



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 3, 2020 – 02:12 PM EST

PDB ID : 6TBM
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/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB 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.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

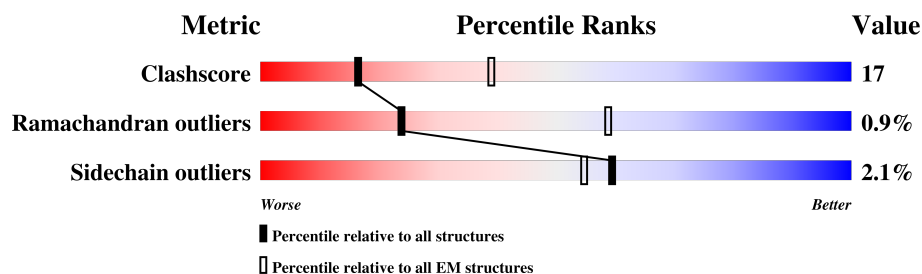
1 Overall quality at a glance

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)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	M	240	37% 33% 6% 25%
2	A	448	31% 7% 61%
3	C	698	9% . 86%
4	F	517	33% 7% 59%
5	D	341	37% 21% . 39%
6	E	1191	10% . . 87%
7	J	217	36% 7% 56%
8	K	609	17% 7% . 75%
9	G	722	52% 20% . 28%

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Mol	Chain	Length	Quality of chain
10	H	485	<div><div></div><div>69%17%13%</div></div>
11	I	153	<div><div></div><div>65%16%20%</div></div>
12	L	3825	<div><div></div><div>66%11%22%</div></div>
13	B	722	<div><div></div><div>10%89%</div></div>
14	N	400	<div><div></div><div>72%12%16%</div></div>
15	R	76	<div><div></div><div>84%16%</div></div>
16	Q	502	<div><div></div><div>77%18%</div></div>
17	O	123	<div><div></div><div>59%37%5%</div></div>
18	P	96	<div><div></div><div>59%34%6%</div></div>

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-binding protein.

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		

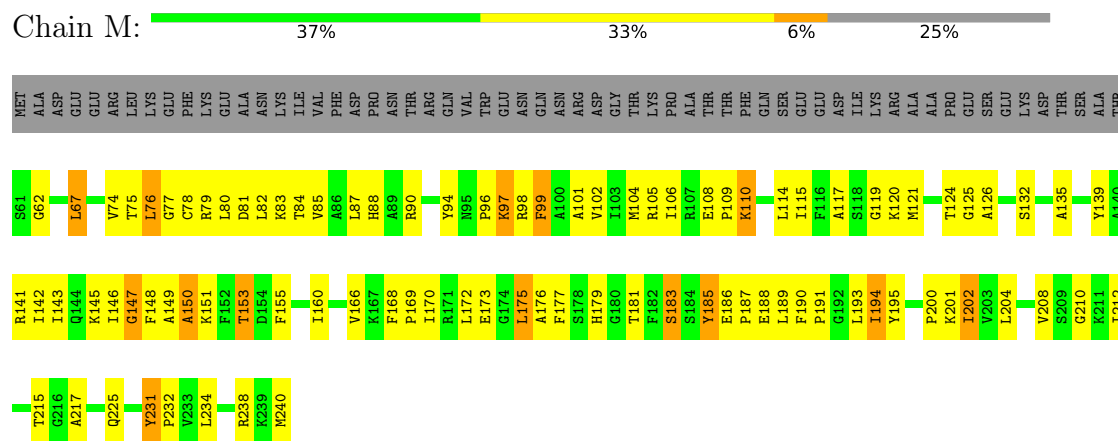
- Molecule 19 is water.

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

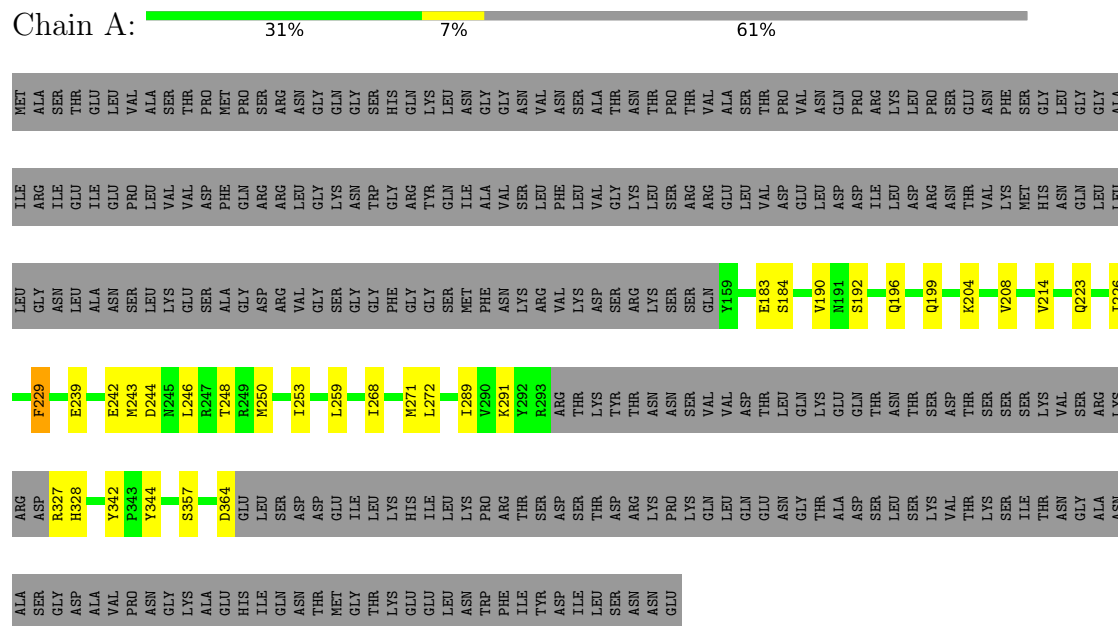
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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-binding protein



- Molecule 2: Transcriptional coactivator HFI1/ADA1



- Molecule 3: Subunit of SAGA histone acetyltransferase complex

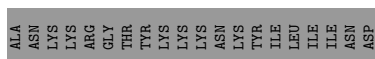


[illegible]

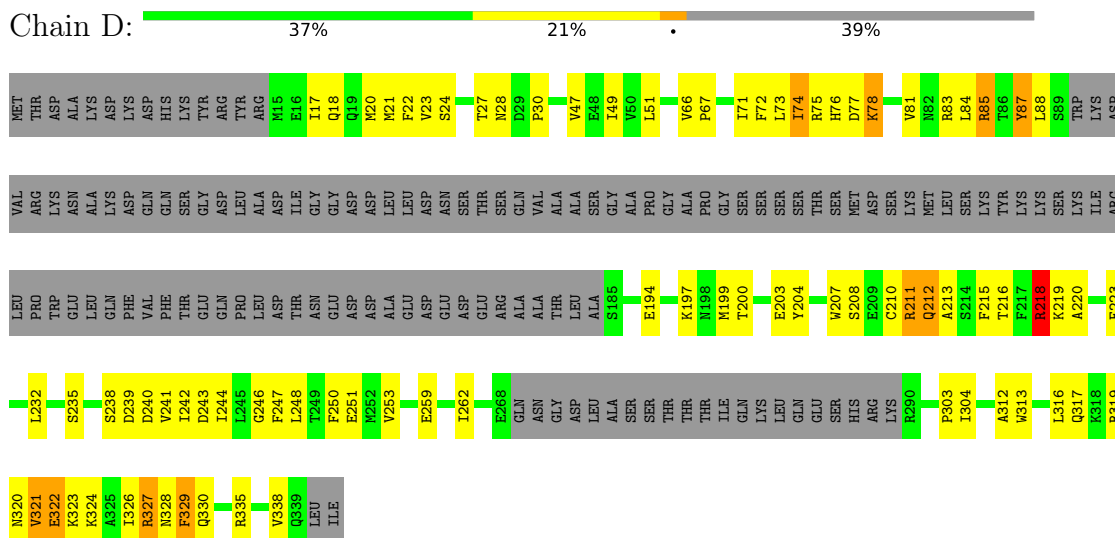
- Molecule 4: Spt20

Chain F: 33% 7% 59%

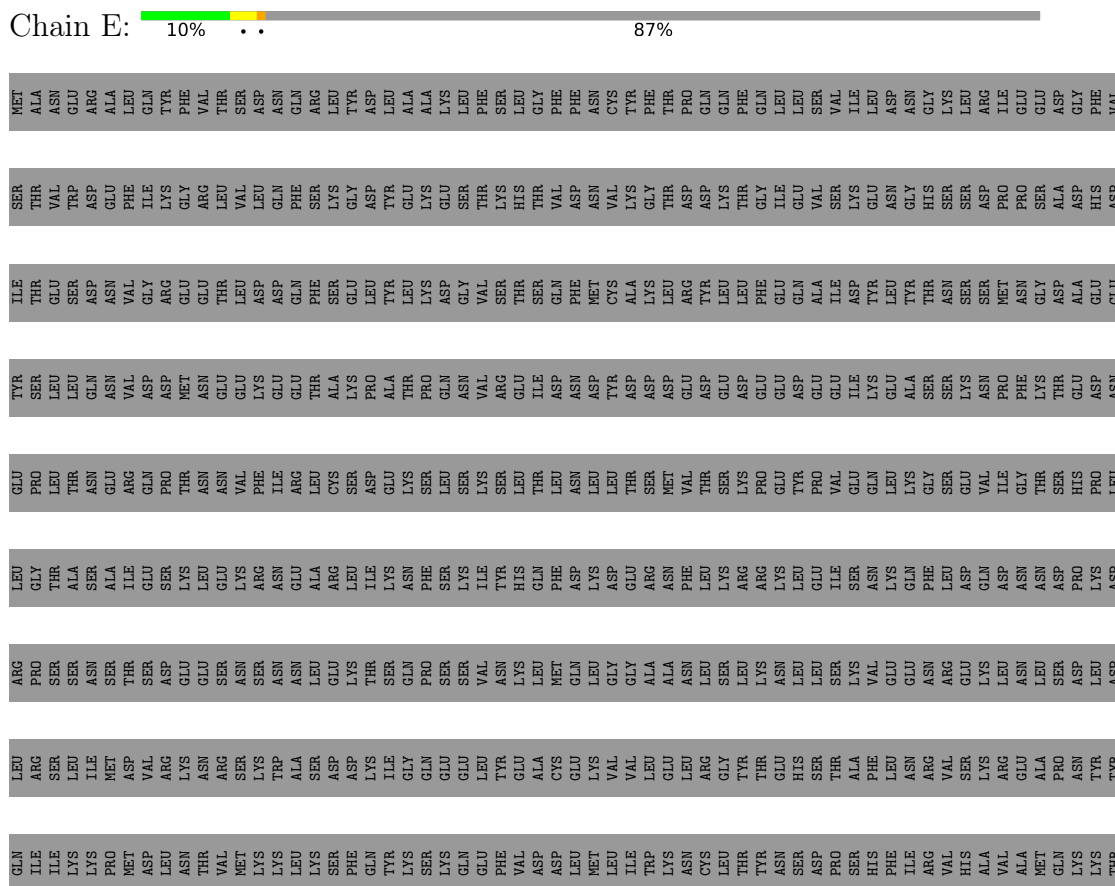
GLN	ASN	ASP	THR	THR	LYS	MET
HIS	LEU	ASP	ASN	ASN	THR	SER
ASN	THR	SER	ASN	GLU	TVR	GLN
GLN	PRO	GLN	THR	LYS	K64	ILE
HIS	GLN	GLN	THR	LYS	P80	GLN
GLN	LYS	GLY	GLU	PRO	L83	SER
GLN	ALA	SER	PRO	THR	T84	GLN
ASN	ALA	SER	SER	LYS	F85	VAL
GLN	ILE	VAL	THR	THR	E89	GLY
ASP	GLN	THR	PRO	ALA	F111	ALA
GLU	GLN	SER	VAL	K184	V115	LYS
LEU	ARG	SER	K184	L195	R93	ASN
LEU	MET	GLN	F324	I189	F94	ASN
SER	SER	GLN	M325	L190	G95	THR
SER	ILE	GLN	R326	R191	F111	ALA
ASP	GLN	GLY	R326	L195	F111	GLN
ASP	GLY	ARG	R396	L195	V115	PRO
LYS	ARG	GLY	R396	D200	E118	GLN
LYS	ALA	GLU	GLU	L201	E119	ALA
ILE	PRO	ARG	GLN	L202	P122	GLN
LYS	PRO	LEU	LEU	Y203	K129	GLN
PRO	GLN	GLN	GLN	Q204	V133	ARG
GLN	GLN	GLN	SER	T205	Q134	PRO
ALA	GLN	SER	GLY	F212	E137	ILE
ALA	GLN	GLY	GLY	L218	L142	ASN
LYS	PRO	GLY	GLY	N219	R143	GLY
ASN	ASP	GLY	GLY	E223	R148	SER
GLN	GLN	SER	GLY	N277	HIS	VAL
GLN	GLN	LEU	GLN	A278	LEU	THR
MET	GLN	GLN	PRO	D279	VAL	LEU
THR	GLN	GLY	GLY	T282	ALA	SER
LEU	PRO	GLN	ILE	TVR	HIS	GLN
HIS	GLN	ILE	PRO	ARG	ASP	ASN
GLN	GLN	PRO	PRO	LYS	ILE	LEU
ASN	ALA	GLY	MET	LYS	ASP	THR
VAL	MET	MET	MET	HIS	ALA	GLN
ALA	SER	LEU	LEU	GLU	LYS	GLN
GLY	GLN	SER	SER	ASP	ASP	GLN
THR	ARG	PHE	THR	MET	GLN	ARG
ILE	GLN	SER	SER	GLN	GLN	LEU
PRO	GLN	SER	ASN	HIS	VAL	LEU
SER	GLN	THR	THR	GLY	SER	GLN
ALA	GLN	GLY	GLY	S295	GLN	GLN
GLU	GLN	ASN	ASN	L304	LYS	LYS
SER	GLN	MET	MET	S305	VAL	VAL
THR	LEU	THR	THR	D306	LEU	LEU
PRO	TYR	ASN	ASN	R307	SER	HIS
PRO	PRO	THR	THR	PHE	ALA	GLN
THR	THR	GLN	GLN	ASP	ASN	GLN
ALA	GLN	ASP	ASP	THR	GLN	LYS



- Molecule 5: Subunit of the SAGA and SAGA-like transcriptional regulatory complexes, interacts with Spt15p to act




- Molecule 6: Subunit of the SAGA transcriptional regulatory complex, involved in proper assembly of the complex



[illegible]

- Molecule 7: Transcription initiation factor TFIID subunit 10

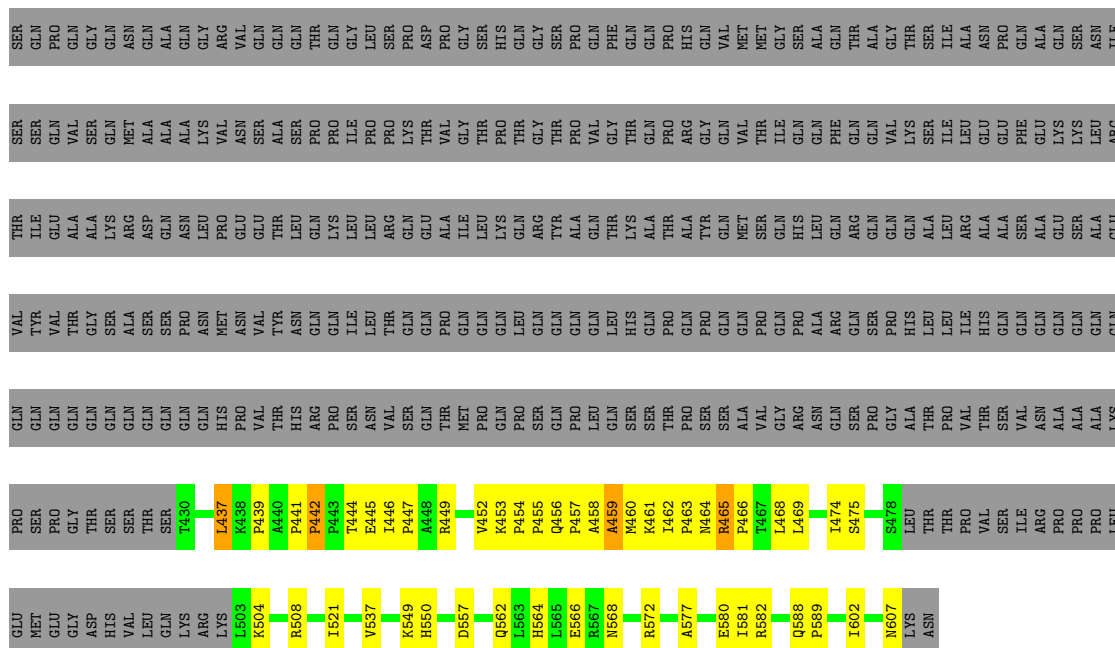
Chain J:  36% 7% 56%

[illegible]

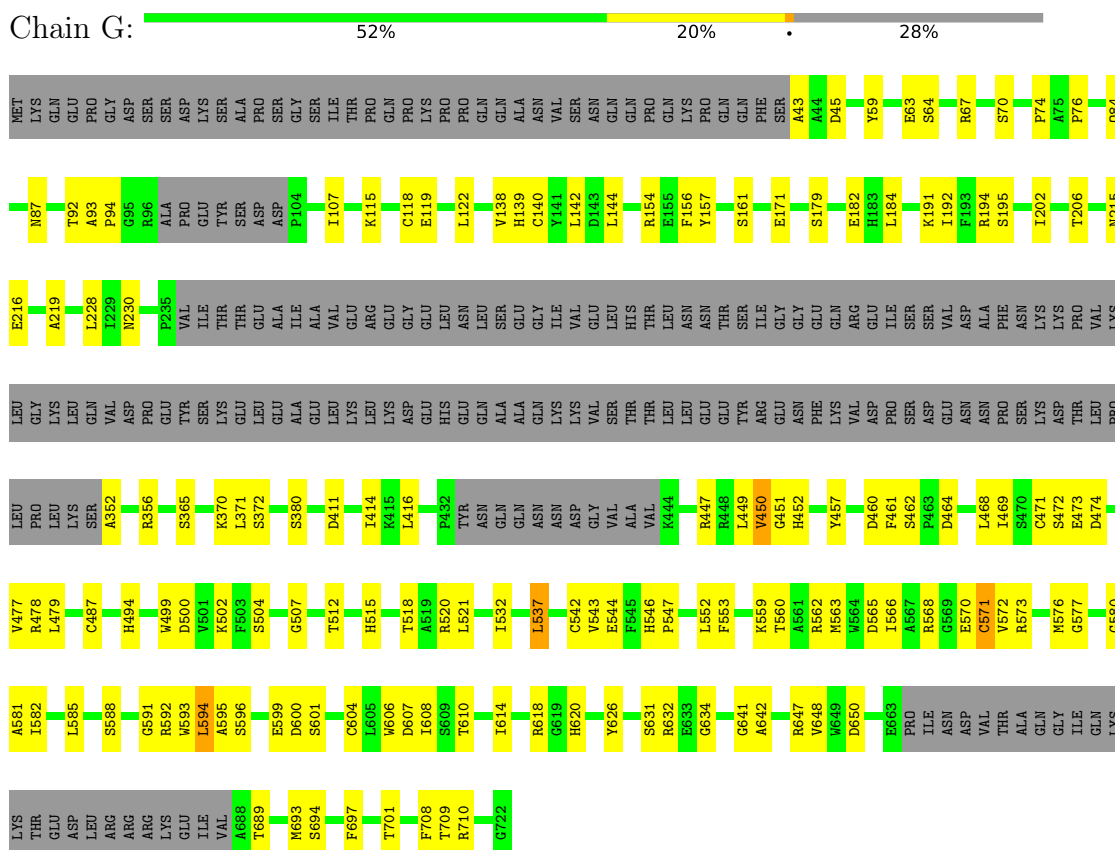
- Molecule 8: Subunit (61/68 kDa) of TFIID and SAGA complexes

Chain K: 17% 7% 75%

[illegible]

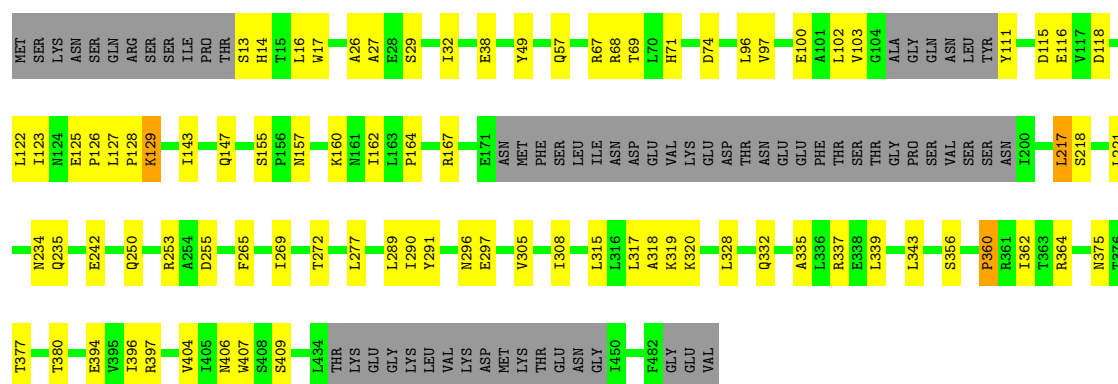


- Molecule 9: Subunit (90 kDa) of TFIID and SAGA complexes



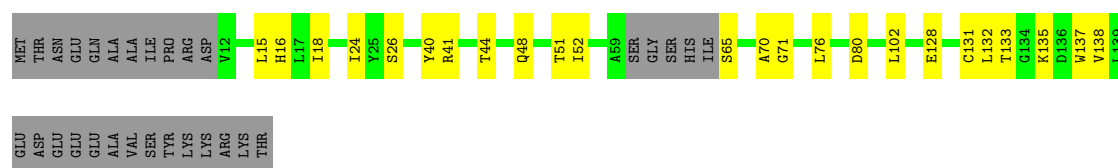
- Molecule 10: Subunit (60 kDa) of TFIID and SAGA complexes





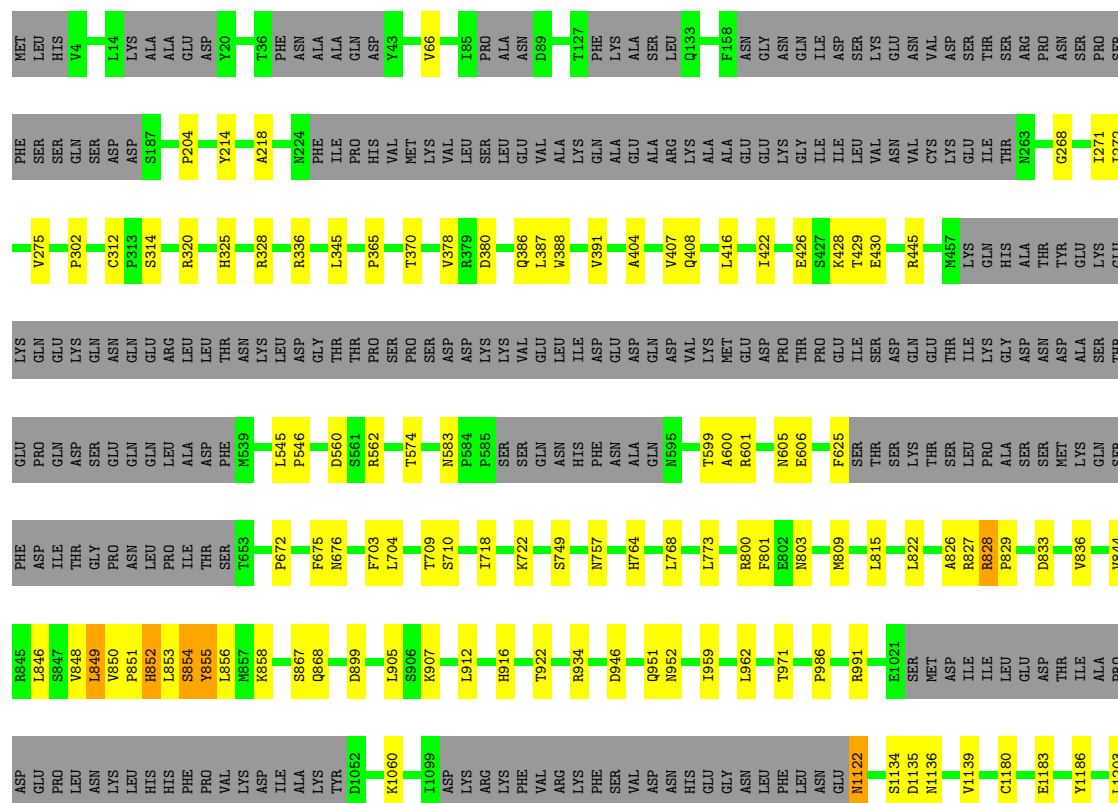
- Molecule 11: Subunit (17 kDa) of TFIID and SAGA complexes, involved in RNA polymerase II transcription initiation

Chain I: 65% 16% 20%

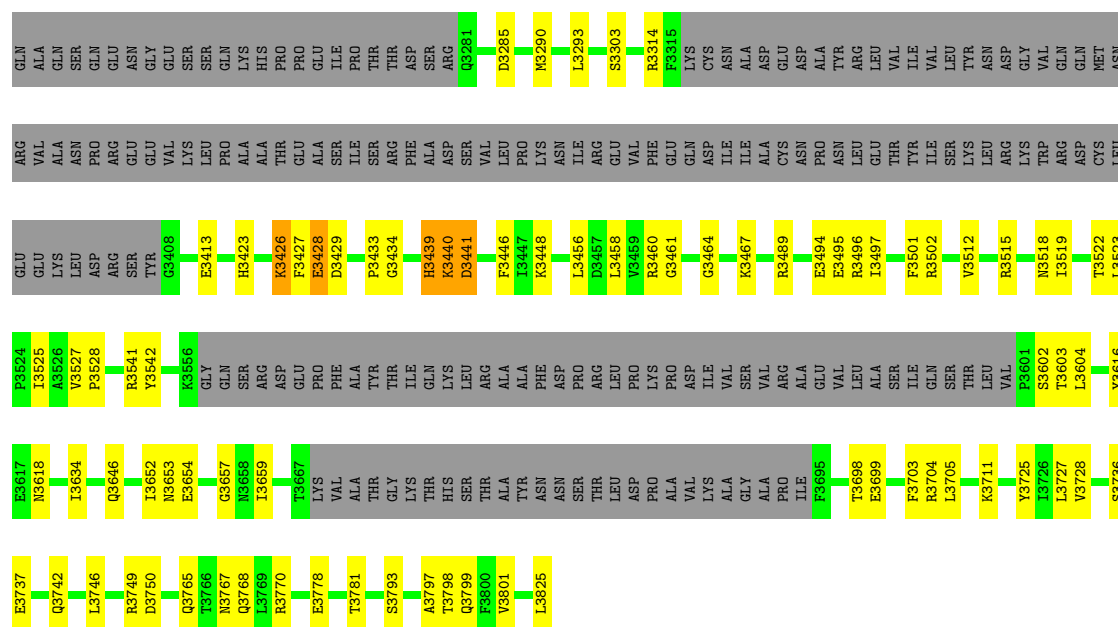


- Molecule 12: Transcription-associated protein

Chain L: 66% 11% 22%



SER	K3101	GLN	D2896	Q2803	P2602	L2490	LYS	L2190	GLY	A1811	K1685	K1495	ASP	D1204
SER	L3102	GLU	I2897	G2804	N2603	S2491	THR	ARG	ASP	K1822	K1686	K1501	ALA	I1205
ASN	L3103	ALA	N2898	F2805		PRO	ASP	ASP	ASP	K1823	L1680	K1502	GLU	P1206
GLN	S3111	PHE	I2899	S2806	N2633	GLU	PHE	ASP	SER	T1824	L1681	L1506	GLU	F1210
ASP		LYS	N2900	Q2807	L2665	ASN	PRO	ASN	SER	R1978	R1684	L1507	SER	R1219
THR	H3126	LEU	N2901	K2808	E2666	THR	THR	SER	SER	V1994	A1508	A1509	LEU	R1220
ALA		ARG	V2904	D2810		LEU	LEU	ASN	ASN	MET	S1690	W1509	VAL	A1221
ASP		GLU	T2905	T2811	M2669	SER	ARG	THR	THR	SER	P1691	A1510	SER	L1222
SER		GLN	W2906	L2812	F2677	PRO	GLY	GLN	THR	ASN	L1692	A1511	ALA	R1226
VAL		ALA	R2907	L2813		GLM	GLY	GLY	SER	R1840	T1514	L1515	HIS	R1226
LYS	P3131	LYS	V2810	V2815	T2680	SER	PRO	SER	GLU	A1848	F1694	Q1516	ARG	L1243
ASN	V3132	CYS	S2816	S2817		ILE	PRO	GLU	ASP		Q1698	Q1517	ILE	L1243
THR	W3133	HIS	R2817	L2818	Y2687	THR	GLU	TYR	TYR	P1855	E1701	D1522	GLU	T1256
ASN		TYR	G2912			GLU	LEU	GLU	GLU	D1860	L1716	M1525	HIS	R1257
ASN	I3136	GLN	V2913	G2822	T2690	GLY	ALA	VAL	SER	M1861	G1717	M1526	SER	S1262
PRO	V3139	ASN	I2914	G2823	F2396	THR	PRO	GLU	GLY	R1862	H1718	N1526	ASP	S1263
GLN	N2915	SER	N2915	K2829		ALA	VAL	ASN	THR	K1863	F1724	Q1530	GLY	D1275
PRO	R2916	SER	R2916		L2708	ARG	VAL	SER	THR	D1864	K1727	H1540	THR	N1278
THR	M2919	LEU	M2919	R2836	F2721	GLU	GLU	GLU	THR			H1541	THR	R1284
ARG	PHE	ASN	PHE	G2843	P2722	GLU	LEU	GLU	THR			L1542	THR	R1284
VAL	VAL	GLY	VAL	L2844	Y2737	LEU	ALA	GLU	GLU			P1543	THR	S1295
PRO	PRO	VAL	PRO	Q2849	E2740	GLU	VAL	SER	PRO	A1884	P1734	H1547	THR	M1305
GLN	VAL	LEU	LEU	L2854	K2741	LYS	LYS	GLU	GLU	Y1886	F1735	L1548	THR	L1314
THR	ILE	GLM	GLM	L2854	W2745	ALA	THR	ASN	THR	V1887	L1737	M1563	THR	L1317
THR	GLN	GLN	GLN	S2858		PRO	GLM	SER	GLY	F1895		V1422	THR	S1307
ALA	S2865	THR	V2865	Q2869	T2749	ASN	GLN	VAL	THR			V1423	THR	K1310
GLU	V2869	THR	V2869	L2861	E2750	I2521	LYS	LYS	THR			F1424	THR	K1310
ASP	S2862	GLY	S2862	S2862	L2751	L2522	THR	TRP	PRO			Q1568	THR	S1314
LYS		ASN	ASN	S2862		D2523	GLU	SER	GLU			R1582	THR	L1314
THR		GLY	GLY	V2865	T2758	H2528	L2428	GLY	VAL			S1587	THR	L1317
THR		THR	THR	V2865	L2762	F2531	L2433	ASN	THR			F1588	THR	R1323
ALA		ASN	ASN	V2865	R2767	L2532	L2437	GLN	THR			V1608	THR	N1333
GLN		GLM	GLM	L2879	GLY	T2539	L2440	GLY	LEU			G1609	THR	G1340
ASP		ASN	ASN	K2880	ASP	A2540	L2441	ASP	GLU			L1610	THR	L1343
VAL		LEU	LEU	L2881	W2771	G2541	L2446	PHE	SER			D1446	LEU	F1347
LYS		ASP	ASP	V2882	L2776		E2446	ALA	ASP			S1623	LYS	E1352
SER		VAL	VAL	L2883	L2778	I2548	L2447	ASN	ASP			R1626	LYS	F1352
SER		LYS	LYS	Q2884	K2783	N2560	D2448	GLN	ASP			G1629	LEU	L1354
THR		THR	THR	Q2884	L2788	A2572	I2449	PRO	SER			H1632	LEU	R1356
LYS		THR	THR	L2889	P2789	D2572	R2452	ARG	GLU			Q1633	THR	L1357
ILE		ILE	ILE	R2887	T2790	D2592	L2465	ILE	PRO			H1632	THR	L1489
THR		TYR	TYR	E2888	R2791	Y2593	L2475	TRP	ALA			Q1633	GLY	PHE
THR		VAL	VAL	L2889	R2792	Y2594	Q2476	LYS	GLU			GLY	ASN	ILE
THR		LYS	LYS	Q2884	Q2794	I2595	Q2476	PRO	ASP			ALA	ASN	E1360
GLN		ASP	ASP	R2887	Q2797	R2596	Y2479	THR	THR			LEU	GLU	L1364
ALA		ASN	ASN	E2888	T2798	Q2597	R2489	THR	GLY			E1639	TYR	PHE
GLU		GLU	GLU	R2889		R2601								VAL
PRO		ILE	ILE		L2802									



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

Chain B:  10% . 89%





4 Experimental information

Property	Value	Source
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

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 > 2$	RMSZ	# $ Z > 2$
1	M	0.88	2/1442 (0.1%)	0.78	2/1942 (0.1%)
10	H	0.38	0/3315	0.60	0/4500
11	I	0.44	0/1006	0.63	0/1374
12	L	0.33	0/22712	0.54	0/30825
13	B	0.64	0/370	0.70	1/509 (0.2%)
15	R	0.83	1/619 (0.2%)	0.75	0/833
16	Q	0.71	0/3897	1.09	15/5265 (0.3%)
17	O	0.79	0/931	1.13	2/1250 (0.2%)
18	P	0.75	0/747	1.01	0/1011
2	A	0.44	0/1319	0.60	0/1794
3	C	0.53	0/774	0.75	0/1039
4	F	0.34	0/1718	0.58	0/2335
5	D	0.51	0/1641	0.65	0/2213
6	E	0.45	0/1246	0.62	0/1667
7	J	0.47	0/779	0.60	0/1051
8	K	0.42	0/1213	0.66	0/1647
9	G	0.52	0/4177	0.60	0/5661
All	All	0.47	3/47906 (0.0%)	0.67	20/64916 (0.0%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	194	ILE	C-N	27.38	1.97	1.34
1	M	183	SER	C-N	6.38	1.48	1.34
15	R	24	GLU	CB-CG	-5.25	1.42	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	61	TYR	CB-CG-CD1	9.83	126.90	121.00
16	Q	61	TYR	CB-CG-CD2	-9.38	115.37	121.00
1	M	62	GLY	N-CA-C	6.94	130.46	113.10
16	Q	78	ARG	NE-CZ-NH1	-6.80	116.90	120.30
13	B	527	PRO	N-CA-CB	6.57	111.18	103.30
17	O	119	GLY	N-CA-C	6.39	129.07	113.10
16	Q	240	PHE	CB-CG-CD1	6.28	125.20	120.80
1	M	194	ILE	CA-C-N	-6.13	103.71	117.20
16	Q	41	TYR	CB-CG-CD1	6.09	124.65	121.00
16	Q	396	ARG	NE-CZ-NH1	5.95	123.27	120.30
16	Q	384	ARG	NE-CZ-NH2	5.87	123.23	120.30
16	Q	78	ARG	NE-CZ-NH2	5.72	123.16	120.30
16	Q	187	PHE	CB-CG-CD1	5.58	124.71	120.80
16	Q	174	ARG	NE-CZ-NH2	5.57	123.09	120.30
16	Q	240	PHE	CB-CG-CD2	-5.31	117.08	120.80
16	Q	38	TYR	CA-CB-CG	5.28	123.44	113.40
16	Q	187	PHE	CB-CG-CD2	-5.18	117.18	120.80
16	Q	41	TYR	CB-CG-CD2	-5.13	117.92	121.00
17	O	118	GLY	C-N-CA	5.12	133.06	122.30
16	Q	392	PHE	CB-CG-CD2	-5.08	117.24	120.80

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	102	0
2	A	1300	0	1254	30	0
3	C	761	0	779	194	0
4	F	1682	0	1622	30	0
5	D	1616	0	1558	122	0
6	E	1232	0	1276	40	0
7	J	768	0	754	11	0
8	K	1192	0	1214	89	0
9	G	4075	0	3934	102	0
10	H	3263	0	3258	69	0
11	I	981	0	982	18	0
12	L	22318	0	20960	376	0
13	B	373	0	190	2	0
14	N	1648	0	382	61	0
15	R	611	0	636	20	0
16	Q	3817	0	3772	521	0
17	O	922	0	897	411	0
18	P	735	0	743	191	0
19	Q	8	0	0	10	0
19	R	83	0	0	7	0
All	All	48800	0	45702	1602	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 (1602) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:38:LEU:HD13	16:Q:210:ARG:CZ	1.21	1.54
3:C:34:LEU:CD2	16:Q:446:PHE:HE1	0.95	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:9:THR:CG2	18:P:10:LYS:CE	1.86	1.41
3:C:39:ARG:HH11	16:Q:148:ILE:CG2	1.29	1.41
17:O:11:TRP:CE2	18:P:86:ILE:HD12	1.55	1.40
14:N:207:UNK:C	14:N:208:UNK:N	1.79	1.40
16:Q:182:THR:N	17:O:44:ASP:CB	1.70	1.40
17:O:11:TRP:CD1	18:P:83:LEU:CD2	1.93	1.39
16:Q:482:VAL:HG12	17:O:49:LYS:N	1.30	1.39
16:Q:78:ARG:NH2	18:P:23:TYR:HE2	1.15	1.39
17:O:27:ILE:CD1	18:P:59:PHE:HA	1.53	1.38
16:Q:479:ILE:HG23	17:O:47:SER:CB	1.53	1.38
16:Q:78:ARG:NH2	18:P:23:TYR:CE2	1.88	1.38
16:Q:472:PHE:CD2	17:O:46:ILE:CG1	2.06	1.38
17:O:55:ARG:C	18:P:52:THR:HG21	1.01	1.37
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
17:O:55:ARG:C	18:P:52:THR:CG2	1.96	1.34
17:O:19:LEU:HD23	18:P:67:GLU:CG	1.57	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:ASP:CB	16:Q:243:THR:O	1.75	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:472:PHE:CB	17:O:46:ILE:HG13	1.60	1.31
16:Q:106:TRP:HD1	17:O:20:ARG:CZ	1.41	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
17:O:11:TRP:HE1	18:P:83:LEU:CA	1.46	1.26
16:Q:178:LEU:CD1	17:O:37:ILE:CD1	2.02	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
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
17:O:56:LEU:N	18:P:52:THR:HG21	1.55	1.20
3:C:50:ILE:N	16:Q:214:LEU:HD11	1.53	1.20
16:Q:479:ILE:CG2	17:O:47:SER:CA	1.91	1.20
12:L:828:ARG:H	12:L:829:PRO:HD3	1.06	1.20
16:Q:472:PHE:CZ	17:O:45:GLN:CB	2.23	1.20
16:Q:416:PHE:CE1	18:P:35:TYR:CD2	2.29	1.20
17:O:27:ILE:HD13	18:P:59:PHE:CA	1.71	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
16:Q:182:THR:CB	17:O:44:ASP:CB	2.13	1.19
3:C:49:PRO:CG	16:Q:237:PHE:CE1	2.24	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
1:M:194:ILE:C	1:M:195:TYR:N	1.97	1.17
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:51:LEU:HD23	16:Q:214:LEU:HD23	1.27	1.16
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
17:O:22:ILE:HD12	18:P:43:ILE:CD1	1.75	1.13
19:R:153:HOH:O	16:Q:326:LYS:HB3	1.44	1.13
3:C:40:TYR:CB	16:Q:214:LEU:HD21	1.78	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
17:O:11:TRP:CE2	18:P:86:ILE:CD1	2.32	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
3:C:40:TYR:HB3	16:Q:214:LEU:HD21	1.33	1.11
16:Q:474:PHE:CD2	17:O:47:SER:CB	2.33	1.11
3:C:39:ARG:NH1	16:Q:147:PHE:C	2.03	1.11
16:Q:93:CYS:SG	17:O:20:ARG:HB2	1.89	1.11
5:D:212:GLN:HE21	5:D:212:GLN:HA	1.12	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
3:C:49:PRO:C	16:Q:214:LEU:CD1	2.19	1.10
14:N:501:UNK:HA	14:N:505:UNK:HA	1.30	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
16:Q:482:VAL:CG2	17:O:49:LYS:HD2	1.61	1.07
8:K:469:LEU:HD13	12:L:2788:ILE:HG22	1.30	1.07
8:K:468:LEU:HB3	12:L:2829:LYS:HZ1	1.05	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:501:GLN:HB2	18:P:31:ARG:HH22	1.17	1.05
16:Q:464:ILE:HD11	17:O:46:ILE:CG2	1.86	1.05
16:Q:482:VAL:HG23	17:O:49:LYS:HD2	1.29	1.05
3:C:54:CYS:SG	16:Q:215:SER:O	2.13	1.05
5:D:78:LYS:HA	5:D:78:LYS:HE3	1.38	1.05
17:O:11:TRP:NE1	18:P:83:LEU:HD23	1.71	1.05
16:Q:472:PHE:CG	17:O:46:ILE:HG13	1.90	1.04
15:R:4:PHE:CE1	16:Q:377:ARG:NH1	2.25	1.04
8:K:468:LEU:HB3	12:L:2829:LYS:NZ	1.70	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:472:PHE:HB3	17:O:47:SER:C	1.51	1.03
16:Q:482:VAL:CG1	17:O:49:LYS:H	1.70	1.03
16:Q:464:ILE:HG13	17:O:46:ILE:CD1	1.87	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
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:479:ILE:O	17:O:68:HIS:CE1	2.12	1.02
16:Q:472:PHE:CE1	17:O:45:GLN:HB3	1.94	1.02
17:O:54:GLN:NE2	18:P:49:SER:N	2.07	1.01
3:C:38:LEU:CD2	16:Q:210:ARG:CD	2.18	1.01
16:Q:93:CYS:SG	17:O:20:ARG:CD	2.49	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:52:GLN:HE21	16:Q:153:GLN:HG3	0.94	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:482:VAL:HG12	17:O:49:LYS:CA	1.73	1.00
16:Q:479:ILE:HB	17:O:68:HIS:HE1	0.83	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:CD1	16:Q:211:ASP:O	2.09	0.99
3:C:51:LEU:HG	16:Q:214:LEU:HB3	1.43	0.99
5:D:66:VAL:HG12	5:D:67:PRO:HD2	1.44	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
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
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
16:Q:182:THR:CB	17:O:44:ASP:HB3	1.77	0.95
19:R:165:HOH:O	16:Q:355:LEU:HD11	1.63	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:H	12:L:849:LEU:HD12	1.31	0.95
16:Q:481:LEU:HD12	17:O:50:GLU:H	1.28	0.95
16:Q:479:ILE:CB	17:O:68:HIS:HE1	1.70	0.95
16:Q:482:VAL:CG1	17:O:49:LYS:N	2.26	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:88:HIS:C	14:N:515:UNK:C	2.35	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:473:LYS:N	17:O:47:SER:O	2.00	0.93
16:Q:130:TYR:CD2	17:O:28:LEU:HD12	2.04	0.93
3:C:54:CYS:SG	16:Q:215:SER:C	2.47	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:NE2	5:D:212:GLN:HA	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
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:52:GLN:HE21	16:Q:153:GLN:CG	1.82	0.92
3:C:34:LEU:HD21	16:Q:446:PHE:CD1	2.03	0.92
16:Q:78:ARG:CZ	18:P:23:TYR:CD2	2.53	0.92
12:L:828:ARG:N	12:L:829:PRO:HD3	1.83	0.91
1:M:172:LEU:HB3	1:M:193:LEU:HD13	1.50	0.91
1:M:99:PHE:CE2	1:M:101:ALA:HB3	2.05	0.91
16:Q:464:ILE:HG13	17:O:46:ILE:HD12	0.92	0.91
12:L:2916:ARG:HB2	12:L:2916:ARG:NH2	1.84	0.91
3:C:39:ARG:CD	16:Q:147:PHE:CE1	2.52	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
9:G:546:HIS:CD2	9:G:547:PRO:HD2	2.06	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:40:TYR:HB2	16:Q:214:LEU:HD21	1.54	0.89
3:C:34:LEU:HD13	16:Q:446:PHE:CE1	2.08	0.89
19:R:153:HOH:O	16:Q:326:LYS:CG	2.21	0.88
9:G:543:VAL:HG22	9:G:552:LEU:HD11	1.55	0.88
8:K:468:LEU:CB	12:L:2829:LYS:HZ1	1.87	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
17:O:54:GLN:HE22	18:P:48:GLN:C	1.76	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:93:CYS:HG	17:O:20:ARG:HD2	1.37	0.88
16:Q:464:ILE:CD1	17:O:46:ILE:HG21	2.01	0.88
16:Q:444:GLN:NE2	18:P:35:TYR:CE2	2.38	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:H	6:E:938:ILE:HD12	1.38	0.87
16:Q:472:PHE:CG	17:O:46:ILE:CG1	2.54	0.87
17:O:11:TRP:NE1	18:P:86:ILE:HD12	1.90	0.87
17:O:9:THR:CG2	18:P:10:LYS:NZ	2.38	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
3:C:50:ILE:C	16:Q:214:LEU:HD11	1.95	0.86
5:D:216:THR:CG2	5:D:246:GLY:HA3	2.06	0.86
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
17:O:56:LEU:N	18:P:52:THR:CG2	2.33	0.86
12:L:2854:LEU:HD13	12:L:2906:TRP:CH2	2.11	0.85
16:Q:125:ASP:OD1	17:O:24:ILE:HD13	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:78:ARG:NH2	18:P:23:TYR:CD2	2.42	0.85
16:Q:472:PHE:CB	17:O:46:ILE:C	2.43	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
17:O:19:LEU:CD2	18:P:67:GLU:CA	2.45	0.85
16:Q:474:PHE:CE1	17:O:48:LEU:HG	2.11	0.85
15:R:4:PHE:CZ	16:Q:377:ARG:CZ	2.44	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
17:O:19:LEU:HD21	18:P:67:GLU:CB	2.07	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:472:PHE:CD2	17:O:46:ILE:HG13	1.92	0.83
16:Q:464:ILE:HD12	17:O:46:ILE:HD13	0.84	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:G:537:LEU:H	9:G:537:LEU:HD12	1.46	0.81
1:M:82:LEU:HD13	1:M:101:ALA:HA	1.61	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
16:Q:474:PHE:CE1	17:O:47:SER:HB3	2.16	0.81
3:C:51:LEU:CD2	16:Q:214:LEU:HD23	2.10	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
16:Q:472:PHE:CD2	17:O:46:ILE:N	2.49	0.80
3:C:45:ASN:HD21	16:Q:171:ASP:HA	1.44	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
9:G:478:ARG:NH1	9:G:487:CYS:SG	2.55	0.80
3:C:55:LEU:HD23	16:Q:160:ILE:HG12	1.63	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
16:Q:282:ASP:CG	19:Q:603:HOH:O	2.19	0.79
16:Q:130:TYR:HB3	17:O:28:LEU:HD11	1.64	0.79
3:C:51:LEU:CD1	16:Q:215:SER:OG	2.31	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
17:O:51:ILE:CG2	18:P:45:ARG:HG3	2.12	0.79
16:Q:182:THR:HG21	17:O:45:GLN:H	1.47	0.79
3:C:51:LEU:CG	16:Q:214:LEU:HB3	2.13	0.79
16:Q:315:SER:CB	19:Q:605:HOH:O	2.31	0.79
17:O:9:THR:HG21	18:P:10:LYS:CD	2.13	0.79
16:Q:464:ILE:HD11	17:O:46:ILE:CB	2.13	0.79
16:Q:88:LEU:HB3	18:P:11:GLN:HG2	1.65	0.79
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:176:ALA:HB2	1:M:193:LEU:HD11	1.65	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:482:VAL:CG1	17:O:49:LYS:CA	2.48	0.77
16:Q:470:ASN:HA	17:O:51:ILE:H	1.50	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
12:L:2593:TYR:H	12:L:2596:ARG:HG2	1.48	0.77
3:C:45:ASN:ND2	16:Q:171:ASP:CA	2.48	0.77
16:Q:479:ILE:O	17:O:68:HIS:NE2	2.16	0.77
12:L:1122:ASN:HD22	12:L:1122:ASN:N	1.82	0.76
3:C:44:ASN:OD1	16:Q:174:ARG:HG3	1.85	0.76
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
12:L:2854:LEU:HD13	12:L:2906:TRP:HH2	1.49	0.76
1:M:101:ALA:HB1	1:M:115:ILE:O	1.85	0.76
2:A:239:GLU:OE1	2:A:239:GLU:N	2.18	0.76
3:C:50:ILE:C	16:Q:214:LEU:CD1	2.54	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:37:PRO:O	16:Q:467:ARG:NH2	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NE2	12:L:2884:GLN:HA	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:49:PRO:C	16:Q:214:LEU:HD12	2.07	0.75
3:C:45:ASN:ND2	16:Q:171:ASP:HA	2.01	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
16:Q:107:LYS:HZ3	17:O:13:CYS:HA	1.50	0.74
2:A:327:ARG:NH1	2:A:328:HIS:O	2.20	0.74
10:H:129:LYS:HA	10:H:129:LYS:HZ2	1.52	0.74
17:O:9:THR:HG21	18:P:10:LYS:HD2	1.69	0.74
5:D:322:GLU:HA	5:D:322:GLU:OE2	1.87	0.74
14:N:223:UNK:H	14:N:230:UNK:CB	2.00	0.74
16:Q:474:PHE:HZ	17:O:46:ILE:HB	1.50	0.74
16:Q:78:ARG:HH12	18:P:27:SER:CB	1.99	0.74
17:O:55:ARG:O	18:P:52:THR:HG23	1.84	0.74
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:HD11	18:P:51:VAL:C	2.07	0.74
16:Q:130:TYR:HE2	17:O:25:ASN:OD1	1.70	0.73
9:G:414:ILE:HB	9:G:449:LEU:HB2	1.68	0.73
17:O:19:LEU:HD23	18:P:67:GLU:HG3	0.78	0.73
17:O:11:TRP:CG	18:P:86:ILE:HD12	2.23	0.73
3:C:49:PRO:CG	16:Q:237:PHE:HE1	1.85	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:78:ARG:NE	18:P:23:TYR:HD2	1.86	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
12:L:1417:ARG:HA	12:L:1420:ILE:HD12	1.70	0.73
3:C:49:PRO:HG2	16:Q:237:PHE:HE1	0.98	0.73
3:C:38:LEU:HB2	16:Q:210:ARG:NH2	2.03	0.73
8:K:453:LYS:C	8:K:455:PRO:HD2	2.08	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:N	9:G:537:LEU:HD12	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:CE	5:D:78:LYS:HA	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:N	12:L:849:LEU:HD12	2.03	0.72
17:O:54:GLN:HE21	18:P:49:SER:HA	1.53	0.72
17:O:54:GLN:NE2	18:P:48:GLN:C	2.40	0.72
16:Q:481:LEU:CD1	17:O:50:GLU:H	2.01	0.72
3:C:51:LEU:HD11	16:Q:211:ASP:C	2.09	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:50:ILE:CA	16:Q:214:LEU:HD12	2.18	0.72
3:C:38:LEU:HD12	16:Q:210:ARG:NH1	2.03	0.72
5:D:317:GLN:C	5:D:319:ARG:H	1.93	0.72
5:D:73:LEU:O	5:D:73:LEU:HD23	1.89	0.72
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
16:Q:130:TYR:CG	17:O:28:LEU:HD11	2.24	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:90:ARG:HH11	14:N:513:UNK:CB	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:87:LEU:CD1	14:N:490:UNK:CA	2.66	0.70
3:C:49:PRO:C	16:Q:214:LEU:HD13	2.11	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
16:Q:472:PHE:HE2	17:O:50:GLU:OE2	1.74	0.70
3:C:39:ARG:CD	16:Q:147:PHE:HE1	1.96	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
5:D:21:MET:CE	5:D:250:PHE:HA	2.21	0.70
17:O:19:LEU:HD23	18:P:67:GLU:CB	2.19	0.70
16:Q:88:LEU:HB2	18:P:11:GLN:HG2	1.73	0.70
16:Q:479:ILE:C	17:O:68:HIS:CE1	2.52	0.69
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:49:PRO:HG2	16:Q:237:PHE:CD1	2.21	0.69
8:K:550:HIS:NE2	11:I:80:ASP:OD1	2.25	0.69
8:K:466:PRO:CA	12:L:2791:PRO:HG2	2.19	0.69
3:C:39:ARG:HH22	16:Q:150:GLN:HE21	1.40	0.69
16:Q:178:LEU:CB	17:O:37:ILE:HD13	2.22	0.69
8:K:580:GLU:O	11:I:65:SER:N	2.25	0.69
16:Q:472:PHE:HB3	17:O:46:ILE:C	2.10	0.69
6:E:948:GLN:OE1	6:E:948:GLN:HA	1.93	0.69
16:Q:472:PHE:CE2	17:O:50:GLU:OE2	2.45	0.69
3:C:47:ASP:HB3	16:Q:243:THR:HB	1.73	0.69
4:F:202:LEU:O	4:F:205:THR:OG1	2.08	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
8:K:456:GLN:HA	12:L:2669:MET:HG3	1.74	0.68
3:C:39:ARG:NE	16:Q:147:PHE:CD1	2.62	0.68
9:G:581:ALA:HB3	9:G:599:GLU:HG2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
17:O:55:ARG:HB3	18:P:52:THR:HG22	1.74	0.68
16:Q:78:ARG:CZ	18:P:23:TYR:CE2	2.71	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
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
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
5:D:320:ASN:C	5:D:322:GLU:H	1.95	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
6:E:817:GLY:N	7:J:69:GLU:OE2	2.26	0.67
12:L:849:LEU:CD1	12:L:849:LEU:H	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:21:MET:HE2	5:D:253:VAL:HG21	1.77	0.67
5:D:66:VAL:HG12	5:D:67:PRO:CD	2.22	0.67
11:I:48:GLN:O	11:I:51:THR:OG1	2.11	0.67
8:K:447:PRO:HG3	12:L:2788:ILE:HG23	1.77	0.67
16:Q:338:GLU:OE2	19:Q:601:HOH:O	0.66	0.66
16:Q:91:LEU:HD23	17:O:13:CYS:CB	2.25	0.66
3:C:34:LEU:HD21	16:Q:446:PHE:HD1	1.60	0.66
9:G:157:TYR:O	9:G:161:SER:N	2.28	0.66
8:K:453:LYS:HG2	8:K:455:PRO:CD	2.26	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:HA	6:E:946:LYS:HE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
16:Q:182:THR:HG21	17:O:45:GLN:N	2.12	0.65
16:Q:78:ARG:HD3	18:P:23:TYR:CD2	2.32	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
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
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
16:Q:472:PHE:CB	17:O:47:SER:C	2.36	0.65
16:Q:76:ARG:HH22	18:P:18:VAL:C	1.99	0.65
11:I:128:GLU:OE1	11:I:128:GLU:N	2.28	0.64
16:Q:482:VAL:O	17:O:49:LYS:C	2.35	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
1:M:82:LEU:HB3	1:M:94:TYR:HE2	1.60	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
9:G:154:ARG:NH2	9:G:179:SER:OG	2.31	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
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:56:LEU:HD13	18:P:51:VAL:HB	1.80	0.64
17:O:7:GLN:HG2	18:P:83:LEU:HD22	1.79	0.64
17:O:55:ARG:CB	18:P:52:THR:HG22	2.27	0.64
3:C:51:LEU:HD12	16:Q:215:SER:CA	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
14:N:184:UNK:CB	14:N:237:UNK:HA	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:11:TRP:CZ2	18:P:86:ILE:CD1	2.81	0.63
16:Q:315:SER:HB2	19:Q:605:HOH:O	1.97	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
5:D:73:LEU:HD23	5:D:73:LEU:C	2.19	0.63
14:N:221:UNK:HA	14:N:229:UNK:O	1.97	0.63
17:O:55:ARG:CB	18:P:52:THR:CG2	2.77	0.63
8:K:468:LEU:C	12:L:2829:LYS:HZ3	2.01	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
12:L:365:PRO:HB3	12:L:407:VAL:HG11	1.81	0.63
3:C:38:LEU:CG	16:Q:210:ARG:CD	2.77	0.63
12:L:2854:LEU:HD13	12:L:2906:TRP:CZ2	2.33	0.62
17:O:15:MET:CE	18:P:74:VAL:HG21	2.28	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
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:HD12	5:D:17:ILE:N	2.14	0.62
12:L:2880:LYS:HD2	12:L:2880:LYS:H	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
10:H:217:LEU:HD12	10:H:218:SER:H	1.65	0.62
8:K:439:PRO:HB3	12:L:916:HIS:CE1	2.34	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
5:D:49:ILE:HG23	5:D:73:LEU:HD13	1.82	0.61
3:C:51:LEU:HD11	16:Q:211:ASP:HA	1.82	0.61
3:C:39:ARG:NH2	16:Q:150:GLN:HE21	1.97	0.61
16:Q:472:PHE:HZ	17:O:45:GLN:CG	2.13	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
3:C:38:LEU:CG	16:Q:210:ARG:HD2	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:M:115:ILE:HD13	1:M:121:MET:SD	2.40	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:HD3	5:D:78:LYS:O	2.01	0.61
15:R:12:THR:HG21	16:Q:379:LYS:HE3	1.83	0.61
5:D:320:ASN:C	5:D:322:GLU:N	2.53	0.61
17:O:56:LEU:HD11	18:P:52:THR:H	0.45	0.60
5:D:21:MET:HE1	5:D:250:PHE:HA	1.82	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
2:A:289:ILE:O	6:E:958:LEU:HD21	2.01	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
12:L:2907:ARG:NH1	12:L:2907:ARG:HG2	2.10	0.60
3:C:44:ASN:OD1	16:Q:174:ARG:CG	2.49	0.60
16:Q:478:ARG:CG	17:O:68:HIS:HD2	2.14	0.60
5:D:76:HIS:C	5:D:78:LYS:N	2.53	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
5:D:76:HIS:C	5:D:78:LYS:H	2.04	0.60
9:G:518:THR:HG21	11:I:102:LEU:HD22	1.82	0.60
10:H:277:LEU:O	10:H:320:LYS:NZ	2.34	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
12:L:853:LEU:O	12:L:855:TYR:N	2.35	0.60
16:Q:184:LEU:CD1	17:O:44:ASP:O	2.39	0.60
16:Q:479:ILE:HA	17:O:47:SER:HG	1.65	0.60
1:M:188:GLU:HA	1:M:188:GLU:OE2	2.02	0.60
1:M:185:TYR:OH	5:D:211:ARG:HD3	2.02	0.59
5:D:21:MET:HE3	5:D:250:PHE:HA	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:38:LEU:CD1	16:Q:210:ARG:CD	2.75	0.59
5:D:317:GLN:C	5:D:319:ARG:N	2.55	0.59
8:K:437:LEU:H	8:K:437:LEU:HD23	1.67	0.59
1:M:202:ILE:HD11	1:M:217:ALA:HB2	1.84	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
3:C:39:ARG:NE	16:Q:148:ILE:HG22	2.17	0.59
3:C:38:LEU:HD12	16:Q:210:ARG:CZ	2.19	0.59
4:F:119:GLU:N	4:F:119:GLU:OE1	2.36	0.59
8:K:469:LEU:CD1	12:L:2788:ILE:HG22	2.14	0.59
12:L:848:VAL:C	12:L:851:PRO:HD2	2.23	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
12:L:3440:LYS:HG3	12:L:3446:PHE:CE1	2.38	0.59
12:L:3767:ASN:OD1	12:L:3770:ARG:NH2	2.35	0.59
12:L:3704:ARG:NH2	12:L:3825:LEU:O	2.36	0.59
16:Q:139:TYR:CZ	17:O:24:ILE:CG2	2.86	0.59
3:C:59:ILE:CG2	16:Q:170:ILE:HD11	2.32	0.59
3:C:55:LEU:CD2	16:Q:160:ILE:HG12	2.30	0.59
1:M:90:ARG:NH1	14:N:513:UNK:CB	2.66	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
3:C:44:ASN:CG	16:Q:174:ARG:HG3	2.23	0.59
12:L:2805:PHE:CZ	12:L:2812:LEU:HG	2.38	0.58
17:O:22:ILE:HG21	18:P:43:ILE:HG13	1.85	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:CD1	2.33	0.58
10:H:100:GLU:OE2	10:H:111:TYR:N	2.35	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
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
10:H:162:ILE:HG22	10:H:164:PRO:HD2	1.86	0.58
10:H:38:GLU:N	10:H:38:GLU:OE1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:190:PHE:HB3	5:D:88:LEU:HG	1.84	0.58
3:C:52:GLN:CD	16:Q:153:GLN:HG3	2.21	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
6:E:946:LYS:HD2	6:E:946:LYS:N	2.17	0.58
4:F:83:LEU:O	4:F:142:LEU:HD13	2.03	0.58
1:M:168:PHE:CD1	1:M:238:ARG:HG3	2.39	0.58
14:N:493:UNK:HA	14:N:510:UNK:O	2.03	0.58
12:L:2601:ARG:HE	12:L:2601:ARG:N	2.02	0.58
16:Q:138:ASP:OD2	18:P:58:THR:HA	2.03	0.58
15:R:14:THR:OG1	16:Q:364:SER:HB3	2.04	0.58
3:C:51:LEU:HD11	16:Q:211:ASP:CA	2.32	0.58
3:C:51:LEU:HG	16:Q:214:LEU:C	2.24	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
5:D:87:TYR:C	5:D:87:TYR:CD1	2.77	0.57
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: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
12:L:905:LEU:HD22	12:L:922:THR:HG23	1.85	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
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:HB2	10:H:129:LYS:HZ3	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:108:GLU:HA	1:M:110:LYS:H	1.70	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
1:M:87:LEU:O	1:M:90:ARG:HG2	2.04	0.57
17:O:15:MET:HE1	18:P:74:VAL:HG21	1.87	0.57
17:O:19:LEU:HD13	18:P:70:ALA:HB1	1.86	0.57
16:Q:107:LYS:HG2	17:O:20:ARG:CZ	2.34	0.57
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
12:L:2880:LYS:CD	12:L:2880:LYS:N	2.67	0.56
1:M:191:PRO:HB3	5:D:212:GLN:CG	2.34	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
3:C:288:LEU:HD21	3:C:292:THR:HG21	1.87	0.56
9:G:546:HIS:HB2	9:G:553:PHE:CE1	2.35	0.56
12:L:2880:LYS:HE3	12:L:2880:LYS:CA	2.35	0.56
12:L:2880:LYS:HD2	12:L:2880:LYS:N	2.20	0.56
12:L:853:LEU:O	12:L:856:LEU:N	2.37	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
12:L:3433:PRO:HB2	12:L:3527:VAL:HG11	1.86	0.56
8:K:456:GLN:HG3	12:L:2677:PHE:CE2	2.41	0.56
1:M:74:VAL:HG23	1:M:155:PHE:HA	1.87	0.56
6:E:932:HIS:O	6:E:935:SER:HB2	2.04	0.56
8:K:460:MET:N	8:K:460:MET:SD	2.76	0.56
12:L:3174:ARG:NH1	12:L:3290:MET:SD	2.79	0.56
12:L:302:PRO:HD3	12:L:336:ARG:HH22	1.71	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
5:D:320:ASN:HB3	5:D:324:LYS:HB2	1.89	0.55
12:L:3439:HIS:C	12:L:3440:LYS:HG2	2.27	0.55
12:L:946:ASP:O	12:L:951:GLN:NE2	2.39	0.55
12:L:583:ASN:ND2	12:L:600:ALA:O	2.39	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:188:ILE:HG23	17:O:90:THR:HG22	1.88	0.55
3:C:42:ILE:HD12	16:Q:176:PRO:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:182:THR:CG2	17:O:45:GLN:N	2.69	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
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
17:O:26:ASN:ND2	18:P:47:THR:HB	2.22	0.55
3:C:39:ARG:CZ	16:Q:147:PHE:C	2.70	0.55
5:D:88:LEU:HD13	5:D:88:LEU:C	2.27	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: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
5:D:212:GLN:CA	5:D:212:GLN:HE21	2.02	0.55
1:M:143:ILE:O	1:M:150:ALA:HB2	2.06	0.55
1:M:189:LEU:HD21	5:D:81:VAL:HG12	1.87	0.55
3:C:39:ARG:HE	16:Q:148:ILE:HG22	1.71	0.54
5:D:238:SER:OG	5:D:240:ASP:OD1	2.11	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
1:M:187:PRO:CB	5:D:211:ARG:HB2	2.37	0.54
1:M:83:LYS:O	1:M:87:LEU:HG	2.07	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
2:A:208:VAL:HG21	2:A:214:VAL:HG11	1.88	0.54
1:M:99:PHE:CZ	1:M:114:LEU:HD12	2.43	0.54
17:O:7:GLN:HG2	18:P:83:LEU:HD23	1.88	0.54
5:D:22:PHE:CE2	5:D:30:PRO:HD3	2.43	0.54
1:M:189:LEU:HD13	5:D:84:LEU:HD13	1.89	0.54
12:L:822:LEU:HD22	12:L:1186:TYR:H	1.72	0.54
12:L:3458:LEU:N	12:L:3458:LEU:HD23	2.22	0.54
1:M:115:ILE:CD1	1:M:121:MET:SD	2.95	0.54
16:Q:205:HIS:CE1	17:O:46:ILE:HG22	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:199:MET:HA	5:D:203:GLU:CB	2.37	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
10:H:394:GLU:OE1	10:H:394:GLU:N	2.40	0.54
12:L:2916:ARG:HB2	12:L:2916:ARG:HH21	1.71	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
8:K:464:ASN:OD1	12:L:2669:MET:SD	2.65	0.54
5:D:216:THR:CG2	5:D:243:ASP:HA	2.38	0.54
3:C:51:LEU:CD2	16:Q:214:LEU:HB3	2.38	0.54
1:M:90:ARG:HD2	14:N:513:UNK:CB	2.38	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
16:Q:93:CYS:SG	17:O:20:ARG:CG	2.95	0.54
5:D:17:ILE:HD12	5:D:17:ILE:H	1.72	0.54
12:L:3428:GLU:HG2	12:L:3429:ASP:H	1.73	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
17:O:23:VAL:HG21	18:P:63:ILE:HD12	1.90	0.53
19:R:165:HOH:O	16:Q:355:LEU:CD1	2.39	0.53
12:L:1522:ASP:N	12:L:1522:ASP:OD1	2.41	0.53
16:Q:78:ARG:NE	18:P:23:TYR:CD2	2.70	0.53
5:D:317:GLN:HA	5:D:317:GLN:NE2	2.22	0.53
5:D:66:VAL:HG13	5:D:67:PRO:HD2	1.87	0.53
8:K:468:LEU:C	12:L:2829:LYS:NZ	2.61	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:188:ILE:HG23	17:O:90:THR:CG2	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:340:ALA:HB3	19:Q:601:HOH:O	2.09	0.53
9:G:521:LEU:O	9:G:521:LEU:HD23	2.08	0.53
12:L:959:ILE:HG21	12:L:2449:ILE:HD12	1.91	0.53
3:C:48:ARG:HH12	16:Q:216:GLY:HA2	1.74	0.53
16:Q:474:PHE:CD2	16:Q:479:ILE:HD12	2.44	0.53
5:D:84:LEU:HD23	5:D:84:LEU:C	2.29	0.53
10:H:406:ASN:O	10:H:409:SER:OG	2.15	0.53
12:L:1278:ASN:O	12:L:1284:ARG:NH2	2.42	0.53
12:L:345:LEU:O	12:L:386:GLN:NE2	2.42	0.53
16:Q:106:TRP:HB3	17:O:20:ARG:NH2	2.23	0.53
17:O:22:ILE:HG23	18:P:44:ASN:OD1	2.08	0.53
16:Q:472:PHE:CD2	17:O:46:ILE:CA	2.92	0.53
3:C:39:ARG:HH22	16:Q:150:GLN:NE2	2.05	0.53
3:C:47:ASP:HB3	16:Q:243:THR:C	2.25	0.53
5:D:313:TRP:O	5:D:317:GLN:HG2	2.08	0.53
5:D:323:LYS:O	5:D:323:LYS:HG3	2.08	0.53
10:H:217:LEU:HD12	10:H:218:SER:O	2.08	0.53
12:L:3101:LYS:O	12:L:3742:GLN:NE2	2.42	0.53
12:L:416:LEU:HD11	12:L:574:THR:HB	1.91	0.53
1:M:173:GLU:HG2	5:D:197:LYS:CA	2.29	0.53
1:M:188:GLU:OE1	5:D:85:ARG:CZ	2.57	0.53
16:Q:474:PHE:CA	17:O:47:SER:OG	2.50	0.53
9:G:546:HIS:CG	9:G:547:PRO:CD	2.92	0.52
9:G:76:PRO:O	9:G:592:ARG:NH1	2.42	0.52
1:M:84:THR:HA	1:M:87:LEU:HD12	1.90	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
5:D:21:MET:HE2	5:D:253:VAL:CG2	2.38	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
9:G:521:LEU:C	9:G:521:LEU:HD23	2.30	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
9:G:562:ARG:HB3	9:G:571:CYS:SG	2.49	0.52
3:C:42:ILE:CD1	16:Q:176:PRO:HA	2.40	0.52
3:C:51:LEU:N	16:Q:214:LEU:CD1	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:326:ILE:HD12	5:D:326:ILE:C	2.30	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
12:L:852:HIS:CG	12:L:852:HIS:O	2.62	0.52
17:O:24:ILE:HG13	18:P:59:PHE:CZ	2.45	0.52
2:A:223:GLN:HA	2:A:223:GLN:OE1	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
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
12:L:846:LEU:HA	12:L:850:VAL:CB	2.39	0.52
8:K:442:PRO:CD	12:L:912:LEU:HD22	2.36	0.52
5:D:218:ARG:C	5:D:220:ALA:H	2.12	0.52
8:K:602:ILE:O	8:K:607:ASN:N	2.43	0.52
8:K:468:LEU:CB	12:L:2829:LYS:NZ	2.58	0.52
15:R:12:THR:HG21	16:Q:379:LYS:CE	2.39	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
1:M:185:TYR:HD1	1:M:185:TYR:C	2.13	0.52
16:Q:106:TRP:HD1	17:O:20:ARG:NH1	1.97	0.52
15:R:63:LYS:NZ	19:R:103:HOH:O	2.29	0.52
9:G:202:ILE:HD11	9:G:206:THR:HG21	1.92	0.51
9:G:84:GLN:OE1	9:G:215:ASN:O	2.28	0.51
10:H:27:ALA:HB1	10:H:32:ILE:CD1	2.35	0.51
1:M:102:VAL:HG12	1:M:115:ILE:HB	1.92	0.51
16:Q:178:LEU:HD22	17:O:37:ILE:CG2	2.38	0.51
9:G:607:ASP:HB2	9:G:614:ILE:HG13	1.92	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
12:L:672:PRO:HA	12:L:675:PHE:HB3	1.93	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
16:Q:182:THR:CG2	17:O:45:GLN:H	2.19	0.51
19:R:153:HOH:O	16:Q:326:LYS:CB	2.11	0.51
6:E:947:PHE:HD1	6:E:947:PHE:O	1.94	0.51
12:L:2805:PHE:CE1	12:L:2812:LEU:HG	2.46	0.51
12:L:899:ASP:OD1	12:L:899:ASP:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2601:ARG:O	12:L:2603:ASN:N	2.43	0.51
12:L:986:PRO:O	12:L:991:ARG:NH2	2.44	0.51
2:A:364:ASP:OD1	2:A:364:ASP:N	2.42	0.51
6:E:935:SER:OG	6:E:940:LYS:HB2	2.11	0.51
4:F:200:ASP:HA	4:F:203:TYR:HE2	1.75	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
3:C:49:PRO:HG3	16:Q:237:PHE:CE1	2.36	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
12:L:809:MET:HE1	12:L:844:VAL:HG21	1.92	0.51
17:O:15:MET:HE3	18:P:74:VAL:HG21	1.93	0.51
16:Q:70:GLU:OE1	18:P:24:ASP:HA	2.11	0.51
5:D:74:ILE:HG13	5:D:78:LYS:HB3	1.92	0.51
9:G:650:ASP:HB3	9:G:693:MET:HE2	1.93	0.51
8:K:461:LYS:HZ1	12:L:2792:ARG:NH2	2.09	0.51
12:L:3456:LEU:HD12	12:L:3467:LYS:HB3	1.93	0.51
1:M:105:ARG:O	1:M:106:ILE:HG23	2.10	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:2802:LEU:HD11	12:L:2858:SER:HB2	1.93	0.51
12:L:562:ARG:NH1	12:L:625:PHE:O	2.44	0.51
2:A:246:LEU:O	2:A:250:MET:HG3	2.11	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
16:Q:472:PHE:CE2	17:O:50:GLU:CD	2.83	0.51
2:A:192:SER:O	2:A:196:GLN:NE2	2.44	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
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
12:L:2415:THR:HA	12:L:2418:MET:HE3	1.93	0.50
4:F:326:ARG:HG2	12:L:2751:LEU:HD11	1.92	0.50
15:R:75:GLY:HA2	16:Q:270:GLU:OE2	2.11	0.50
9:G:565:ASP:HB3	9:G:568:ARG:HB3	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:2802:LEU:HD22	12:L:2854:LEU:HD12	1.92	0.50
12:L:703:PHE:O	12:L:709:THR:OG1	2.29	0.50
1:M:170:ILE:HD13	1:M:234:LEU:HD22	1.93	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
1:M:185:TYR:CD1	1:M:185:TYR:C	2.84	0.50
2:A:246:LEU:HG	2:A:250:MET:HE2	1.93	0.50
5:D:78:LYS:C	5:D:78:LYS:HE3	2.31	0.50
12:L:1507:LEU:HA	12:L:1510:ALA:HB3	1.92	0.50
16:Q:472:PHE:CZ	17:O:50:GLU:HG2	2.44	0.50
16:Q:90:SER:H	18:P:14:GLN:NE2	2.10	0.50
16:Q:464:ILE:C	17:O:46:ILE:CD1	2.80	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
3:C:38:LEU:HD22	16:Q:210:ARG:HD2	0.55	0.50
1:M:67:LEU:HD13	1:M:160:ILE:HG23	1.94	0.50
17:O:26:ASN:HB2	18:P:47:THR:HG21	1.94	0.50
4:F:122:PRO:HG3	4:F:195:LEU:HD23	1.93	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
1:M:142:ILE:HA	1:M:145:LYS:HE3	1.94	0.50
10:H:290:ILE:HG22	10:H:343:LEU:HD11	1.93	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:469:ILE:HD11	9:G:479:LEU:HD12	1.93	0.49
9:G:122:LEU:HD21	10:H:291:TYR:CD1	2.46	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:CD	12:L:2880:LYS:H	2.23	0.49
17:O:56:LEU:CA	18:P:52:THR:CG2	2.90	0.49
12:L:2797:GLN:HG2	12:L:2818:LEU:HD21	1.93	0.49
1:M:80:LEU:HD21	1:M:143:ILE:HD12	1.93	0.49
16:Q:107:LYS:CA	17:O:20:ARG:HH22	2.26	0.49
3:C:47:ASP:CG	16:Q:243:THR:HB	2.32	0.49
10:H:96:LEU:HD23	10:H:97:VAL:N	2.27	0.49
17:O:34:ARG:NH1	18:P:57:PRO:CA	2.69	0.49
16:Q:107:LYS:HG2	17:O:20:ARG:NH1	2.27	0.49
5:D:67:PRO:O	5:D:71:ILE:HG22	2.12	0.49
4:F:200:ASP:HA	4:F:203:TYR:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:L:428:LYS:HG3	12:L:430:GLU:CG	2.42	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
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
3:C:56:SER:HB2	16:Q:156:ARG:HD3	1.94	0.49
5:D:329:PHE:N	5:D:329:PHE:CD1	2.80	0.49
4:F:279:ASP:O	8:K:521:ILE:HD11	2.12	0.49
13:B:556:VAL:O	13:B:557:VAL:C	2.50	0.49
3:C:306:SER:OG	3:C:307:VAL:N	2.45	0.49
5:D:319:ARG:HG3	5:D:320:ASN:H	1.77	0.49
12:L:3175:THR:HG21	12:L:3528:PRO:HB2	1.94	0.49
1:M:82:LEU:CD1	1:M:101:ALA:HA	2.37	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
12:L:1364:LEU:O	12:L:1391:ARG:NH1	2.45	0.49
1:M:108:GLU:HA	1:M:109:PRO:C	2.31	0.49
16:Q:472:PHE:CB	17:O:46:ILE:CG1	2.55	0.49
2:A:190:VAL:HG22	2:A:192:SER:H	1.77	0.49
6:E:946:LYS:CA	6:E:946:LYS:CE	2.91	0.49
12:L:2475:LEU:O	12:L:2479:TYR:N	2.44	0.49
1:M:175:LEU:O	1:M:179:HIS:HB2	2.13	0.49
3:C:48:ARG:NH1	16:Q:216:GLY:HA2	2.27	0.48
5:D:78:LYS:O	5:D:78:LYS:CD	2.61	0.48
4:F:223:GLU:N	4:F:223:GLU:OE1	2.46	0.48
11:I:133:THR:O	11:I:135:LYS:N	2.44	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
3:C:34:LEU:C	16:Q:467:ARG:HG2	2.32	0.48
9:G:139:HIS:ND1	9:G:228:LEU:HD22	2.29	0.48
8:K:564:HIS:ND1	8:K:568:ASN:OD1	2.44	0.48
12:L:545:LEU:HD12	12:L:546:PRO:HD2	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:LEU:CG	16:Q:210:ARG:CZ	2.89	0.48
16:Q:93:CYS:H	17:O:17:ASN:CG	2.14	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
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
12:L:387:LEU:HD21	12:L:422:ILE:HG12	1.95	0.48
17:O:19:LEU:CD1	18:P:70:ALA:CB	2.91	0.48
17:O:7:GLN:HG3	18:P:86:ILE:CB	2.41	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
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
1:M:96:PRO:O	1:M:98:ARG:N	2.47	0.48
16:Q:259:TRP:NE1	17:O:114:ASP:OD1	2.42	0.48
4:F:115:VAL:HG13	4:F:190:LEU:HD11	1.96	0.47
9:G:184:LEU:O	9:G:191:LYS:NZ	2.41	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
8:K:458:ALA:O	8:K:459:ALA:HB2	2.14	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
1:M:194:ILE:CA	1:M:195:TYR:N	2.76	0.47
9:G:650:ASP:HB3	9:G:693:MET:CE	2.43	0.47
17:O:55:ARG:HB3	18:P:52:THR:CG2	2.41	0.47
16:Q:315:SER:HB3	19:Q:605:HOH:O	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:1262:SER:OG	12:L:1263:SER:N	2.47	0.47
12:L:1855:PRO:HA	12:L:1862:ARG:HH22	1.79	0.47
8:K:468:LEU:O	12:L:2790:THR:HG22	2.14	0.47
12:L:853:LEU:N	12:L:853:LEU:HD23	2.28	0.47
3:C:50:ILE:C	16:Q:214:LEU:CG	2.83	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
3:C:54:CYS:HG	16:Q:215:SER:C	1.90	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:328:ASN:ND2	6:E:963:ASN:OD1	2.48	0.47
5:D:47:VAL:O	5:D:51:LEU:HD23	2.14	0.47
5:D:73:LEU:CD2	5:D:73:LEU:C	2.82	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:CE	2.45	0.47
6:E:947:PHE:CD1	6:E:947:PHE:C	2.88	0.47
4:F:118:GLU:O	4:F:191:ARG:N	2.45	0.47
9:G:472:SER:OG	9:G:474:ASP:OD1	2.28	0.47
4:F:304:LEU:CD2	8:K:475:SER:HB2	2.45	0.47
12:L:1417:ARG:HG2	12:L:1418:VAL:N	2.29	0.47
12:L:867:SER:OG	12:L:868:GLN:N	2.48	0.47
3:C:55:LEU:HD23	16:Q:160:ILE:CG1	2.41	0.47
4:F:189:ILE:C	4:F:190:LEU:HD12	2.35	0.47
8:K:566:GLU:O	8:K:572:ARG:NH1	2.46	0.47
12:L:1684:ARG:HH12	12:L:1692:LEU:HD13	1.80	0.47
12:L:854:SER:C	12:L:856:LEU:H	2.18	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
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
12:L:3798:THR:OG1	12:L:3799:GLN:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:82:LEU:HG	1:M:117:ALA:HB2	1.97	0.47
16:Q:478:ARG:HD3	17:O:76:ASN:HD21	1.79	0.47
9:G:546:HIS:NE2	9:G:547:PRO:HD2	2.29	0.47
10:H:157:ASN:HD22	10:H:160:LYS:HZ3	1.62	0.47
12:L:1134:SER:OG	12:L:1135:ASP:N	2.47	0.47
12:L:2808:GLN:OE1	12:L:2808:GLN:HA	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:1203:LEU:HD22	12:L:1210:PHE:CE2	2.50	0.47
12:L:1848:ALA:HB2	12:L:1887:VAL:HG23	1.97	0.47
12:L:312:CYS:O	12:L:320:ARG:NH2	2.47	0.47
16:Q:464:ILE:C	17:O:46:ILE:HD11	2.36	0.47
15:R:46:ALA:CA	16:Q:331:PRO:O	2.50	0.47
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:504:LYS:O	8:K:508:ARG:NH1	2.48	0.46
12:L:853:LEU:O	12:L:854:SER:C	2.54	0.46
8:K:441:PRO:CA	12:L:912:LEU:HD21	2.33	0.46
1:M:151:LYS:O	1:M:153:THR:HG22	2.15	0.46
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:N	12:L:952:ASN:OD1	2.48	0.46
16:Q:472:PHE:HZ	17:O:45:GLN:CD	2.18	0.46
15:R:71:LEU:HD12	16:Q:397:PHE:HB2	1.97	0.46
16:Q:130:TYR:CE2	17:O:25:ASN:OD1	2.59	0.46
17:O:34:ARG:NH1	18:P:57:PRO:CG	2.55	0.46
16:Q:416:PHE:CE2	18:P:35:TYR:O	2.69	0.46
5:D:75:ARG:O	5:D:75:ARG:HG2	2.16	0.46
4:F:137:GLU:O	9:G:59:TYR:N	2.45	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:2601:ARG:O	12:L:2602:PRO:C	2.53	0.46
12:L:2959:HIS:HA	12:L:3512:VAL:HG11	1.96	0.46
2:A:357:SER:O	2:A:357:SER:OG	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:2812:LEU:HD11	12:L:2862:SER:HB2	1.97	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
16:Q:472:PHE:CB	17:O:47:SER:N	2.73	0.46
8:K:588:GLN:NE2	8:K:589:PRO:O	2.45	0.46
8:K:465:ARG:O	12:L:2829:LYS:HE2	2.16	0.46
12:L:853:LEU:HD23	12:L:853:LEU:H	1.80	0.46
12:L:934:ARG:HG2	12:L:934:ARG:H	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
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
1:M:117:ALA:C	1:M:119:GLY:H	2.19	0.46
17:O:7:GLN:HG3	18:P:86:ILE:CG2	2.45	0.46
15:R:4:PHE:CE1	16:Q:362:LEU:HD13	2.51	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
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:17:ILE:N	5:D:17:ILE:CD1	2.79	0.45
9:G:709:THR:HG22	9:G:710:ARG:H	1.80	0.45
7:J:58:THR:N	7:J:61:GLU:OE2	2.49	0.45
12:L:1608:VAL:O	12:L:1617:ARG:NH2	2.49	0.45
12:L:828:ARG:N	12:L:829:PRO:CD	2.57	0.45
1:M:172:LEU:HB2	5:D:204:TYR:CE2	2.52	0.45
17:O:11:TRP:CG	18:P:86:ILE:CD1	2.94	0.45
16:Q:472:PHE:CG	17:O:46:ILE:N	2.80	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:CD2	12:L:3458:LEU:H	2.28	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:1136:ASN:HB3	12:L:1139:VAL:HG12	1.96	0.45
12:L:2807:GLN:OE1	12:L:2807:GLN:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:827:ARG:HH21	12:L:829:PRO:HB3	1.80	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
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
17:O:24:ILE:CG1	18:P:59:PHE:CE1	2.94	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
16:Q:91:LEU:CD2	17:O:13:CYS:HG	2.19	0.45
8:K:562:GLN:CD	8:K:577:ALA:HB3	2.36	0.45
12:L:1916:ASP:OD1	12:L:1916:ASP:N	2.49	0.45
1:M:166:VAL:HG22	1:M:210:GLY:O	2.17	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
4:F:326:ARG:HD3	12:L:2751:LEU:HD21	1.97	0.45
12:L:854:SER:C	12:L:856:LEU:N	2.69	0.45
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:3461:GLY:N	12:L:3464:GLY:O	2.50	0.45
14:N:221:UNK:HA	14:N:230:UNK:CB	2.47	0.45
3:C:49:PRO:HB2	16:Q:214:LEU:HD13	1.97	0.45
1:M:189:LEU:HD13	5:D:84:LEU:HD22	1.98	0.45
9:G:697:PHE:O	10:H:147:GLN:NE2	2.50	0.45
12:L:1543:PRO:O	12:L:1547:HIS:NE2	2.49	0.45
8:K:465:ARG:HG3	12:L:2844:LEU:CD1	2.47	0.45
12:L:3494:GLU:HA	12:L:3497:ILE:HG12	1.99	0.45
12:L:962:LEU:HG	12:L:2572:ALA:HB2	1.98	0.45
1:M:124:THR:CG2	1:M:125:GLY:N	2.80	0.45
16:Q:35:ASP:HA	16:Q:38:TYR:CD2	2.52	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
1:M:135:ALA:O	1:M:139:TYR:CD2	2.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:107:ILE:HD11	9:G:140:CYS:HB2	1.99	0.45
8:K:437:LEU:H	8:K:437:LEU:CD2	2.28	0.45
14:N:83:UNK:C	14:N:506:UNK:C	2.95	0.45
2:A:342:TYR:HD1	2:A:344:TYR:HH	1.64	0.44
6:E:946:LYS:CD	6:E:946:LYS:N	2.79	0.44
9:G:450:VAL:HG22	9:G:451:GLY:N	2.29	0.44
4:F:305:SER:O	8:K:452:VAL:HG21	2.16	0.44
3:C:39:ARG:NH1	16:Q:148:ILE:HG23	2.06	0.44
8:K:465:ARG:H	8:K:465:ARG:HD3	1.83	0.44
12:L:1425:PHE:C	12:L:1427:SER:N	2.70	0.44
12:L:1780:TYR:HA	12:L:1783:ILE:HG22	1.99	0.44
12:L:1876:ASP:N	12:L:1876:ASP:OD1	2.51	0.44
12:L:2539:THR:HG23	12:L:2541:GLY: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
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:1340:CYS:HA	12:L:1343:LEU:HD13	1.98	0.44
12:L:214:TYR:O	12:L:218:ALA:N	2.49	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
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
3:C:38:LEU:HD21	16:Q:210:ARG:HG2	1.99	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
9:G:63:GLU:OE1	9:G:64:SER:OG	2.31	0.44
8:K:465:ARG:O	12:L:2791:PRO:HG3	2.18	0.44
12:L:1610:LEU:O	12:L:1617:ARG:NH2	2.51	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
5:D:24:SER:HB3	5:D:210:CYS:CB	2.48	0.44
12:L:1356:ARG:NE	12:L:1356:ARG:N	2.65	0.44
12:L:1358:VAL:O	12:L:1359:GLN:C	2.56	0.44
12:L:1727:LYS:HD2	12:L:1734:PRO:HG3	1.99	0.44
1:M:78:CYS:SG	1:M:80:LEU:HD11	2.57	0.44
3:C:38:LEU:CB	16:Q:210:ARG:CZ	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1358:VAL:O	12:L:1360:GLU:N	2.51	0.44
12:L:3522:THR:OG1	12:L:3522:THR:O	2.33	0.44
12:L:404:ALA:HB3	12:L:407:VAL:HG22	1.99	0.44
17:O:26:ASN:CB	18:P:47:THR:HG21	2.48	0.44
16:Q:137:GLY:O	18:P:60:SER:OG	2.27	0.44
9:G:74:PRO:HB3	9:G:610:THR:CG2	2.47	0.44
12:L:2437:LEU:HA	12:L:2440:ILE:HD12	2.00	0.44
8:K:461:LYS:HZ2	12:L:2792:ARG:NE	2.16	0.44
12:L:2897:ILE:HA	12:L:2897:ILE:HD12	1.86	0.44
12:L:722:LYS:HG2	12:L:768:LEU:HD21	2.00	0.44
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
6:E:880:LYS:C	6:E:881:LEU:HD12	2.38	0.43
8:K:557:ASP:OD1	8:K:557:ASP:N	2.46	0.43
8:K:461:LYS:HD2	12:L:2762:LEU:HD11	1.99	0.43
1:M:76:LEU:O	1:M:78:CYS:N	2.51	0.43
13:B:413:ASP:O	13:B:414:ASP:C	2.56	0.43
3:C:59:ILE:HG22	16:Q:170:ILE:HD11	1.99	0.43
5:D:259:GLU:HA	5:D:262:ILE:HD12	2.00	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
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
1:M:126:ALA:HB3	1:M:132:SER:OG	2.19	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
1:M:79:ARG:O	1:M:80:LEU:HD12	2.17	0.43
16:Q:130:TYR:CE2	17:O:28:LEU:HD12	2.51	0.43
3:C:48:ARG:HG3	16:Q:238:LYS:HG2	2.00	0.43
10:H:318:ALA:HB3	10:H:337:ARG:NH1	2.32	0.43
12:L:3765:GLN:HB3	12:L:3768:GLN:HB3	2.00	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
14:N:207:UNK:CA	14:N:208:UNK:CB	2.96	0.43
5:D:321:VAL:HG12	5:D:321:VAL:O	2.17	0.43
8:K:469:LEU:N	8:K:469:LEU:HD23	2.33	0.43
12:L:3541:ARG:HB2	12:L:3654:GLU:HB2	2.01	0.43
12:L:773:LEU:HD13	12:L:815:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:200:PRO:HD3	1:M:225:GLN:OE1	2.18	0.43
17:O:11:TRP:CD1	18:P:83:LEU:HG	2.51	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: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
1:M:88:HIS:CB	14:N:515:UNK:O	2.56	0.43
12:L:2523:ASP:OD1	12:L:2523:ASP:N	2.42	0.43
3:C:51:LEU:HD12	16:Q:215:SER:H	1.81	0.43
5:D:207:TRP:C	5:D:207:TRP:CD1	2.91	0.43
5:D:17:ILE:HG22	5:D:21:MET:SD	2.59	0.43
4:F:204:GLN:HA	4:F:204:GLN:OE1	2.19	0.43
9:G:92:THR:OG1	9:G:93:ALA:N	2.51	0.43
7:J:206:TYR:HB3	7:J:207:GLY:H	1.71	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
12:L:560:ASP:OD1	12:L:560:ASP:N	2.51	0.43
3:C:36:ASN:CB	16:Q:467:ARG:NH2	2.81	0.43
2:A:243:MET:CB	2:A:268:ILE:HD12	2.49	0.43
1:M:177:PHE:CB	5:D:194:GLU:HA	2.49	0.43
6:E:883:SER:O	6:E:886:SER:OG	2.28	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
14:N:181:UNK:O	14:N:198:UNK:CB	2.67	0.43
5:D:319:ARG:HD2	5:D:319:ARG:HA	1.65	0.42
6:E:929:LEU:CD1	6:E:955:ILE:HG22	2.49	0.42
6:E:950:VAL:HG23	6:E:950:VAL:O	2.19	0.42
6:E:885:VAL:HG13	10:H:128:PRO:HG2	2.01	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
12:L:1060:LYS:HA	12:L:1060:LYS:HD2	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
3:C:51:LEU:HD12	16:Q:211:ASP:O	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:129:LYS:CB	10:H:129:LYS:HZ3	2.31	0.42
10:H:129:LYS:CB	10:H:129:LYS:NZ	2.82	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
2:A:183:GLU:O	2:A:184:SER:OG	2.26	0.42
10:H:317:LEU:HD12	10:H:318:ALA:N	2.34	0.42
8:K:581:ILE:HD12	11:I:52:ILE:HD11	2.01	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
12:L:848:VAL:O	12:L:851:PRO:HD2	2.19	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:N	8:K:437:LEU:HD23	2.32	0.42
12:L:3111:SER:O	12:L:3111:SER:OG	2.33	0.42
12:L:846:LEU:CA	12:L:850:VAL:HB	2.45	0.42
12:L:907:LYS:HB3	12:L:907:LYS:HE3	1.83	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
9:G:416:LEU:N	9:G:447:ARG:O	2.52	0.42
10:H:242:GLU:N	10:H:242:GLU:OE1	2.52	0.42
12:L:1356:ARG:CA	12:L:1356:ARG:NE	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:HG2	12:L:2889:ARG:O	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:HA	5:D:72:PHE:HD1	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
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
10:H:315:LEU:O	10:H:318:ALA:HB2	2.20	0.42
8:K:582:ARG:NH1	11:I:71:GLY:O	2.52	0.42
7:J:116:TYR:OH	7:J:120:ARG:NH2	2.53	0.42
12:L:2476:GLN:HG2	12:L:2548:ILE:HD12	2.02	0.42
12:L:2592:ASP:OD1	12:L:2592:ASP:N	2.53	0.42
12:L:2740:GLU:HB2	12:L:2745:TRP:CH2	2.55	0.42
1:M:186:GLU:HB3	1:M:189:LEU:HB2	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:M:187:PRO:HB3	5:D:211:ARG:HB2	2.02	0.42
3:C:253:ARG:NH2	10:H:49:TYR:OH	2.51	0.42
10:H:67:ARG:NH2	10:H:74:ASP:OD1	2.53	0.42
12:L:1863:LYS:HD2	12:L:1863:LYS:HA	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
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
2:A:259:LEU:HD21	8:K:549:LYS:HB2	2.02	0.41
12:L:3149:LYS:HD3	12:L:3149:LYS:HA	1.89	0.41
12:L:328:ARG:HH11	12:L:370:THR:HG22	1.84	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:3634:ILE:HD12	12:L:3703:PHE:HB2	2.02	0.41
12:L:718:ILE:HD12	12:L:718:ILE:HA	1.95	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
3:C:41:ARG:HB3	16:Q:173:SER:HB3	2.02	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
8:K:469:LEU:CD2	12:L:2790:THR:HG23	2.50	0.41
8:K:442:PRO:HB3	12:L:2817:ARG:NH1	2.35	0.41
12:L:3603:THR:HG22	12:L:3711:LYS:HG2	2.01	0.41
1:M:74:VAL:HG23	1:M:155:PHE:CA	2.49	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:HB2	12:L:1444:LYS:HE3	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
9:G:709:THR:HG22	9:G:710:ARG:N	2.35	0.41
8:K:466:PRO:HA	12:L:2791:PRO:CG	2.23	0.41
1:M:146:ILE:O	1:M:147:GLY:C	2.58	0.41
3:C:52:GLN:CG	16:Q:153:GLN:HG3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:44:ASN:OD1	16:Q:174:ARG:CD	2.69	0.41
1:M:185:TYR:HD2	5:D:204:TYR:HH	1.64	0.41
1:M:189:LEU:CD1	5:D:84:LEU:HD13	2.49	0.41
6:E:934:GLU:O	6:E:936:LYS:N	2.45	0.41
9:G:460:ASP:OD1	9:G:461:PHE:N	2.54	0.41
8:K:454:PRO:CD	8:K:455:PRO:HD2	2.50	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
12:L:388:TRP:HA	12:L:391:VAL:HG12	2.03	0.41
17:O:11:TRP:CE2	18:P:86:ILE:CG1	2.97	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
9:G:563:MET:HE3	9:G:608:ILE:HD13	2.03	0.41
10:H:129:LYS:NZ	10:H:129:LYS:CA	2.82	0.41
12:L:1629:GLY:HA2	12:L:1632:HIS:HD2	1.86	0.41
12:L:268:GLY:O	12:L:272:ILE:N	2.53	0.41
12:L:2794:GLN:HG2	12:L:2822:GLY:HA3	2.02	0.41
12:L:672:PRO:O	12:L:676:ASN:ND2	2.54	0.41
1:M:84:THR:O	1:M:87:LEU:HB2	2.20	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
1:M:231:TYR:HB3	1:M:232:PRO:HD3	2.03	0.41
2:A:242:GLU:O	2:A:243:MET:C	2.58	0.41
4:F:133:VAL:HG23	4:F:134:GLN:CD	2.41	0.41
10:H:396:ILE:HG23	10:H:397:ARG:N	2.36	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
3:C:51:LEU:CG	16:Q:214:LEU:CG	2.97	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
11:I:51:THR:HG22	11:I:76:LEU:HD21	2.03	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:314:SER:OG	12:L:314:SER:O	2.33	0.41
12:L:853:LEU:CD2	12:L:853:LEU:H	2.34	0.41
12:L:858:LYS:HB2	12:L:858:LYS:HE3	1.87	0.41
10:H:335:ALA:O	10:H:339:LEU:HD23	2.20	0.41
16:Q:107:LYS:HZ2	17:O:13:CYS:HA	1.83	0.41
2:A:199:GLN:NE2	3:C:305:PHE:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:460:MET:HG3	12:L:2758:THR:CG2	2.51	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:325:HIS:HA	12:L:328:ARG:HB3	2.03	0.40
12:L:3604:LEU:HD12	12:L:3604:LEU:HA	1.93	0.40
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
12:L:2687:TYR:HB2	12:L:2690:THR:HG22	2.02	0.40
12:L:2817:ARG:HD2	12:L:2817:ARG:HA	1.91	0.40
12:L:2907:ARG:HH11	12:L:2907:ARG:CG	2.25	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
3:C:49:PRO:CD	16:Q:238:LYS:HA	2.52	0.40
6:E:944:ASP:N	6:E:944:ASP:OD1	2.54	0.40
4:F:85:PHE:N	4:F:143:ARG:O	2.46	0.40
9:G:588:SER:HB3	9:G:593:TRP:HB2	2.04	0.40
10:H:127:LEU:HD12	10:H:127:LEU:C	2.39	0.40
10:H:217:LEU:HB2	10:H:221:LEU:HD22	2.02	0.40
12:L:1611:ASP:OD1	12:L:1611:ASP:N	2.53	0.40
12:L:833:ASP:HA	12:L:836:VAL:HG12	2.03	0.40
1:M:78:CYS:SG	1:M:80:LEU:CD1	3.10	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
9:G:45:ASP:OD1	9:G:45:ASP:N	2.55	0.40
8:K:461:LYS:HE2	8:K:463:PRO:HD2	2.03	0.40
12:L:2783:LYS:HD3	12:L:2783:LYS:HA	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
9:G:182:GLU:N	9:G:182:GLU:OE1	2.49	0.40
12:L:3778:GLU:HA	12:L:3781:THR:HG22	2.04	0.40
1:M:85:VAL:HG11	1:M:143:ILE:HG22	2.04	0.40
1:M:88:HIS:CA	14:N:515:UNK:C	2.98	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%)	3	30
2	A	169/448 (38%)	151 (89%)	18 (11%)	0	100	100
3	C	89/698 (13%)	83 (93%)	6 (7%)	0	100	100
4	F	202/517 (39%)	177 (88%)	24 (12%)	1 (0%)	31	74
5	D	203/341 (60%)	177 (87%)	19 (9%)	7 (3%)	4	33
6	E	150/1191 (13%)	135 (90%)	13 (9%)	2 (1%)	13	54
7	J	92/217 (42%)	82 (89%)	9 (10%)	1 (1%)	16	58
8	K	150/609 (25%)	125 (83%)	23 (15%)	2 (1%)	13	54
9	G	512/722 (71%)	448 (88%)	63 (12%)	1 (0%)	49	85
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%)	27	70
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%)	13	54
17	O	115/123 (94%)	103 (90%)	6 (5%)	6 (5%)	2	25
18	P	88/96 (92%)	85 (97%)	3 (3%)	0	100	100
All	All	5980/10965 (54%)	5381 (90%)	548 (9%)	51 (1%)	24	61

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%)	10	34
2	A	134/394 (34%)	132 (98%)	2 (2%)	67	85
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%)	154 (93%)	12 (7%)	16	46
6	E	142/1101 (13%)	136 (96%)	6 (4%)	32	61
7	J	85/183 (46%)	84 (99%)	1 (1%)	74	87
8	K	133/524 (25%)	130 (98%)	3 (2%)	53	76
9	G	439/635 (69%)	430 (98%)	9 (2%)	56	78
10	H	352/438 (80%)	348 (99%)	4 (1%)	76	88
11	I	104/130 (80%)	103 (99%)	1 (1%)	78	89
12	L	2156/3450 (62%)	2114 (98%)	42 (2%)	60	80
15	R	70/68 (103%)	69 (99%)	1 (1%)	69	85
16	Q	431/449 (96%)	425 (99%)	6 (1%)	69	85
17	O	103/109 (94%)	102 (99%)	1 (1%)	78	89
18	P	85/91 (93%)	85 (100%)	0	100	100
All	All	4816/9181 (52%)	4714 (98%)	102 (2%)	59	78

All (102) 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	185	TYR
1	M	202	ILE
1	M	215	THR
1	M	231	TYR
1	M	240	MET
2	A	229	PHE
2	A	291	LYS
5	D	18	GLN
5	D	74	ILE
5	D	78	LYS
5	D	83	ARG
5	D	85	ARG
5	D	87	TYR
5	D	211	ARG
5	D	212	GLN
5	D	218	ARG
5	D	322	GLU
5	D	329	PHE
5	D	338	VAL
6	E	933	ILE
6	E	940	LYS
6	E	942	MET
6	E	946	LYS
6	E	948	GLN
6	E	949	LYS
7	J	205	GLU
8	K	437	LEU
8	K	449	ARG
8	K	465	ARG
9	G	115	LYS
9	G	194	ARG
9	G	230	ASN
9	G	452	HIS
9	G	537	LEU

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Mol	Chain	Res	Type
9	G	542	CYS
9	G	560	THR
9	G	571	CYS
9	G	594	LEU
10	H	129	LYS
10	H	217	LEU
10	H	360	PRO
10	H	364	ARG
11	I	16	HIS
12	L	429	THR
12	L	800	ARG
12	L	849	LEU
12	L	852	HIS
12	L	971	THR
12	L	1122	ASN
12	L	1278	ASN
12	L	1314	LEU
12	L	1323	ARG
12	L	1356	ARG
12	L	1358	VAL
12	L	1413	ARG
12	L	1417	ARG
12	L	1419	LYS
12	L	1424	PHE
12	L	1548	LYS
12	L	1665	LYS
12	L	1680	LEU
12	L	2427	ARG
12	L	2489	ARG
12	L	2595	ILE
12	L	2633	ASN
12	L	2807	GLN
12	L	2878	GLU
12	L	2880	LYS
12	L	2881	ARG
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

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Mol	Chain	Res	Type
12	L	2916	ARG
12	L	3314	ARG
12	L	3426	LYS
12	L	3440	LYS
12	L	3441	ASP
12	L	3489	ARG
12	L	3502	ARG
12	L	3542	TYR
12	L	3646	GLN
15	R	60	ASN
16	Q	38	TYR
16	Q	57	ASN
16	Q	61	TYR
16	Q	187	PHE
16	Q	254	LEU
16	Q	397	PHE
17	O	42	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	91	ASN
1	M	95	ASN
1	M	179	HIS
2	A	227	HIS
3	C	52	GLN
5	D	212	GLN
5	D	317	GLN
9	G	391	ASN
10	H	64	HIS
10	H	157	ASN
10	H	306	HIS
12	L	1632	HIS
12	L	2633	ASN
12	L	2698	GLN
12	L	2884	GLN
15	R	2	GLN
15	R	25	ASN
15	R	60	ASN
15	R	62	GLN
15	R	68	HIS
16	Q	110	HIS

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Mol	Chain	Res	Type
16	Q	150	GLN
16	Q	205	HIS
16	Q	466	ASN
17	O	26	ASN
17	O	52	ASN
17	O	54	GLN
17	O	76	ASN
18	P	14	GLN
18	P	36	GLN

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	15,16	3,3,3	0.68	0	1,2,2	1.36	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	15,16	-	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 carbohydrates 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 [i](#)

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