



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:34 AM UTC

PDB ID : 8XZV / pdb_00008xzv
EMDB ID : EMD-38799
Title : Architecture of the spinach plastid-encoded RNA polymerase
Authors : Wang, G.-L.; Yu, L.-J.; Lu, C.
Deposited on : 2024-01-21
Resolution : 3.16 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

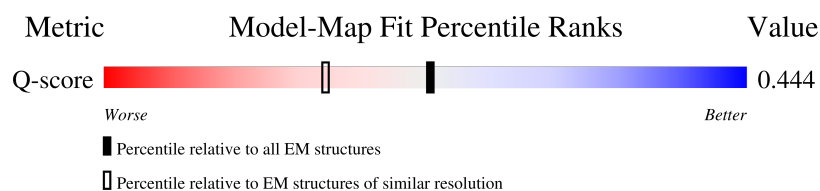
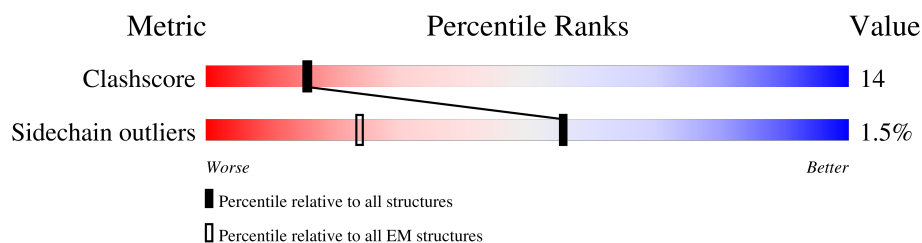
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.16 Å.

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



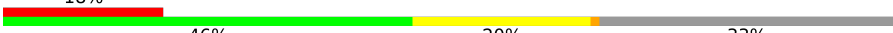
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14474 (2.66 - 3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	335	
1	O	335	
2	B	1070	
3	C	677	
4	D	1357	

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Mol	Chain	Length	Quality of chain
5	E	472	
6	F	181	
6	R	181	
7	G	518	
8	H	892	
9	I	490	
10	K	324	
11	L	284	
12	M	273	
13	N	678	
14	P	170	
15	Q	143	
16	S	583	
17	J	774	

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 58999 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	225	Total	C	N	O	S	0	0
			1775	1123	309	333	10		
1	O	223	Total	C	N	O	S	0	0
			1761	1115	307	329	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1070	Total	C	N	O	S	0	0
			8517	5403	1505	1575	34		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	677	Total	C	N	O	S	0	0
			5507	3525	969	985	28		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta''.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	1216	Total	C	N	O	S	1	0
			8374	5215	1551	1582	26		

- Molecule 5 is a protein called Fructokinase-like 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	382	Total	C	N	O	S	0	0
			3079	1957	521	584	17		

- Molecule 6 is a protein called Thioredoxin-like protein CITRX, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	116	Total	C	N	O	S	0	0
			940	596	154	181	9		
6	R	116	Total	C	N	O	S	0	0
			940	596	154	181	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	21	PHE	SER	conflict	UNP A0A9R0J865
R	21	PHE	SER	conflict	UNP A0A9R0J865

- Molecule 7 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	237	Total	C	N	O	S	0	0
			2009	1273	354	374	8		

- Molecule 8 is a protein called pTAC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	595	Total	C	N	O	S	0	0
			4653	2944	823	860	26		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	892	ALA	SER	conflict	UNP A0A9R0IP63

- Molecule 9 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 14 iso-form X2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	413	Total	C	N	O	S	0	0
			3373	2162	575	615	21		

- Molecule 10 is a protein called pTAC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	214	Total	C	N	O	S	0	0
			1803	1137	320	339	7		

- Molecule 11 is a protein called superoxide dismutase.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	224	Total	C	N	O	S	0	0
			1817	1176	299	338	4		

- Molecule 12 is a protein called superoxide dismutase.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	215	Total	C	N	O	S	0	0
			1763	1145	294	318	6		

- Molecule 13 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	475	Total	C	N	O	S	0	0
			4032	2565	693	756	18		

- Molecule 14 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	105	Total	C	N	O	S	0	0
			840	525	148	162	5		

- Molecule 15 is a protein called pTAC18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	104	Total	C	N	O	S	0	0
			902	587	156	157	2		

- Molecule 16 is a protein called Fructokinase-like 2, chloroplastic isoform X2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	344	Total	C	N	O	S	0	0
			2695	1721	462	494	18		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	114	VAL	-	insertion	UNP A0A9R0K4E6
S	115	LEU	-	insertion	UNP A0A9R0K4E6
S	116	HIS	-	insertion	UNP A0A9R0K4E6
S	117	THR	-	insertion	UNP A0A9R0K4E6
S	118	GLU	-	insertion	UNP A0A9R0K4E6
S	119	MET	-	insertion	UNP A0A9R0K4E6

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Chain	Residue	Modelled	Actual	Comment	Reference
S	120	LYS	-	insertion	UNP A0A9R0K4E6
S	121	LEU	-	insertion	UNP A0A9R0K4E6
S	122	PHE	-	insertion	UNP A0A9R0K4E6
S	123	SER	-	insertion	UNP A0A9R0K4E6

- Molecule 17 is a protein called MurE.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	546	Total	C	N	O	S	0	0
			4218	2640	726	826	26		

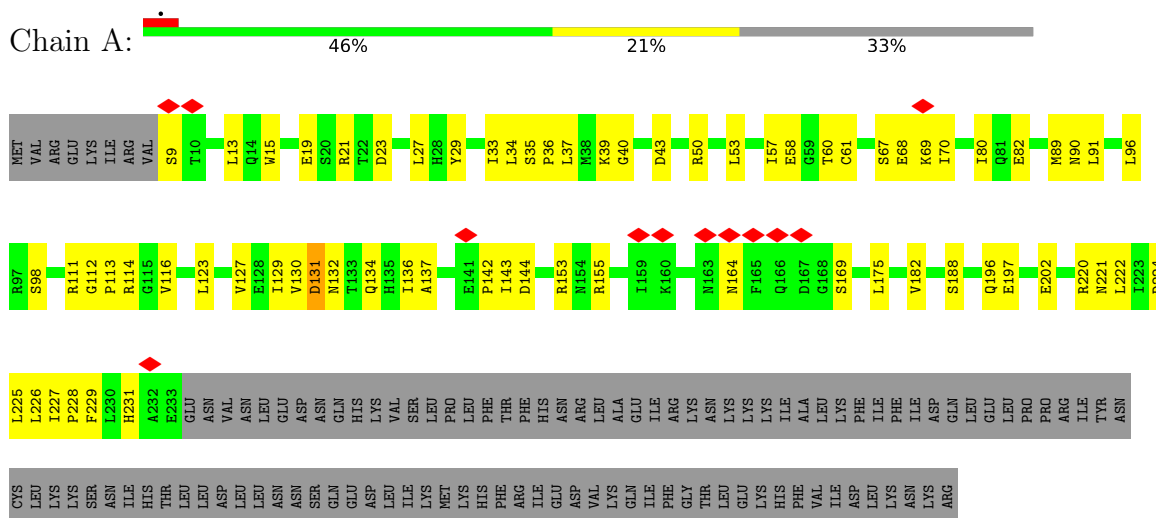
- Molecule 18 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
18	L	1	Total	Fe	0
			1	1	

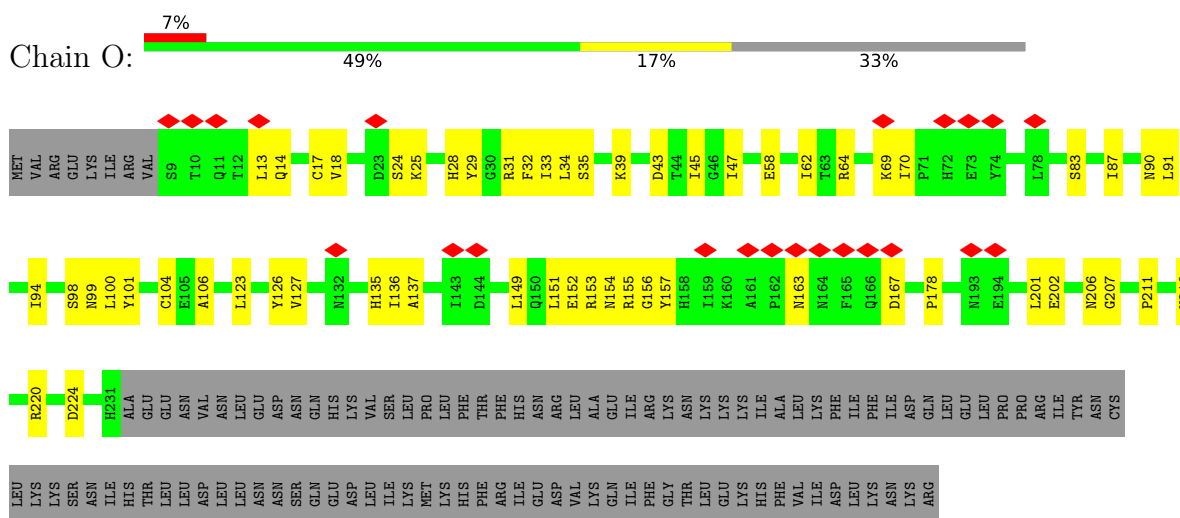
3 Residue-property plots

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

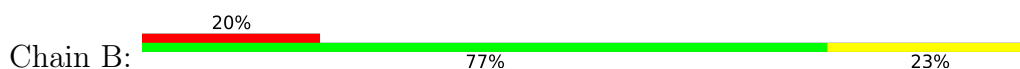
- Molecule 1: DNA-directed RNA polymerase subunit alpha

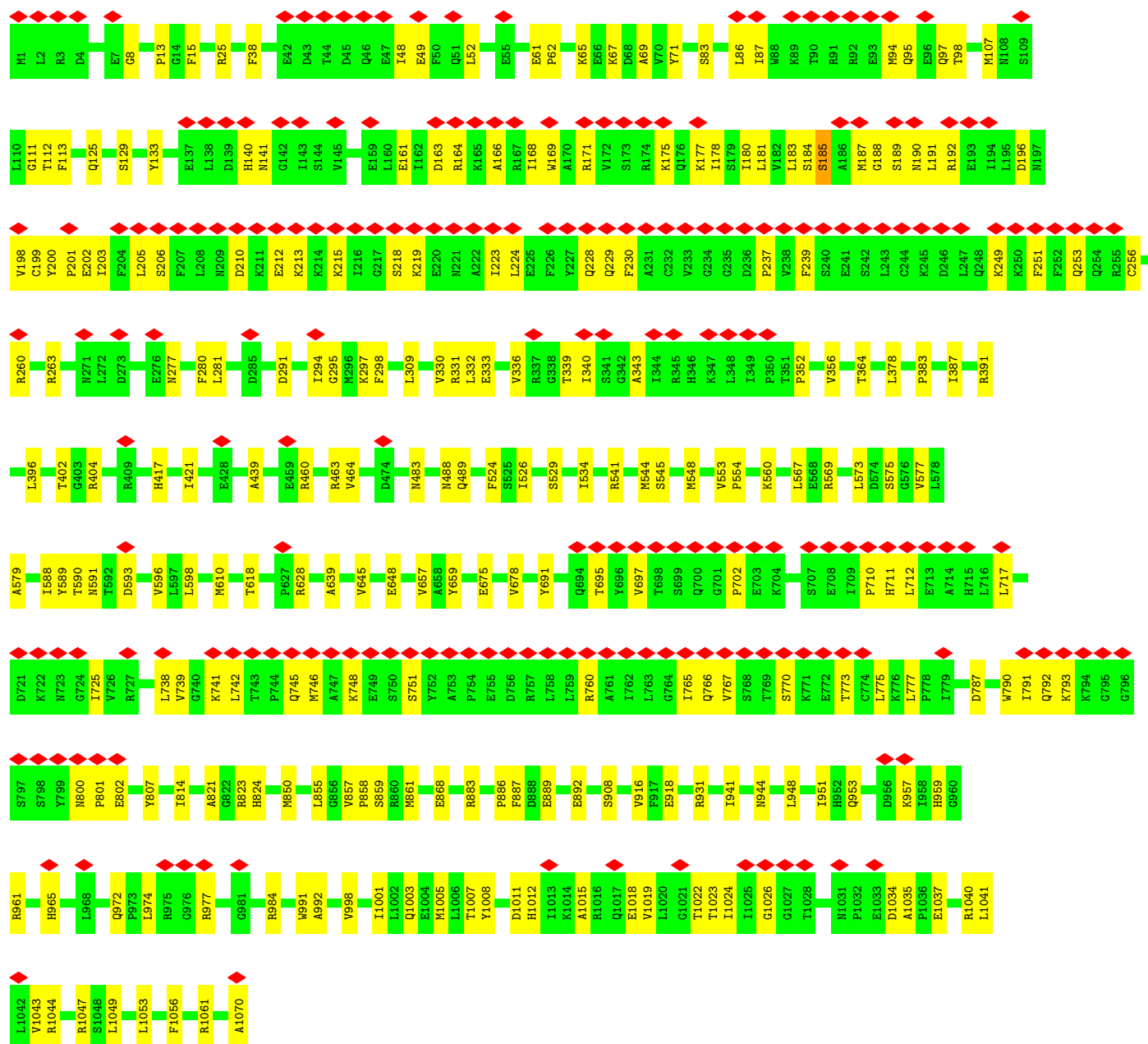


- Molecule 1: DNA-directed RNA polymerase subunit alpha

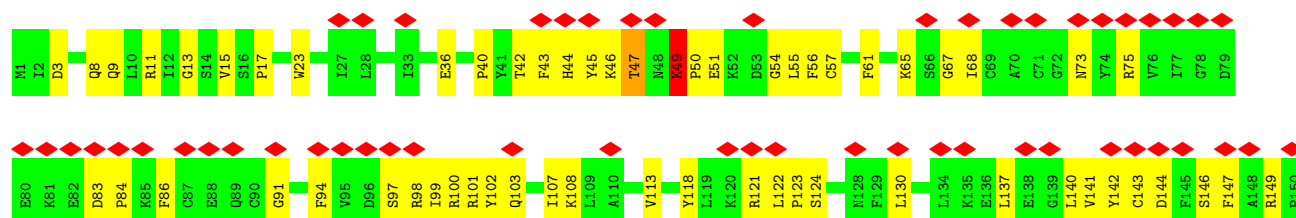


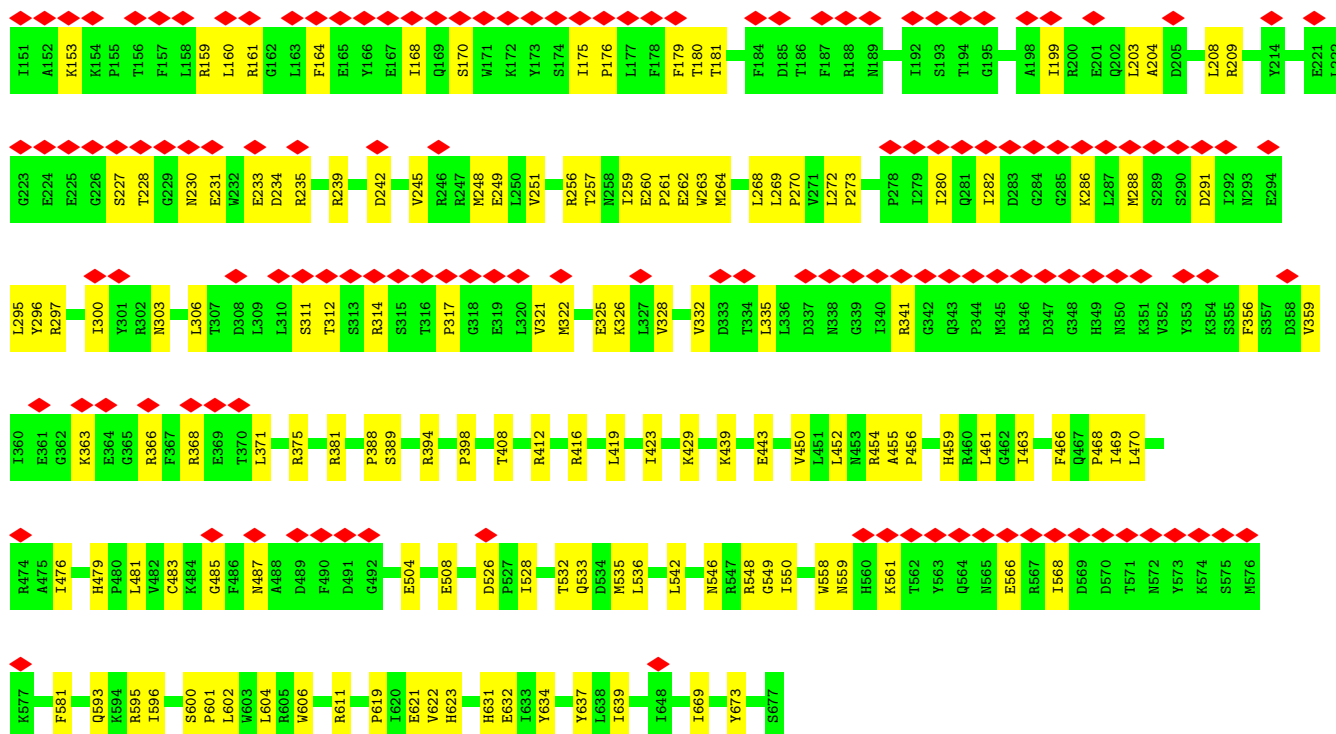
- Molecule 2: DNA-directed RNA polymerase subunit beta



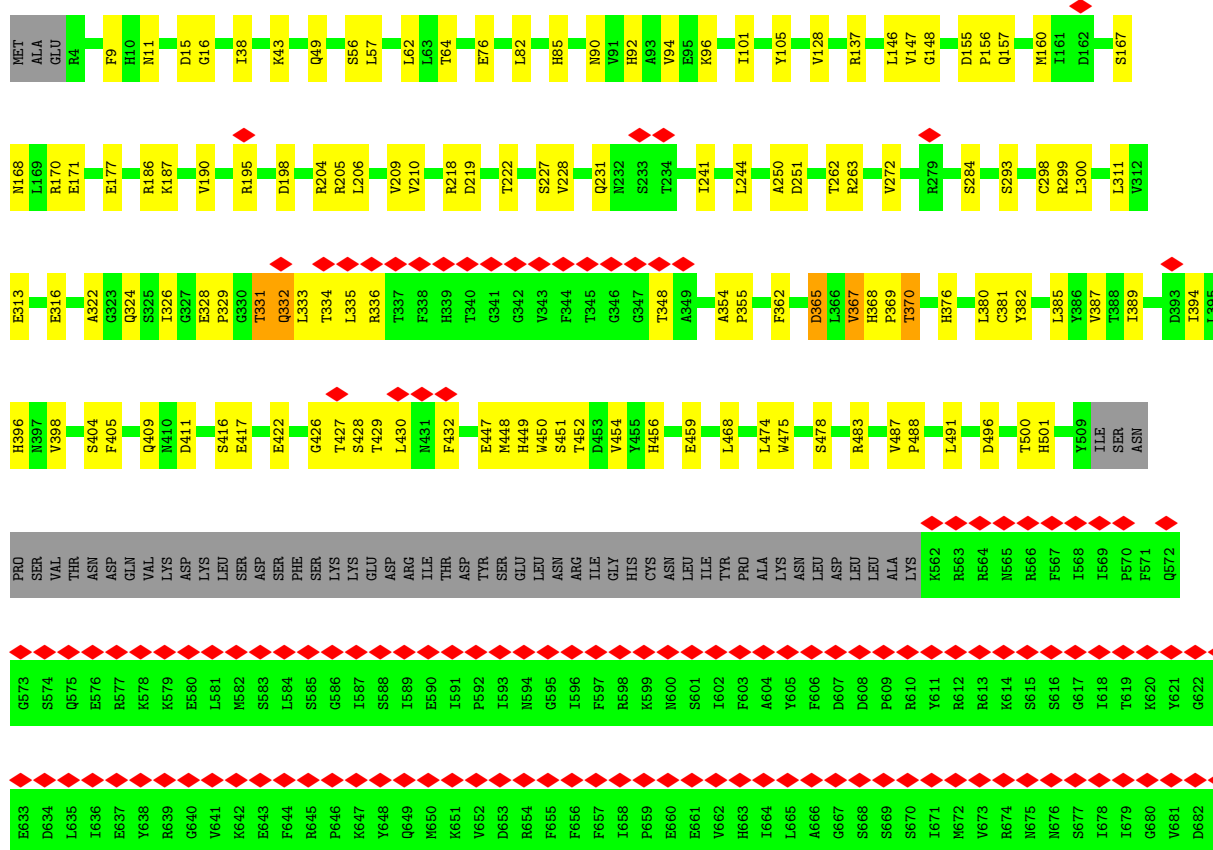
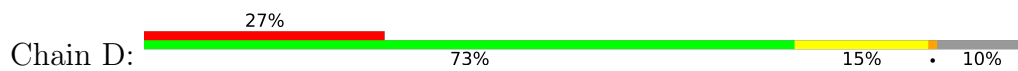


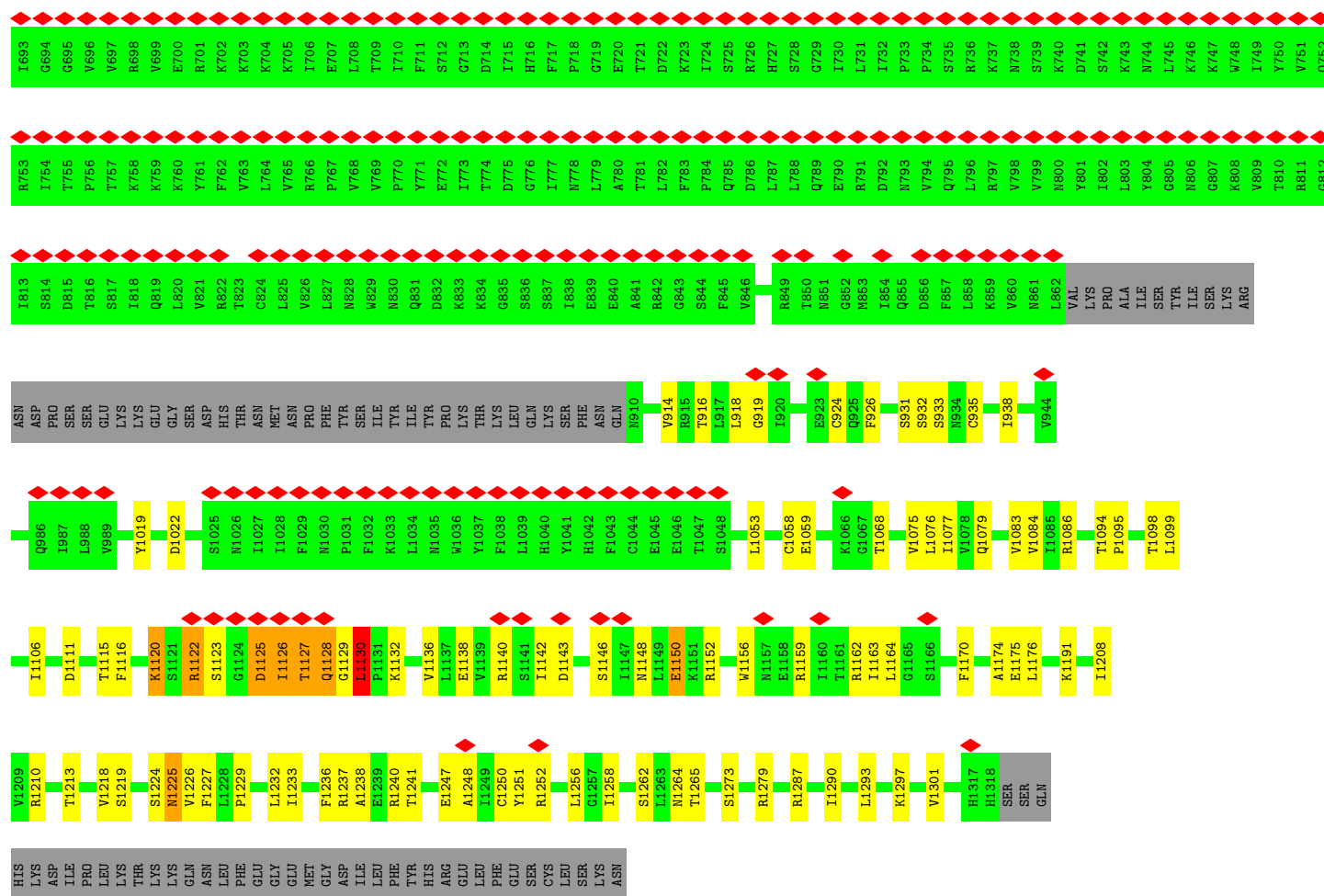
• Molecule 3: DNA-directed RNA polymerase subunit beta'





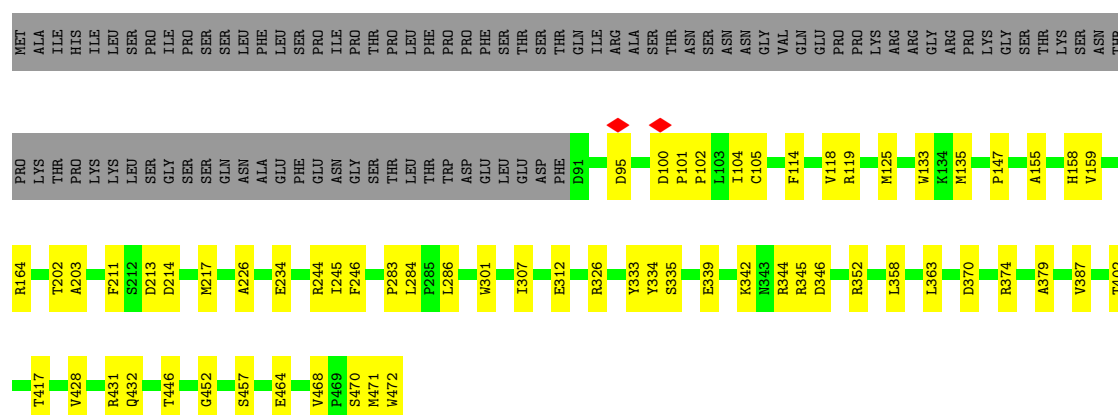
• Molecule 4: DNA-directed RNA polymerase subunit beta”





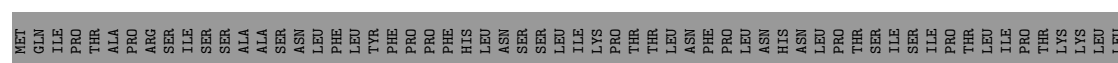
• Molecule 5: Fructokinase-like 1, chloroplastic

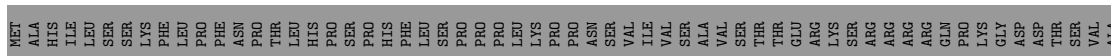
Chain E: 67% 14% 19%

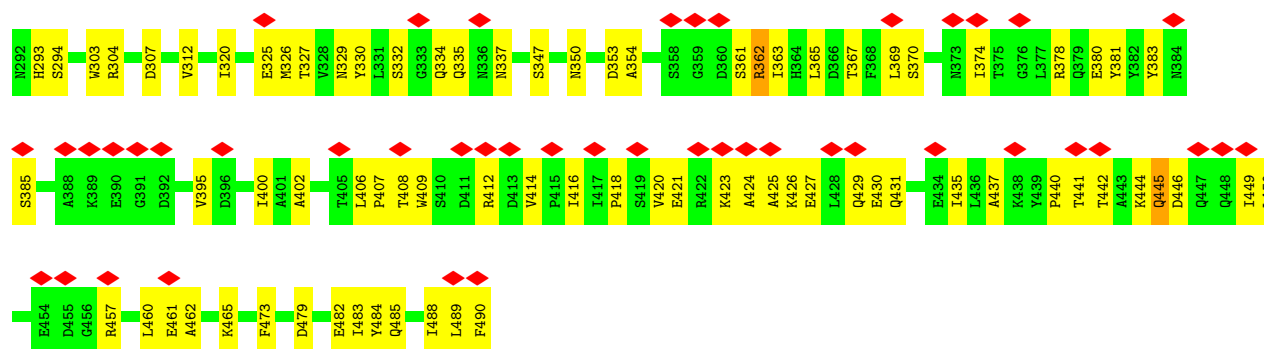


• Molecule 6: Thioredoxin-like protein CITRX, chloroplastic

Chain F: 49% 15% 36%

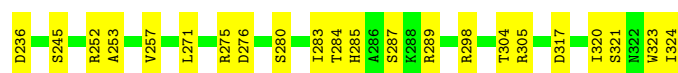
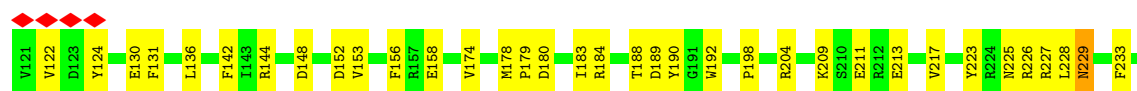
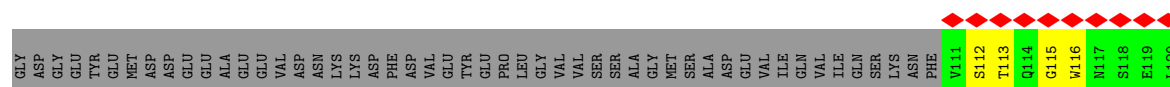
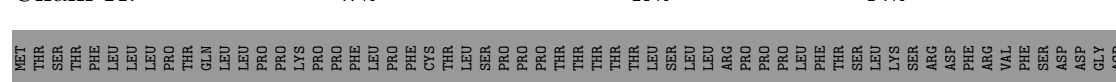






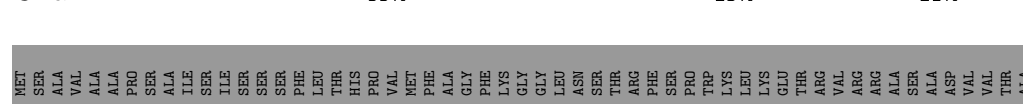
• Molecule 10: pTAC6

Chain K:



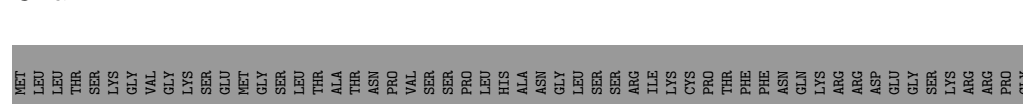
• Molecule 11: superoxide dismutase

Chain L:

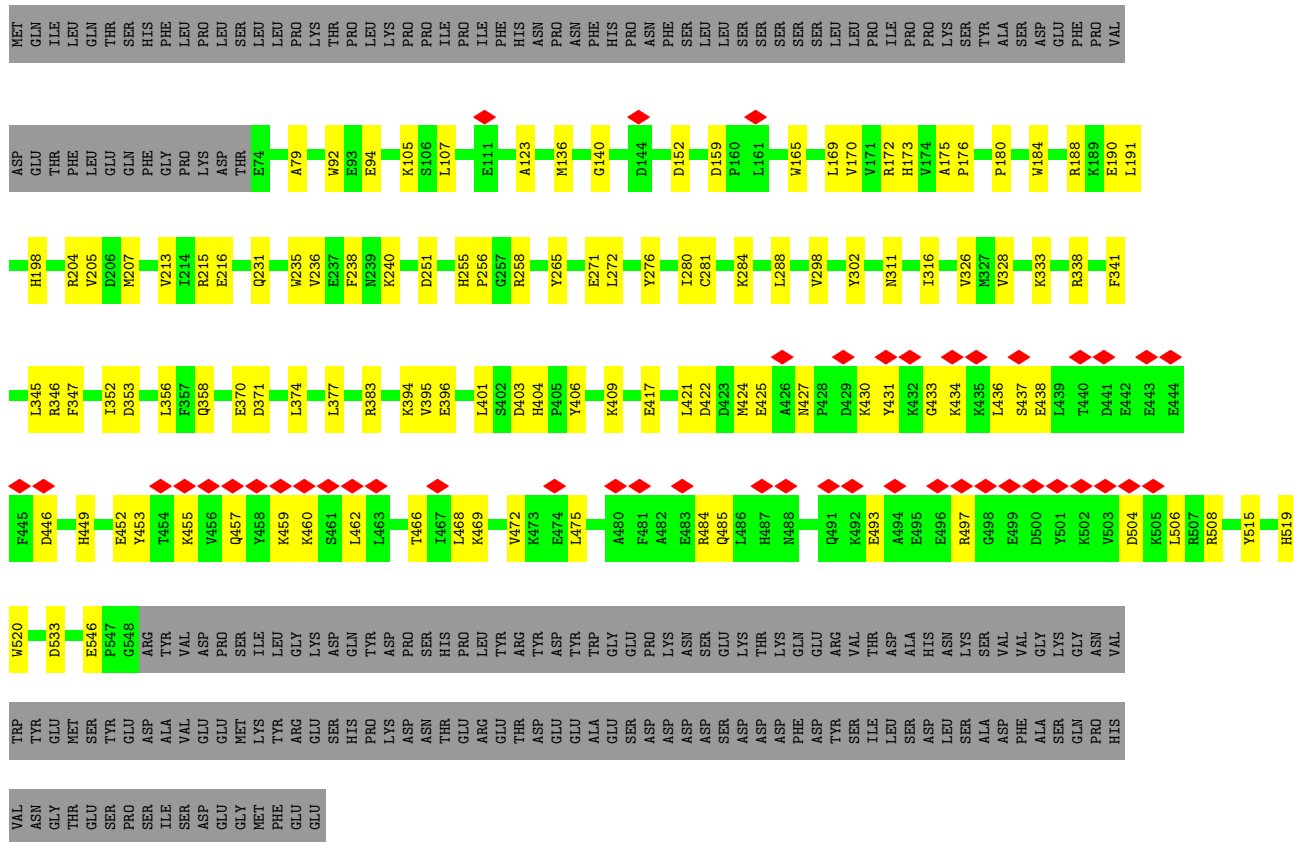


• Molecule 12: superoxide dismutase

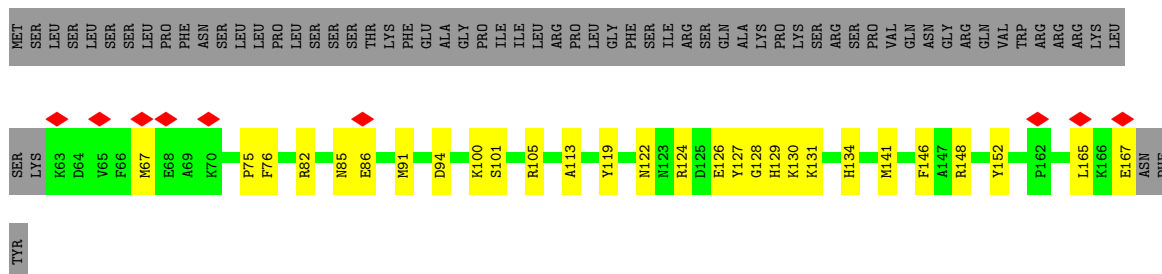
Chain M:



● Molecule 13: Protein PLASTID TRANSCRIPTIONALLY ACTIVE 10

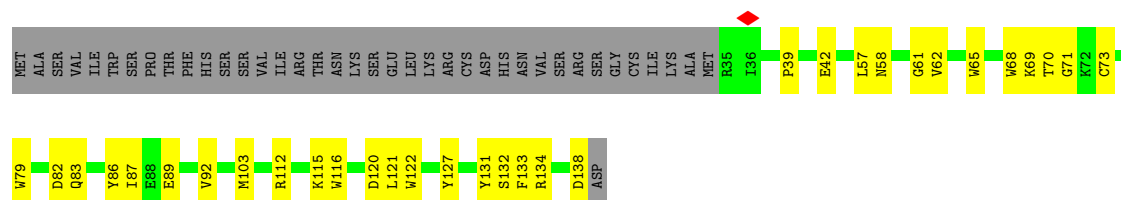


- Molecule 14: Protein PLASTID TRANSCRIPTIONALLY ACTIVE 7

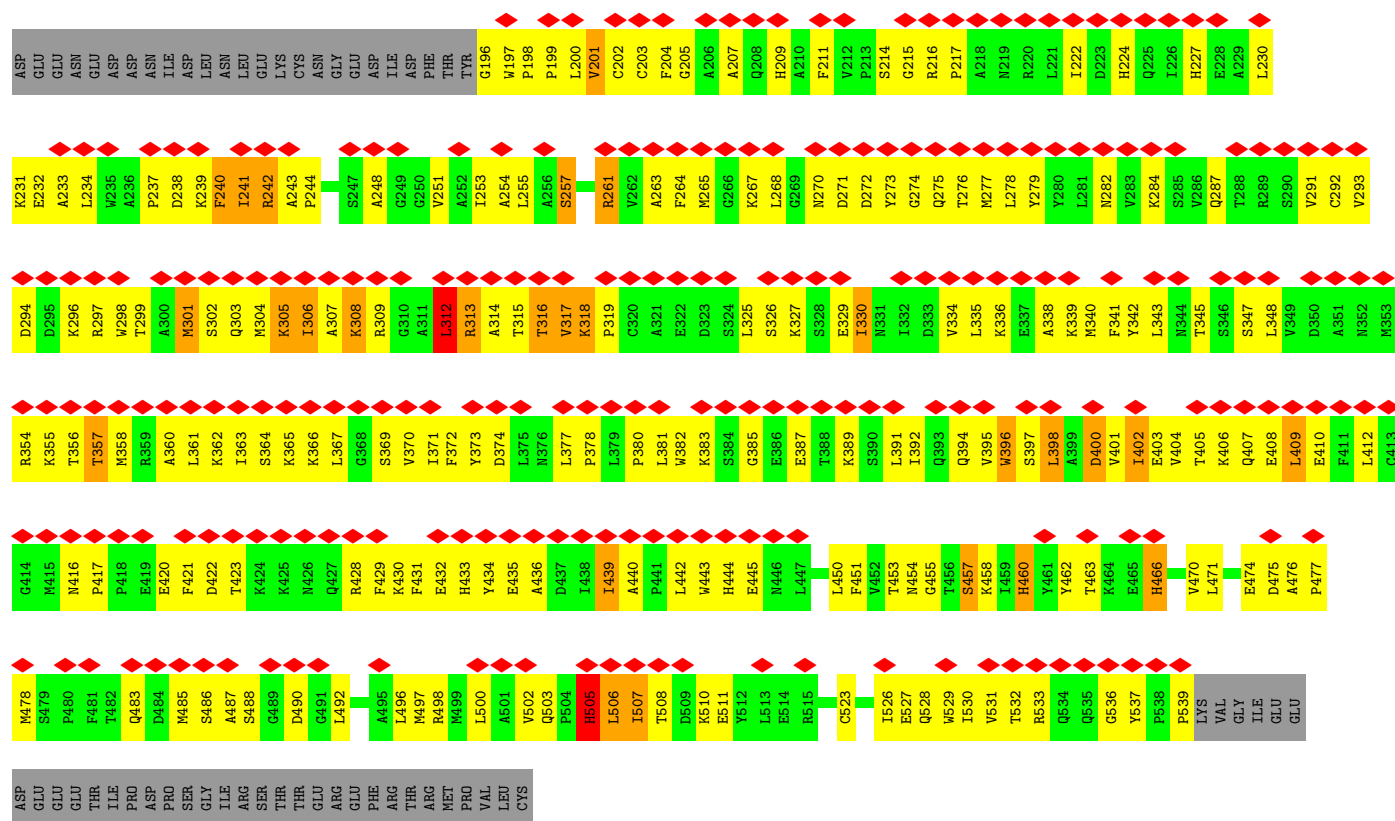
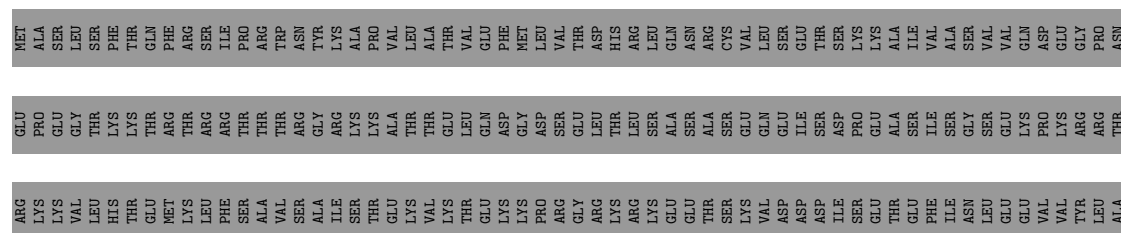
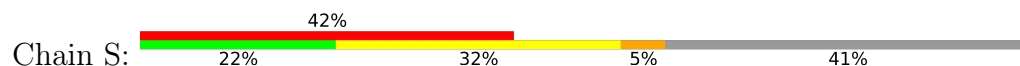


- Molecule 15: pTAC18

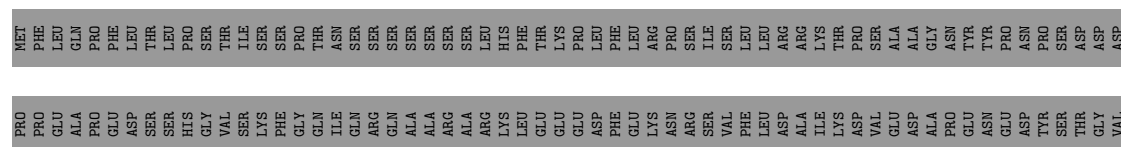




• Molecule 16: Fructokinase-like 2, chloroplastic isoform X2



• Molecule 17: MurE



SER	GLN	P241	R301	T361	V421	I481	S541	T601	L662	A723
GLY	GLY	S242	G302	A362	M422	V482	G542	P602	D663	G724
SER	LEU	F243	A303	A363	E423	M483	L543	D603	I664	K725
GLY	ARG	F244	A304	H364	A424	V484	L544	A604	L665	G726
ASP	VAL	K244	V304	L364	A424	D485	G545	L605	D666	H727
ASP	VAL	M245	A305	L365	S425	D486	R546	S606	D667	E728
LEU	ASP	T246	V306	L366	S426	D487	R547	R607	M668	A729
PHE	VAL	L247	V307	K367	M427	P487	H548	L608	L669	Y730
GLY	ASP	A248	A308	T368	E428	M488	M548	L609	A670	Y731
ASP	GLY	E249	S309	K369	L429	A489	I549	D610	G671	V732
ASP	LYS	L250	K310	Y370	T430	A490	Y550	L609	G671	V732
LYS	LYS	A248	S309	T368	L429	A489	Y550	D610	G671	V732
ASP	GLY	E249	K310	Y370	T430	A490	Y550	D610	G671	V732
ALA	GLU	L251	E311	E371	H431	F491	N551	S611	I672	D733
ILE	PHE	D252	T312	A372	T432	F492	I552	V612	G673	G734
ALA	ASP	E253	D313	K373	R433	I493	L553	R613	W674	G735
GLN	ASP	C254	D314	G374	C434	A494	A554	E614	T675	D736
LYS	ASP	K255	E315	L375	E435	Q495	A555	L615	M676	K736
ARG	ASP	V256	E316	R376	E436	Q496	V556	L616	Q677	K737
LYS	ILE	T257	T317	T377	L437	M497	T557	Q616	D678	E738
GLY	ASP	V257	G318	K378	D438	P498	V558	P617	Y679	F739
LEU	VAL	P258	L318	K379	D439	M499	G559	R618	L680	F740
LYS	VAL	I259	G319	M380	F439	M499	G559	R619	K681	D741
GLY	SER	S260	C320	M380	D440	V500	I560	I620	H682	D742
LEU	GLU	V261	K321	S381	I441	P501	A561	I621	G683	R743
LEU	GLY	V262	A322	S382	A442	V502	V562	T622	E684	R743
LYS	LYS	G263	L323	V383	V443	L503	G563	V623	E684	E744
PRO	ASN	D264	V324	A384	F444	T504	A564	I624	M685	E745
ASN	GLY	L265	I325	Y385	T445	F505	P565	G625	D686	C746
PRO	SER	E266	V326	Y386	T446	A506	L566	S626	Y687	R747
PRO	SER	V267	E327	Y387	L447	L507	E567	G627	P689	E748
LYS	SER	E268	D328	H388	S448	E508	D568	G628	P690	A749
GLU	PHE	I269	T329	G389	R449	M509	I569	E629	L691	L750
ARG	VAL	T270	N330	D390	D450	K510	V570	K630	P692	G751
VAL	ALA	G271	A331	N391	M451	D511	A571	E631	M693	Y752
GLU	SER	I272	A332	K392	S452	A512	G572	R632	G694	V753
VAL	PHE	E273	L333	L393	H453	D513	I573	G633	H695	L754
ALA	ASP	H274	P334	D394	F454	V514	E574	K634	R696	E755
ASP	ASP	D275	A335	F395	Q455	H515	E575	R635	L697	L756
GLU	PHE	S276	L336	P396	Q456	H516	V576	P636	F698	H757
LEU	ASP	R277	A337	E397	M457	L517	D577	M637	L699	Q758
GLY	SER	L278	A338	A398	E458	L518	V578	L638	H700	G760
GLU	GLU	V279	A339	N399	E459	F519	V579	A639	D701	I761
VAL	VAL	N280	F340	P400	E460	E520	P580	K640	I702	R762
ASP	ASP	S281	R341	D401	F461	L521	G581	V641	R703	T763
LEU	SER	G282	R342	A402	R462	S522	R582	A642	R704	S764
GLU	GLU	D283	Y343	V403	V463	L523	C583	D644	V707	E765
ILE	ILE	L284	P344	L404	A464	F524	E584	K645	R708	G766
ASP	ASP	F285	T345	V405	Q465	E525	V585	S646	C709	P767
LEU	PHE	C287	K346	Q406	A466	T526	I586	D647	V710	W768
GLY	ASP	C288	S347	K407	K467	T527	D587	V648	A711	R769
ASP	ASP	V289	S349	M409	L468	V528	E588	T649	A712	L770
LEU	LEU	D290	V350	A410	F469	L529	E589	M650	M713	P771
GLU	GLU	G291	I351	K411	S470	V530	Q590	L651	G714	E772
GLU	GLU	N292	G352	M412	R471	N531	A591	T652	E715	G773
ASP	ASP	L293	I353	L413	M472	T532	F592	S653	E716	H774
LEU	LEU	C294	T354	H414	V473	P533	G593	D654	G717	
ASP	ASP	L295	G355	N415	D474	Q534	V594	N655	D718	
LEU	LEU	I296	T356	Q416	P475	G535	I595	Q656	M719	
ASP	ASP	E297	H357	T417	D476	L536	V596	G657	V720	
GLU	GLU	A298	G358	E418	R477	E537	D597	S658	W721	
ASP	ASP	D299	K359	A419	R479	I539	A599	E659	V722	
LEU	LEU	K300	T360	V420	K480	S540	R600			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	180924	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.697	Depositor
Minimum map value	-1.051	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.23	Depositor
Map size ($\text{\AA}$)	563.2, 563.2, 563.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.18	0/1810	0.38	0/2454
1	O	0.12	0/1796	0.33	0/2435
2	B	0.13	0/8691	0.33	1/11741 (0.0%)
3	C	0.15	0/5636	0.36	2/7617 (0.0%)
4	D	0.24	0/8497	0.48	4/11580 (0.0%)
5	E	0.12	0/3154	0.30	0/4268
6	F	0.12	0/956	0.30	0/1292
6	R	0.23	0/956	0.57	0/1292
7	G	0.14	0/2062	0.34	0/2781
8	H	0.29	0/4745	0.49	1/6417 (0.0%)
9	I	0.13	0/3456	0.39	0/4675
10	K	0.12	0/1849	0.32	0/2507
11	L	0.28	0/1877	0.47	2/2558 (0.1%)
12	M	0.11	0/1820	0.30	0/2478
13	N	0.11	0/4139	0.28	0/5582
14	P	0.14	0/857	0.41	0/1152
15	Q	0.18	0/932	0.52	0/1261
16	S	0.36	0/2756	0.86	8/3731 (0.2%)
17	J	0.14	0/4293	0.38	0/5820
All	All	0.19	0/60282	0.42	18/81641 (0.0%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	333	LEU	N-CA-C	-10.90	99.79	112.87
4	D	332	GLN	N-CA-C	-10.65	98.95	112.90
2	B	185	SER	N-CA-C	-8.75	102.74	112.72
4	D	1130	LEU	CA-C-N	-8.14	110.56	119.19
4	D	1130	LEU	C-N-CA	-8.14	110.56	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	334	TYR	N-CA-C	-8.03	98.64	110.52
3	C	49	LYS	N-CA-C	-7.40	98.78	110.10
16	S	241	ILE	N-CA-C	-7.33	105.69	112.43
16	S	257	SER	N-CA-C	-7.30	103.02	110.97
16	S	505	HIS	N-CA-C	-7.12	101.79	112.54
16	S	439	ILE	N-CA-C	-6.46	106.94	113.47
16	S	242	ARG	N-CA-C	-6.38	105.48	113.20
16	S	240	PHE	N-CA-C	-6.34	104.59	112.90
11	L	205	ASP	CA-C-N	-6.18	113.11	121.71
11	L	205	ASP	C-N-CA	-6.18	113.11	121.71
16	S	312	LEU	N-CA-C	6.04	117.54	110.41
16	S	409	LEU	N-CA-C	-5.45	107.64	114.56
3	C	45	TYR	N-CA-C	-5.07	106.35	112.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1775	0	1783	61	0
1	O	1761	0	1772	44	0
2	B	8517	0	8571	177	0
3	C	5507	0	5546	164	0
4	D	8374	0	7240	200	0
5	E	3079	0	2992	46	0
6	F	940	0	934	21	0
6	R	940	0	934	95	0
7	G	2009	0	1967	58	0
8	H	4653	0	4517	160	0
9	I	3373	0	3321	98	0
10	K	1803	0	1752	53	0
11	L	1817	0	1720	54	0
12	M	1763	0	1698	34	0
13	N	4032	0	3891	88	0
14	P	840	0	804	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	Q	902	0	870	23	0
16	S	2695	0	2712	293	0
17	J	4218	0	4148	166	0
18	L	1	0	0	0	0
All	All	58999	0	57172	1653	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 14.

All (1653) 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)
6:R:142:MET:HE1	16:S:314:ALA:HB3	1.23	1.15
8:H:96:MET:HB2	8:H:101:LEU:HB2	1.33	1.05
6:R:160:ASP:HA	16:S:305:LYS:HB3	1.42	1.00
16:S:270:ASN:O	16:S:275:GLN:HG3	1.63	0.98
16:S:304:MET:HE1	16:S:316:THR:HA	1.43	0.98
16:S:421:PHE:HB2	16:S:433:HIS:HB3	1.52	0.91
9:I:445:GLN:HG2	9:I:449:ILE:HB	1.55	0.89
3:C:17:PRO:HB3	3:C:268:LEU:HD23	1.56	0.87
8:H:70:ARG:HH22	8:H:104:GLY:H	1.23	0.86
6:R:103:TRP:CE2	16:S:241:ILE:HG13	2.11	0.86
16:S:304:MET:CE	16:S:316:THR:HA	2.06	0.85
8:H:430:ASP:HB3	17:J:673:GLY:H	1.41	0.84
6:R:143:GLN:CG	16:S:315:THR:HA	2.08	0.82
8:H:70:ARG:NH2	8:H:104:GLY:H	1.76	0.82
5:E:446:THR:HG21	5:E:452:GLY:HA3	1.61	0.82
4:D:432:PHE:HB2	4:D:1123:SER:HB3	1.60	0.81
8:H:404:LEU:HD13	8:H:803:GLY:HA3	1.59	0.81
16:S:304:MET:HE1	16:S:316:THR:CA	2.11	0.81
6:R:142:MET:CE	16:S:314:ALA:HB3	2.09	0.80
16:S:385:GLY:HA2	16:S:412:LEU:HD23	1.64	0.79
1:A:60:THR:HG21	1:A:98:SER:HB3	1.64	0.79
16:S:317:VAL:HG22	16:S:318:LYS:HG3	1.65	0.79
8:H:74:MET:HG3	9:I:489:LEU:HD22	1.66	0.78
3:C:54:GLY:H	3:C:57:CYS:HB2	1.47	0.78
16:S:270:ASN:H	16:S:274:GLY:HA3	1.49	0.78
16:S:199:PRO:HB3	16:S:339:LYS:CG	2.14	0.77
4:D:262:THR:HB	9:I:143:MET:HE1	1.66	0.77
6:R:143:GLN:HG2	16:S:315:THR:HA	1.65	0.77
2:B:859:SER:HB3	4:D:137:ARG:HD3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:758:ALA:HA	8:H:763:TRP:HB3	1.67	0.77
16:S:251:VAL:HG22	16:S:490:ASP:HA	1.65	0.76
4:D:449:HIS:HE1	13:N:92:TRP:HD1	1.33	0.76
2:B:589:TYR:HB3	2:B:596:VAL:HB	1.67	0.75
16:S:354:ARG:HB3	16:S:358:MET:HE1	1.67	0.75
3:C:389:SER:HB2	14:P:167:GLU:OE2	1.86	0.75
11:L:141:LYS:HB2	11:L:259:SER:HB3	1.67	0.75
17:J:640:LYS:HB2	17:J:672:ILE:HG21	1.68	0.75
6:R:88:ARG:NH1	6:R:157:PRO:O	2.20	0.75
2:B:941:ILE:HG22	4:D:56:SER:HB3	1.69	0.74
12:M:242:PHE:HA	12:M:246:LEU:HB2	1.68	0.74
16:S:389:LYS:HG2	16:S:396:TRP:CZ2	2.22	0.74
13:N:452:GLU:HG3	13:N:468:LEU:HA	1.70	0.74
17:J:306:VAL:HG11	17:J:318:LEU:HD12	1.69	0.74
8:H:155:ARG:HB3	8:H:158:ARG:HB2	1.69	0.74
16:S:317:VAL:HG13	16:S:318:LYS:H	1.53	0.73
9:I:445:GLN:HG3	9:I:446:ASP:H	1.53	0.73
16:S:345:THR:HG22	16:S:378:PRO:HD2	1.68	0.73
3:C:161:ARG:HH12	17:J:684:GLU:HG2	1.53	0.73
8:H:732:PHE:CD2	8:H:743:MET:HE3	2.24	0.73
16:S:478:MET:HE1	16:S:529:TRP:HB2	1.71	0.73
7:G:257:VAL:HG13	10:K:323:TRP:HE1	1.53	0.73
3:C:50:PRO:HB3	3:C:56:PHE:HB2	1.72	0.72
9:I:230:CYS:HB2	9:I:257:MET:HE1	1.71	0.72
1:O:62:ILE:HG21	1:O:149:LEU:HD12	1.72	0.72
16:S:308:LYS:HE2	16:S:312:LEU:HA	1.71	0.72
2:B:107:MET:HE3	2:B:111:GLY:HA2	1.70	0.72
3:C:669:ILE:HD11	4:D:38:ILE:HD11	1.70	0.72
16:S:270:ASN:ND2	16:S:294:ASP:O	2.21	0.72
17:J:596:VAL:HG23	17:J:723:ALA:HA	1.72	0.72
11:L:196:ASN:HB3	11:L:199:ASN:ND2	2.04	0.71
1:A:39:LYS:O	1:O:155:ARG:NH2	2.23	0.71
9:I:334:GLN:OE1	9:I:335:GLN:N	2.22	0.71
1:A:68:GLU:HG2	1:A:69:LYS:HG2	1.72	0.71
16:S:304:MET:HE2	16:S:304:MET:HA	1.72	0.71
3:C:40:PRO:HB2	3:C:297:ARG:HG3	1.71	0.70
1:A:228:PRO:HG3	1:O:13:LEU:HB3	1.74	0.70
3:C:108:LYS:O	3:C:303:ASN:ND2	2.25	0.70
11:L:197:ALA:C	11:L:199:ASN:H	1.99	0.70
15:Q:70:THR:OG1	15:Q:73:CYS:SG	2.50	0.70
1:A:220:ARG:HE	16:S:477:PRO:HD2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:332:GLN:C	4:D:334:THR:N	2.48	0.70
17:J:329:THR:O	17:J:333:LEU:HB2	1.91	0.70
2:B:760:ARG:HA	2:B:765:ILE:HB	1.73	0.70
16:S:199:PRO:HB3	16:S:339:LYS:HG3	1.71	0.70
4:D:1152:ARG:NH1	8:H:732:PHE:O	2.25	0.70
9:I:114:LYS:HG2	9:I:115:ASP:H	1.55	0.70
7:G:188:LEU:HB3	7:G:193:LYS:HG2	1.73	0.70
17:J:411:LYS:O	17:J:415:ASN:HB2	1.90	0.70
8:H:743:MET:HB3	8:H:746:ARG:HE	1.56	0.69
2:B:751:SER:HB2	3:C:65:LYS:HE2	1.74	0.69
1:A:112:GLY:HA3	1:A:142:PRO:HA	1.74	0.69
17:J:481:ILE:HD11	17:J:561:ALA:HB2	1.74	0.69
11:L:177:GLN:O	11:L:246:ARG:NH1	2.23	0.69
8:H:113:VAL:HG11	9:I:416:ILE:HA	1.75	0.68
17:J:387:VAL:HA	17:J:412:MET:HE1	1.75	0.68
2:B:161:GLU:HB3	2:B:169:TRP:HE1	1.57	0.68
3:C:459:HIS:NE2	3:C:485:GLY:O	2.26	0.68
1:A:123:LEU:HD11	1:A:129:ILE:HG23	1.76	0.68
13:N:506:LEU:HD12	13:N:508:ARG:H	1.58	0.68
16:S:370:VAL:HG13	16:S:400:ASP:CG	2.19	0.68
11:L:196:ASN:HB3	11:L:199:ASN:CG	2.18	0.67
16:S:268:LEU:HA	16:S:277:MET:HE2	1.76	0.67
3:C:43:PHE:HA	3:C:50:PRO:HA	1.77	0.67
3:C:86:PHE:HB3	3:C:91:GLY:HA2	1.77	0.67
3:C:261:PRO:O	3:C:264:MET:HG3	1.94	0.67
8:H:801:THR:HA	8:H:805:CYS:HB3	1.77	0.67
16:S:341:PHE:HB3	16:S:371:ILE:HG23	1.74	0.67
16:S:370:VAL:HG13	16:S:400:ASP:HB2	1.77	0.67
2:B:1023:THR:O	3:C:412:ARG:NH2	2.21	0.67
5:E:104:ILE:HD11	5:E:417:THR:HG21	1.77	0.67
2:B:191:LEU:O	2:B:192:ARG:NH1	2.27	0.67
4:D:62:LEU:HB2	4:D:170:ARG:HD3	1.77	0.67
8:H:843:ILE:O	8:H:844:ILE:C	2.38	0.67
16:S:297:ARG:HG3	16:S:318:LYS:HE3	1.77	0.67
8:H:756:THR:HA	8:H:759:ASP:HB3	1.75	0.67
2:B:554:PRO:HD2	2:B:618:THR:HG21	1.76	0.66
3:C:416:ARG:HH12	14:P:128:GLY:HA3	1.60	0.66
4:D:387:VAL:HG23	4:D:398:VAL:HB	1.77	0.66
7:G:217:THR:HG23	7:G:220:GLU:OE1	1.96	0.66
1:O:14:GLN:H	1:O:35:SER:HB3	1.60	0.66
11:L:197:ALA:HB3	13:N:520:TRP:CD1	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:343:LEU:HD12	16:S:373:TYR:HE1	1.60	0.66
3:C:209:ARG:HB3	8:H:470:VAL:HB	1.76	0.66
8:H:74:MET:HE3	8:H:74:MET:HA	1.76	0.66
10:K:275:ARG:HB2	10:K:280:SER:HB3	1.77	0.66
16:S:340:MET:HE1	16:S:401:VAL:HB	1.78	0.66
17:J:307:VAL:HG22	17:J:325:ILE:HG12	1.77	0.66
5:E:213:ASP:OD1	5:E:214:ASP:N	2.28	0.66
3:C:593:GLN:NE2	1:O:156:GLY:O	2.27	0.66
5:E:339:GLU:OE1	5:E:344:ARG:NH1	2.28	0.66
13:N:455:LYS:HD2	13:N:462:LEU:HD23	1.78	0.66
17:J:380:MET:HB3	17:J:422:MET:HG2	1.78	0.66
4:D:241:ILE:HG12	4:D:272:VAL:HG11	1.79	0.65
6:R:100:TYR:HB2	6:R:104:CYS:SG	2.36	0.65
17:J:669:LEU:HD21	17:J:674:TRP:HB3	1.78	0.65
17:J:516:PRO:HA	17:J:530:VAL:HA	1.78	0.65
2:B:1026:GLY:HA3	14:P:124:ARG:CZ	2.27	0.65
4:D:474:LEU:HG	4:D:1099:LEU:HD21	1.78	0.65
4:D:1224:SER:OG	4:D:1225:ASN:N	2.28	0.65
16:S:374:ASP:HA	16:S:403:GLU:HB2	1.79	0.65
1:O:106:ALA:HB3	1:O:149:LEU:HB2	1.79	0.65
2:B:402:THR:HG23	2:B:404:ARG:H	1.62	0.65
3:C:412:ARG:HH11	14:P:124:ARG:HH22	1.45	0.65
4:D:478:SER:O	4:D:1086:ARG:NH1	2.29	0.65
6:R:143:GLN:HG3	16:S:315:THR:HA	1.77	0.64
16:S:239:LYS:HA	16:S:242:ARG:CB	2.27	0.64
2:B:553:VAL:HG22	2:B:951:ILE:HD12	1.79	0.64
8:H:314:HIS:CG	8:H:756:THR:HG21	2.32	0.64
8:H:430:ASP:HB3	17:J:673:GLY:N	2.13	0.64
9:I:329:ASN:ND2	9:I:332:SER:OG	2.30	0.64
13:N:493:GLU:O	13:N:497:ARG:NH2	2.31	0.64
1:A:220:ARG:NH2	16:S:478:MET:SD	2.71	0.64
3:C:394:ARG:NH1	14:P:86:GLU:O	2.26	0.64
8:H:732:PHE:HD2	8:H:743:MET:HE3	1.61	0.64
6:R:78:LEU:HD13	6:R:128:VAL:HG11	1.79	0.64
2:B:331:ARG:NH1	2:B:364:THR:OG1	2.30	0.64
4:D:57:LEU:HD11	4:D:128:VAL:HG22	1.80	0.64
16:S:304:MET:HE1	16:S:316:THR:N	2.13	0.64
6:R:95:LEU:HG	6:R:153:ILE:HB	1.78	0.64
2:B:15:PHE:HB2	2:B:387:ILE:HD12	1.78	0.64
2:B:332:LEU:O	2:B:336:VAL:HG23	1.98	0.64
11:L:85:HIS:NE2	12:M:233:ASN:OD1	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:416:ARG:NH2	14:P:127:TYR:O	2.31	0.64
4:D:355:PRO:HD2	4:D:389:ILE:HD12	1.78	0.64
8:H:485:ARG:HD3	8:H:485:ARG:C	2.22	0.64
8:H:345:ARG:O	8:H:348:LYS:HB3	1.97	0.64
16:S:273:TYR:HB2	16:S:299:THR:HB	1.79	0.64
17:J:367:LYS:HD3	17:J:379:MET:HE3	1.78	0.64
2:B:417:HIS:HB3	2:B:421:ILE:HB	1.79	0.64
4:D:148:GLY:N	4:D:168:ASN:OD1	2.31	0.64
16:S:394:GLN:O	16:S:398:LEU:HB2	1.98	0.64
2:B:725:ILE:HG23	2:B:739:VAL:HG22	1.79	0.64
1:A:227:ILE:HD11	16:S:529:TRP:CH2	2.34	0.63
11:L:59:LEU:HD22	11:L:87:ARG:HE	1.64	0.63
6:R:143:GLN:HE21	16:S:314:ALA:C	2.06	0.63
11:L:186:VAL:HG12	11:L:227:PRO:HA	1.79	0.63
1:O:43:ASP:O	1:O:47:ILE:HG13	1.99	0.63
6:R:88:ARG:HH22	16:S:306:ILE:HG21	1.62	0.63
6:R:136:TYR:OH	16:S:383:LYS:NZ	2.27	0.63
6:R:141:ASP:O	16:S:313:ARG:HA	1.97	0.63
4:D:332:GLN:C	4:D:334:THR:H	2.06	0.63
4:D:432:PHE:HB2	4:D:1123:SER:CB	2.26	0.63
16:S:302:SER:O	16:S:319:PRO:HA	1.98	0.63
17:J:640:LYS:HD3	17:J:672:ILE:HD12	1.81	0.63
2:B:48:ILE:HG21	2:B:340:ILE:HD11	1.81	0.63
3:C:533:GLN:OE1	4:D:137:ARG:NH2	2.27	0.63
16:S:440:ALA:HA	16:S:443:TRP:CD1	2.34	0.63
17:J:518:LYS:HB3	17:J:529:LEU:HB2	1.80	0.63
4:D:168:ASN:HB2	4:D:171:GLU:HG3	1.80	0.63
6:R:143:GLN:HG2	16:S:314:ALA:O	1.99	0.63
6:R:163:ARG:HD2	16:S:304:MET:HB2	1.79	0.63
17:J:369:MET:HA	17:J:572:GLY:HA3	1.80	0.62
7:G:194:ASP:OD1	7:G:199:ARG:NH1	2.32	0.62
10:K:148:ASP:OD2	10:K:152:ASP:N	2.28	0.62
10:K:131:PHE:HD2	10:K:142:PHE:HB3	1.64	0.62
2:B:260:ARG:HH12	2:B:277:ASN:HA	1.64	0.62
8:H:758:ALA:CA	8:H:763:TRP:HB3	2.30	0.62
16:S:203:CYS:HB3	16:S:248:ALA:HB1	1.80	0.62
3:C:532:THR:HG22	3:C:533:GLN:H	1.64	0.62
4:D:82:LEU:HD21	4:D:96:LYS:HA	1.82	0.62
8:H:319:PRO:HG2	8:H:761:TRP:HD1	1.65	0.62
13:N:175:ALA:O	13:N:198:HIS:NE2	2.31	0.62
13:N:180:PRO:HD3	13:N:191:LEU:HD21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:GLU:OE1	1:A:90:ASN:ND2	2.32	0.62
6:R:163:ARG:H	16:S:303:GLN:HA	1.64	0.62
16:S:402:ILE:HG22	16:S:450:LEU:HB2	1.81	0.62
1:A:220:ARG:HG2	16:S:477:PRO:HG2	1.82	0.62
3:C:296:TYR:O	3:C:300:ILE:HG13	1.99	0.62
3:C:257:THR:HG23	3:C:259:ILE:H	1.63	0.62
7:G:208:VAL:HG23	7:G:209:LYS:H	1.64	0.62
1:O:58:GLU:HA	1:O:154:ASN:O	2.00	0.62
6:R:146:GLY:HA3	16:S:211:PHE:CZ	2.35	0.62
16:S:239:LYS:HA	16:S:242:ARG:HB2	1.82	0.62
17:J:650:MET:HE3	17:J:651:LEU:H	1.64	0.62
16:S:200:LEU:H	16:S:338:ALA:HA	1.65	0.62
8:H:483:LYS:O	8:H:487:ARG:NH1	2.32	0.62
2:B:1026:GLY:HA3	14:P:124:ARG:NH2	2.15	0.61
6:R:160:ASP:HA	16:S:305:LYS:CB	2.25	0.61
17:J:516:PRO:HB3	17:J:528:VAL:HG13	1.82	0.61
2:B:972:GLN:NE2	2:B:1011:ASP:OD1	2.33	0.61
3:C:621:GLU:OE1	10:K:275:ARG:NH1	2.32	0.61
4:D:205:ARG:NH1	4:D:1138:GLU:OE2	2.33	0.61
8:H:376:ARG:HD2	8:H:471:GLU:HG3	1.82	0.61
13:N:105:LYS:HE3	13:N:123:ALA:HB2	1.83	0.61
4:D:328:GLU:HB3	4:D:329:PRO:HD3	1.82	0.61
8:H:758:ALA:CB	8:H:763:TRP:HB3	2.30	0.61
16:S:360:ALA:O	16:S:364:SER:N	2.33	0.61
2:B:488:ASN:OD1	2:B:489:GLN:N	2.32	0.61
16:S:392:ILE:O	16:S:394:GLN:N	2.34	0.61
16:S:487:ALA:HB1	16:S:490:ASP:HB2	1.83	0.61
9:I:88:ILE:HG13	14:P:67:MET:HE1	1.83	0.61
17:J:363:ALA:HB1	17:J:379:MET:HE1	1.82	0.61
17:J:719:MET:SD	17:J:721:VAL:HG23	2.40	0.61
4:D:432:PHE:CB	4:D:1123:SER:HB3	2.31	0.61
8:H:785:LEU:HA	8:H:788:LYS:HB3	1.82	0.61
12:M:104:ASP:OD2	13:N:188:ARG:NH2	2.32	0.61
13:N:417:GLU:HG3	13:N:475:LEU:HD11	1.83	0.61
3:C:168:ILE:HG22	3:C:170:SER:H	1.65	0.61
4:D:474:LEU:HD11	4:D:1099:LEU:HD11	1.81	0.61
2:B:959:HIS:CD2	2:B:977:ARG:HG2	2.35	0.60
8:H:63:SER:OG	8:H:64:ALA:N	2.32	0.60
16:S:298:TRP:CB	16:S:301:MET:HG3	2.30	0.60
6:F:104:CYS:HB2	6:F:147:LEU:HD13	1.82	0.60
8:H:282:GLU:HA	8:H:285:ASN:HD22	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:203:LEU:HB2	9:I:223:MET:HE3	1.82	0.60
6:R:103:TRP:HZ3	6:R:147:LEU:HD11	1.66	0.60
3:C:282:ILE:HD11	3:C:288:MET:HG3	1.84	0.60
3:C:673:TYR:OH	9:I:95:ARG:NH1	2.35	0.60
4:D:426:GLY:O	4:D:427:THR:OG1	2.15	0.60
17:J:526:THR:HB	17:J:541:SER:O	2.02	0.60
4:D:1126:ILE:HG23	4:D:1127:THR:H	1.65	0.60
8:H:430:ASP:OD2	17:J:671:GLY:N	2.34	0.60
17:J:273:GLU:HA	17:J:403:VAL:HG11	1.84	0.60
17:J:646:SER:O	17:J:695:HIS:ND1	2.35	0.60
2:B:931:ARG:O	1:O:47:ILE:HD13	2.01	0.60
5:E:464:GLU:OE1	7:G:238:ARG:NH1	2.33	0.60
4:D:64:THR:OG1	4:D:170:ARG:NH2	2.34	0.60
16:S:254:ALA:HA	16:S:537:TYR:HB3	1.83	0.60
3:C:122:LEU:HB2	3:C:123:PRO:HD2	1.84	0.60
9:I:363:ILE:O	9:I:409:TRP:N	2.33	0.60
17:J:635:ARG:HG2	17:J:636:PRO:HD3	1.82	0.60
17:J:691:LEU:O	17:J:692:PRO:C	2.45	0.60
3:C:256:ARG:NH2	8:H:294:ALA:O	2.35	0.60
3:C:282:ILE:HB	3:C:286:LYS:HB2	1.81	0.60
4:D:329:PRO:O	4:D:332:GLN:HG2	2.01	0.60
4:D:1143:ASP:HA	4:D:1146:SER:HB2	1.84	0.60
13:N:404:HIS:HD2	13:N:519:HIS:HB2	1.66	0.60
5:E:431:ARG:NH2	5:E:470:SER:O	2.34	0.60
2:B:787:ASP:HB3	2:B:807:TYR:HD2	1.66	0.59
3:C:99:ILE:HD11	3:C:103:GLN:HG2	1.84	0.59
5:E:470:SER:OG	7:G:231:GLU:OE1	2.20	0.59
1:A:224:ASP:CG	16:S:478:MET:HB3	2.26	0.59
4:D:405:PHE:HB2	4:D:422:GLU:HB3	1.83	0.59
9:I:215:GLN:HG3	9:I:444:LYS:HZ3	1.67	0.59
6:F:94:PRO:HB3	6:F:181:MET:HG2	1.83	0.59
11:L:252:ILE:HA	11:L:255:GLU:HB2	1.83	0.59
16:S:466:HIS:HD2	16:S:510:LYS:HD3	1.67	0.59
16:S:276:THR:HA	16:S:279:TYR:HD2	1.68	0.59
2:B:163:ASP:H	2:B:166:ALA:HB3	1.68	0.59
2:B:742:LEU:HD22	2:B:770:SER:HB2	1.85	0.59
3:C:381:ARG:HH12	3:C:455:ALA:HB2	1.66	0.59
4:D:316:GLU:OE2	14:P:105:ARG:NH2	2.35	0.59
13:N:424:MET:HG3	13:N:434:LYS:HG3	1.84	0.59
16:S:364:SER:OG	16:S:365:LYS:NZ	2.30	0.59
3:C:311:SER:O	3:C:314:ARG:NH1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:427:GLU:HA	9:I:430:GLU:HB2	1.84	0.59
16:S:204:PHE:HB3	16:S:343:LEU:HD21	1.85	0.59
3:C:306:LEU:HD22	3:C:328:VAL:HG21	1.84	0.59
17:J:267:VAL:HG23	17:J:321:LYS:HE3	1.84	0.59
2:B:790:TRP:HE1	2:B:802:GLU:HG2	1.68	0.59
3:C:398:PRO:HD3	3:C:476:ILE:HG12	1.85	0.59
4:D:449:HIS:CD2	4:D:451:SER:HB2	2.38	0.59
5:E:345:ARG:NH2	5:E:370:ASP:OD2	2.35	0.59
10:K:122:VAL:HG12	10:K:124:TYR:H	1.67	0.59
2:B:1043:VAL:HG23	2:B:1053:LEU:HB3	1.85	0.58
3:C:419:LEU:O	3:C:429:LYS:NZ	2.36	0.58
3:C:504:GLU:HG3	14:P:113:ALA:HB1	1.85	0.58
4:D:459:GLU:N	4:D:459:GLU:OE1	2.35	0.58
8:H:727:ASP:O	8:H:728:ASP:C	2.45	0.58
16:S:305:LYS:HE2	16:S:306:ILE:O	2.03	0.58
16:S:348:LEU:HD13	16:S:392:ILE:HG21	1.85	0.58
1:A:129:ILE:HD12	1:A:131:ASP:O	2.02	0.58
4:D:483:ARG:NH2	4:D:924:CYS:SG	2.76	0.58
6:R:154:SER:H	6:R:181:MET:HE3	1.68	0.58
16:S:370:VAL:HG13	16:S:400:ASP:CB	2.33	0.58
2:B:792:GLN:HB2	2:B:800:ASN:HB3	1.85	0.58
7:G:396:ASP:OD1	7:G:396:ASP:N	2.36	0.58
15:Q:62:VAL:HG11	15:Q:86:TYR:HD2	1.67	0.58
17:J:690:PRO:HB2	17:J:694:GLY:HA2	1.84	0.58
2:B:1061:ARG:HH12	8:H:230:THR:HG23	1.68	0.58
4:D:92:HIS:CE1	4:D:94:VAL:HB	2.39	0.58
16:S:298:TRP:HB2	16:S:301:MET:HG3	1.85	0.58
4:D:227:SER:HA	4:D:284:SER:HA	1.83	0.58
13:N:457:GLN:HG3	13:N:459:LYS:H	1.69	0.58
16:S:271:ASP:CG	16:S:272:ASP:H	2.11	0.58
16:S:406:LYS:HB3	16:S:454:ASN:CG	2.27	0.58
2:B:657:VAL:HG22	2:B:850:MET:HB3	1.86	0.58
4:D:449:HIS:CE1	13:N:92:TRP:HD1	2.17	0.58
5:E:95:ASP:OD1	5:E:95:ASP:N	2.36	0.58
8:H:769:LEU:HA	8:H:772:ARG:HE	1.69	0.58
9:I:337:ASN:ND2	9:I:353:ASP:OD2	2.37	0.58
6:R:150:LEU:HD12	6:R:164:THR:HG22	1.86	0.58
3:C:175:ILE:O	3:C:179:PHE:N	2.31	0.58
7:G:189:SER:OG	7:G:190:GLU:N	2.37	0.58
13:N:452:GLU:OE2	13:N:469:LYS:NZ	2.34	0.58
1:O:123:LEU:HB3	1:O:127:VAL:HG23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:J:691:LEU:HD13	17:J:692:PRO:HD2	1.85	0.58
3:C:280:ILE:HB	3:C:288:MET:HB2	1.86	0.58
3:C:306:LEU:HD21	3:C:325:GLU:HG3	1.85	0.58
9:I:164:PRO:O	9:I:165:LYS:HG3	2.04	0.58
12:M:155:GLY:H	12:M:158:GLN:HE22	1.51	0.58
14:P:86:GLU:N	14:P:86:GLU:OE1	2.36	0.58
3:C:65:LYS:HB3	3:C:68:ILE:HB	1.84	0.58
16:S:335:LEU:HB2	16:S:363:ILE:HG22	1.85	0.58
17:J:302:GLY:HA2	17:J:320:CYS:HB2	1.85	0.58
11:L:151:GLU:HG3	11:L:267:TYR:HE2	1.68	0.57
11:L:244:ASN:ND2	12:M:88:GLN:OE1	2.37	0.57
17:J:338:ALA:O	17:J:343:TYR:N	2.34	0.57
8:H:801:THR:HG22	8:H:802:ILE:H	1.69	0.57
16:S:345:THR:HG21	16:S:377:LEU:HD22	1.86	0.57
1:A:21:ARG:NH1	1:A:23:ASP:OD1	2.38	0.57
3:C:593:GLN:OE1	3:C:595:ARG:NE	2.27	0.57
6:R:142:MET:HE3	6:R:142:MET:HA	1.86	0.57
16:S:199:PRO:HB3	16:S:339:LYS:HD2	1.87	0.57
16:S:341:PHE:H	16:S:372:PHE:HB2	1.70	0.57
3:C:504:GLU:O	3:C:508:GLU:HG2	2.04	0.57
9:I:116:ILE:HG12	9:I:320:ILE:HB	1.85	0.57
9:I:210:ASP:OD2	9:I:457:ARG:NH1	2.37	0.57
6:R:95:LEU:HD22	6:R:126:MET:HE2	1.85	0.57
2:B:548:MET:HE3	2:B:821:ALA:HB1	1.86	0.57
2:B:892:GLU:O	7:G:235:ARG:NH2	2.36	0.57
16:S:422:ASP:OD1	16:S:423:THR:N	2.36	0.57
2:B:198:VAL:HG21	2:B:291:ASP:HB2	1.87	0.57
3:C:230:ASN:HB3	3:C:233:GLU:HG2	1.87	0.57
9:I:81:ALA:HA	9:I:103:GLU:HB2	1.85	0.57
6:R:66:ALA:N	6:R:69:VAL:O	2.38	0.57
6:R:160:ASP:CA	16:S:305:LYS:HB3	2.26	0.57
16:S:343:LEU:HD12	16:S:373:TYR:CE1	2.40	0.57
16:S:500:LEU:HA	16:S:506:LEU:HD22	1.87	0.57
17:J:608:LEU:HD21	17:J:721:VAL:HG21	1.85	0.57
5:E:119:ARG:NH1	5:E:312:GLU:OE1	2.32	0.57
16:S:325:LEU:HB3	16:S:356:THR:HG21	1.86	0.57
16:S:396:TRP:HZ3	16:S:412:LEU:HD13	1.69	0.57
16:S:435:GLU:HG3	16:S:436:ALA:H	1.69	0.57
17:J:654:ASP:OD1	17:J:703:ARG:NE	2.37	0.57
1:A:29:TYR:HE1	1:A:202:GLU:HG2	1.70	0.57
2:B:908:SER:HB2	2:B:916:VAL:HB	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1047:ARG:NH2	2:B:1070:ALA:O	2.38	0.57
16:S:205:GLY:HA2	16:S:347:SER:HB3	1.87	0.57
16:S:405:THR:HA	16:S:454:ASN:H	1.68	0.57
17:J:272:ILE:HD13	17:J:341:PHE:HE2	1.70	0.57
2:B:256:CYS:HB3	2:B:281:LEU:HB2	1.86	0.57
16:S:345:THR:CG2	16:S:378:PRO:HD2	2.35	0.57
16:S:200:LEU:HD21	16:S:263:ALA:N	2.19	0.56
16:S:387:GLU:O	16:S:391:LEU:HB3	2.05	0.56
1:A:227:ILE:HD11	16:S:529:TRP:HH2	1.69	0.56
3:C:566:GLU:HG3	3:C:568:ILE:H	1.71	0.56
3:C:8:GLN:HB3	4:D:1293:LEU:HD12	1.85	0.56
4:D:1156:TRP:HA	4:D:1159:ARG:HG2	1.87	0.56
5:E:217:MET:HG3	6:F:84:THR:HG22	1.87	0.56
13:N:437:SER:OG	13:N:438:GLU:OE1	2.23	0.56
16:S:255:LEU:HD13	16:S:498:ARG:HB2	1.88	0.56
17:J:314:ILE:HG22	17:J:323:LEU:HD23	1.87	0.56
17:J:519:PHE:HE1	17:J:549:ILE:HG13	1.69	0.56
17:J:586:ILE:O	17:J:590:GLN:NE2	2.34	0.56
13:N:346:ARG:NH2	13:N:353:ASP:OD2	2.37	0.56
6:R:175:ASP:O	6:R:179:ASN:N	2.38	0.56
3:C:181:THR:HB	17:J:769:ARG:HH22	1.70	0.56
4:D:1170:PHE:HE2	4:D:1251:TYR:CD2	2.23	0.56
11:L:81:HIS:HE1	11:L:232:ASP:OD2	1.87	0.56
3:C:140:LEU:HA	3:C:146:SER:HB2	1.88	0.56
4:D:105:TYR:HE1	4:D:348:THR:HG22	1.71	0.56
13:N:316:ILE:HD13	13:N:352:ILE:HD12	1.87	0.56
6:R:104:CYS:HB3	6:R:108:ILE:HG12	1.87	0.56
16:S:242:ARG:HH21	16:S:474:GLU:HG3	1.71	0.56
5:E:118:VAL:HB	5:E:284:LEU:HD12	1.88	0.56
10:K:136:LEU:HD23	10:K:245:SER:HB2	1.86	0.56
2:B:67:LYS:O	2:B:71:TYR:HB2	2.05	0.56
2:B:697:VAL:HA	2:B:702:PRO:HA	1.87	0.56
5:E:147:PRO:HG2	5:E:402:THR:HA	1.87	0.56
11:L:132:ASN:ND2	11:L:219:ASN:OD1	2.35	0.56
16:S:531:VAL:HG12	16:S:532:THR:HG23	1.88	0.56
2:B:391:ARG:NH2	2:B:439:ALA:O	2.39	0.56
3:C:153:LYS:HZ1	8:H:454:LYS:H	1.54	0.56
3:C:159:ARG:HA	17:J:767:PRO:HG2	1.87	0.56
3:C:363:LYS:HA	3:C:368:ARG:HG3	1.88	0.56
3:C:546:ASN:OD1	3:C:548:ARG:NH2	2.38	0.56
1:O:28:HIS:HB3	1:O:211:PRO:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1163:ILE:HG13	4:D:1164:LEU:HD12	1.88	0.56
8:H:451:ARG:HG2	17:J:680:LEU:HD12	1.87	0.56
11:L:197:ALA:C	11:L:199:ASN:N	2.64	0.56
15:Q:120:ASP:O	15:Q:122:TRP:HD1	1.88	0.56
16:S:276:THR:HA	16:S:279:TYR:CD2	2.41	0.56
16:S:458:LYS:HA	16:S:471:LEU:HA	1.87	0.56
2:B:169:TRP:CD2	2:B:178:ILE:HD11	2.41	0.55
4:D:1170:PHE:CZ	4:D:1174:ALA:HB2	2.42	0.55
8:H:487:ARG:HH11	8:H:487:ARG:HG2	1.71	0.55
9:I:88:ILE:O	9:I:92:ARG:NH1	2.38	0.55
9:I:111:PHE:HE1	9:I:325:GLU:HG3	1.70	0.55
6:R:83:ILE:HA	6:R:86:LEU:HD22	1.88	0.55
17:J:687:TYR:C	17:J:689:PRO:HD3	2.31	0.55
2:B:961:ARG:NH2	2:B:965:HIS:O	2.38	0.55
2:B:1037:GLU:OE2	3:C:102:TYR:OH	2.23	0.55
4:D:195:ARG:HD2	4:D:334:THR:HG23	1.89	0.55
16:S:526:ILE:HA	16:S:529:TRP:CZ2	2.42	0.55
3:C:269:LEU:HD12	3:C:270:PRO:HD2	1.87	0.55
4:D:409:GLN:HG3	7:G:222:TRP:CZ2	2.42	0.55
7:G:316:ILE:HG21	7:G:327:GLU:HG3	1.87	0.55
8:H:79:SER:HA	8:H:82:ARG:HB2	1.89	0.55
9:I:304:ARG:NH1	9:I:307:ASP:OD1	2.40	0.55
16:S:406:LYS:O	16:S:410:GLU:N	2.39	0.55
3:C:144:ASP:CG	3:C:326:LYS:HG3	2.32	0.55
17:J:247:LEU:HB3	17:J:265:LEU:HB3	1.89	0.55
2:B:223:ILE:HB	2:B:228:GLN:HG3	1.88	0.55
3:C:291:ASP:O	3:C:295:LEU:HD12	2.07	0.55
7:G:350:ASP:OD1	7:G:351:ILE:N	2.39	0.55
11:L:273:PHE:O	11:L:277:ARG:HG3	2.05	0.55
12:M:264:ASN:ND2	13:N:356:LEU:O	2.34	0.55
6:R:91:ARG:NH2	6:R:93:VAL:O	2.39	0.55
16:S:361:LEU:HD13	16:S:398:LEU:HD22	1.88	0.55
2:B:198:VAL:HG23	2:B:199:CYS:H	1.72	0.55
2:B:712:LEU:HD23	2:B:717:LEU:HD11	1.89	0.55
4:D:313:GLU:OE1	14:P:105:ARG:NE	2.39	0.55
8:H:805:CYS:SG	8:H:806:ALA:N	2.79	0.55
9:I:362:ARG:HB3	9:I:409:TRP:HB3	1.89	0.55
12:M:188:TRP:NE1	12:M:203:THR:OG1	2.38	0.55
16:S:199:PRO:HB3	16:S:339:LYS:CD	2.37	0.55
3:C:159:ARG:HD2	17:J:762:ASP:HB3	1.89	0.55
4:D:1075:VAL:HG13	4:D:1083:VAL:HG13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:209:PRO:HG2	12:M:216:PRO:HG3	1.89	0.55
6:R:143:GLN:HE22	16:S:313:ARG:HE	1.55	0.55
9:I:169:ASP:OD2	9:I:264:GLN:NE2	2.34	0.55
2:B:889:GLU:O	7:G:235:ARG:NH2	2.41	0.54
2:B:1044:ARG:NH2	2:B:1070:ALA:OXT	2.41	0.54
3:C:245:VAL:HG21	4:D:1229:PRO:HD2	1.88	0.54
6:F:95:LEU:HB3	6:F:153:ILE:HB	1.89	0.54
8:H:71:LEU:HA	8:H:74:MET:HB2	1.89	0.54
16:S:240:PHE:HD1	16:S:240:PHE:H	1.55	0.54
16:S:488:SER:OG	16:S:528:GLN:NE2	2.35	0.54
2:B:181:LEU:HG	2:B:183:LEU:H	1.73	0.54
2:B:185:SER:HB3	2:B:251:PHE:HZ	1.73	0.54
4:D:1132:LYS:O	4:D:1136:VAL:HG12	2.07	0.54
10:K:184:ARG:HH12	10:K:227:ARG:HH11	1.54	0.54
16:S:239:LYS:HE2	16:S:242:ARG:HH22	1.72	0.54
16:S:466:HIS:CD2	16:S:510:LYS:HD3	2.42	0.54
8:H:838:PRO:C	8:H:840:TYR:H	2.14	0.54
11:L:242:PHE:O	11:L:245:ARG:HG2	2.08	0.54
16:S:327:LYS:HA	16:S:330:ILE:HD12	1.89	0.54
3:C:121:ARG:HH21	4:D:1279:ARG:HB2	1.72	0.54
3:C:204:ALA:HB2	3:C:262:GLU:HG2	1.89	0.54
3:C:454:ARG:HG2	3:C:456:PRO:HD2	1.88	0.54
8:H:451:ARG:HH22	17:J:679:TYR:HD2	1.54	0.54
11:L:274:ALA:HA	11:L:277:ARG:HD2	1.88	0.54
16:S:268:LEU:HD22	16:S:277:MET:HG2	1.88	0.54
17:J:690:PRO:HA	17:J:695:HIS:O	2.07	0.54
1:A:9:SER:N	16:S:511:GLU:OE1	2.39	0.54
2:B:590:THR:HG22	2:B:628:ARG:HE	1.71	0.54
3:C:42:THR:HA	3:C:55:LEU:HB2	1.89	0.54
6:F:92:ASN:N	6:F:92:ASN:OD1	2.41	0.54
7:G:304:VAL:HG11	7:G:334:MET:HG3	1.88	0.54
7:G:350:ASP:OD2	7:G:352:ARG:NH1	2.41	0.54
8:H:313:ASP:OD2	8:H:316:ARG:NH2	2.41	0.54
15:Q:62:VAL:HG11	15:Q:86:TYR:CD2	2.42	0.54
17:J:534:GLN:NE2	17:J:564:ALA:O	2.40	0.54
2:B:383:PRO:HG3	2:B:577:VAL:HG21	1.89	0.54
3:C:159:ARG:HB2	17:J:770:LEU:H	1.71	0.54
3:C:249:GLU:OE2	4:D:1287:ARG:NH1	2.41	0.54
3:C:317:PRO:HG2	3:C:321:VAL:HG23	1.90	0.54
5:E:374:ARG:HE	5:E:387:VAL:HG22	1.72	0.54
8:H:321:MET:HE3	8:H:356:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:451:ARG:NH2	17:J:666:ASP:OD1	2.37	0.54
6:R:146:GLY:HA3	16:S:211:PHE:CE1	2.42	0.54
16:S:278:LEU:O	16:S:282:ASN:ND2	2.35	0.54
1:A:229:PHE:CE1	1:O:34:LEU:HD21	2.43	0.54
2:B:112:THR:HG21	2:B:378:LEU:HD22	1.89	0.54
11:L:198:VAL:O	11:L:201:LYS:N	2.28	0.54
6:R:76:LYS:HG2	6:R:78:LEU:HD12	1.90	0.54
16:S:214:SER:HG	16:S:382:TRP:CG	2.26	0.54
16:S:239:LYS:H	16:S:242:ARG:HB2	1.71	0.54
4:D:1224:SER:HB2	4:D:1247:GLU:HG2	1.90	0.54
2:B:184:SER:HB3	2:B:188:GLY:HA3	1.89	0.54
3:C:312:THR:HG22	3:C:312:THR:O	2.08	0.54
16:S:362:LYS:H	16:S:362:LYS:HD2	1.70	0.54
16:S:371:ILE:HG21	16:S:373:TYR:CZ	2.43	0.54
6:R:83:ILE:HD11	6:R:97:ILE:HD13	1.89	0.54
6:R:154:SER:H	6:R:181:MET:CE	2.20	0.54
16:S:303:GLN:NE2	16:S:318:LYS:O	2.41	0.54
16:S:377:LEU:HB3	16:S:381:LEU:HB2	1.89	0.54
17:J:586:ILE:HD11	17:J:743:ARG:HD3	1.89	0.54
3:C:542:LEU:HD13	4:D:49:GLN:HG2	1.90	0.53
7:G:364:GLU:OE2	7:G:368:LYS:NZ	2.41	0.53
9:I:427:GLU:O	9:I:431:GLN:N	2.37	0.53
13:N:431:TYR:O	13:N:433:GLY:N	2.40	0.53
1:O:28:HIS:HD2	1:O:207:GLY:HA2	1.73	0.53
1:O:83:SER:O	1:O:87:ILE:HG13	2.08	0.53
15:Q:134:ARG:NH1	15:Q:138:ASP:OD1	2.40	0.53
16:S:420:GLU:HA	16:S:432:GLU:HA	1.90	0.53
3:C:322:MET:O	3:C:326:LYS:HG2	2.09	0.53
8:H:174:ARG:NH2	9:I:380:GLU:OE2	2.42	0.53
16:S:239:LYS:HE2	16:S:242:ARG:NH2	2.23	0.53
3:C:208:LEU:HB3	3:C:251:VAL:HG13	1.91	0.53
3:C:312:THR:HA	3:C:314:ARG:HH11	1.73	0.53
4:D:209:VAL:HG12	4:D:210:VAL:HG13	1.89	0.53
6:R:82:GLU:O	6:R:86:LEU:HD13	2.08	0.53
16:S:227:HIS:HB3	16:S:230:LEU:HB2	1.89	0.53
16:S:402:ILE:HG12	16:S:403:GLU:N	2.24	0.53
16:S:463:THR:OG1	16:S:466:HIS:ND1	2.39	0.53
4:D:155:ASP:OD1	4:D:156:PRO:HD2	2.09	0.53
8:H:481:GLU:HA	8:H:484:ILE:HB	1.90	0.53
8:H:785:LEU:O	8:H:789:ILE:HG22	2.08	0.53
9:I:406:LEU:HG	9:I:408:THR:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:305:ARG:NH2	10:K:324:ILE:O	2.41	0.53
16:S:201:VAL:HG12	16:S:340:MET:HB3	1.89	0.53
16:S:400:ASP:OD1	16:S:400:ASP:N	2.42	0.53
16:S:450:LEU:HG	16:S:462:TYR:HB2	1.91	0.53
2:B:196:ASP:HB3	2:B:201:PRO:HG3	1.91	0.53
7:G:206:PRO:HA	7:G:209:LYS:HD2	1.90	0.53
11:L:201:LYS:O	11:L:203:SER:N	2.41	0.53
13:N:403:ASP:O	13:N:519:HIS:ND1	2.42	0.53
2:B:1056:PHE:HB2	3:C:9:GLN:HB3	1.90	0.53
3:C:153:LYS:HZ1	8:H:454:LYS:N	2.07	0.53
4:D:450:TRP:CD1	4:D:454:VAL:HB	2.44	0.53
8:H:82:ARG:HH12	9:I:418:PRO:HB3	1.74	0.53
10:K:148:ASP:OD2	10:K:153:VAL:HG22	2.09	0.53
1:O:28:HIS:CD2	1:O:207:GLY:HA2	2.43	0.53
16:S:200:LEU:HD23	16:S:201:VAL:N	2.24	0.53
16:S:326:SER:H	16:S:329:GLU:HB3	1.74	0.53
17:J:276:SER:HB3	17:J:294:CYS:HB3	1.89	0.53
17:J:722:VAL:HG21	17:J:746:CYS:SG	2.49	0.53
1:A:19:GLU:HG2	1:A:29:TYR:HE2	1.72	0.53
4:D:1152:ARG:HH12	8:H:731:TRP:HB3	1.73	0.53
12:M:190:VAL:HG12	12:M:216:PRO:HA	1.90	0.53
16:S:241:ILE:O	16:S:244:PRO:HD3	2.09	0.53
16:S:298:TRP:HB3	16:S:301:MET:SD	2.48	0.53
4:D:64:THR:HA	4:D:147:VAL:HG13	1.90	0.53
4:D:1232:LEU:HD22	4:D:1264:ASN:HD22	1.74	0.53
8:H:495:ASN:HB3	8:H:498:PRO:HD2	1.90	0.53
8:H:376:ARG:NH2	8:H:472:THR:OG1	2.42	0.52
10:K:228:LEU:HD12	10:K:233:PHE:HE2	1.73	0.52
6:R:162:ILE:HG22	16:S:301:MET:HB2	1.91	0.52
17:J:362:ALA:N	17:J:551:ASN:HD21	2.06	0.52
3:C:141:VAL:O	3:C:143:CYS:N	2.42	0.52
4:D:1094:THR:HG22	13:N:107:LEU:HD13	1.91	0.52
1:O:98:SER:HB2	1:O:127:VAL:HG12	1.90	0.52
17:J:651:LEU:HD13	17:J:665:LEU:HD22	1.91	0.52
17:J:653:SER:O	17:J:731:GLN:NE2	2.40	0.52
2:B:1024:ILE:HG21	3:C:423:ILE:HD11	1.90	0.52
6:F:87:VAL:O	6:F:91:ARG:NH1	2.43	0.52
12:M:188:TRP:HB2	12:M:201:VAL:HG12	1.92	0.52
12:M:196:LYS:HB3	12:M:265:LEU:HD23	1.92	0.52
17:J:285:PHE:CD2	17:J:306:VAL:HG23	2.45	0.52
1:A:222:LEU:O	1:A:226:LEU:HG	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:175:ILE:HG13	3:C:176:PRO:HD3	1.90	0.52
4:D:491:LEU:O	13:N:383:ARG:NH1	2.43	0.52
8:H:775:ARG:NH2	8:H:778:SER:O	2.43	0.52
11:L:110:VAL:O	11:L:112:ARG:N	2.43	0.52
8:H:431:TYR:O	8:H:432:MET:HB3	2.08	0.52
11:L:197:ALA:O	11:L:199:ASN:N	2.41	0.52
12:M:166:SER:HB3	12:M:168:PRO:HD2	1.91	0.52
6:R:96:ILE:HD11	6:R:152:PHE:CE1	2.45	0.52
17:J:669:LEU:HD23	17:J:674:TRP:HE3	1.75	0.52
4:D:1053:LEU:HD11	13:N:288:LEU:HB3	1.91	0.52
5:E:105:CYS:HB3	5:E:246:PHE:HA	1.91	0.52
8:H:109:HIS:CE1	8:H:142:THR:HA	2.45	0.52
10:K:180:ASP:OD1	10:K:180:ASP:N	2.36	0.52
6:R:139:ALA:O	6:R:144:VAL:HB	2.10	0.52
16:S:200:LEU:HD21	16:S:263:ALA:H	1.74	0.52
4:D:1156:TRP:HE3	4:D:1159:ARG:HD3	1.73	0.52
9:I:445:GLN:HG3	9:I:446:ASP:N	2.24	0.52
13:N:421:LEU:HD23	13:N:484:ARG:HH11	1.73	0.52
2:B:1012:HIS:HB3	2:B:1015:ALA:HB3	1.92	0.52
2:B:1015:ALA:O	2:B:1019:VAL:HG12	2.10	0.52
3:C:44:HIS:CD2	3:C:46:LYS:H	2.28	0.52
4:D:428:SER:O	4:D:428:SER:OG	2.28	0.52
4:D:454:VAL:HG22	4:D:468:LEU:HG	1.91	0.52
8:H:802:ILE:HG13	8:H:803:GLY:H	1.75	0.52
11:L:104:GLY:O	11:L:105:LEU:HD23	2.10	0.52
12:M:119:TYR:HB2	12:M:128:PHE:CD1	2.45	0.52
6:R:87:VAL:HG11	16:S:308:LYS:HZ3	1.74	0.52
16:S:463:THR:HG1	16:S:466:HIS:HD1	1.55	0.52
17:J:703:ARG:O	17:J:707:VAL:HG22	2.09	0.52
3:C:180:THR:OG1	3:C:181:THR:N	2.41	0.51
6:F:114:LEU:HD11	6:F:150:LEU:HD21	1.92	0.51
10:K:152:ASP:HB3	10:K:184:ARG:HG3	1.91	0.51
12:M:149:GLY:HA2	12:M:247:VAL:HG12	1.93	0.51
1:O:29:TYR:OH	1:O:202:GLU:OE2	2.26	0.51
16:S:340:MET:HE2	16:S:372:PHE:CD2	2.44	0.51
16:S:385:GLY:HA2	16:S:412:LEU:HA	1.92	0.51
16:S:440:ALA:HA	16:S:443:TRP:HD1	1.75	0.51
2:B:463:ARG:HG3	2:B:464:VAL:HG23	1.92	0.51
4:D:262:THR:OG1	4:D:263:ARG:N	2.43	0.51
8:H:281:THR:O	8:H:285:ASN:ND2	2.43	0.51
9:I:99:VAL:HG12	9:I:326:MET:HE1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:434:LYS:HG2	13:N:436:LEU:HG	1.93	0.51
6:R:103:TRP:CG	16:S:241:ILE:HG21	2.45	0.51
2:B:161:GLU:HB3	2:B:169:TRP:NE1	2.24	0.51
2:B:610:MET:HE3	2:B:610:MET:HA	1.92	0.51
2:B:648:GLU:OE1	2:B:883:ARG:NH2	2.39	0.51
4:D:187:LYS:O	4:D:187:LYS:HG3	2.09	0.51
7:G:318:LYS:NZ	7:G:322:GLU:OE2	2.43	0.51
8:H:328:VAL:HG11	8:H:357:LEU:HD11	1.92	0.51
8:H:395:GLN:HB3	8:H:396:PRO:HD3	1.92	0.51
8:H:396:PRO:HG3	8:H:797:GLY:H	1.75	0.51
12:M:164:PHE:HD2	12:M:170:PHE:HB2	1.75	0.51
13:N:457:GLN:OE1	13:N:460:LYS:N	2.44	0.51
16:S:299:THR:O	16:S:301:MET:HG2	2.09	0.51
16:S:334:VAL:HG12	16:S:335:LEU:HG	1.93	0.51
3:C:526:ASP:OD1	3:C:526:ASP:N	2.40	0.51
10:K:276:ASP:N	10:K:276:ASP:OD1	2.43	0.51
17:J:665:LEU:HA	17:J:668:MET:HG3	1.92	0.51
4:D:1175:GLU:OE2	8:H:746:ARG:HD3	2.10	0.51
10:K:130:GLU:OE2	10:K:144:ARG:NH2	2.39	0.51
13:N:213:VAL:HG12	13:N:215:ARG:HB2	1.93	0.51
13:N:424:MET:HB3	13:N:434:LYS:HE3	1.92	0.51
13:N:504:ASP:N	13:N:504:ASP:OD1	2.42	0.51
1:O:135:HIS:NE2	1:O:137:ALA:O	2.44	0.51
17:J:351:ILE:HG12	17:J:441:ILE:HB	1.92	0.51
1:A:144:ASP:N	1:A:144:ASP:OD1	2.42	0.51
4:D:76:GLU:OE1	7:G:234:SER:OG	2.29	0.51
4:D:167:SER:OG	4:D:177:GLU:OE1	2.29	0.51
4:D:362:PHE:HB3	4:D:387:VAL:HG12	1.92	0.51
16:S:198:PRO:O	16:S:199:PRO:C	2.53	0.51
16:S:358:MET:HA	16:S:361:LEU:HG	1.92	0.51
8:H:337:ILE:O	8:H:338:ARG:C	2.54	0.51
8:H:725:ASN:O	8:H:727:ASP:N	2.44	0.51
8:H:791:SER:O	8:H:795:GLU:HG2	2.11	0.51
9:I:293:HIS:CD2	9:I:330:TYR:H	2.29	0.51
14:P:131:LYS:O	14:P:134:HIS:N	2.43	0.51
6:R:142:MET:HE2	16:S:304:MET:HG3	1.93	0.51
16:S:453:THR:HG22	16:S:455:GLY:H	1.76	0.51
17:J:429:LEU:HD23	17:J:467:LYS:HB3	1.92	0.51
2:B:125:GLN:NE2	2:B:396:LEU:O	2.38	0.51
3:C:581:PHE:HD2	3:C:602:LEU:HD13	1.75	0.51
4:D:416:SER:OG	4:D:417:GLU:N	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:102:PRO:HB3	5:E:244:ARG:HG3	1.93	0.51
13:N:172:ARG:HG3	13:N:173:HIS:H	1.75	0.51
6:R:103:TRP:CZ3	6:R:147:LEU:HD11	2.45	0.51
16:S:308:LYS:HB3	16:S:313:ARG:O	2.11	0.51
8:H:435:TYR:HA	8:H:438:GLU:OE1	2.11	0.51
13:N:255:HIS:CD2	13:N:256:PRO:HD2	2.45	0.51
1:A:15:TRP:HA	1:A:33:ILE:O	2.11	0.51
4:D:228:VAL:HG21	4:D:244:LEU:HD21	1.93	0.51
4:D:1111:ASP:OD1	4:D:1111:ASP:N	2.43	0.51
6:R:117:LEU:HD21	6:R:174:ARG:NE	2.27	0.51
6:R:142:MET:HB2	6:R:144:VAL:HG23	1.92	0.51
16:S:291:VAL:CG2	16:S:293:VAL:HG13	2.41	0.51
17:J:521:LEU:HD21	17:J:545:GLY:H	1.76	0.51
7:G:257:VAL:HG22	10:K:323:TRP:HZ2	1.75	0.50
8:H:225:HIS:HB2	8:H:253:VAL:HG21	1.94	0.50
16:S:345:THR:HG21	16:S:377:LEU:CD2	2.41	0.50
16:S:358:MET:HE3	16:S:394:GLN:HB2	1.92	0.50
1:A:112:GLY:O	1:A:114:ARG:N	2.44	0.50
4:D:222:THR:O	4:D:263:ARG:NH2	2.43	0.50
4:D:916:THR:HG22	4:D:918:LEU:HB2	1.94	0.50
13:N:425:GLU:OE2	13:N:484:ARG:HG2	2.11	0.50
13:N:425:GLU:OE1	13:N:485:GLN:NE2	2.44	0.50
15:Q:62:VAL:HA	15:Q:65:TRP:CE2	2.46	0.50
16:S:244:PRO:HD2	16:S:485:MET:O	2.11	0.50
16:S:431:PHE:O	16:S:432:GLU:HG2	2.11	0.50
17:J:584:GLU:O	17:J:743:ARG:NH1	2.44	0.50
11:L:93:LEU:O	11:L:97:ILE:HG12	2.12	0.50
11:L:199:ASN:HA	13:N:520:TRP:CZ2	2.46	0.50
15:Q:57:LEU:O	15:Q:61:GLY:N	2.44	0.50
15:Q:68:TRP:HB2	15:Q:131:TYR:HE2	1.76	0.50
16:S:201:VAL:HG11	16:S:342:TYR:CE1	2.47	0.50
16:S:238:ASP:HB2	16:S:240:PHE:CE1	2.47	0.50
16:S:485:MET:HG3	16:S:528:GLN:HG2	1.92	0.50
17:J:545:GLY:O	17:J:549:ILE:HG12	2.11	0.50
2:B:738:LEU:HD11	2:B:777:LEU:HD13	1.94	0.50
4:D:926:PHE:HB2	4:D:1106:ILE:HG13	1.93	0.50
9:I:140:LEU:HD13	9:I:141:PRO:HA	1.93	0.50
13:N:546:GLU:HB3	15:Q:116:TRP:CD2	2.46	0.50
6:R:87:VAL:HG11	16:S:308:LYS:NZ	2.26	0.50
16:S:267:LYS:HD2	16:S:292:CYS:H	1.77	0.50
2:B:1001:ILE:O	2:B:1005:MET:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:170:ILE:HA	6:F:173:MET:HE3	1.93	0.50
8:H:827:THR:OG1	8:H:828:THR:N	2.43	0.50
13:N:338:ARG:NH2	13:N:371:ASP:OD2	2.33	0.50
1:O:100:LEU:HD13	1:O:126:TYR:CE2	2.46	0.50
17:J:354:THR:OG1	17:J:465:GLN:OE1	2.29	0.50
4:D:328:GLU:O	4:D:329:PRO:C	2.53	0.50
5:E:352:ARG:NH1	5:E:379:ALA:O	2.45	0.50
8:H:218:GLU:HA	8:H:221:LYS:HE2	1.94	0.50
9:I:252:ASP:N	9:I:252:ASP:OD1	2.43	0.50
11:L:100:THR:OG1	11:L:101:GLU:N	2.45	0.50
16:S:253:ILE:HD11	16:S:284:LYS:HD3	1.94	0.50
17:J:516:PRO:HD3	17:J:553:LEU:HD11	1.93	0.50
2:B:169:TRP:HB3	2:B:180:ILE:HD13	1.93	0.50
2:B:228:GLN:NE2	2:B:229:GLN:OE1	2.45	0.50
2:B:787:ASP:HB3	2:B:807:TYR:CD2	2.46	0.50
4:D:1233:ILE:HB	4:D:1237:ARG:HG2	1.93	0.50
4:D:1247:GLU:N	4:D:1247:GLU:OE1	2.45	0.50
2:B:249:LYS:HA	2:B:253:GLN:HB3	1.93	0.50
2:B:984:ARG:HB2	3:C:375:ARG:HD2	1.93	0.50
3:C:73:ASN:OD1	3:C:73:ASN:N	2.45	0.50
4:D:1077:ILE:HG22	4:D:1079:GLN:HG3	1.93	0.50
8:H:379:ARG:NH1	8:H:481:GLU:OE2	2.44	0.50
9:I:228:HIS:C	9:I:230:CYS:H	2.20	0.50
10:K:317:ASP:O	10:K:321:SER:OG	2.29	0.50
13:N:255:HIS:CE1	13:N:341:PHE:HE1	2.30	0.50
1:A:164:ASN:O	1:A:169:SER:OG	2.23	0.50
2:B:529:SER:HB2	2:B:567:LEU:HD22	1.94	0.50
8:H:395:GLN:OE1	8:H:396:PRO:HD3	2.11	0.50
11:L:180:SER:OG	11:L:235:GLU:OE1	2.29	0.50
13:N:255:HIS:HE1	13:N:341:PHE:HE1	1.59	0.50
1:A:227:ILE:HG22	1:A:228:PRO:HD3	1.94	0.49
2:B:824:HIS:NE2	2:B:868:GLU:OE1	2.38	0.49
4:D:1191:LYS:HE2	4:D:1191:LYS:HA	1.93	0.49
5:E:468:VAL:HG11	7:G:231:GLU:HB3	1.94	0.49
9:I:134:LEU:HD12	9:I:175:LEU:HB3	1.93	0.49
11:L:108:GLU:HB3	11:L:112:ARG:HH12	1.77	0.49
16:S:239:LYS:HA	16:S:242:ARG:HB3	1.93	0.49
17:J:245:MET:HE1	17:J:250:LEU:HD13	1.95	0.49
1:A:35:SER:HB2	1:A:36:PRO:HD2	1.94	0.49
4:D:935:CYS:HG	5:E:334:TYR:HD1	1.58	0.49
8:H:463:GLY:HA3	8:H:466:TYR:CE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:764:THR:HA	8:H:767:ARG:HB2	1.93	0.49
16:S:305:LYS:HG2	16:S:317:VAL:HB	1.94	0.49
16:S:403:GLU:HA	16:S:451:PHE:O	2.12	0.49
17:J:376:ARG:HE	17:J:388:HIS:HB2	1.78	0.49
1:A:98:SER:HB2	1:A:127:VAL:HG22	1.94	0.49
1:A:116:VAL:HG12	1:A:136:ILE:HG23	1.93	0.49
2:B:332:LEU:HD11	2:B:356:VAL:HG13	1.94	0.49
2:B:489:GLN:HA	5:E:471:MET:HE2	1.94	0.49
4:D:1148:ASN:O	4:D:1152:ARG:HG2	2.13	0.49
9:I:365:LEU:HG	9:I:408:THR:HB	1.93	0.49
12:M:187:VAL:HG12	12:M:220:LEU:HB3	1.94	0.49
6:R:91:ARG:C	6:R:155:PRO:HG3	2.37	0.49
16:S:377:LEU:HG	16:S:408:GLU:HG2	1.93	0.49
4:D:1240:ARG:HH21	8:H:309:LEU:HG	1.78	0.49
9:I:304:ARG:HD2	14:P:100:LYS:HG2	1.94	0.49
9:I:426:LYS:O	9:I:429:GLN:HG2	2.11	0.49
10:K:184:ARG:N	10:K:225:ASN:OD1	2.35	0.49
11:L:267:TYR:CZ	11:L:271:LYS:HD2	2.48	0.49
6:R:162:ILE:HG22	16:S:301:MET:CB	2.42	0.49
16:S:201:VAL:HG11	16:S:342:TYR:CZ	2.48	0.49
17:J:505:PHE:HD2	17:J:553:LEU:HB3	1.77	0.49
4:D:430:LEU:CD1	4:D:1122:ARG:HD3	2.42	0.49
9:I:267:CYS:SG	9:I:282:ASN:HB3	2.52	0.49
10:K:211:GLU:N	10:K:211:GLU:OE1	2.46	0.49
17:J:687:TYR:HB2	17:J:688:TYR:CZ	2.48	0.49
7:G:245:THR:HG22	7:G:269:THR:HG21	1.93	0.49
7:G:297:MET:HG2	7:G:316:ILE:HD11	1.94	0.49
8:H:386:ALA:O	8:H:389:THR:OG1	2.28	0.49
8:H:474:PHE:CE2	8:H:477:ARG:HA	2.47	0.49
10:K:184:ARG:HD2	10:K:226:ARG:O	2.13	0.49
1:O:13:LEU:HA	1:O:35:SER:OG	2.12	0.49
17:J:272:ILE:HG12	17:J:403:VAL:HG13	1.95	0.49
2:B:746:MET:HE2	2:B:746:MET:N	2.27	0.49
3:C:389:SER:OG	14:P:167:GLU:OE1	2.30	0.49
8:H:485:ARG:NH2	8:H:773:PRO:HA	2.27	0.49
9:I:412:ARG:O	9:I:412:ARG:NH1	2.41	0.49
6:R:141:ASP:OD1	16:S:313:ARG:HA	2.12	0.49
6:R:163:ARG:HD3	16:S:302:SER:HB3	1.94	0.49
2:B:129:SER:O	2:B:133:TYR:OH	2.25	0.49
2:B:464:VAL:HG13	5:E:135:MET:HE1	1.93	0.49
4:D:1226:VAL:HG13	8:H:300:VAL:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:451:ARG:HD2	17:J:680:LEU:HB2	1.94	0.49
12:M:120:ASN:HB2	12:M:123:ASN:O	2.12	0.49
16:S:204:PHE:HD2	16:S:357:THR:HG23	1.78	0.49
16:S:453:THR:HG22	16:S:455:GLY:N	2.28	0.49
2:B:330:VAL:O	2:B:333:GLU:HG3	2.12	0.49
11:L:107:LEU:HD23	11:L:108:GLU:H	1.78	0.49
1:O:100:LEU:HD12	1:O:101:TYR:H	1.78	0.49
3:C:3:ASP:OD1	3:C:3:ASP:N	2.37	0.49
3:C:122:LEU:HD21	4:D:1279:ARG:HD3	1.94	0.49
8:H:314:HIS:NE2	8:H:753:ASN:HA	2.27	0.49
8:H:427:TYR:HA	8:H:834:ARG:CZ	2.43	0.49
8:H:808:ILE:HG21	8:H:824:ILE:HD13	1.94	0.49
15:Q:79:TRP:NE1	15:Q:83:GLN:OE1	2.40	0.49
16:S:370:VAL:HG11	16:S:401:VAL:HG23	1.93	0.49
17:J:306:VAL:HG13	17:J:306:VAL:O	2.13	0.49
3:C:160:LEU:H	17:J:767:PRO:HG2	1.78	0.48
4:D:932:SER:O	5:E:335:SER:OG	2.27	0.48
7:G:356:ASP:OD1	7:G:356:ASP:N	2.44	0.48
8:H:493:LEU:HB3	8:H:514:GLU:HB2	1.95	0.48
2:B:263:ARG:NH2	2:B:280:PHE:O	2.46	0.48
4:D:370:THR:HG21	4:D:380:LEU:HD12	1.95	0.48
4:D:1227:PHE:CZ	4:D:1241:THR:HG21	2.49	0.48
16:S:202:CYS:O	16:S:342:TYR:N	2.44	0.48
16:S:202:CYS:HB3	16:S:265:MET:CG	2.43	0.48
16:S:450:LEU:HD11	16:S:462:TYR:HD2	1.78	0.48
1:A:91:LEU:HD12	1:A:136:ILE:HD11	1.93	0.48
2:B:861:MET:HG2	4:D:146:LEU:HD21	1.95	0.48
3:C:479:HIS:HE1	4:D:43:LYS:HE2	1.77	0.48
4:D:298:CYS:SG	4:D:299:ARG:N	2.86	0.48
4:D:432:PHE:C	4:D:1123:SER:HB3	2.39	0.48
6:F:143:GLN:O	6:F:163:ARG:NH1	2.39	0.48
1:A:131:ASP:CG	1:A:134:GLN:HG3	2.39	0.48
4:D:299:ARG:HH21	4:D:311:LEU:HB3	1.78	0.48
4:D:429:THR:O	4:D:430:LEU:HG	2.14	0.48
4:D:1058:CYS:SG	4:D:1059:GLU:N	2.86	0.48
4:D:1262:SER:O	4:D:1265:THR:OG1	2.25	0.48
8:H:96:MET:HE2	8:H:96:MET:HB3	1.78	0.48
9:I:446:ASP:O	9:I:449:ILE:HG22	2.13	0.48
6:R:103:TRP:CZ2	16:S:215:GLY:HA2	2.47	0.48
16:S:207:ALA:HB2	16:S:264:PHE:CZ	2.49	0.48
16:S:239:LYS:CA	16:S:242:ARG:HB2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:327:LYS:HE3	16:S:355:LYS:HB3	1.95	0.48
16:S:345:THR:HG23	16:S:381:LEU:HD23	1.96	0.48
17:J:364:HIS:HA	17:J:367:LYS:HE2	1.94	0.48
17:J:552:ILE:O	17:J:556:VAL:HG12	2.14	0.48
4:D:1237:ARG:NH1	8:H:305:GLU:OE2	2.30	0.48
13:N:251:ASP:OD2	13:N:258:ARG:NH1	2.38	0.48
2:B:229:GLN:HG3	2:B:239:PHE:HA	1.96	0.48
4:D:157:GLN:O	4:D:157:GLN:HG2	2.13	0.48
16:S:363:ILE:HA	16:S:366:LYS:HG2	1.96	0.48
17:J:282:GLY:H	17:J:303:ALA:HA	1.77	0.48
3:C:239:ARG:HG3	3:C:239:ARG:HH11	1.79	0.48
4:D:231:GLN:HA	4:D:231:GLN:NE2	2.29	0.48
7:G:257:VAL:HG22	10:K:323:TRP:CZ2	2.48	0.48
12:M:181:LEU:HB2	12:M:202:LYS:HD3	1.95	0.48
14:P:91:MET:HE1	14:P:134:HIS:CD2	2.48	0.48
16:S:274:GLY:O	16:S:277:MET:HB3	2.12	0.48
17:J:643:THR:O	17:J:695:HIS:ND1	2.47	0.48
1:A:188:SER:HB2	7:G:351:ILE:HD13	1.96	0.48
2:B:823:ARG:NH2	2:B:868:GLU:OE2	2.36	0.48
2:B:998:VAL:HG12	3:C:508:GLU:HB3	1.96	0.48
3:C:107:ILE:HG12	3:C:269:LEU:HB3	1.95	0.48
9:I:347:SER:HB3	9:I:350:ASN:HB3	1.96	0.48
16:S:224:HIS:HA	16:S:227:HIS:HE1	1.79	0.48
16:S:475:ASP:OD1	16:S:477:PRO:HD3	2.13	0.48
3:C:230:ASN:O	3:C:234:ASP:N	2.44	0.48
13:N:425:GLU:HB3	13:N:434:LYS:HZ2	1.77	0.48
16:S:340:MET:HE3	16:S:340:MET:HA	1.94	0.48
1:A:220:ARG:HA	1:A:220:ARG:HD2	1.61	0.48
2:B:184:SER:HB3	2:B:188:GLY:CA	2.44	0.48
3:C:67:GLY:HA2	3:C:94:PHE:HB3	1.95	0.48
4:D:92:HIS:HE1	4:D:94:VAL:HB	1.77	0.48
9:I:431:GLN:O	9:I:435:ILE:N	2.43	0.48
10:K:252:ARG:NH1	10:K:253:ALA:O	2.47	0.48
13:N:159:ASP:OD1	13:N:159:ASP:N	2.46	0.48
13:N:404:HIS:CD2	13:N:519:HIS:HB2	2.49	0.48
14:P:126:GLU:OE2	14:P:130:LYS:NZ	2.46	0.48
17:J:744:GLU:O	17:J:747:ARG:HG3	2.14	0.48
2:B:560:LYS:HG3	2:B:645:VAL:HG13	1.96	0.47
3:C:483:CYS:O	3:C:487:ASN:N	2.47	0.47
4:D:322:ALA:O	4:D:326:ILE:HG13	2.14	0.47
4:D:1098:THR:O	4:D:1098:THR:OG1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:113:VAL:HA	8:H:116:VAL:HG12	1.96	0.47
16:S:263:ALA:HB1	16:S:287:GLN:HB3	1.96	0.47
16:S:400:ASP:O	16:S:402:ILE:N	2.46	0.47
17:J:480:LYS:HZ2	17:J:500:VAL:HB	1.78	0.47
16:S:227:HIS:ND1	16:S:230:LEU:HD22	2.29	0.47
17:J:400:PRO:HB2	17:J:404:LEU:HD13	1.96	0.47
3:C:637:TYR:HE2	3:C:639:ILE:HD11	1.79	0.47
4:D:85:HIS:ND1	4:D:90:ASN:OD1	2.47	0.47
4:D:1129:GLY:O	4:D:1130:LEU:C	2.56	0.47
8:H:342:ARG:HH21	8:H:770:LYS:NZ	2.12	0.47
8:H:382:GLU:CD	8:H:382:GLU:H	2.22	0.47
9:I:421:GLU:HA	9:I:425:ALA:HB3	1.96	0.47
10:K:228:LEU:HD12	10:K:233:PHE:CE2	2.49	0.47
13:N:311:ASN:OD1	13:N:358:GLN:NE2	2.48	0.47
16:S:318:LYS:HE3	16:S:318:LYS:HB2	1.26	0.47
16:S:478:MET:N	16:S:483:GLN:HE22	2.12	0.47
17:J:364:HIS:O	17:J:367:LYS:HG2	2.14	0.47
17:J:583:CYS:N	17:J:596:VAL:O	2.46	0.47
1:A:224:ASP:OD1	16:S:478:MET:HB3	2.14	0.47
1:A:227:ILE:HD12	1:A:227:ILE:HA	1.67	0.47
3:C:549:GLY:HA3	10:K:304:THR:HG21	1.94	0.47
8:H:150:PHE:HB3	8:H:155:ARG:HB2	1.97	0.47
9:I:133:MET:HE2	9:I:285:VAL:HG12	1.97	0.47
13:N:136:MET:O	13:N:140:GLY:N	2.46	0.47
6:R:138:PHE:CE2	16:S:312:LEU:HD11	2.50	0.47
1:A:40:GLY:HA3	1:O:157:TYR:HD2	1.79	0.47
2:B:297:LYS:HG2	2:B:298:PHE:HD1	1.79	0.47
2:B:711:HIS:CE1	2:B:765:ILE:HG23	2.50	0.47
3:C:623:HIS:N	3:C:631:HIS:O	2.47	0.47
4:D:487:VAL:HG23	4:D:488:PRO:HD3	1.96	0.47
7:G:393:ARG:O	7:G:397:PHE:HB2	2.14	0.47
8:H:726:ASP:O	8:H:727:ASP:C	2.57	0.47
9:I:101:PHE:HD1	9:I:110:VAL:HG22	1.80	0.47
6:R:96:ILE:HA	6:R:151:TYR:O	2.14	0.47
6:R:99:PHE:CZ	6:R:142:MET:HG2	2.49	0.47
6:R:103:TRP:HB3	16:S:233:ALA:HB3	1.95	0.47
16:S:308:LYS:CE	16:S:312:LEU:HA	2.44	0.47
3:C:388:PRO:O	4:D:43:LYS:NZ	2.45	0.47
4:D:381:CYS:SG	4:D:404:SER:HB2	2.54	0.47
4:D:1094:THR:HB	4:D:1095:PRO:HD2	1.97	0.47
4:D:1218:VAL:HA	4:D:1251:TYR:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:133:TRP:HE3	6:F:108:ILE:HG13	1.80	0.47
6:F:160:ASP:OD1	6:F:160:ASP:N	2.46	0.47
13:N:453:TYR:CE2	13:N:455:LYS:HG2	2.49	0.47
14:P:75:PRO:HB2	14:P:76:PHE:CD1	2.49	0.47
6:R:96:ILE:HB	6:R:127:ILE:HG12	1.96	0.47
16:S:291:VAL:HG22	16:S:293:VAL:HG13	1.96	0.47
1:A:155:ARG:NH2	1:O:39:LYS:O	2.42	0.47
2:B:185:SER:HB3	2:B:251:PHE:CZ	2.49	0.47
3:C:75:ARG:NH2	3:C:83:ASP:OD1	2.43	0.47
3:C:371:LEU:HD22	4:D:1301:VAL:HG13	1.97	0.47
3:C:479:HIS:CD2	3:C:481:LEU:HB2	2.49	0.47
4:D:311:LEU:HD12	9:I:273:ARG:HH22	1.79	0.47
4:D:376:HIS:CD2	7:G:224:ASN:HB3	2.50	0.47
4:D:1232:LEU:HD21	4:D:1256:LEU:HD21	1.97	0.47
8:H:435:TYR:HB3	17:J:632:ARG:NH2	2.30	0.47
8:H:837:SER:N	8:H:838:PRO:HD2	2.29	0.47
10:K:198:PRO:HG3	10:K:209:LYS:HG3	1.97	0.47
13:N:272:LEU:HD22	13:N:333:LYS:HE3	1.97	0.47
1:O:31:ARG:HA	1:O:201:LEU:O	2.14	0.47
16:S:216:ARG:HG2	16:S:217:PRO:HD3	1.95	0.47
16:S:343:LEU:HB2	16:S:373:TYR:HD1	1.80	0.47
17:J:578:ALA:HB1	17:J:584:GLU:HG3	1.96	0.47
1:A:60:THR:HG22	1:A:153:ARG:HB2	1.97	0.47
7:G:349:THR:HG22	7:G:360:MET:HE1	1.96	0.47
9:I:485:GLN:HA	9:I:488:ILE:HD11	1.96	0.47
10:K:148:ASP:N	10:K:148:ASP:OD1	2.46	0.47
13:N:515:TYR:HE1	15:Q:69:LYS:HE2	1.80	0.47
14:P:94:ASP:OD1	14:P:141:MET:HE2	2.14	0.47
14:P:100:LYS:HE3	14:P:100:LYS:HB2	1.60	0.47
6:R:176:ILE:HG13	16:S:273:TYR:CE2	2.50	0.47
16:S:408:GLU:N	16:S:408:GLU:OE1	2.48	0.47
16:S:416:ASN:HB3	16:S:417:PRO:HD3	1.97	0.47
16:S:478:MET:HE1	16:S:529:TRP:CG	2.50	0.47
17:J:275:ASP:O	17:J:279:VAL:HG23	2.14	0.47
1:A:23:ASP:HB2	1:A:27:LEU:HD23	1.96	0.47
3:C:245:VAL:HA	3:C:248:MET:CE	2.45	0.47
4:D:186:ARG:O	4:D:190:VAL:HG23	2.15	0.47
17:J:371:GLU:HA	17:J:375:LEU:O	2.15	0.47
17:J:518:LYS:HD3	17:J:529:LEU:HD23	1.97	0.47
17:J:609:LEU:O	17:J:613:ARG:HG2	2.15	0.47
2:B:200:TYR:HE2	2:B:203:ILE:H	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1019:VAL:HA	2:B:1022:THR:HG22	1.95	0.47
3:C:546:ASN:HD22	3:C:601:PRO:HB3	1.79	0.47
9:I:420:VAL:HG23	9:I:420:VAL:O	2.15	0.47
13:N:328:VAL:HG21	13:N:345:LEU:HD13	1.97	0.47
1:O:91:LEU:HD23	1:O:94:ILE:HD11	1.97	0.47
6:R:85:GLU:HA	6:R:88:ARG:HB2	1.97	0.47
6:R:88:ARG:HA	6:R:88:ARG:HD3	1.73	0.47
6:R:145:ARG:HA	16:S:380:PRO:HD3	1.97	0.47
16:S:340:MET:HE1	16:S:370:VAL:HG12	1.97	0.47
16:S:363:ILE:HA	16:S:366:LYS:HD3	1.97	0.47
4:D:62:LEU:HD23	4:D:128:VAL:HG21	1.97	0.46
4:D:332:GLN:O	4:D:336:ARG:HB2	2.14	0.46
4:D:1213:THR:O	4:D:1213:THR:OG1	2.30	0.46
4:D:1227:PHE:CE2	4:D:1241:THR:HG21	2.50	0.46
8:H:432:MET:HA	8:H:432:MET:HE2	1.96	0.46
12:M:178:ALA:O	12:M:235:ARG:NH1	2.33	0.46
16:S:486:SER:O	16:S:528:GLN:HA	2.14	0.46
17:J:608:LEU:HD23	17:J:609:LEU:HD22	1.96	0.46
2:B:991:TRP:HB3	4:D:324:GLN:HE21	1.80	0.46
3:C:75:ARG:HH21	3:C:84:PRO:HD2	1.79	0.46
4:D:1170:PHE:HZ	4:D:1252:ARG:O	1.97	0.46
9:I:144:PHE:CD1	9:I:175:LEU:HD11	2.51	0.46
16:S:216:ARG:HH11	16:S:217:PRO:HD3	1.80	0.46
17:J:285:PHE:HD2	17:J:306:VAL:HG23	1.80	0.46
5:E:100:ASP:HB3	5:E:101:PRO:HD3	1.95	0.46
7:G:227:LYS:O	7:G:229:ASP:N	2.35	0.46
1:O:178:PRO:O	1:O:206:ASN:N	2.41	0.46
6:R:114:LEU:HD11	6:R:150:LEU:HD22	1.97	0.46
16:S:402:ILE:HG12	16:S:403:GLU:H	1.80	0.46
17:J:609:LEU:HB3	17:J:645:LYS:HD2	1.96	0.46
2:B:387:ILE:HG12	2:B:575:SER:HA	1.98	0.46
2:B:1034:ASP:OD1	2:B:1035:ALA:N	2.47	0.46
2:B:1040:ARG:O	2:B:1044:ARG:HG2	2.15	0.46
4:D:1219:SER:N	4:D:1250:CYS:O	2.49	0.46
7:G:298:ALA:O	7:G:301:SER:OG	2.30	0.46
8:H:395:GLN:HB3	8:H:396:PRO:CD	2.44	0.46
9:I:378:ARG:HA	9:I:381:TYR:CE1	2.50	0.46
10:K:229:ASN:O	10:K:229:ASN:ND2	2.44	0.46
16:S:377:LEU:HD13	16:S:381:LEU:HB3	1.97	0.46
2:B:213:LYS:NZ	2:B:218:SER:O	2.48	0.46
2:B:991:TRP:HH2	4:D:204:ARG:HG2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:250:ALA:O	4:D:263:ARG:NH1	2.38	0.46
4:D:935:CYS:SG	5:E:334:TYR:HD1	2.39	0.46
8:H:347:LEU:HD23	8:H:347:LEU:HA	1.73	0.46
9:I:130:LEU:HD13	9:I:303:TRP:HH2	1.81	0.46
9:I:441:THR:OG1	9:I:442:THR:N	2.47	0.46
15:Q:112:ARG:HG3	15:Q:112:ARG:O	2.16	0.46
17:J:719:MET:SD	17:J:720:VAL:N	2.89	0.46
1:A:80:ILE:HG22	1:A:82:GLU:H	1.80	0.46
3:C:97:SER:O	3:C:100:ARG:HB2	2.16	0.46
4:D:931:SER:HG	4:D:933:SER:HG	1.63	0.46
10:K:271:LEU:N	10:K:284:THR:O	2.48	0.46
6:R:97:ILE:HG22	6:R:128:VAL:HG23	1.97	0.46
16:S:361:LEU:O	16:S:365:LYS:HG2	2.15	0.46
16:S:432:GLU:HG3	16:S:434:TYR:CE2	2.50	0.46
4:D:430:LEU:CB	4:D:1122:ARG:HA	2.46	0.46
8:H:129:ARG:HD2	8:H:129:ARG:HA	1.75	0.46
9:I:220:GLU:OE2	9:I:224:ARG:NH2	2.40	0.46
17:J:507:LEU:HD23	17:J:550:TYR:HE1	1.81	0.46
17:J:693:ASN:C	17:J:695:HIS:H	2.24	0.46
2:B:391:ARG:HE	2:B:526:ILE:HD11	1.81	0.46
4:D:449:HIS:NE2	4:D:451:SER:HB2	2.30	0.46
8:H:83:ASN:ND2	8:H:85:ASP:OD2	2.49	0.46
8:H:116:VAL:HG23	8:H:149:LEU:HD22	1.96	0.46
9:I:361:SER:O	9:I:362:ARG:HG3	2.16	0.46
13:N:422:ASP:OD1	13:N:484:ARG:NH2	2.48	0.46
3:C:36:GLU:OE1	3:C:108:LYS:N	2.49	0.46
3:C:558:TRP:HA	10:K:298:ARG:HH11	1.80	0.46
7:G:242:ASP:OD1	7:G:243:VAL:N	2.49	0.46
9:I:363:ILE:H	9:I:407:PRO:HB2	1.81	0.46
16:S:204:PHE:CD2	16:S:357:THR:HG23	2.51	0.46
17:J:656:GLN:HB2	17:J:664:ILE:HG13	1.98	0.46
4:D:376:HIS:HD2	7:G:224:ASN:HB3	1.80	0.46
5:E:211:PHE:HZ	6:F:87:VAL:HG12	1.81	0.46
10:K:189:ASP:OD1	10:K:189:ASP:N	2.49	0.46
11:L:81:HIS:CE1	11:L:236:HIS:CD2	3.04	0.46
12:M:150:GLU:O	12:M:249:TRP:NE1	2.46	0.46
15:Q:87:ILE:HG23	15:Q:127:TYR:CE2	2.50	0.46
15:Q:132:SER:O	15:Q:134:ARG:HG3	2.15	0.46
16:S:358:MET:HG2	16:S:394:GLN:HG2	1.98	0.46
17:J:613:ARG:NH1	17:J:645:LYS:HB3	2.31	0.46
1:A:67:SER:HB2	1:A:70:ILE:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:659:TYR:O	4:D:56:SER:OG	2.26	0.45
5:E:114:PHE:CZ	6:F:146:GLY:HA3	2.51	0.45
17:J:718:ASP:OD1	17:J:718:ASP:N	2.44	0.45
1:A:37:LEU:O	1:A:197:GLU:HG2	2.17	0.45
2:B:957:LYS:O	2:B:977:ARG:NH2	2.49	0.45
8:H:111:LEU:HD12	8:H:127:SER:HB3	1.98	0.45
8:H:244:THR:HG21	8:H:280:ASP:HB2	1.99	0.45
8:H:474:PHE:HE1	8:H:480:GLU:HB2	1.81	0.45
9:I:114:LYS:HG2	9:I:115:ASP:N	2.28	0.45
9:I:460:LEU:O	9:I:461:GLU:HB3	2.16	0.45
17:J:623:VAL:HB	17:J:722:VAL:HA	1.98	0.45
3:C:389:SER:OG	14:P:167:GLU:CD	2.58	0.45
4:D:1238:ALA:HB1	4:D:1251:TYR:CE1	2.51	0.45
11:L:107:LEU:HD23	11:L:108:GLU:N	2.30	0.45
6:R:76:LYS:O	6:R:77:LYS:HG3	2.16	0.45
16:S:198:PRO:HA	16:S:199:PRO:HD2	1.84	0.45
16:S:478:MET:HB2	16:S:478:MET:HE2	1.54	0.45
17:J:621:ILE:HA	17:J:648:VAL:O	2.16	0.45
1:A:225:LEU:HB3	1:O:45:ILE:HD11	1.97	0.45
3:C:242:ASP:O	3:C:245:VAL:HG12	2.17	0.45
3:C:389:SER:HB2	14:P:167:GLU:CD	2.41	0.45
3:C:470:LEU:HA	3:C:470:LEU:HD23	1.81	0.45
8:H:285:ASN:HD21	8:H:320:ASN:HD21	1.63	0.45
8:H:775:ARG:NE	8:H:778:SER:OG	2.48	0.45
9:I:381:TYR:HB3	9:I:400:ILE:HD11	1.98	0.45
10:K:192:TRP:CD1	10:K:213:GLU:HB3	2.52	0.45
11:L:65:PRO:HG2	11:L:68:ALA:HB3	1.98	0.45
1:O:216:TYR:CE1	16:S:539:PRO:HD2	2.51	0.45
16:S:199:PRO:HG3	16:S:339:LYS:HD2	1.99	0.45
16:S:214:SER:O	16:S:241:ILE:HD11	2.16	0.45
16:S:241:ILE:O	16:S:241:ILE:HG22	2.16	0.45
1:A:39:LYS:HB3	1:A:39:LYS:HE3	1.68	0.45
3:C:245:VAL:CG2	4:D:1229:PRO:HD2	2.47	0.45
7:G:334:MET:HG2	7:G:335:LEU:HD22	1.98	0.45
8:H:104:GLY:O	8:H:105:PRO:C	2.59	0.45
2:B:541:ARG:O	2:B:545:SER:OG	2.27	0.45
5:E:363:LEU:HD23	5:E:363:LEU:HA	1.84	0.45
9:I:195:PRO:O	9:I:258:TRP:NE1	2.46	0.45
10:K:156:PHE:O	10:K:158:GLU:N	2.49	0.45
11:L:56:LYS:HA	11:L:56:LYS:HD2	1.37	0.45
1:O:90:ASN:ND2	1:O:136:ILE:O	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:ASN:H	2:B:215:LYS:HD3	1.82	0.45
4:D:1022:ASP:N	13:N:298:VAL:O	2.49	0.45
5:E:234:GLU:H	5:E:234:GLU:HG2	1.68	0.45
8:H:378:GLY:HA2	8:H:474:PHE:CZ	2.52	0.45
6:R:103:TRP:CD2	16:S:241:ILE:HG13	2.52	0.45
16:S:231:LYS:O	16:S:234:LEU:HG	2.17	0.45
16:S:396:TRP:CZ3	16:S:412:LEU:HD13	2.49	0.45
16:S:470:VAL:HG12	16:S:471:LEU:H	1.81	0.45
17:J:247:LEU:HB2	17:J:267:VAL:HG13	1.98	0.45
17:J:354:THR:HB	17:J:468:LEU:HD22	1.98	0.45
1:A:116:VAL:HB	1:A:137:ALA:HB3	1.98	0.45
1:A:169:SER:OG	1:A:169:SER:O	2.34	0.45
2:B:183:LEU:HD23	2:B:224:LEU:HA	1.98	0.45
4:D:331:THR:C	4:D:334:THR:H	2.25	0.45
8:H:340:ALA:O	8:H:341:ILE:C	2.59	0.45
9:I:420:VAL:HG23	9:I:424:ALA:H	1.81	0.45
16:S:360:ALA:HA	16:S:363:ILE:HB	1.98	0.45
17:J:588:GLU:N	17:J:590:GLN:OE1	2.48	0.45
17:J:605:LEU:O	17:J:609:LEU:HD23	2.17	0.45
2:B:49:GLU:HB3	2:B:87:ILE:HB	1.98	0.45
3:C:130:LEU:HD11	3:C:203:LEU:HD12	1.99	0.45
8:H:346:ALA:O	8:H:347:LEU:C	2.60	0.45
8:H:810:ARG:O	8:H:814:LYS:NZ	2.49	0.45
12:M:64:LYS:O	13:N:204:ARG:NH2	2.49	0.45
17:J:505:PHE:CD2	17:J:553:LEU:HB3	2.51	0.45
3:C:11:ARG:HG2	4:D:1290:ILE:HG12	1.99	0.45
3:C:118:TYR:O	3:C:124:SER:OG	2.33	0.45
4:D:1142:ILE:O	4:D:1146:SER:OG	2.28	0.45
16:S:406:LYS:HE3	16:S:432:GLU:HG2	1.98	0.45
16:S:523:CYS:O	16:S:527:GLU:HG2	2.17	0.45
16:S:530:ILE:HD13	16:S:536:GLY:HA2	1.99	0.45
17:J:521:LEU:HG	17:J:615:LEU:HD11	1.98	0.45
17:J:687:TYR:HB2	17:J:688:TYR:CE1	2.51	0.45
4:D:918:LEU:HB3	4:D:919[A]:GLY:H	1.62	0.44
4:D:918:LEU:HB3	4:D:919[B]:GLY:H	1.62	0.44
4:D:1219:SER:H	4:D:1251:TYR:HA	1.82	0.44
10:K:271:LEU:HD13	10:K:289:ARG:HB3	2.00	0.44
16:S:492:LEU:O	16:S:496:LEU:HD12	2.16	0.44
17:J:380:MET:HA	17:J:385:TYR:CE1	2.53	0.44
2:B:857:VAL:HB	2:B:858:PRO:HD3	1.99	0.44
4:D:500:THR:O	4:D:501:HIS:ND1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:472:TRP:CD1	5:E:472:TRP:C	2.95	0.44
11:L:93:LEU:HD22	11:L:127:ALA:HA	1.99	0.44
11:L:95:LYS:HA	11:L:98:VAL:HG23	1.99	0.44
14:P:141:MET:HE3	14:P:146:PHE:CD2	2.52	0.44
17:J:379:MET:HB3	17:J:386:TYR:H	1.81	0.44
2:B:855:LEU:HD22	4:D:137:ARG:HB3	1.98	0.44
4:D:1170:PHE:CZ	4:D:1252:ARG:HA	2.52	0.44
15:Q:62:VAL:HG13	15:Q:65:TRP:CE3	2.52	0.44
6:R:95:LEU:HB2	6:R:126:MET:HG2	1.99	0.44
16:S:268:LEU:HD12	16:S:278:LEU:HG	2.00	0.44
16:S:330:ILE:HG13	16:S:356:THR:HG23	1.98	0.44
17:J:489:ALA:HB3	17:J:490:PRO:HD3	2.00	0.44
2:B:97:GLN:HG2	2:B:352:PRO:HG2	1.99	0.44
3:C:439:LYS:O	3:C:443:GLU:HB2	2.18	0.44
8:H:104:GLY:HA2	9:I:490:PHE:CD2	2.52	0.44
8:H:427:TYR:HA	8:H:834:ARG:NH2	2.32	0.44
8:H:724:GLU:HB2	8:H:726:ASP:OD2	2.18	0.44
9:I:414:VAL:O	9:I:414:VAL:HG13	2.18	0.44
10:K:115:GLY:HA3	10:K:116:TRP:HA	1.64	0.44
13:N:427:ASN:HB3	13:N:430:LYS:HG2	1.99	0.44
6:R:92:ASN:N	6:R:92:ASN:OD1	2.49	0.44
16:S:200:LEU:HD21	16:S:263:ALA:HB3	2.00	0.44
17:J:333:LEU:HB3	17:J:334:PRO:HD3	1.99	0.44
17:J:605:LEU:HD22	17:J:605:LEU:H	1.82	0.44
2:B:65:LYS:O	2:B:69:ALA:N	2.47	0.44
2:B:83:SER:HA	2:B:98:THR:HA	1.99	0.44
8:H:319:PRO:HG2	8:H:761:TRP:CD1	2.49	0.44
9:I:362:ARG:HA	9:I:407:PRO:HB3	2.00	0.44
16:S:239:LYS:N	16:S:242:ARG:HB2	2.32	0.44
17:J:537:LEU:HD22	17:J:566:LEU:HB3	1.99	0.44
17:J:600:ARG:HH12	17:J:655:ASN:HD22	1.65	0.44
2:B:177:LYS:HZ3	2:B:230:PHE:HD2	1.64	0.44
4:D:1019:TYR:HA	13:N:280:ILE:O	2.17	0.44
4:D:1138:GLU:HB3	4:D:1140:ARG:HD3	2.00	0.44
5:E:457:SER:OG	7:G:374:ASP:OD2	2.35	0.44
7:G:208:VAL:HG23	7:G:209:LYS:N	2.30	0.44
7:G:217:THR:OG1	7:G:219:GLU:CD	2.61	0.44
8:H:387:LEU:HA	8:H:390:MET:HE3	2.00	0.44
13:N:446:ASP:HB3	13:N:449:HIS:CE1	2.53	0.44
13:N:475:LEU:HD12	13:N:475:LEU:HA	1.81	0.44
16:S:402:ILE:HD13	16:S:404:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:LEU:O	2:B:205:LEU:HD12	2.17	0.44
2:B:230:PHE:CE1	2:B:237:PRO:HG2	2.53	0.44
3:C:461:LEU:HD12	3:C:528:ILE:HG12	2.00	0.44
6:F:80:ALA:O	6:F:84:THR:HG23	2.16	0.44
9:I:294:SER:HB3	9:I:327:THR:HG21	1.99	0.44
6:R:143:GLN:HG3	16:S:315:THR:CA	2.45	0.44
3:C:99:ILE:CD1	3:C:103:GLN:HG2	2.47	0.44
4:D:105:TYR:CE1	4:D:348:THR:HG22	2.53	0.44
4:D:447:GLU:OE2	4:D:1086:ARG:NH2	2.51	0.44
8:H:758:ALA:HB1	8:H:764:THR:H	1.83	0.44
9:I:214:LEU:HD21	9:I:219:LEU:HD23	1.99	0.44
9:I:369:LEU:O	9:I:374:ILE:N	2.51	0.44
9:I:383:TYR:CD2	9:I:395:VAL:HG21	2.52	0.44
13:N:406:TYR:CE1	13:N:409:LYS:HE2	2.52	0.44
16:S:198:PRO:HG2	16:S:261:ARG:HB2	1.99	0.44
2:B:61:GLU:HG2	2:B:62:PRO:HD2	2.00	0.44
2:B:210:ASP:C	2:B:212:GLU:H	2.25	0.44
2:B:1015:ALA:HA	2:B:1018:GLU:CD	2.43	0.44
4:D:365:ASP:OD1	4:D:365:ASP:N	2.51	0.44
5:E:202:THR:HA	5:E:226:ALA:HB3	2.00	0.44
6:F:68:HIS:HB2	7:G:409:LYS:NZ	2.32	0.44
9:I:172:LEU:HD23	9:I:263:ALA:HB1	1.99	0.44
13:N:190:GLU:CD	13:N:231:GLN:HE21	2.25	0.44
1:O:104:CYS:SG	1:O:151:LEU:HB2	2.58	0.44
2:B:309:LEU:HD23	2:B:309:LEU:HA	1.80	0.43
4:D:394:ILE:HB	4:D:396:HIS:CE1	2.53	0.43
9:I:383:TYR:CE1	9:I:385:SER:HA	2.53	0.43
11:L:74:SER:O	11:L:77:THR:OG1	2.33	0.43
11:L:132:ASN:HD21	11:L:219:ASN:CG	2.24	0.43
11:L:179:GLY:O	11:L:246:ARG:NH2	2.51	0.43
6:R:151:TYR:HA	6:R:163:ARG:HA	1.99	0.43
16:S:405:THR:HG22	16:S:454:ASN:H	1.82	0.43
17:J:360:THR:O	17:J:364:HIS:ND1	2.30	0.43
2:B:202:GLU:HG3	2:B:205:LEU:HD23	2.00	0.43
3:C:394:ARG:HD3	3:C:469:ILE:HD13	2.00	0.43
3:C:532:THR:H	3:C:535:MET:HE3	1.83	0.43
9:I:367:THR:HB	9:I:484:TYR:HE1	1.83	0.43
13:N:370:GLU:N	13:N:370:GLU:OE1	2.52	0.43
1:O:17:CYS:HB2	1:O:32:PHE:HD1	1.82	0.43
16:S:423:THR:HG21	16:S:430:LYS:HA	1.99	0.43
17:J:472:MET:HG3	17:J:480:LYS:HE3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:188:GLY:O	2:B:189:SER:C	2.62	0.43
7:G:308:LYS:HE2	7:G:308:LYS:HB2	1.73	0.43
8:H:289:GLN:OE1	8:H:322:ARG:NH2	2.50	0.43
9:I:247:LYS:O	9:I:248:ARG:HG2	2.18	0.43
11:L:94:ASN:O	11:L:98:VAL:HG23	2.18	0.43
6:R:87:VAL:O	6:R:88:ARG:NH1	2.51	0.43
17:J:596:VAL:HA	17:J:723:ALA:HB2	1.99	0.43
17:J:602:PRO:HG3	17:J:634:LYS:HB2	2.00	0.43
2:B:591:ASN:C	2:B:593:ASP:H	2.26	0.43
3:C:550:ILE:H	10:K:304:THR:HG21	1.83	0.43
7:G:303:TRP:O	7:G:342:GLU:HB3	2.19	0.43
8:H:476:GLN:HG2	8:H:810:ARG:NH2	2.33	0.43
8:H:487:ARG:O	8:H:491:ARG:N	2.50	0.43
9:I:420:VAL:O	9:I:424:ALA:N	2.46	0.43
13:N:395:VAL:O	13:N:395:VAL:HG12	2.19	0.43
1:O:202:GLU:OE1	14:P:82:ARG:NH2	2.52	0.43
6:R:107:CYS:SG	6:R:147:LEU:HD13	2.57	0.43
16:S:202:CYS:HB3	16:S:265:MET:HG2	2.00	0.43
1:A:89:MET:HE2	1:A:89:MET:HA	1.99	0.43
2:B:742:LEU:HD23	2:B:742:LEU:HA	1.85	0.43
2:B:1044:ARG:HA	2:B:1044:ARG:HD3	1.74	0.43
3:C:44:HIS:CB	3:C:49:LYS:HD3	2.49	0.43
3:C:245:VAL:HA	3:C:248:MET:HE2	2.01	0.43
5:E:101:PRO:O	5:E:164:ARG:NH1	2.45	0.43
8:H:302:ASP:OD1	8:H:302:ASP:N	2.49	0.43
8:H:343:HIS:O	8:H:344:PHE:C	2.59	0.43
10:K:257:VAL:HG22	10:K:283:ILE:HD12	1.99	0.43
13:N:165:TRP:CE3	13:N:169:LEU:HD11	2.54	0.43
13:N:472:VAL:HA	13:N:475:LEU:HB2	2.01	0.43
16:S:428:ARG:HA	16:S:428:ARG:NE	2.32	0.43
16:S:428:ARG:NE	16:S:429:PHE:H	2.15	0.43
16:S:428:ARG:HE	16:S:429:PHE:H	1.66	0.43
16:S:458:LYS:HG3	16:S:470:VAL:O	2.18	0.43
16:S:476:ALA:HB1	16:S:529:TRP:HB3	2.00	0.43
1:A:111:ARG:HA	1:A:111:ARG:HD3	1.69	0.43
2:B:230:PHE:CD1	2:B:237:PRO:HG2	2.54	0.43
3:C:272:LEU:HD12	3:C:356:PHE:CE1	2.54	0.43
4:D:1146:SER:HA	4:D:1150:GLU:H	1.83	0.43
5:E:125:MET:HE3	5:E:125:MET:HB3	1.84	0.43
8:H:250:LEU:O	8:H:254:GLN:HG3	2.18	0.43
8:H:307:LEU:HD12	8:H:307:LEU:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:131:PHE:CD2	10:K:142:PHE:HB3	2.51	0.43
12:M:215:ILE:HG21	12:M:259:ALA:HB2	2.00	0.43
13:N:515:TYR:HD1	13:N:515:TYR:HA	1.72	0.43
16:S:303:GLN:O	16:S:317:VAL:HG12	2.19	0.43
16:S:405:THR:HG22	16:S:454:ASN:N	2.33	0.43
17:J:693:ASN:ND2	17:J:693:ASN:H	2.16	0.43
2:B:177:LYS:HD2	2:B:177:LYS:HA	1.65	0.43
3:C:227:SER:OG	3:C:228:THR:N	2.51	0.43
4:D:293:SER:O	4:D:1210:ARG:NH2	2.52	0.43
4:D:1170:PHE:CE2	4:D:1251:TYR:O	2.72	0.43
8:H:236:GLU:HA	8:H:240:ARG:O	2.18	0.43
8:H:768:GLU:O	8:H:772:ARG:HG3	2.19	0.43
10:K:174:VAL:HG22	10:K:178:MET:HE3	2.01	0.43
13:N:207:MET:SD	13:N:207:MET:N	2.88	0.43
16:S:307:ALA:HB3	16:S:315:THR:HG22	2.01	0.43
17:J:697:LEU:HD23	17:J:697:LEU:HA	1.84	0.43
17:J:708:ARG:HH12	17:J:756:LEU:HD21	1.83	0.43
2:B:918:GLU:OE1	7:G:355:ARG:NH1	2.42	0.43
2:B:1040:ARG:O	2:B:1043:VAL:HG12	2.18	0.43
9:I:402:ALA:O	9:I:406:LEU:HD22	2.19	0.43
9:I:465:LYS:HD2	9:I:465:LYS:HA	1.58	0.43
12:M:158:GLN:OE1	12:M:158:GLN:N	2.30	0.43
13:N:281:CYS:N	13:N:328:VAL:O	2.40	0.43
14:P:148:ARG:HD2	14:P:152:TYR:HE1	1.83	0.43
6:R:116:MET:HE2	6:R:116:MET:HB2	1.88	0.43
16:S:402:ILE:C	16:S:403:GLU:CD	2.86	0.43
2:B:793:LYS:HB2	2:B:801:PRO:HD2	2.01	0.43
2:B:1007:THR:OG1	2:B:1008:TYR:N	2.52	0.43
4:D:198:ASP:N	4:D:198:ASP:OD1	2.51	0.43
4:D:1273:SER:OG	4:D:1297:LYS:HD3	2.19	0.43
7:G:228:PRO:O	7:G:230:LYS:N	2.52	0.43
8:H:487:ARG:HA	8:H:487:ARG:NE	2.34	0.43
9:I:182:GLN:C	9:I:183:GLU:HG3	2.44	0.43
14:P:91:MET:HE1	14:P:134:HIS:CG	2.54	0.43
15:Q:39:PRO:HD2	15:Q:42:GLU:OE2	2.19	0.43
17:J:521:LEU:HG	17:J:615:LEU:HD21	2.01	0.43
17:J:749:ALA:O	17:J:753:VAL:HG23	2.18	0.43
1:A:53:LEU:HD23	1:A:57:ILE:HD11	2.00	0.43
2:B:777:LEU:HD12	2:B:777:LEU:HA	1.77	0.43
5:E:342:LYS:HA	5:E:342:LYS:HD2	1.91	0.43
10:K:156:PHE:CE1	10:K:183:ILE:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:172:THR:O	11:L:176:THR:HG23	2.19	0.43
15:Q:89:GLU:O	15:Q:127:TYR:HA	2.18	0.43
6:R:137:GLU:O	6:R:141:ASP:HB2	2.19	0.43
17:J:379:MET:HE2	17:J:379:MET:HA	2.00	0.43
1:A:96:LEU:HD23	1:A:129:ILE:HG22	1.99	0.42
2:B:309:LEU:HG	2:B:417:HIS:CE1	2.54	0.42
2:B:1049:LEU:HD11	3:C:356:PHE:HB3	2.00	0.42
4:D:1125:ASP:OD1	4:D:1128:GLN:HG2	2.18	0.42
4:D:1176:LEU:HD21	8:H:742:GLU:HG2	2.01	0.42
13:N:533:ASP:OD2	15:Q:115:LYS:HE2	2.19	0.42
16:S:505:HIS:C	16:S:507:ILE:HG12	2.44	0.42
17:J:636:PRO:HG3	17:J:670:ALA:HB3	2.01	0.42
3:C:619:PRO:HG2	10:K:190:TYR:CZ	2.54	0.42
6:F:152:PHE:HB2	6:F:162:ILE:HB	2.01	0.42
8:H:125:MET:O	8:H:129:ARG:N	2.52	0.42
10:K:174:VAL:HG13	10:K:178:MET:HE2	2.00	0.42
11:L:235:GLU:O	11:L:239:TYR:HB2	2.18	0.42
13:N:434:LYS:HE2	13:N:436:LEU:HD11	2.00	0.42
1:O:100:LEU:HD13	1:O:126:TYR:HE2	1.84	0.42
6:R:108:ILE:O	6:R:112:GLN:HG3	2.19	0.42
16:S:271:ASP:O	16:S:275:GLN:N	2.41	0.42
16:S:297:ARG:HG3	16:S:318:LYS:CE	2.47	0.42
17:J:669:LEU:CB	17:J:676:MET:HE3	2.48	0.42
2:B:675:GLU:O	2:B:678:VAL:HG22	2.19	0.42
2:B:691:TYR:HB3	2:B:775:LEU:HD21	2.00	0.42
3:C:142:TYR:HE1	3:C:341:ARG:HH12	1.67	0.42
3:C:147:PHE:H	3:C:164:PHE:HB2	1.84	0.42
4:D:491:LEU:HD21	13:N:377:LEU:HD22	2.01	0.42
5:E:104:ILE:HD12	5:E:245:ILE:HB	2.01	0.42
9:I:383:TYR:HD2	9:I:395:VAL:HG21	1.84	0.42
9:I:479:ASP:O	9:I:483:ILE:HG12	2.20	0.42
16:S:243:ALA:N	16:S:244:PRO:HD3	2.34	0.42
16:S:412:LEU:HD23	16:S:412:LEU:HA	1.84	0.42
17:J:627:CYS:SG	17:J:631:GLU:HB2	2.60	0.42
17:J:725:LYS:HZ1	17:J:742:ASP:HB2	1.84	0.42
1:A:225:LEU:CB	1:O:45:ILE:HD11	2.50	0.42
2:B:168:ILE:O	2:B:168:ILE:HG13	2.19	0.42
2:B:710:PRO:HD3	2:B:742:LEU:HD11	2.00	0.42
3:C:159:ARG:HG3	17:J:767:PRO:C	2.43	0.42
3:C:459:HIS:HB3	4:D:328:GLU:HG3	2.00	0.42
3:C:558:TRP:CE3	10:K:298:ARG:HD3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1077:ILE:HD12	4:D:1084:VAL:HG21	2.01	0.42
8:H:315:LYS:HE3	8:H:315:LYS:HA	2.02	0.42
9:I:250:ALA:HA	9:I:255:ILE:HD11	2.01	0.42
9:I:307:ASP:O	10:K:204:ARG:NH2	2.53	0.42
11:L:242:PHE:HZ	11:L:252:ILE:HD11	1.85	0.42
1:O:18:VAL:HG22	1:O:33:ILE:HD11	2.00	0.42
14:P:82:ARG:O	14:P:85:ASN:N	2.41	0.42
6:R:78:LEU:HD23	6:R:82:GLU:HB3	2.02	0.42
6:R:103:TRP:HZ2	16:S:215:GLY:HA2	1.85	0.42
6:R:159:LYS:HD3	6:R:159:LYS:HA	1.77	0.42
16:S:214:SER:HB2	16:S:377:LEU:O	2.20	0.42
16:S:313:ARG:HA	16:S:313:ARG:HD2	1.64	0.42
16:S:343:LEU:HA	16:S:343:LEU:HD23	1.66	0.42
16:S:502:VAL:HG23	16:S:503:GLN:HG2	2.01	0.42
17:J:588:GLU:HB2	17:J:750:LEU:HD13	2.01	0.42
1:A:50:ARG:HA	1:A:182:VAL:HG11	2.01	0.42
2:B:569:ARG:HG2	2:B:648:GLU:HG2	2.01	0.42
5:E:301:TRP:CZ2	5:E:358:LEU:HB3	2.54	0.42
9:I:125:ILE:HG23	9:I:312:VAL:HB	2.00	0.42
9:I:354:ALA:HA	9:I:473:PHE:CZ	2.54	0.42
9:I:421:GLU:O	9:I:426:LYS:HB2	2.19	0.42
11:L:58:ASP:OD1	11:L:58:ASP:N	2.37	0.42
13:N:184:TRP:HH2	13:N:238:PHE:HD2	1.68	0.42
13:N:272:LEU:HG	13:N:302:TYR:CD2	2.54	0.42
16:S:409:LEU:HD13	16:S:442:LEU:HD21	2.01	0.42
16:S:478:MET:HE1	16:S:529:TRP:CB	2.43	0.42
17:J:299:ASP:HB2	17:J:318:LEU:HD13	2.01	0.42
17:J:659:GLU:HG3	17:J:664:ILE:HG12	2.02	0.42
1:A:175:LEU:H	1:A:175:LEU:HD23	1.85	0.42
2:B:107:MET:HG3	2:B:113:PHE:CE1	2.54	0.42
2:B:1015:ALA:O	2:B:1018:GLU:HG2	2.20	0.42
4:D:1152:ARG:NH1	8:H:731:TRP:HB3	2.33	0.42
5:E:217:MET:SD	6:F:84:THR:HA	2.59	0.42
7:G:203:PHE:HD2	10:K:321:SER:HB2	1.85	0.42
7:G:212:ILE:HD12	7:G:212:ILE:HA	1.94	0.42
8:H:104:GLY:O	8:H:107:SER:N	2.53	0.42
8:H:463:GLY:HA3	8:H:466:TYR:HE1	1.85	0.42
9:I:79:ASN:O	9:I:103:GLU:N	2.48	0.42
9:I:320:ILE:HD13	9:I:320:ILE:HA	1.93	0.42
9:I:437:ALA:HB3	9:I:440:PRO:HB3	2.02	0.42
9:I:460:LEU:C	9:I:462:ALA:H	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:148:PRO:HB2	11:L:153:LEU:HG	2.01	0.42
1:O:220:ARG:NH2	1:O:224:ASP:OD2	2.52	0.42
6:R:98:ASP:HB2	6:R:150:LEU:HD23	2.02	0.42
6:R:154:SER:HB3	6:R:181:MET:HE3	2.01	0.42
16:S:201:VAL:CG1	16:S:340:MET:HB3	2.49	0.42
17:J:596:VAL:HB	17:J:743:ARG:NH2	2.35	0.42
17:J:650:MET:HE3	17:J:651:LEU:N	2.30	0.42
2:B:965:HIS:HB3	2:B:974:LEU:HD23	2.02	0.42
3:C:46:LYS:O	3:C:47:THR:C	2.61	0.42
4:D:1077:ILE:HA	13:N:288:LEU:O	2.19	0.42
7:G:193:LYS:HA	7:G:193:LYS:HD2	1.79	0.42
8:H:376:ARG:NH1	8:H:471:GLU:HA	2.35	0.42
9:I:262:ILE:HD13	9:I:262:ILE:HA	1.86	0.42
10:K:223:TYR:O	10:K:226:ARG:HG3	2.19	0.42
13:N:236:VAL:HG22	13:N:271:GLU:HG3	2.00	0.42
1:O:24:SER:OG	1:O:25:LYS:N	2.52	0.42
6:R:104:CYS:O	6:R:105:GLY:C	2.62	0.42
16:S:197:TRP:N	16:S:198:PRO:HD2	2.34	0.42
16:S:237:PRO:HG2	16:S:242:ARG:HG3	2.02	0.42
16:S:458:LYS:HZ2	16:S:460:HIS:CE1	2.37	0.42
17:J:273:GLU:O	17:J:285:PHE:N	2.53	0.42
1:A:113:PRO:HD3	1:A:142:PRO:HA	2.02	0.42
2:B:8:GLY:HA2	2:B:13:PRO:HD3	2.00	0.42
2:B:534:ILE:HG22	2:B:886:PRO:HB3	2.01	0.42
4:D:331:THR:O	4:D:335:LEU:HG	2.18	0.42
4:D:448:MET:HA	4:D:475:TRP:O	2.19	0.42
5:E:283:PRO:HD2	5:E:286:LEU:HD22	2.02	0.42
9:I:460:LEU:HD23	9:I:460:LEU:HA	1.87	0.42
11:L:196:ASN:OD1	11:L:199:ASN:ND2	2.53	0.42
11:L:203:SER:HB3	11:L:204:GLU:H	1.68	0.42
12:M:85:TRP:HD1	12:M:141:TRP:NE1	2.18	0.42
12:M:218:ILE:HD11	12:M:252:ALA:HB2	2.02	0.42
13:N:394:LYS:HG3	13:N:396:GLU:HB3	2.02	0.42
15:Q:70:THR:OG1	15:Q:71:GLY:N	2.52	0.42
6:R:117:LEU:HD23	6:R:117:LEU:HA	1.70	0.42
16:S:298:TRP:HB3	16:S:301:MET:HG3	2.00	0.42
16:S:306:ILE:HG22	16:S:308:LYS:HE3	2.02	0.42
16:S:477:PRO:C	16:S:483:GLN:HE22	2.28	0.42
17:J:317:THR:C	17:J:318:LEU:HD22	2.45	0.42
2:B:25:ARG:NH1	2:B:25:ARG:HG2	2.34	0.42
2:B:391:ARG:NE	2:B:526:ILE:HD11	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:622:VAL:HG23	3:C:632:GLU:HG2	2.02	0.42
4:D:496:ASP:O	4:D:914:VAL:HG23	2.20	0.42
4:D:938:ILE:HG23	4:D:1068:THR:HG21	2.02	0.42
5:E:203:ALA:O	6:F:164:THR:HA	2.20	0.42
7:G:217:THR:OG1	7:G:218:SER:N	2.52	0.42
8:H:106:ARG:HH22	9:I:370:SER:HB3	1.85	0.42
8:H:181:VAL:O	8:H:185:VAL:HG23	2.20	0.42
11:L:239:TYR:CE2	12:M:225:HIS:HA	2.54	0.42
16:S:242:ARG:HE	16:S:474:GLU:HG3	1.84	0.42
17:J:321:LYS:HD2	17:J:321:LYS:HA	1.94	0.42
17:J:691:LEU:O	17:J:694:GLY:N	2.52	0.42
1:A:13:LEU:HD11	1:A:34:LEU:HD23	2.01	0.42
2:B:181:LEU:HD13	2:B:219:LYS:HG3	2.02	0.42
2:B:678:VAL:HG12	2:B:814:ILE:HG23	2.01	0.42
2:B:745:GLN:HG2	2:B:748:LYS:HE2	2.01	0.42
2:B:760:ARG:HD3	2:B:767:VAL:HG22	2.02	0.42
3:C:239:ARG:HG3	3:C:239:ARG:NH1	2.34	0.42
3:C:359:VAL:HG12	3:C:366:ARG:HG2	2.02	0.42
3:C:536:LEU:HD21	4:D:16:GLY:HA2	2.02	0.42
3:C:611:ARG:HB3	4:D:9:PHE:H	1.85	0.42
4:D:451:SER:O	4:D:452:THR:HB	2.20	0.42
4:D:475:TRP:NE1	13:N:94:GLU:OE2	2.46	0.42
4:D:1120:LYS:HE2	4:D:1122:ARG:NE	2.35	0.42
12:M:222:LEU:HD13	12:M:235:ARG:HH22	1.85	0.42
1:O:45:ILE:HD13	1:O:45:ILE:HA	1.73	0.42
2:B:294:ILE:HG13	2:B:295:GLY:N	2.35	0.41
2:B:588:ILE:HD13	2:B:598:LEU:HB2	2.02	0.41
2:B:712:LEU:HD12	2:B:712:LEU:HA	1.90	0.41
2:B:1012:HIS:CB	2:B:1015:ALA:HB3	2.50	0.41
3:C:61:PHE:HD1	3:C:103:GLN:HB3	1.85	0.41
3:C:113:VAL:HG11	3:C:332:VAL:HG11	2.02	0.41
3:C:159:ARG:HA	17:J:767:PRO:HB2	2.01	0.41
3:C:443:GLU:HG2	14:P:129:HIS:CD2	2.55	0.41
4:D:218:ARG:HG2	4:D:219:ASP:H	1.85	0.41
4:D:298:CYS:SG	4:D:300:LEU:N	2.90	0.41
4:D:370:THR:CG2	4:D:380:LEU:HD12	2.50	0.41
4:D:1236:PHE:HB3	4:D:1240:ARG:HH11	1.85	0.41
8:H:146:LEU:HD23	8:H:146:LEU:HA	1.89	0.41
8:H:331:PHE:O	8:H:336:VAL:HG23	2.20	0.41
8:H:838:PRO:C	8:H:840:TYR:N	2.78	0.41
11:L:187:TYR:CZ	11:L:207:LYS:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:201:LYS:HE3	11:L:201:LYS:HB2	1.88	0.41
14:P:165:LEU:HD23	14:P:165:LEU:HA	1.90	0.41
6:R:141:ASP:O	16:S:313:ARG:HD2	2.20	0.41
16:S:396:TRP:O	16:S:396:TRP:CG	2.73	0.41
16:S:439:ILE:HG21	16:S:462:TYR:CE2	2.55	0.41
17:J:272:ILE:HG21	17:J:341:PHE:CE2	2.55	0.41
17:J:282:GLY:HA2	17:J:304:VAL:HG13	2.02	0.41
17:J:674:TRP:CH2	17:J:697:LEU:HD11	2.55	0.41
17:J:709:CYS:HA	17:J:712:ALA:HB3	2.01	0.41
3:C:140:LEU:HD23	3:C:199:ILE:HG13	2.02	0.41
3:C:260:GLU:HB2	3:C:263:TRP:CE2	2.55	0.41
6:F:114:LEU:HD23	6:F:114:LEU:HA	1.88	0.41
7:G:187:GLU:HB3	7:G:188:LEU:H	1.75	0.41
7:G:205:ASP:O	7:G:209:LYS:HG3	2.20	0.41
8:H:790:MET:O	8:H:794:ILE:HG13	2.20	0.41
9:I:423:LYS:HB3	9:I:423:LYS:HE2	1.82	0.41
12:M:64:LYS:HE2	12:M:64:LYS:HB2	1.89	0.41
15:Q:92:VAL:CG1	15:Q:121:LEU:HD22	2.50	0.41
6:R:98:ASP:OD1	6:R:99:PHE:N	2.52	0.41
6:R:99:PHE:HE2	6:R:138:PHE:CD2	2.38	0.41
16:S:200:LEU:HD23	16:S:201:VAL:H	1.85	0.41
16:S:296:LYS:HG3	16:S:297:ARG:HH11	1.84	0.41
16:S:305:LYS:CG	16:S:317:VAL:HB	2.50	0.41
16:S:336:LYS:HA	16:S:367:LEU:HD12	2.02	0.41
2:B:171:ARG:NH1	2:B:175:LYS:HA	2.36	0.41
2:B:524:PHE:HE2	2:B:887:PHE:HE2	1.67	0.41
3:C:231:GLU:O	3:C:235:ARG:HG2	2.21	0.41
3:C:450:VAL:HG22	3:C:468:PRO:HD3	2.02	0.41
3:C:452:LEU:HD12	3:C:466:PHE:CD2	2.54	0.41
4:D:332:GLN:HA	4:D:335:LEU:HB2	2.01	0.41
5:E:326:ARG:NH2	5:E:346:ASP:OD2	2.48	0.41
8:H:348:LYS:HB2	8:H:348:LYS:HE2	1.32	0.41
8:H:724:GLU:O	8:H:725:ASN:C	2.63	0.41
10:K:112:SER:OG	10:K:113:THR:N	2.52	0.41
10:K:305:ARG:NH2	10:K:324:ILE:HG23	2.34	0.41
12:M:62:LEU:HG	12:M:93:LEU:HD23	2.02	0.41
1:O:69:LYS:HE2	1:O:69:LYS:HB2	1.77	0.41
16:S:530:ILE:HG21	16:S:536:GLY:CA	2.50	0.41
17:J:514:VAL:HG22	17:J:533:PRO:HD3	2.01	0.41
17:J:725:LYS:NZ	17:J:742:ASP:HB2	2.36	0.41
1:A:142:PRO:C	1:A:143:ILE:HD12	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ASN:O	1:A:224:ASP:HB2	2.20	0.41
3:C:47:THR:O	3:C:49:LYS:N	2.53	0.41
3:C:149:ARG:HD2	3:C:161:ARG:HB2	2.02	0.41
4:D:456:HIS:O	13:N:79:ALA:HB1	2.21	0.41
7:G:380:ILE:HD12	7:G:380:ILE:HA	1.94	0.41
9:I:482:GLU:HA	9:I:485:GLN:HE21	1.85	0.41
16:S:242:ARG:O	16:S:485:MET:SD	2.79	0.41
17:J:549:ILE:HG12	17:J:549:ILE:H	1.68	0.41
17:J:609:LEU:HD12	17:J:645:LYS:CB	2.51	0.41
17:J:688:TYR:N	17:J:689:PRO:HD3	2.35	0.41
2:B:695:THR:HG22	2:B:741:LYS:HD3	2.01	0.41
3:C:98:ARG:O	3:C:101:ARG:HG2	2.20	0.41
3:C:596:ILE:HB	3:C:600:SER:OG	2.21	0.41
3:C:606:TRP:HZ2	3:C:611:ARG:HD3	1.85	0.41
3:C:669:ILE:HD13	3:C:669:ILE:HA	1.84	0.41
4:D:1122:ARG:O	4:D:1123:SER:C	2.62	0.41
8:H:77:LEU:HD12	8:H:92:VAL:HG12	2.03	0.41
8:H:347:LEU:O	8:H:348:LYS:C	2.63	0.41
13:N:240:LYS:HE3	13:N:265:TYR:CE2	2.55	0.41
13:N:272:LEU:HA	13:N:272:LEU:HD23	1.83	0.41
15:Q:65:TRP:CD2	15:Q:132:SER:HB2	2.55	0.41
16:S:222:ILE:HD13	16:S:232:GLU:HB3	2.02	0.41
16:S:339:LYS:HA	16:S:369:SER:HB2	2.01	0.41
16:S:444:HIS:CG	16:S:445:GLU:N	2.88	0.41
17:J:443:VAL:HG13	17:J:481:ILE:HB	2.03	0.41
17:J:682:HIS:ND1	17:J:686:ASP:HB3	2.35	0.41
17:J:708:ARG:NH1	17:J:756:LEU:HD21	2.35	0.41
1:A:43:ASP:OD1	1:A:43:ASP:N	2.53	0.41
1:A:231:HIS:NE2	16:S:530:ILE:HG23	2.35	0.41
2:B:163:ASP:OD1	2:B:164:ARG:NH1	2.54	0.41
3:C:130:LEU:HD22	3:C:137:LEU:HD21	2.03	0.41
3:C:295:LEU:HD22	3:C:335:LEU:HA	2.03	0.41
4:D:474:LEU:HD13	4:D:474:LEU:HA	1.95	0.41
6:F:74:LEU:N	6:F:115:GLU:OE2	2.31	0.41
8:H:260:PRO:HG2	8:H:299:ARG:CZ	2.50	0.41
10:K:188:THR:O	10:K:217:VAL:HG13	2.20	0.41
10:K:285:HIS:CE1	10:K:287:SER:HB3	2.55	0.41
13:N:152:ASP:OD1	13:N:152:ASP:N	2.52	0.41
1:O:98:SER:OG	1:O:99:ASN:N	2.53	0.41
14:P:119:TYR:HA	14:P:122:ASN:ND2	2.36	0.41
15:Q:86:TYR:CD1	15:Q:86:TYR:C	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:J:621:ILE:HG22	17:J:720:VAL:HA	2.02	0.41
2:B:86:LEU:HD23	2:B:95:GLN:NE2	2.35	0.41
2:B:86:LEU:HD23	2:B:95:GLN:HE21	1.85	0.41
2:B:579:ALA:HB3	2:B:639:ALA:HB3	2.03	0.41
4:D:328:GLU:HB3	4:D:329:PRO:CD	2.47	0.41
7:G:223:TRP:HA	7:G:226:ARG:HG3	2.03	0.41
12:M:155:GLY:H	12:M:158:GLN:NE2	2.17	0.41
13:N:170:VAL:HG11	13:N:205:VAL:HG11	2.02	0.41
1:O:152:GLU:OE1	1:O:153:ARG:N	2.54	0.41
6:R:86:LEU:HG	6:R:126:MET:HE3	2.02	0.41
17:J:669:LEU:HB3	17:J:676:MET:HE3	2.02	0.41
1:A:61:CYS:HA	1:A:96:LEU:HD12	2.03	0.41
2:B:38:PHE:CD2	2:B:52:LEU:HD12	2.55	0.41
2:B:223:ILE:O	2:B:228:GLN:HB2	2.21	0.41
2:B:339:THR:O	2:B:343:ALA:N	2.53	0.41
3:C:50:PRO:CB	3:C:56:PHE:HB2	2.47	0.41
4:D:206:LEU:HA	4:D:1258:ILE:HD11	2.03	0.41
4:D:1159:ARG:HH12	8:H:735:ASP:C	2.29	0.41
5:E:158:HIS:CE1	5:E:163:GLY:HA3	2.56	0.41
7:G:294:ILE:HG23	7:G:298:ALA:HB3	2.03	0.41
9:I:234:TRP:O	9:I:238:TRP:HB2	2.20	0.41
9:I:291:LEU:HD11	9:I:312:VAL:HG21	2.01	0.41
9:I:329:ASN:OD1	9:I:330:TYR:N	2.53	0.41
9:I:383:TYR:HE1	9:I:385:SER:HA	1.86	0.41
16:S:202:CYS:HB2	16:S:341:PHE:CG	2.56	0.41
16:S:330:ILE:HD11	16:S:356:THR:HA	2.03	0.41
16:S:398:LEU:HA	16:S:444:HIS:CD2	2.56	0.41
16:S:486:SER:HB2	16:S:533:ARG:NE	2.36	0.41
16:S:506:LEU:C	16:S:507:ILE:HG12	2.44	0.41
17:J:282:GLY:C	17:J:304:VAL:HG22	2.45	0.41
17:J:322:ALA:O	17:J:323:LEU:HD13	2.20	0.41
1:A:58:GLU:HG2	1:A:155:ARG:HB2	2.02	0.41
1:A:220:ARG:NE	16:S:477:PRO:HD2	2.28	0.41
2:B:87:ILE:HG12	2:B:94:MET:HE2	2.03	0.41
2:B:541:ARG:HA	2:B:541:ARG:HD2	1.78	0.41
2:B:544:MET:HB3	2:B:544:MET:HE2	1.75	0.41
3:C:13:GLY:HA3	3:C:259:ILE:HD11	2.03	0.41
3:C:559:ASN:O	3:C:561:LYS:HG2	2.21	0.41
4:D:15:ASP:OD1	4:D:15:ASP:N	2.46	0.41
4:D:368:HIS:CE1	4:D:382:TYR:HD2	2.39	0.41
4:D:411:ASP:OD1	4:D:411:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1148:ASN:OD1	4:D:1152:ARG:NH2	2.54	0.41
5:E:307:ILE:HG13	5:E:363:LEU:HD21	2.03	0.41
5:E:428:VAL:O	5:E:432:GLN:HG2	2.21	0.41
8:H:837:SER:N	8:H:838:PRO:CD	2.84	0.41
11:L:256:ASN:OD1	11:L:256:ASN:N	2.52	0.41
12:M:125:LEU:HB3	12:M:126:PRO:HD2	2.03	0.41
13:N:216:GLU:N	13:N:216:GLU:OE1	2.54	0.41
13:N:284:LYS:HB2	13:N:284:LYS:HE2	1.79	0.41
13:N:326:VAL:HG21	13:N:347:PHE:HE1	1.86	0.41
6:R:110:MET:HE2	6:R:167:LEU:HA	2.03	0.41
6:R:121:TYR:HD2	6:R:125:ALA:HB3	1.86	0.41
16:S:199:PRO:HB3	16:S:339:LYS:CB	2.50	0.41
16:S:239:LYS:HB2	16:S:407:GLN:NE2	2.36	0.41
16:S:304:MET:HE2	16:S:316:THR:HA	1.99	0.41
17:J:507:LEU:HD13	17:J:516:PRO:HG2	2.03	0.41
17:J:533:PRO:HG2	17:J:560:ILE:HG21	2.03	0.41
17:J:624:ILE:HG21	17:J:638:LEU:HD21	2.03	0.41
17:J:635:ARG:HA	17:J:638:LEU:HB3	2.03	0.41
17:J:649:THR:HB	17:J:698:PHE:CD1	2.56	0.41
4:D:101:ILE:HD12	4:D:160:MET:HB2	2.02	0.41
4:D:426:GLY:C	4:D:427:THR:HG1	2.23	0.41
4:D:1159:ARG:HH12	8:H:735:ASP:CA	2.34	0.41
4:D:1248:ALA:HB1	4:D:1250:CYS:SG	2.62	0.41
5:E:155:ALA:O	5:E:159:VAL:HG12	2.20	0.41
7:G:351:ILE:HD12	7:G:351:ILE:HA	1.86	0.41
7:G:417:ARG:HD3	7:G:421:GLU:HG2	2.03	0.41
8:H:792:LYS:HA	8:H:792:LYS:HD2	1.87	0.41
13:N:184:TRP:CD2	13:N:235:TRP:HD1	2.38	0.41
16:S:238:ASP:C	16:S:240:PHE:H	2.29	0.41
16:S:348:LEU:HD11	16:S:395:VAL:HB	2.03	0.41
16:S:444:HIS:CE1	16:S:445:GLU:O	2.74	0.41
17:J:763:THR:HA	17:J:768:TRP:CZ3	2.56	0.41
2:B:460:ARG:NE	2:B:460:ARG:HA	2.36	0.40
2:B:1023:THR:HG22	3:C:408:THR:HB	2.03	0.40
4:D:1076:LEU:HG	4:D:1086:ARG:HB2	2.03	0.40
4:D:1159:ARG:O	4:D:1162:ARG:HG3	2.20	0.40
7:G:260:TYR:CE2	10:K:320:ILE:HG22	2.55	0.40
8:H:452:ARG:HD2	8:H:452:ARG:HA	1.81	0.40
8:H:833:TYR:O	8:H:834:ARG:HB2	2.20	0.40
9:I:304:ARG:HG2	14:P:101:SER:HB3	2.04	0.40
10:K:179:PRO:HG2	10:K:183:ILE:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:275:ARG:HE	10:K:275:ARG:HB3	1.76	0.40
12:M:232:LYS:HD3	12:M:232:LYS:HA	1.82	0.40
13:N:176:PRO:HB3	13:N:276:TYR:HB2	2.02	0.40
6:R:96:ILE:HD11	6:R:152:PHE:HE1	1.85	0.40
6:R:122:GLU:O	6:R:123:LYS:HD3	2.21	0.40
6:R:143:GLN:CG	16:S:315:THR:CA	2.91	0.40
6:R:143:GLN:HE22	16:S:313:ARG:NE	2.18	0.40
16:S:457:SER:O	16:S:458:LYS:C	2.62	0.40
16:S:507:ILE:HG22	16:S:508:THR:H	1.86	0.40
2:B:140:HIS:NE2	2:B:141:ASN:OD1	2.54	0.40
2:B:206:SER:HB2	2:B:210:ASP:C	2.46	0.40
2:B:573:LEU:HD12	7:G:392:TYR:CD1	2.56	0.40
2:B:741:LYS:O	2:B:773:THR:OG1	2.28	0.40
2:B:992:ALA:HB3	3:C:463:ILE:HD12	2.04	0.40
2:B:1003:GLN:O	2:B:1007:THR:HG23	2.21	0.40
4:D:354:ALA:HB3	4:D:416:SER:O	2.22	0.40
4:D:1115:THR:O	4:D:1116:PHE:HB2	2.20	0.40
5:E:333:TYR:CD2	13:N:255:HIS:HB2	2.56	0.40
7:G:325:GLU:H	7:G:325:GLU:HG2	1.62	0.40
8:H:130:ARG:H	8:H:130:ARG:HG2	1.62	0.40
8:H:432:MET:HB2	17:J:671:GLY:CA	2.52	0.40
12:M:151:SER:HA	12:M:167:PHE:CE2	2.56	0.40
6:R:108:ILE:HA	6:R:111:ALA:HB3	2.02	0.40
17:J:279:VAL:HG13	17:J:283:ASP:OD1	2.21	0.40
17:J:653:SER:O	17:J:653:SER:OG	2.30	0.40
3:C:15:VAL:HG11	3:C:23:TRP:CH2	2.56	0.40
3:C:272:LEU:HD23	3:C:273:PRO:N	2.36	0.40
3:C:412:ARG:NH1	14:P:124:ARG:HH22	2.15	0.40
3:C:619:PRO:HB3	3:C:634:TYR:CE1	2.56	0.40
4:D:367:VAL:HG13	4:D:385:LEU:HD11	2.02	0.40
4:D:1226:VAL:O	8:H:301:GLN:NE2	2.55	0.40
8:H:124:ALA:HB1	8:H:146:LEU:HD21	2.02	0.40
8:H:164:ALA:O	8:H:168:LYS:HG2	2.20	0.40
8:H:293:ARG:HE	8:H:293:ARG:HB3	1.77	0.40
15:Q:83:GLN:HB2	15:Q:133:PHE:CE1	2.57	0.40
16:S:196:GLY:HA2	16:S:261:ARG:NH1	2.36	0.40
16:S:270:ASN:OD1	16:S:293:VAL:HG21	2.20	0.40
16:S:304:MET:HE1	16:S:315:THR:C	2.45	0.40
16:S:340:MET:CE	16:S:401:VAL:HB	2.48	0.40
2:B:791:ILE:O	2:B:802:GLU:HA	2.22	0.40
3:C:389:SER:CB	14:P:167:GLU:CD	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:69:VAL:HG22	7:G:409:LYS:HE2	2.03	0.40
8:H:732:PHE:CE2	8:H:743:MET:HE3	2.55	0.40
8:H:744:ARG:HD2	8:H:744:ARG:N	2.37	0.40
11:L:67:ASP:OD1	11:L:67:ASP:N	2.52	0.40
13:N:374:LEU:HD23	13:N:374:LEU:HA	1.94	0.40
1:O:64:ARG:NH2	1:O:163:ASN:O	2.54	0.40
1:O:69:LYS:C	1:O:70:ILE:HD12	2.47	0.40
1:O:167:ASP:OD1	1:O:167:ASP:N	2.35	0.40
6:R:143:GLN:HG3	16:S:315:THR:CB	2.52	0.40
6:R:147:LEU:HD23	6:R:147:LEU:HA	1.95	0.40
16:S:255:LEU:HD22	16:S:497:MET:HG3	2.03	0.40
17:J:324:VAL:O	17:J:324:VAL:HG13	2.21	0.40
2:B:25:ARG:HG2	2:B:25:ARG:HH11	1.87	0.40
2:B:183:LEU:CD1	2:B:190:ASN:HD21	2.35	0.40
2:B:711:HIS:HE1	2:B:766:GLN:H	1.69	0.40
4:D:206:LEU:HD22	4:D:1208:ILE:HD13	2.02	0.40
4:D:329:PRO:O	4:D:331:THR:N	2.55	0.40
8:H:205:LEU:HD23	8:H:205:LEU:HA	1.88	0.40
8:H:807:ILE:O	8:H:810:ARG:HG2	2.21	0.40
10:K:223:TYR:HA	10:K:236:ASP:HB2	2.03	0.40
11:L:75:LYS:HB2	11:L:75:LYS:HE3	1.88	0.40
11:L:220:PRO:HB2	11:L:227:PRO:HG3	2.03	0.40
12:M:139:PHE:CZ	12:M:216:PRO:HB2	2.57	0.40
13:N:188:ARG:HD3	13:N:188:ARG:HA	1.87	0.40
6:R:108:ILE:HA	6:R:108:ILE:HD13	1.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	198/305 (65%)	194 (98%)	4 (2%)	48	68
1	O	197/305 (65%)	197 (100%)	0	100	100
2	B	929/929 (100%)	923 (99%)	6 (1%)	78	81
3	C	599/599 (100%)	595 (99%)	4 (1%)	76	80
4	D	702/1214 (58%)	686 (98%)	16 (2%)	44	66
5	E	336/418 (80%)	336 (100%)	0	100	100
6	F	104/166 (63%)	104 (100%)	0	100	100
6	R	104/166 (63%)	102 (98%)	2 (2%)	50	69
7	G	217/460 (47%)	216 (100%)	1 (0%)	81	82
8	H	470/772 (61%)	457 (97%)	13 (3%)	38	63
9	I	363/437 (83%)	360 (99%)	3 (1%)	73	78
10	K	203/305 (67%)	202 (100%)	1 (0%)	81	82
11	L	189/236 (80%)	184 (97%)	5 (3%)	40	64
12	M	186/235 (79%)	186 (100%)	0	100	100
13	N	433/623 (70%)	431 (100%)	2 (0%)	81	82
14	P	87/147 (59%)	87 (100%)	0	100	100
15	Q	94/130 (72%)	91 (97%)	3 (3%)	34	61
16	S	290/508 (57%)	263 (91%)	27 (9%)	8	29
17	J	462/666 (69%)	458 (99%)	4 (1%)	70	77
All	All	6163/8621 (72%)	6072 (98%)	91 (2%)	55	72

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	VAL
1	A	131	ASP
1	A	132	ASN
1	A	196	GLN
2	B	187	MET
2	B	483	ASN
2	B	944	ASN
2	B	948	LEU
2	B	953	GLN
2	B	1041	LEU

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Mol	Chain	Res	Type
3	C	47	THR
3	C	49	LYS
3	C	51	GLU
3	C	604	LEU
4	D	11	ASN
4	D	251	ASP
4	D	331	THR
4	D	365	ASP
4	D	367	VAL
4	D	369	PRO
4	D	370	THR
4	D	1120	LYS
4	D	1122	ARG
4	D	1125	ASP
4	D	1126	ILE
4	D	1127	THR
4	D	1128	GLN
4	D	1130	LEU
4	D	1150	GLU
4	D	1225	ASN
7	G	217	THR
8	H	87	ILE
8	H	137	VAL
8	H	336	VAL
8	H	338	ARG
8	H	347	LEU
8	H	348	LYS
8	H	492	HIS
8	H	724	GLU
8	H	752	GLU
8	H	763	TRP
8	H	833	TYR
8	H	837	SER
8	H	840	TYR
9	I	362	ARG
9	I	445	GLN
9	I	450	LEU
10	K	229	ASN
11	L	56	LYS
11	L	107	LEU
11	L	177	GLN
11	L	198	VAL

Continued on next page...

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Mol	Chain	Res	Type
11	L	223	TRP
13	N	401	LEU
13	N	466	THR
15	Q	58	ASN
15	Q	82	ASP
15	Q	103	MET
6	R	86	LEU
6	R	149	THR
16	S	201	VAL
16	S	209	HIS
16	S	257	SER
16	S	261	ARG
16	S	301	MET
16	S	305	LYS
16	S	306	ILE
16	S	308	LYS
16	S	309	ARG
16	S	312	LEU
16	S	313	ARG
16	S	316	THR
16	S	317	VAL
16	S	318	LYS
16	S	330	ILE
16	S	357	THR
16	S	396	TRP
16	S	397	SER
16	S	398	LEU
16	S	400	ASP
16	S	402	ILE
16	S	457	SER
16	S	460	HIS
16	S	466	HIS
16	S	505	HIS
16	S	506	LEU
16	S	507	ILE
17	J	497	ASN
17	J	688	TYR
17	J	691	LEU
17	J	693	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	ASN
2	B	95	GLN
2	B	209	ASN
2	B	228	GLN
2	B	229	GLN
2	B	489	GLN
2	B	536	HIS
2	B	551	GLN
2	B	711	HIS
2	B	719	ASN
2	B	944	ASN
2	B	971	GLN
2	B	1054	ASN
2	B	1062	ASN
3	C	7	HIS
3	C	19	GLN
3	C	44	HIS
3	C	479	HIS
3	C	494	GLN
3	C	498	HIS
4	D	10	HIS
4	D	11	ASN
4	D	77	GLN
4	D	118	ASN
4	D	273	ASN
4	D	363	ASN
4	D	376	HIS
4	D	418	GLN
4	D	449	HIS
4	D	1190	GLN
4	D	1196	GLN
5	E	185	ASN
5	E	281	ASN
8	H	254	GLN
8	H	285	ASN
8	H	394	ASN
8	H	476	GLN
8	H	495	ASN
9	I	215	GLN
9	I	237	ASN
9	I	431	GLN
10	K	114	GLN
11	L	86	HIS

Continued on next page...

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Mol	Chain	Res	Type
11	L	116	ASN
11	L	132	ASN
11	L	155	GLN
11	L	177	GLN
11	L	219	ASN
11	L	264	ASN
12	M	109	HIS
12	M	129	ASN
12	M	137	HIS
12	M	250	HIS
13	N	255	HIS
13	N	319	HIS
14	P	134	HIS
14	P	142	ASN
15	Q	128	GLN
6	R	68	HIS
16	S	287	GLN
16	S	407	GLN
16	S	444	HIS
16	S	483	GLN
17	J	357	HIS
17	J	391	ASN
17	J	399	ASN
17	J	406	GLN
17	J	427	ASN
17	J	451	ASN
17	J	478	HIS
17	J	483	ASN
17	J	495	GLN
17	J	548	ASN
17	J	677	GLN
17	J	685	ASN
17	J	693	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

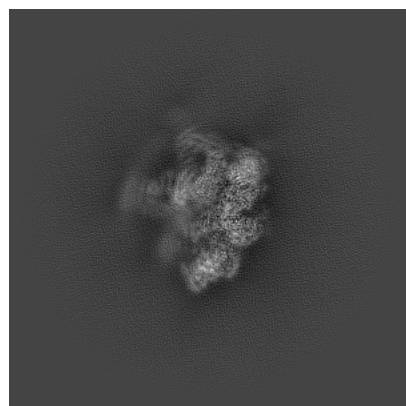
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38799. These allow visual inspection of the internal detail of the map and identification of artifacts.

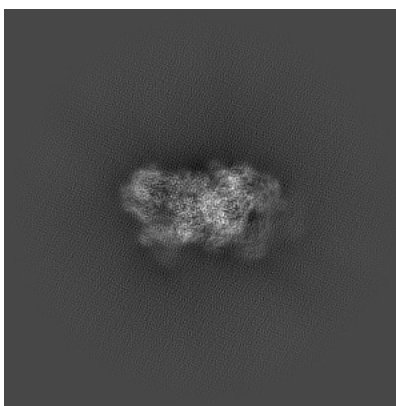
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

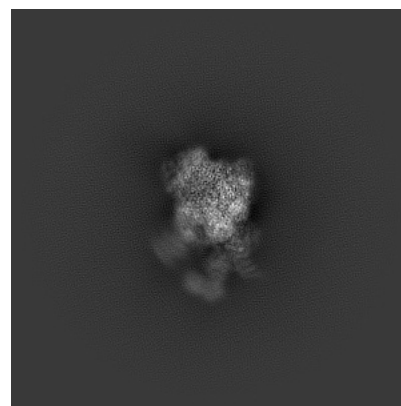
6.1.1 Primary map



X

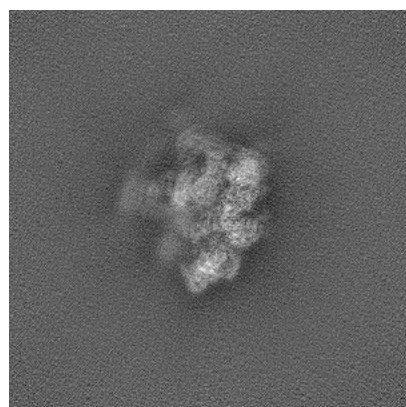


Y

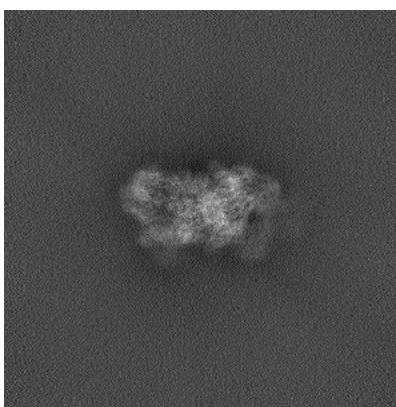


Z

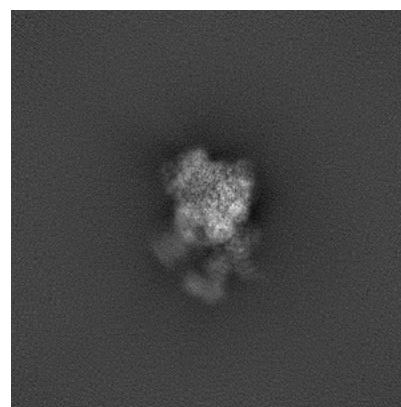
6.1.2 Raw map



X



Y

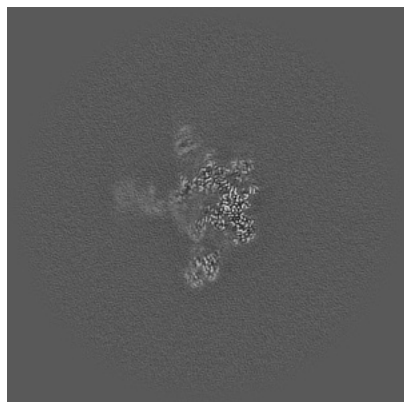


Z

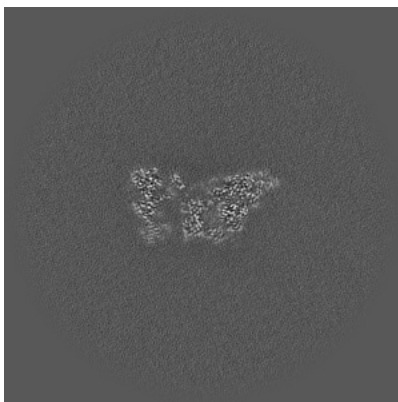
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

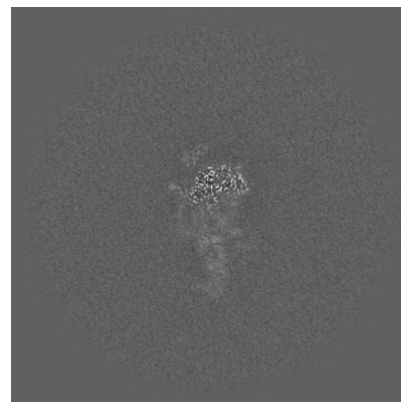
6.2.1 Primary map



X Index: 256

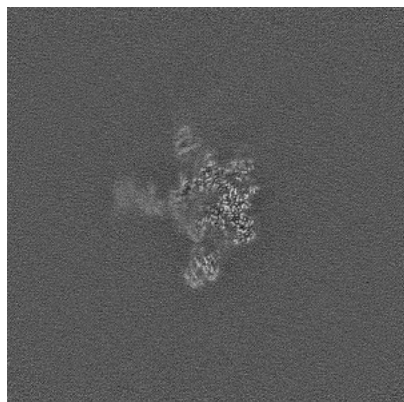


Y Index: 256

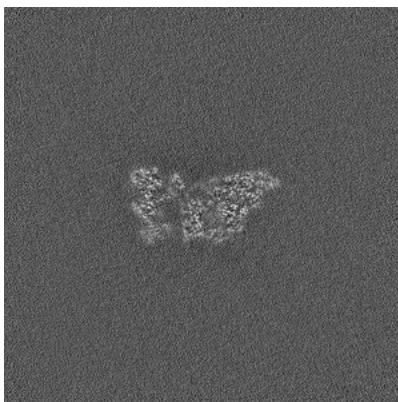


Z Index: 256

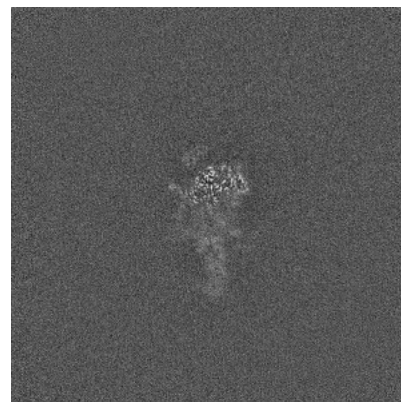
6.2.2 Raw map



X Index: 256



Y Index: 256

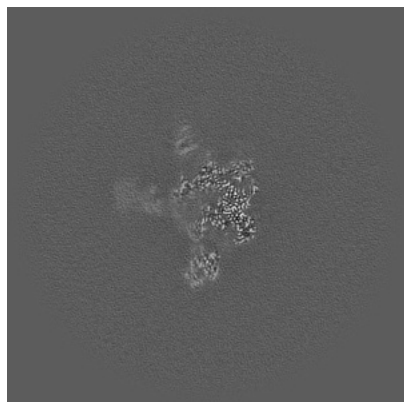


Z Index: 256

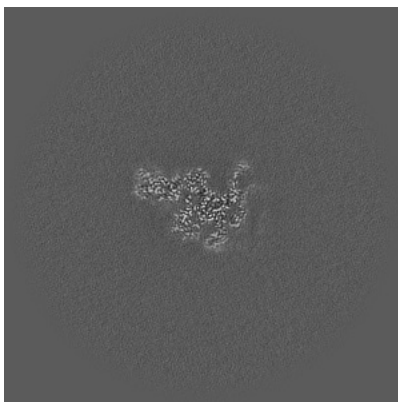
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

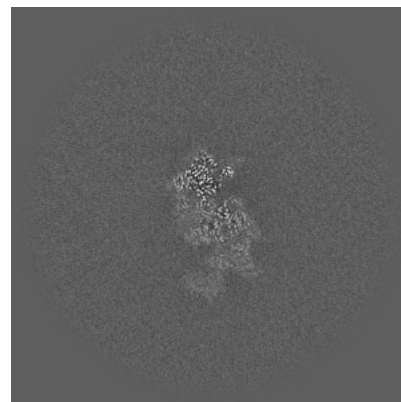
6.3.1 Primary map



X Index: 255

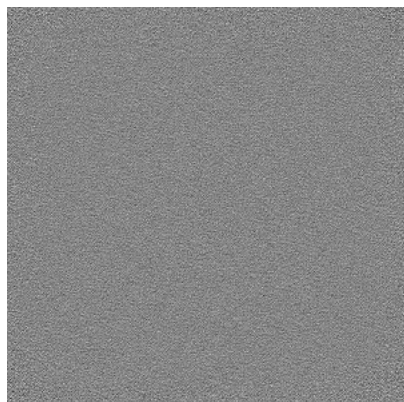


Y Index: 283

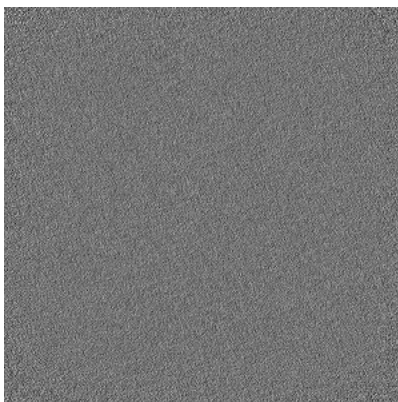


Z Index: 278

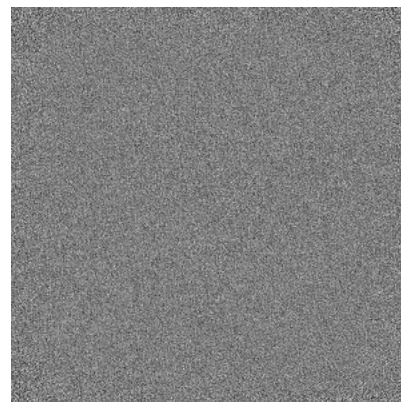
6.3.2 Raw map



X Index: 0



Y Index: 0

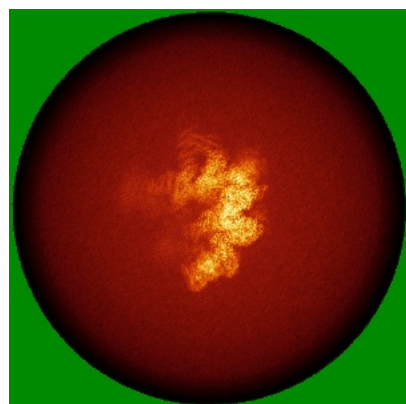


Z Index: 0

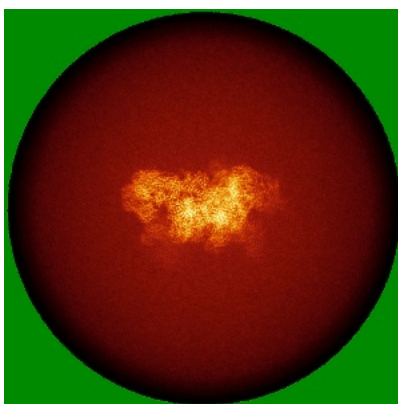
The images above show the largest variance slices of the map in three orthogonal directions.

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

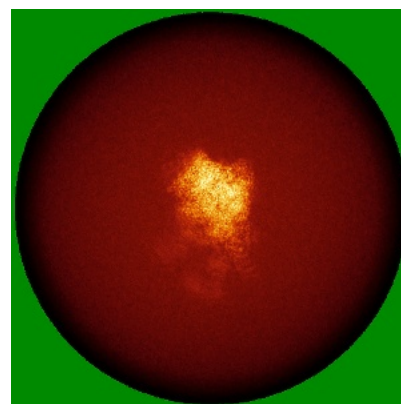
6.4.1 Primary map



X

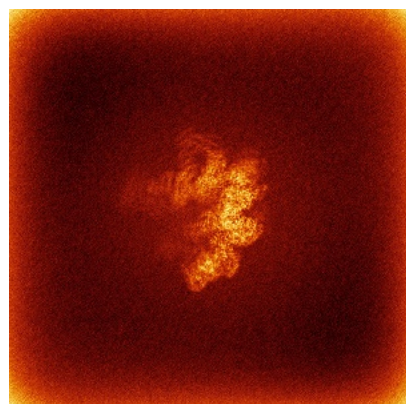


Y

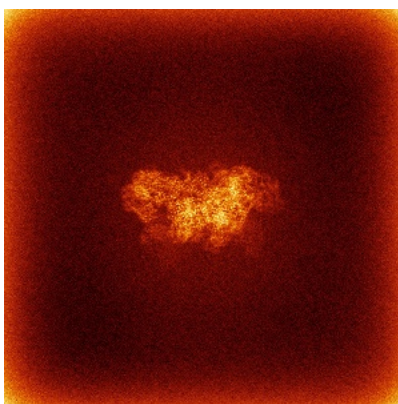


Z

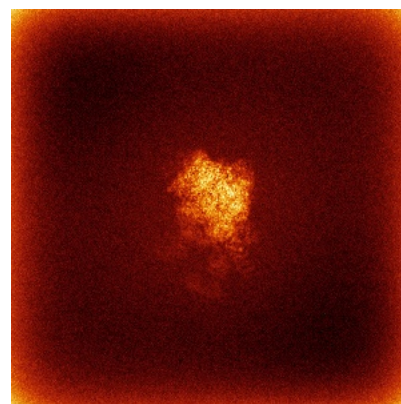
6.4.2 Raw map



X



Y

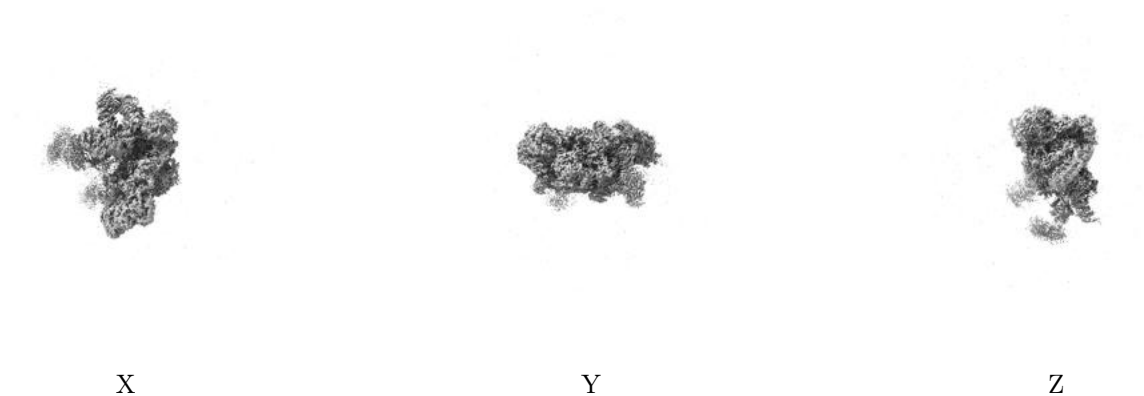


Z

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

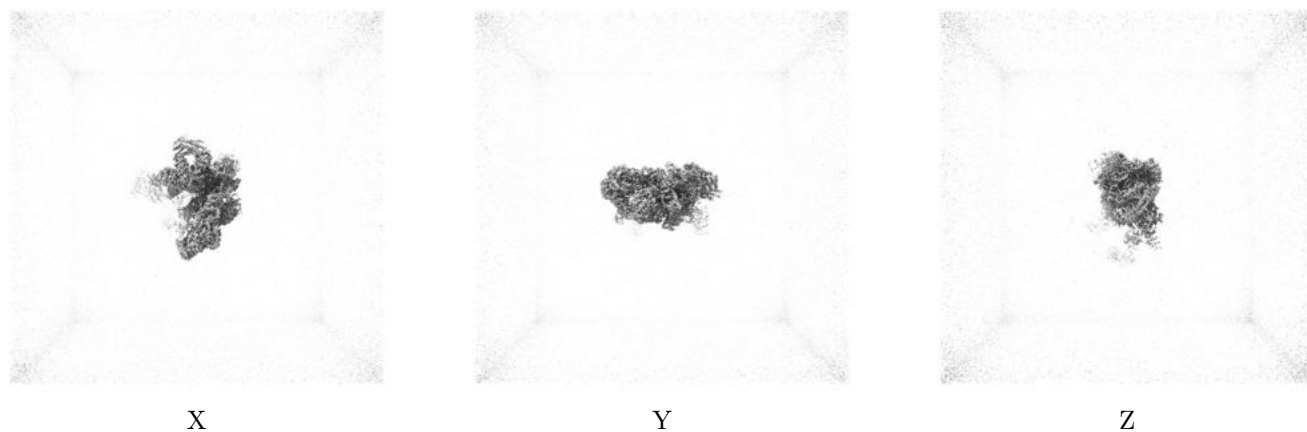
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.23. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

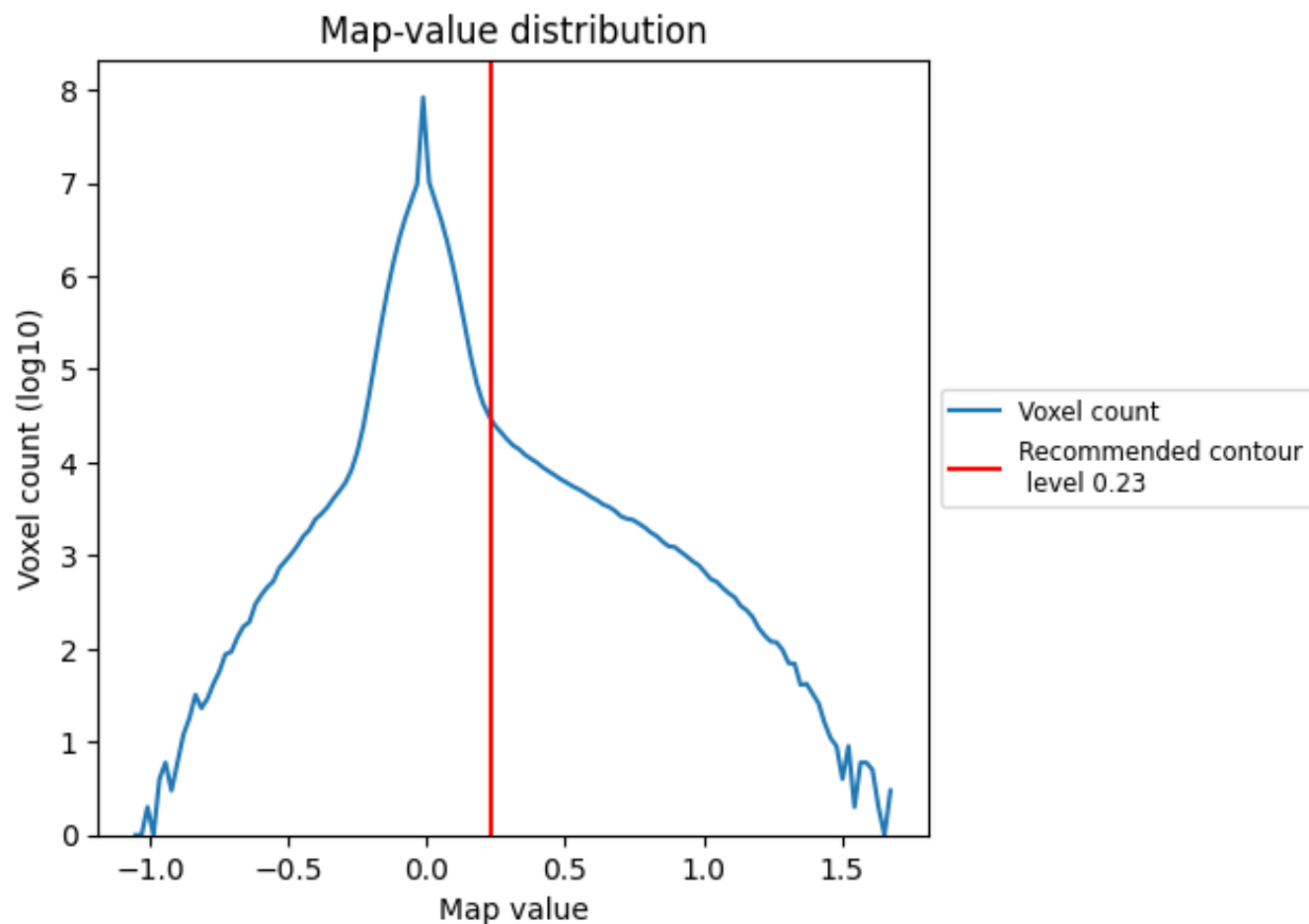
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

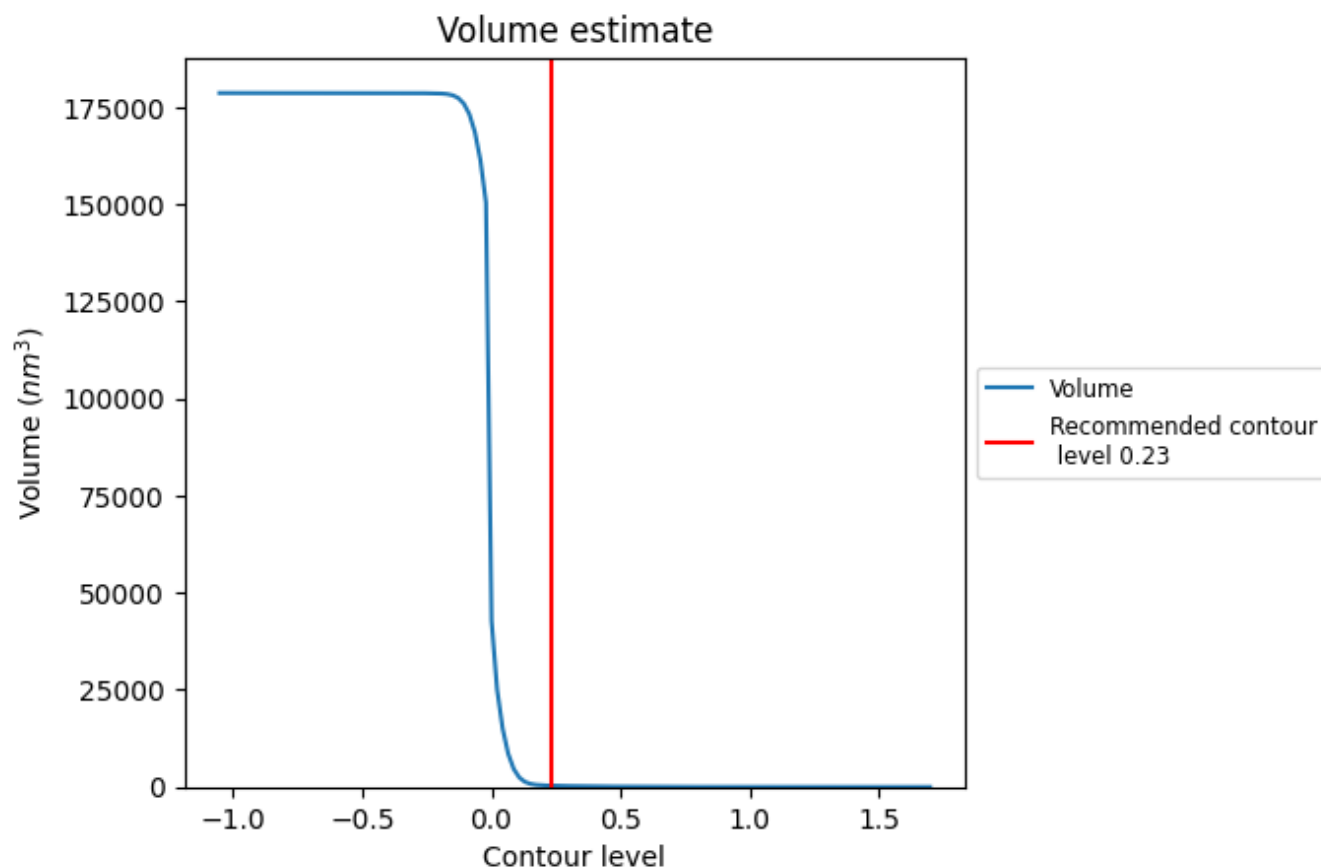
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

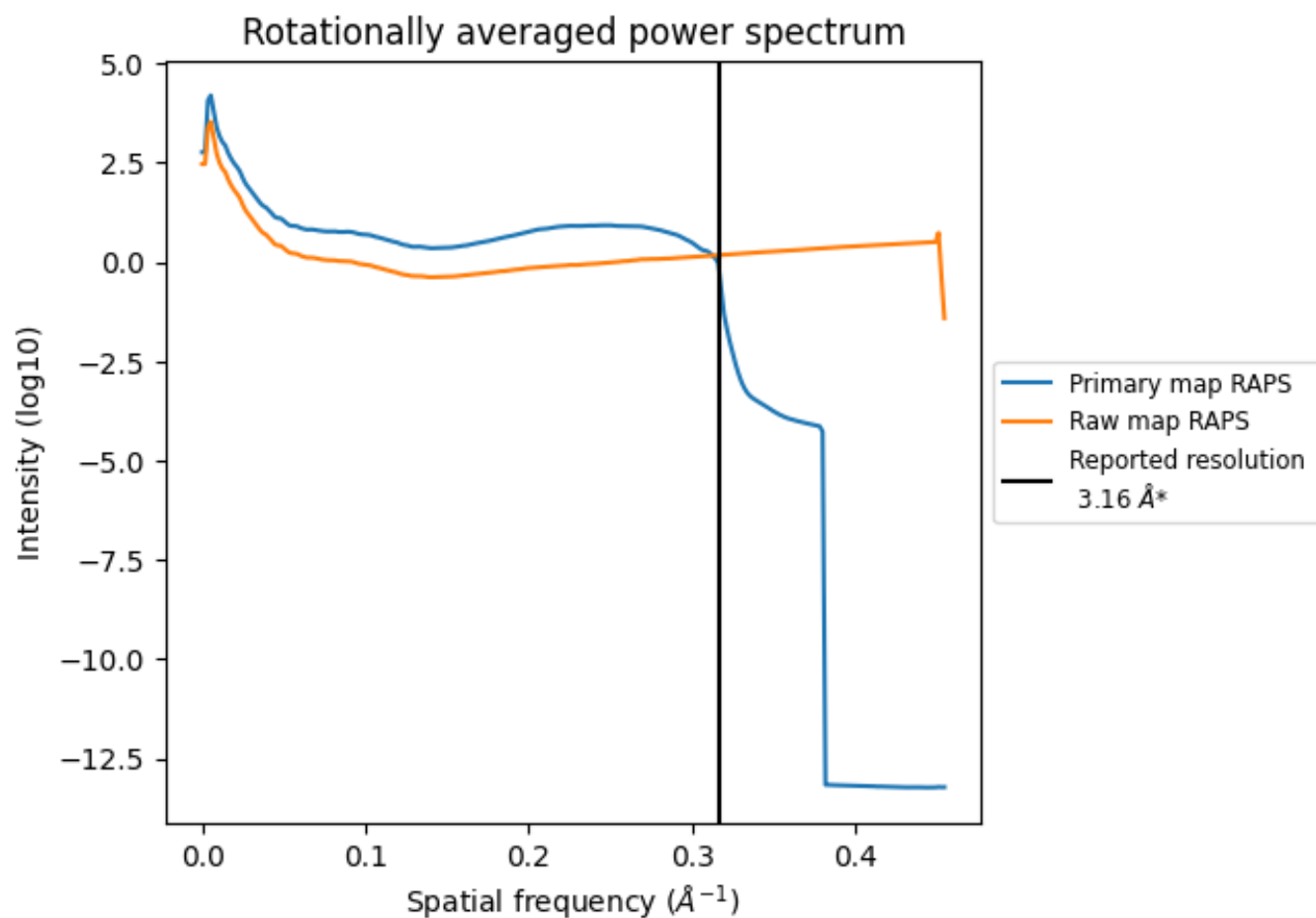
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 331 nm³; this corresponds to an approximate mass of 299 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

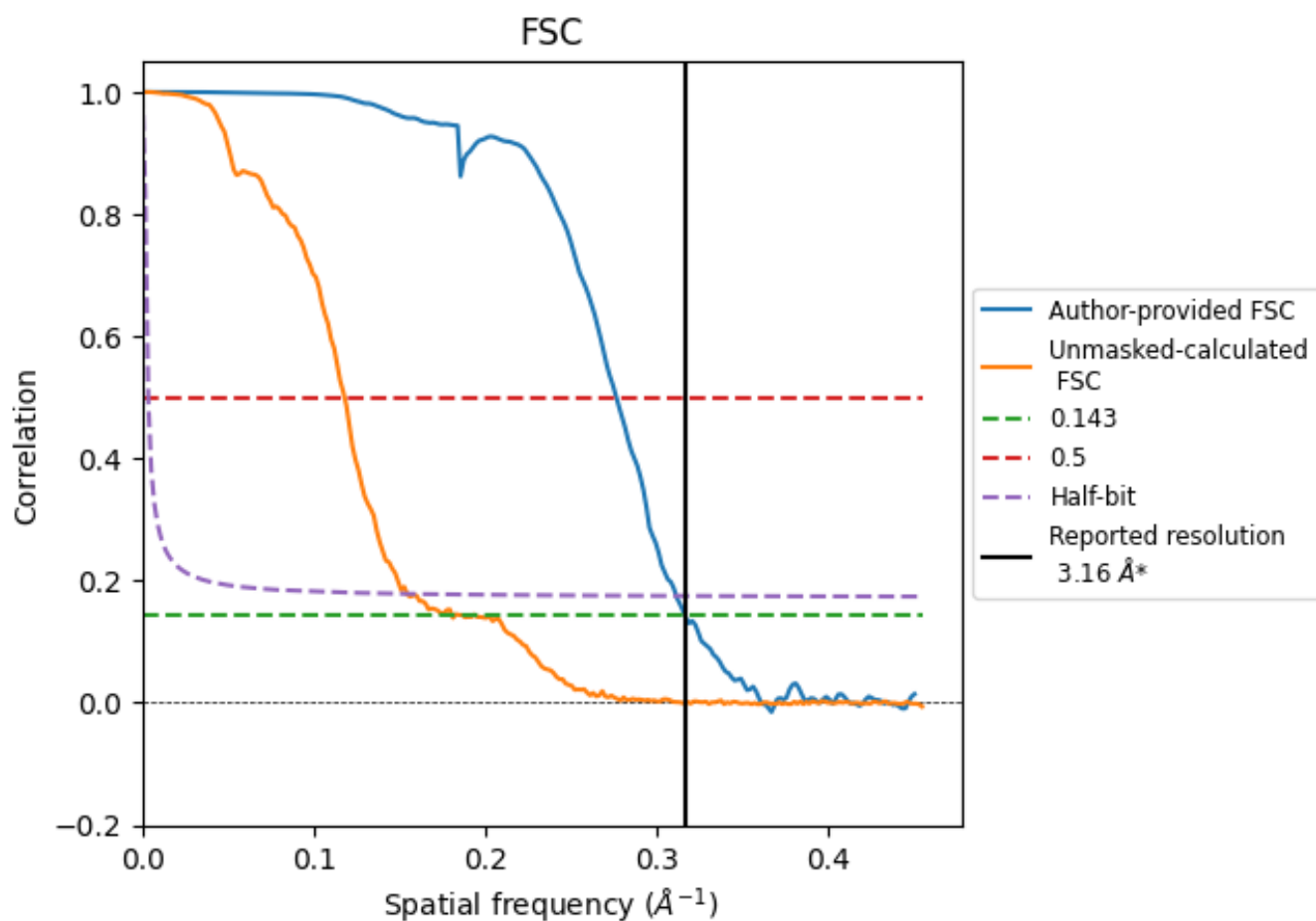


*Reported resolution corresponds to spatial frequency of 0.316 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.316 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

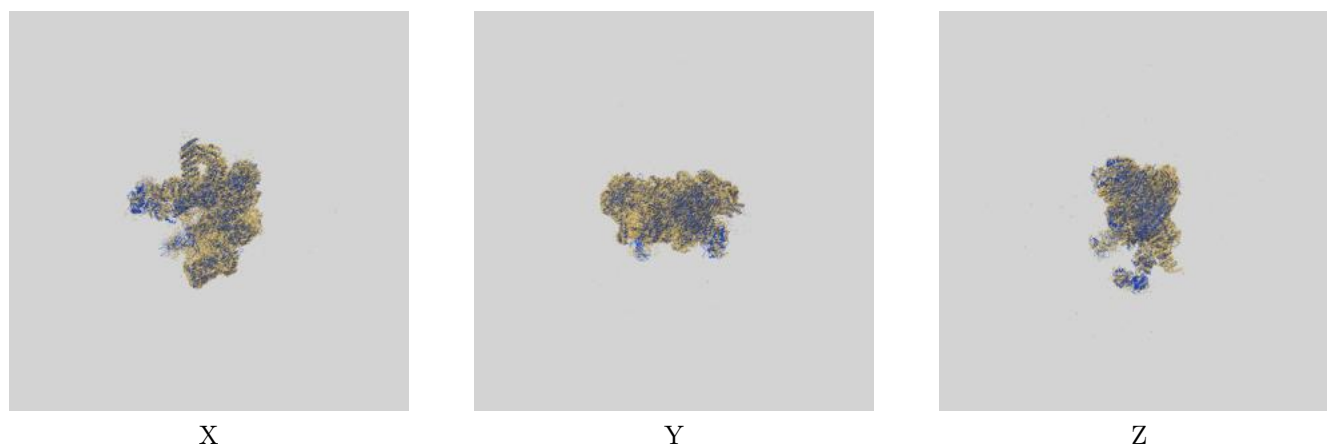
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	3.16	3.62	3.21
Unmasked-calculated*	5.54	8.48	6.48

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.54 differs from the reported value 3.16 by more than 10 %

9 Map-model fit [i](#)

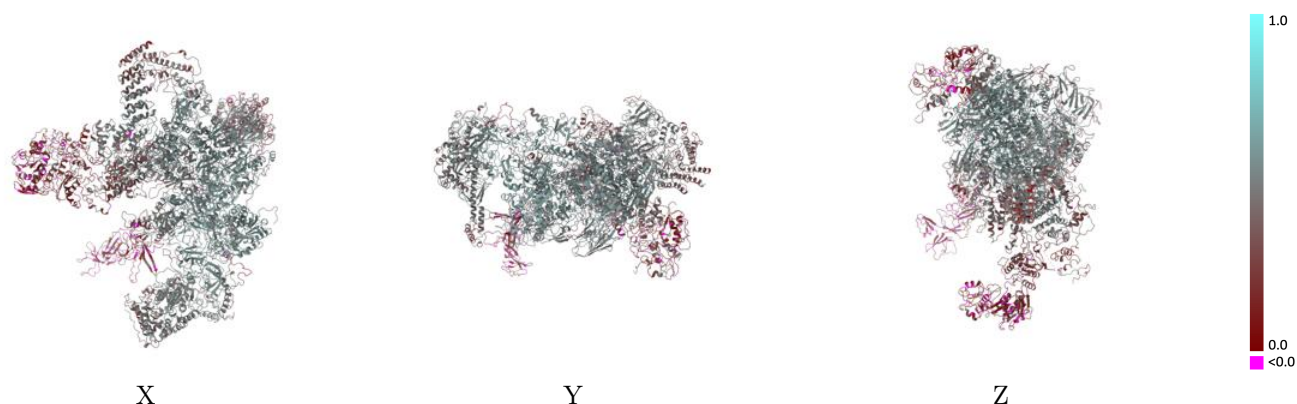
This section contains information regarding the fit between EMDB map EMD-38799 and PDB model 8XZV. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



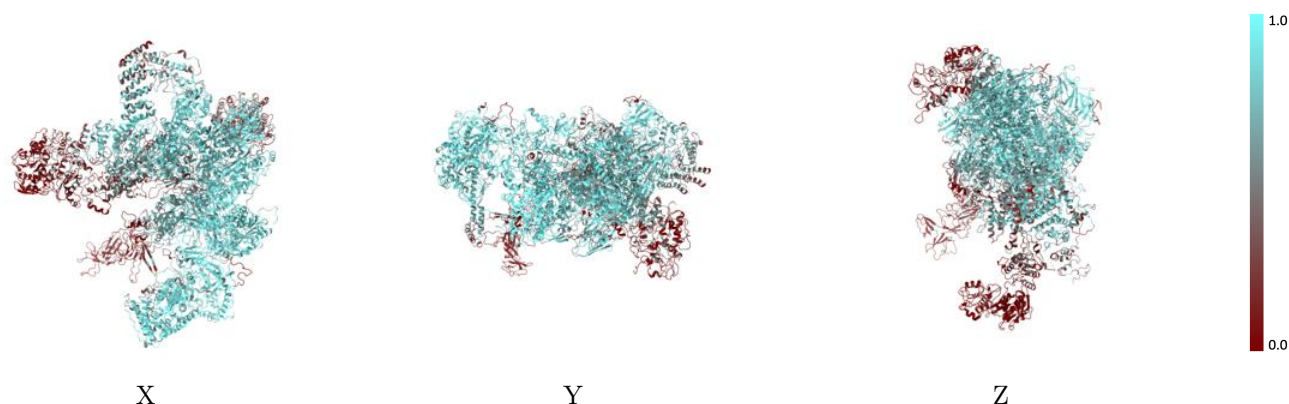
The images above show the 3D surface view of the map at the recommended contour level 0.23 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



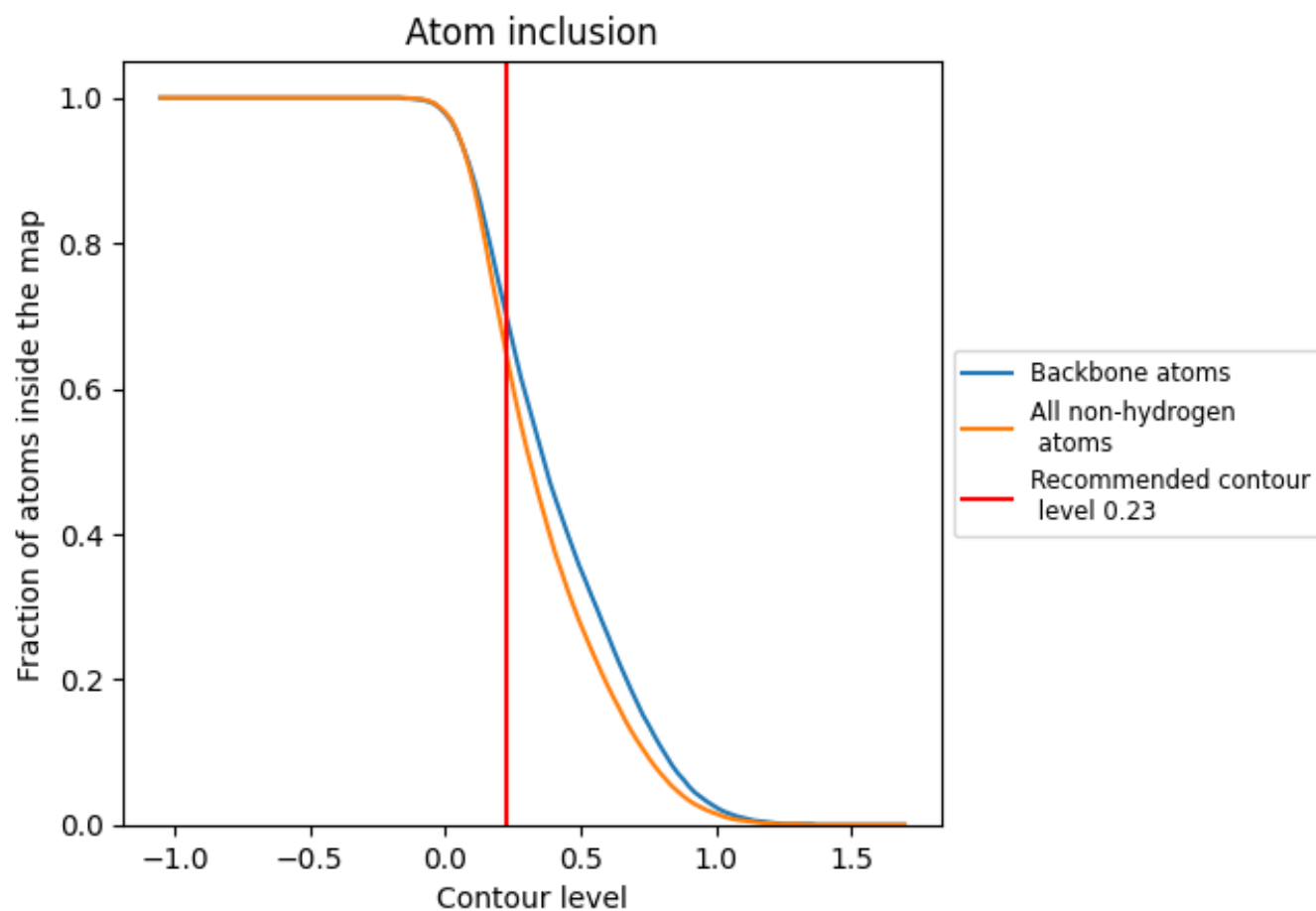
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.23).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.23) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6400	 0.4440
A	 0.7800	 0.5120
B	 0.6730	 0.4890
C	 0.5860	 0.4520
D	 0.6430	 0.4480
E	 0.8980	 0.5620
F	 0.8910	 0.5520
G	 0.8460	 0.5320
H	 0.6020	 0.3940
I	 0.7010	 0.4500
J	 0.1120	 0.2100
K	 0.7830	 0.4900
L	 0.8010	 0.4440
M	 0.8750	 0.5030
N	 0.7810	 0.4970
O	 0.7070	 0.4860
P	 0.7760	 0.5010
Q	 0.8490	 0.5150
R	 0.1770	 0.2940
S	 0.2610	 0.2770

