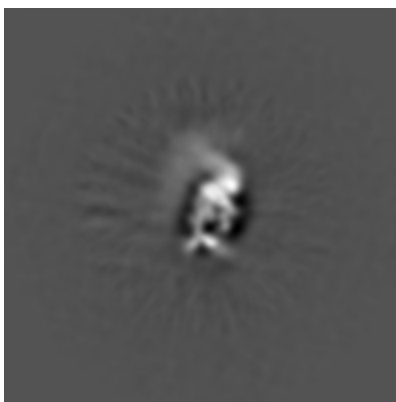
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 128



Y Index: 128



Z Index: 128

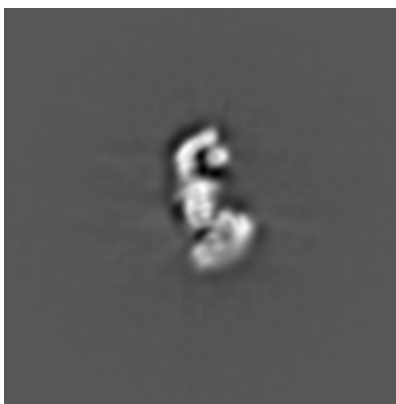
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

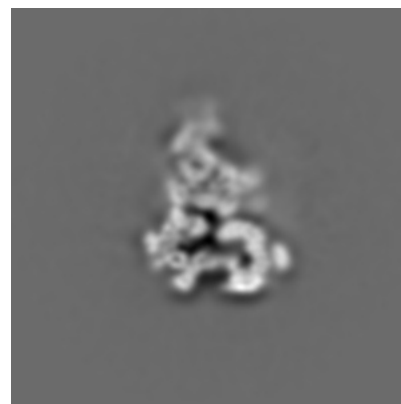
6.3.1 Primary map



X Index: 121



Y Index: 93

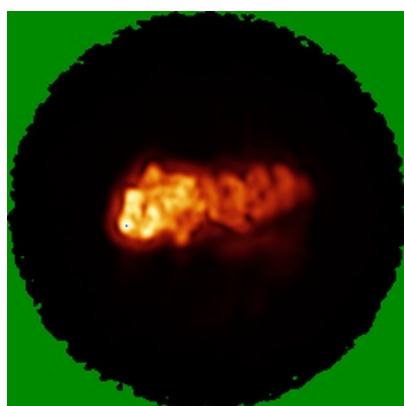


Z Index: 133

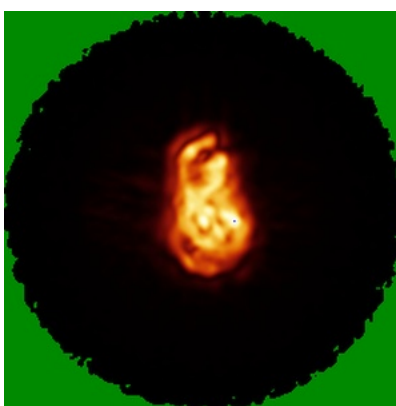
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

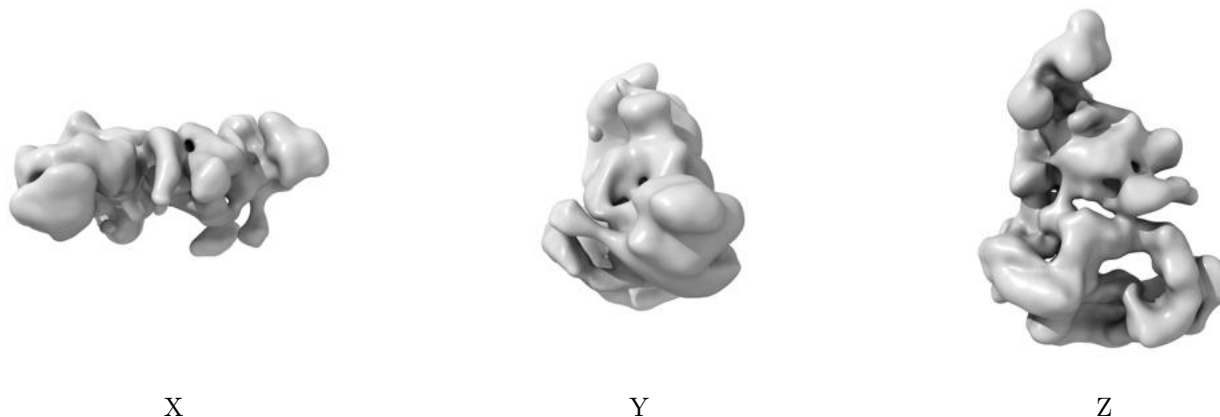


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

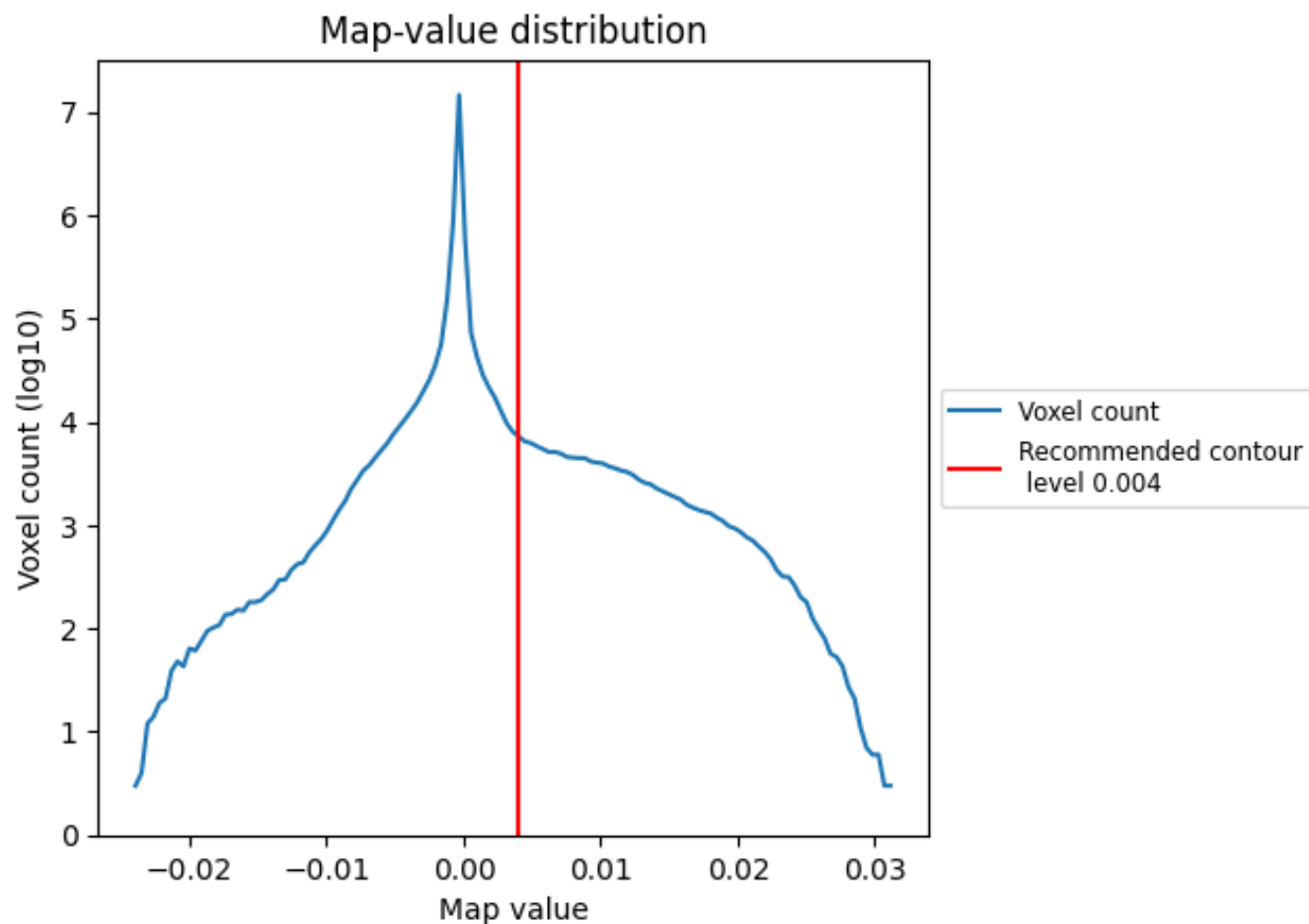
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

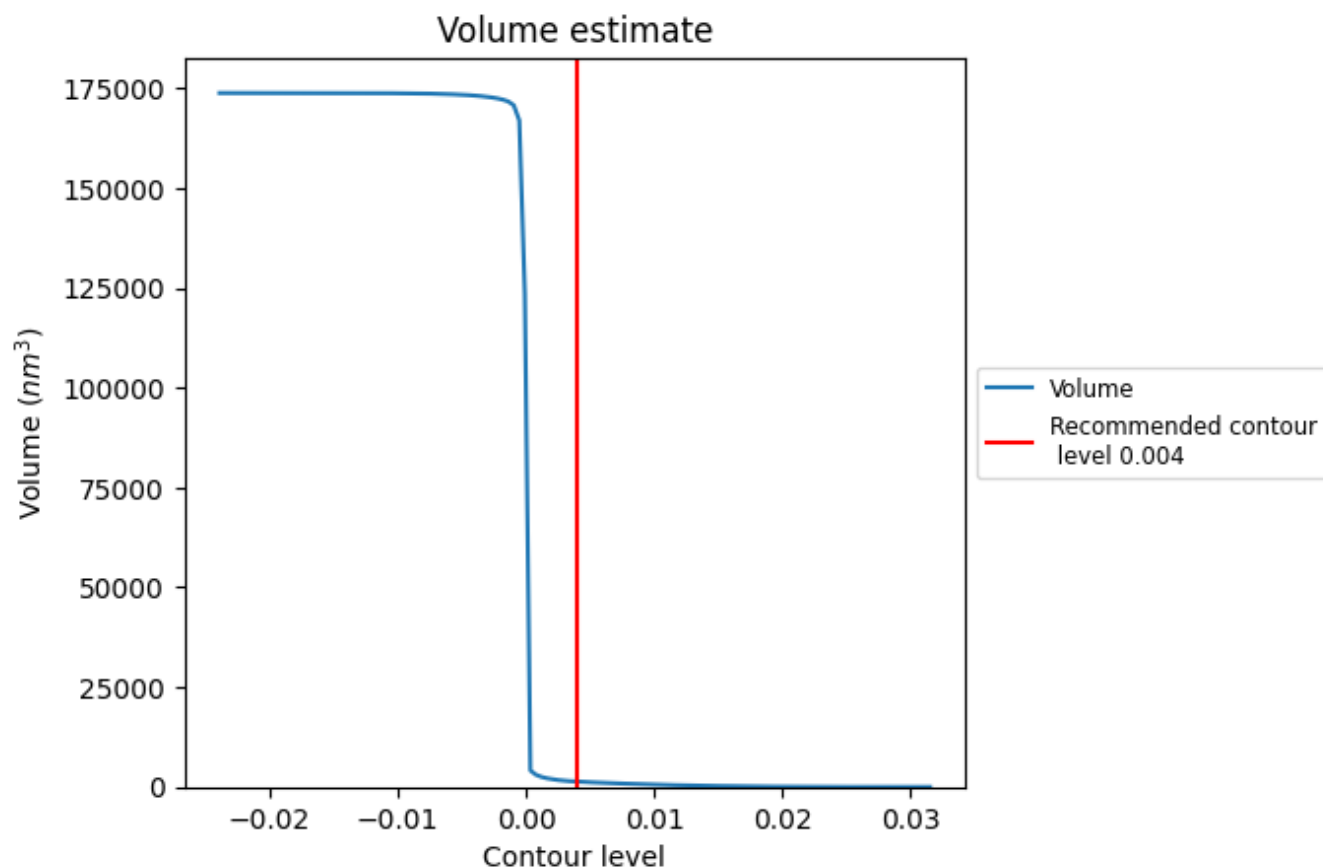
This section contains the results of statistical analysis of the map.

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.

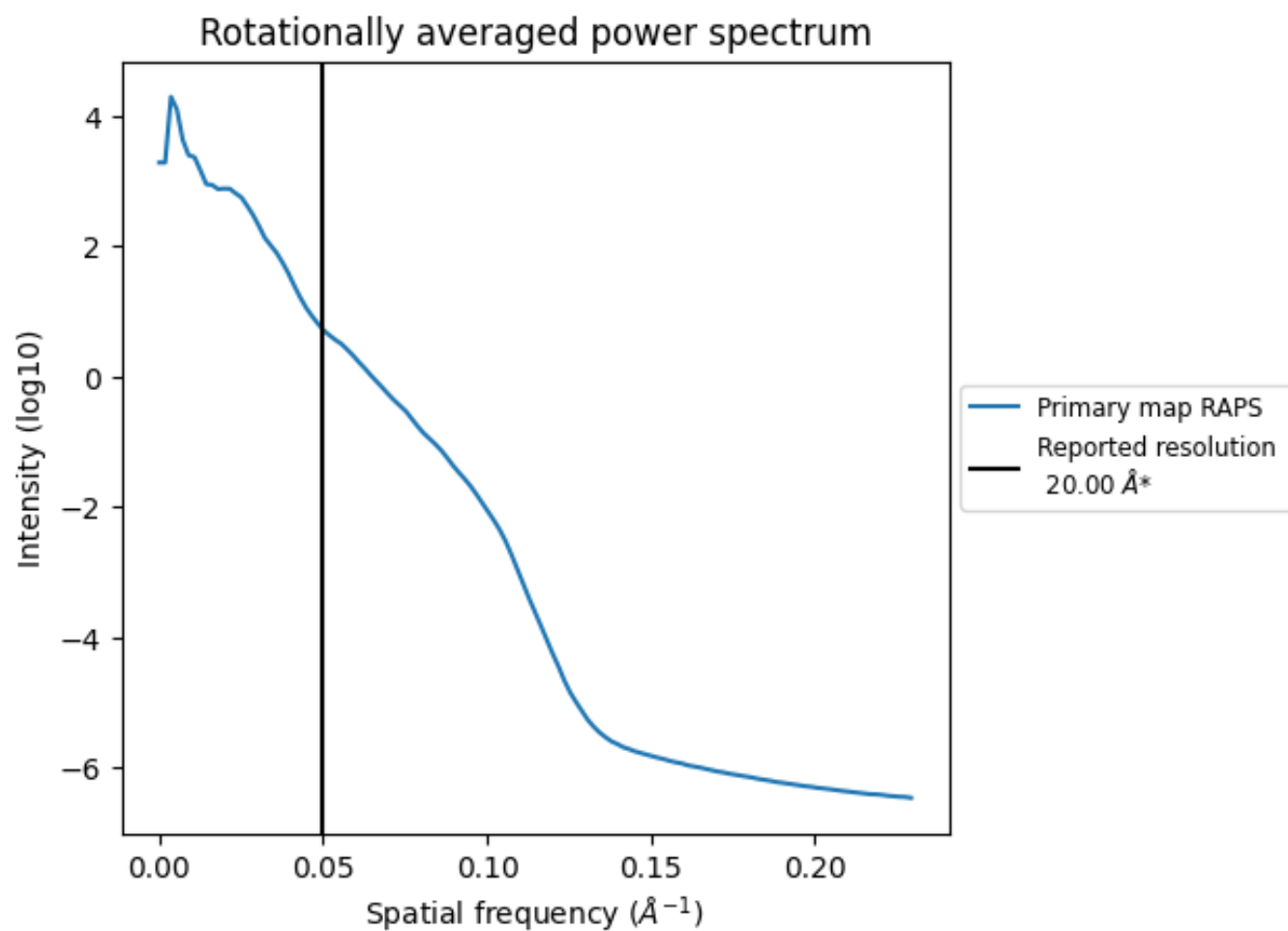
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1341 nm^3 ; this corresponds to an approximate mass of 1211 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 0.050 $\text{\AA}^{-1}$

8 Fourier-Shell correlation

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

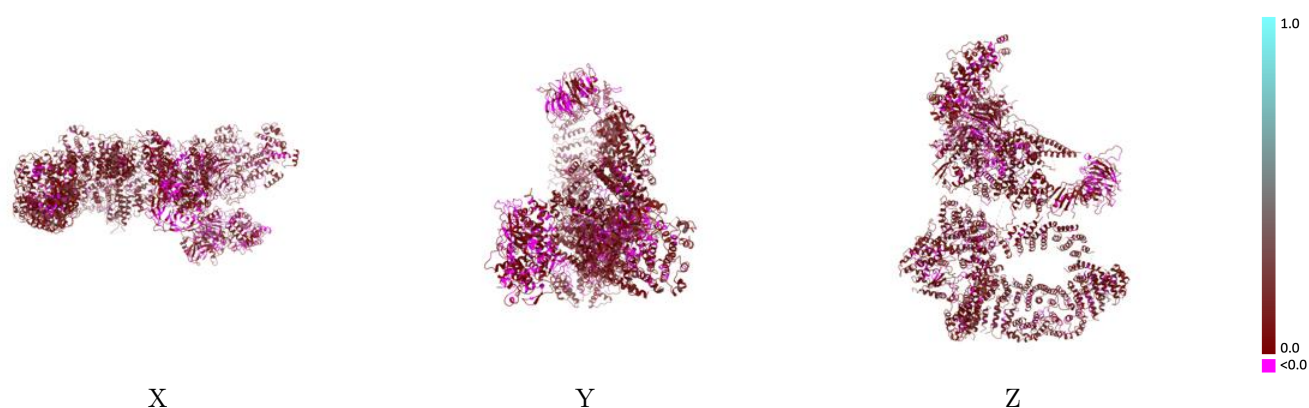
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10446 and PDB model 6TBM. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

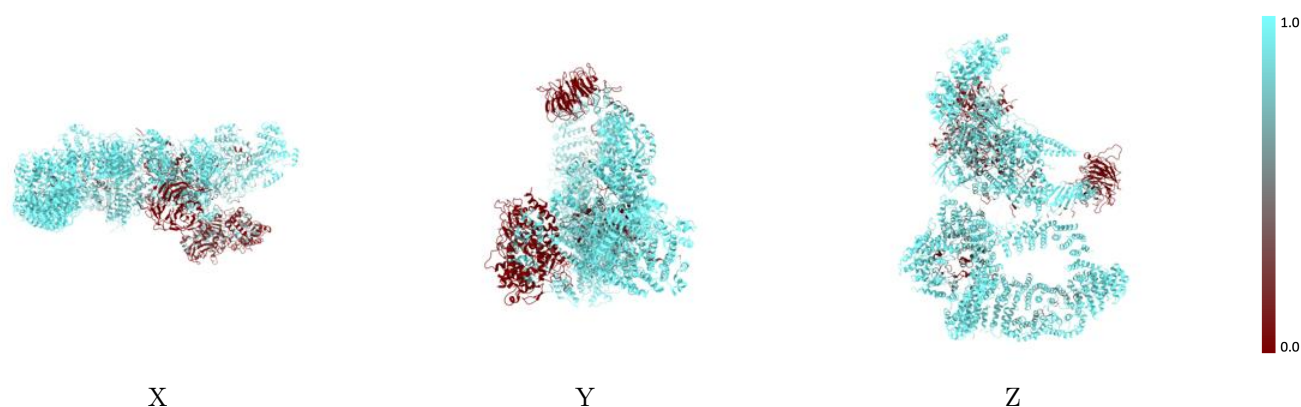
This section was not generated.

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



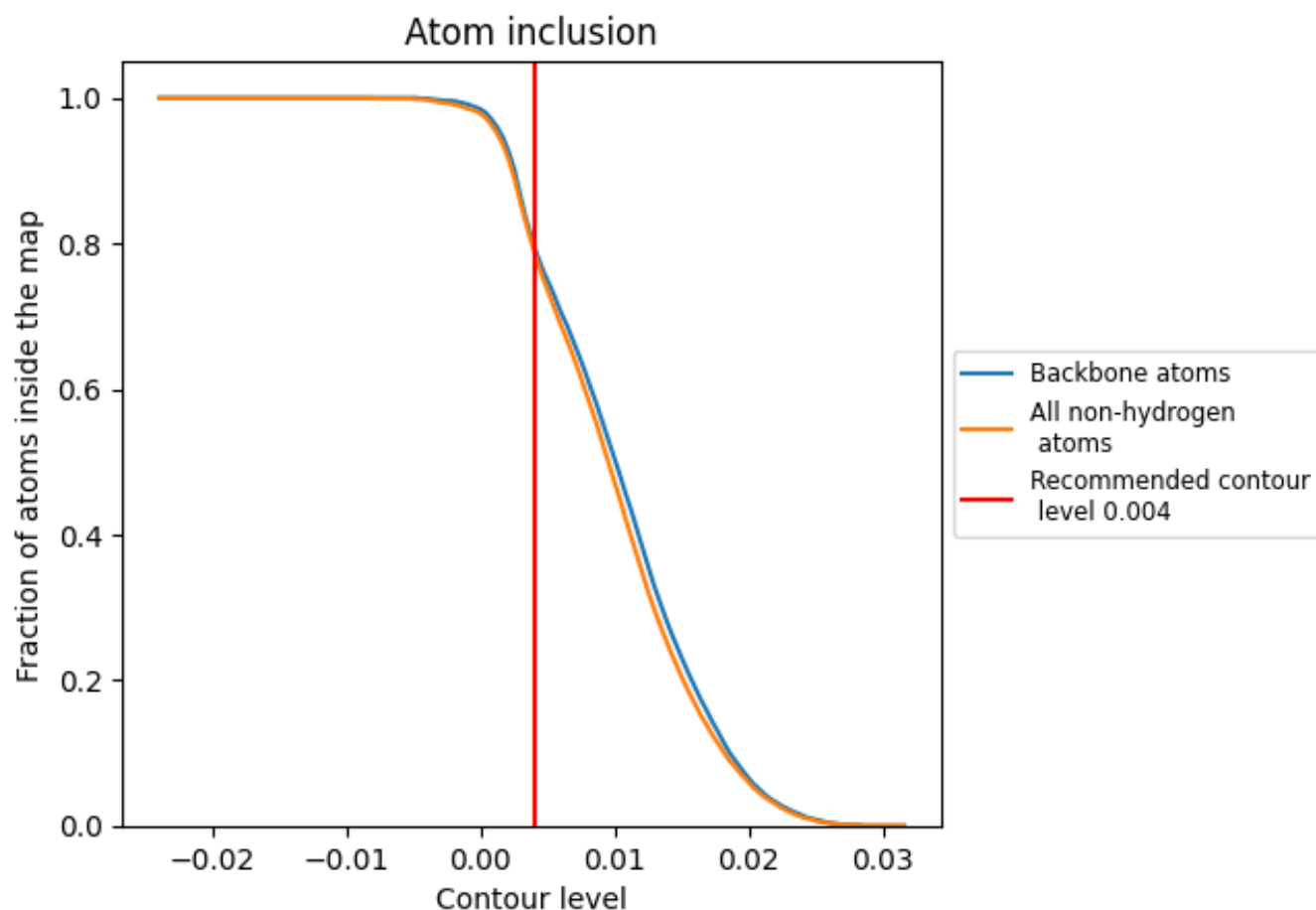
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7880	 0.0800
A	 0.7340	 0.0550
B	 1.0000	 0.1030
C	 0.5900	 0.0520
D	 0.8780	 0.0850
E	 0.9840	 0.1110
F	 0.8990	 0.0920
G	 0.8960	 0.0740
H	 0.9010	 0.0800
I	 0.8680	 0.0710
J	 0.9480	 0.0730
K	 0.8180	 0.0500
L	 0.9280	 0.1010
M	 0.8060	 0.0760
N	 0.0380	 0.0210
O	 0.1700	 0.0130
P	 0.2190	 0.0410
Q	 0.2220	 0.0270
R	 0.3800	 0.0620

