



Full wwPDB EM Validation Report ⓘ

Apr 21, 2026 – 11:55 AM JST

PDB ID : 9K4Z / pdb_00009k4z
EMDB ID : EMD-62075
Title : Structure of substrate-engaged human 26S proteasome RP-CP subcomplex in state ED1.1
Authors : Wu, Z.; Chen, E.; Mao, Y.
Deposited on : 2024-10-21
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

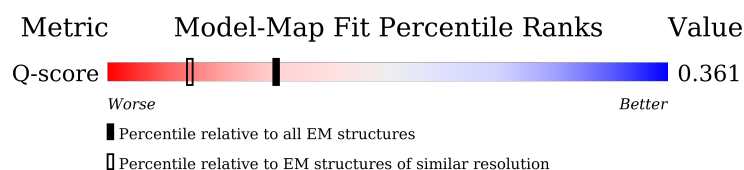
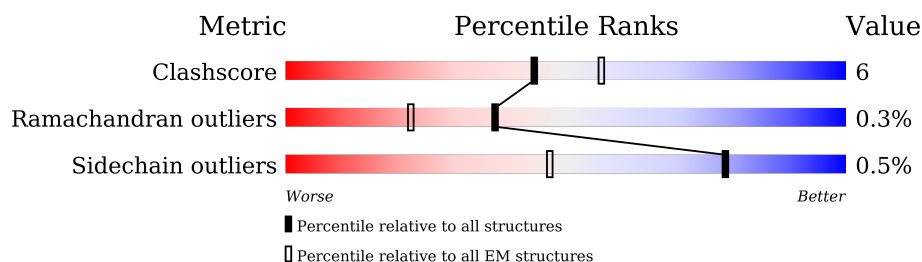
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	433	
2	B	440	
3	C	398	
4	D	418	









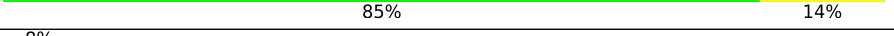
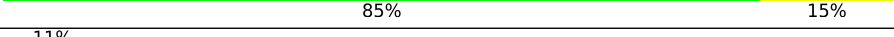
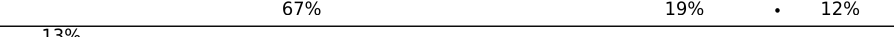


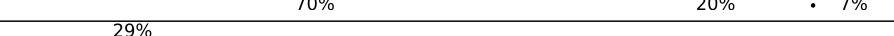



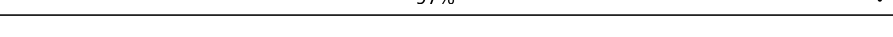
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Mol	Chain	Length	Quality of chain
5	E	403	
6	F	439	
7	G	246	
7	g	246	
8	H	234	
8	h	234	
9	I	261	
9	i	261	
10	J	248	
10	j	248	
11	K	241	
11	k	241	
12	L	263	
12	l	263	
13	M	255	
13	m	255	
14	N	239	
14	n	239	
15	O	277	
15	o	277	
16	P	205	
16	p	205	
17	Q	201	
17	q	201	
18	R	263	

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Mol	Chain	Length	Quality of chain
18	r	263	
19	S	241	
19	s	241	
20	T	264	
20	t	264	
21	U	953	
22	V	534	
23	W	456	
24	X	422	
25	Y	389	
26	Z	324	
27	a	376	
28	b	377	
29	c	310	
30	d	350	
31	e	70	
32	f	908	
33	v	36	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 106334 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 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	413	Total	C	N	O	S	0	0
			3229	2034	566	611	18		

- Molecule 2 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	411	Total	C	N	O	S	0	0
			3207	2022	548	622	15		

- Molecule 3 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	396	Total	C	N	O	S	0	0
			3105	1954	558	576	17		

- Molecule 4 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	380	Total	C	N	O	S	0	0
			3040	1923	524	580	13		

- Molecule 5 is a protein called Proteasome 26S subunit, ATPase 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	389	Total	C	N	O	S	0	0
			3097	1947	552	581	17		

- Molecule 6 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	395	Total	C	N	O	S	0	0
			3098	1951	533	596	18		

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	240	Total	C	N	O	S	0	0
			1867	1187	312	355	13		
7	g	244	Total	C	N	O	S	0	0
			1879	1193	318	355	13		

- Molecule 8 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	232	Total	C	N	O	S	0	0
			1801	1149	304	342	6		
8	h	232	Total	C	N	O	S	0	0
			1805	1154	307	338	6		

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	248	Total	C	N	O	S	0	0
			1933	1222	330	371	10		
9	i	250	Total	C	N	O	S	0	0
			1955	1234	336	375	10		

- Molecule 10 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	239	Total	C	N	O	S	0	0
			1861	1166	327	363	5		
10	j	239	Total	C	N	O	S	0	0
			1861	1168	332	356	5		

- Molecule 11 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	238	Total	C	N	O	S	0	0
			1813	1139	302	361	11		
11	k	234	Total	C	N	O	S	0	0
			1782	1119	295	357	11		

- Molecule 12 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	240	Total	C	N	O	S	0	0
			1876	1175	338	352	11		
12	l	238	Total	C	N	O	S	0	0
			1861	1165	335	350	11		

- Molecule 13 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	242	Total	C	N	O	S	1	0
			1893	1202	323	356	12		
13	m	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	203	Total	C	N	O	S	0	0
			1521	954	259	296	12		
14	n	202	Total	C	N	O	S	0	0
			1510	947	258	293	12		

- Molecule 15 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	220	Total	C	N	O	S	0	0
			1645	1035	278	320	12		
15	o	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		

- Molecule 16 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	204	Total	C	N	O	S	0	0
			1587	1010	264	294	19		
16	p	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

- Molecule 17 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	199	Total	C	N	O	S	1	0
			1591	1019	270	292	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	199	Total	C	N	O	S	0	0
			1578	1012	267	290	9		

- Molecule 18 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		
18	r	201	Total	C	N	O	S	0	0
			1549	977	270	293	9		

- Molecule 19 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	213	Total	C	N	O	S	0	0
			1641	1041	281	309	10		
19	s	213	Total	C	N	O	S	0	0
			1650	1044	283	313	10		

- Molecule 20 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	216	Total	C	N	O	S	0	0
			1683	1062	291	318	12		
20	t	216	Total	C	N	O	S	0	0
			1687	1064	291	320	12		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	878	Total	C	N	O	S	0	0
			6867	4352	1163	1306	46		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	444	Total	C	N	O	S	0	0
			3612	2301	645	653	13		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	441	Total	C	N	O	S	0	0
			3596	2277	613	682	24		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	422	Total	C	N	O	S	0	0
			3335	2116	567	639	13		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	389	Total	C	N	O	S	0	0
			3202	2041	545	598	18		

- Molecule 26 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	286	Total	C	N	O	S	0	0
			2281	1457	392	427	5		

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	373	Total	C	N	O	S	0	0
			2995	1911	510	559	15		

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	191	Total	C	N	O	S	0	0
			1458	910	261	279	8		

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	287	Total	C	N	O	S	0	0
			2260	1430	389	422	19		

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	257	Total	C	N	O	S	0	0
			2116	1371	346	390	9		

- Molecule 31 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	e	50	Total	C	N	O	0	0
			425	260	65	100		

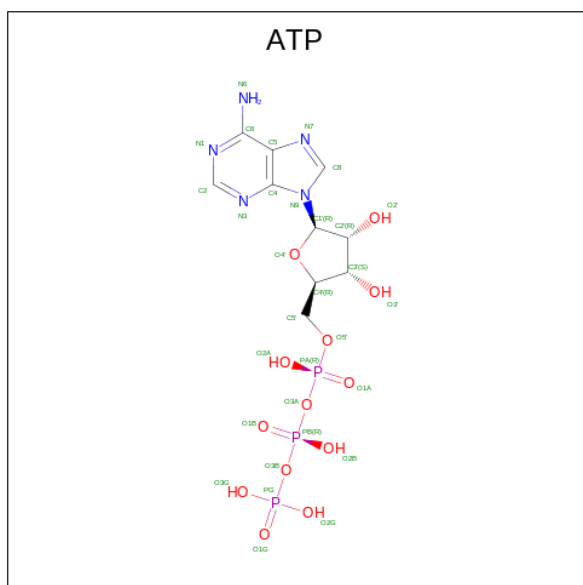
- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	844	Total	C	N	O	S	0	0
			6529	4126	1108	1250	45		

- Molecule 33 is a protein called Substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	v	36	Total	C	N	O	0	0
			180	108	36	36		

- Molecule 34 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
34	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

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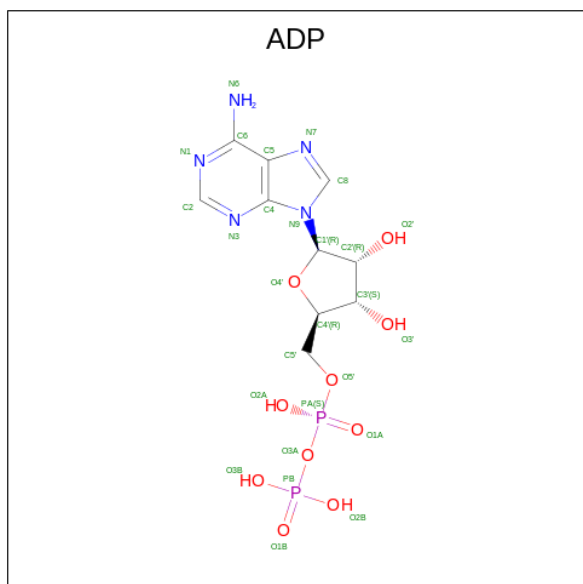
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Mol	Chain	Residues	Atoms					AltConf
34	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
35	A	1	Total	Mg	0
			1	1	
35	B	1	Total	Mg	0
			1	1	
35	C	1	Total	Mg	0
			1	1	
35	D	1	Total	Mg	0
			1	1	

- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
36	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

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Mol	Chain	Residues	Atoms					AltConf
36	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

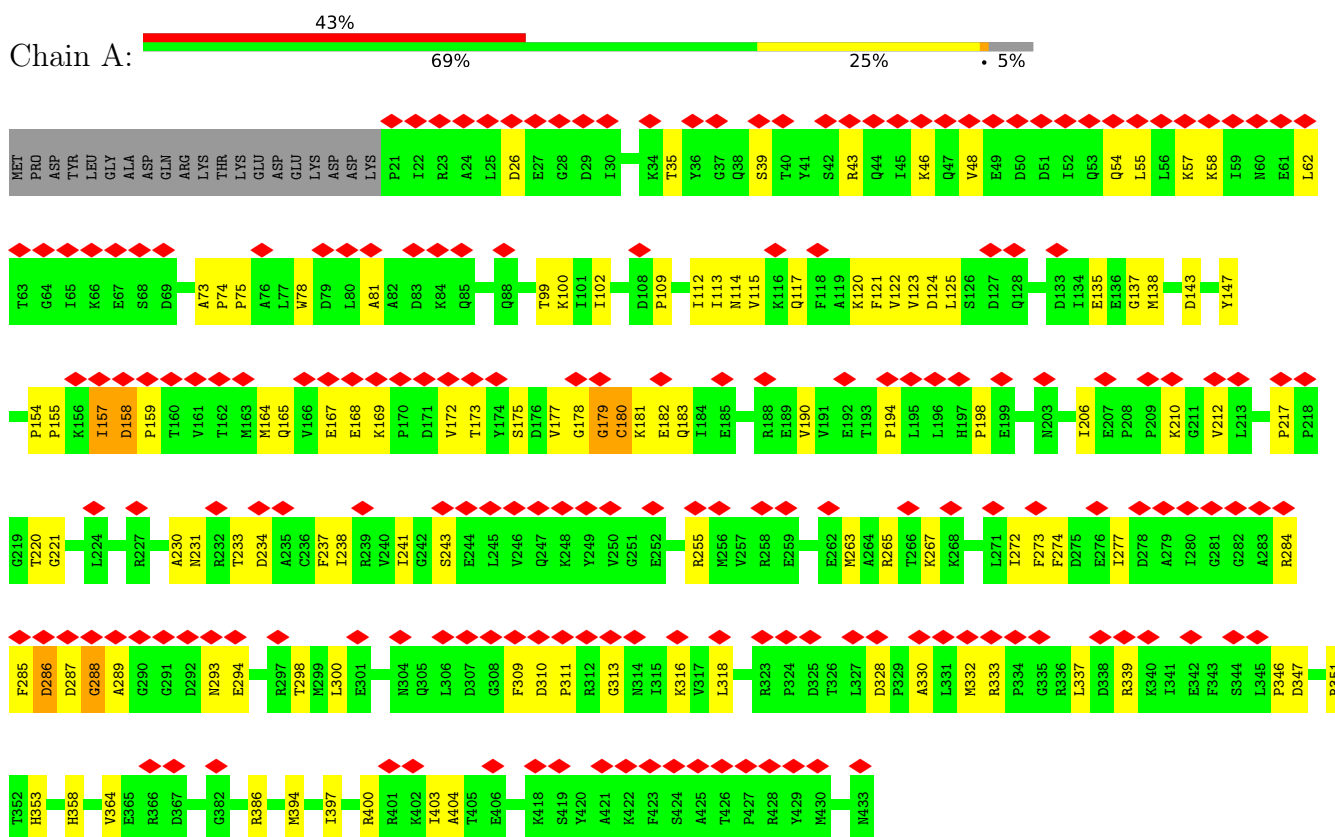
- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
37	c	1	Total	Zn	0
			1	1	

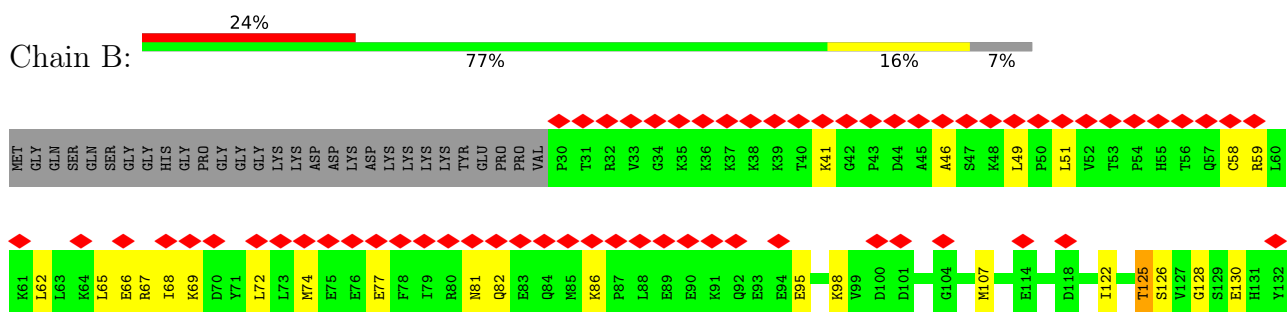
3 Residue-property plots

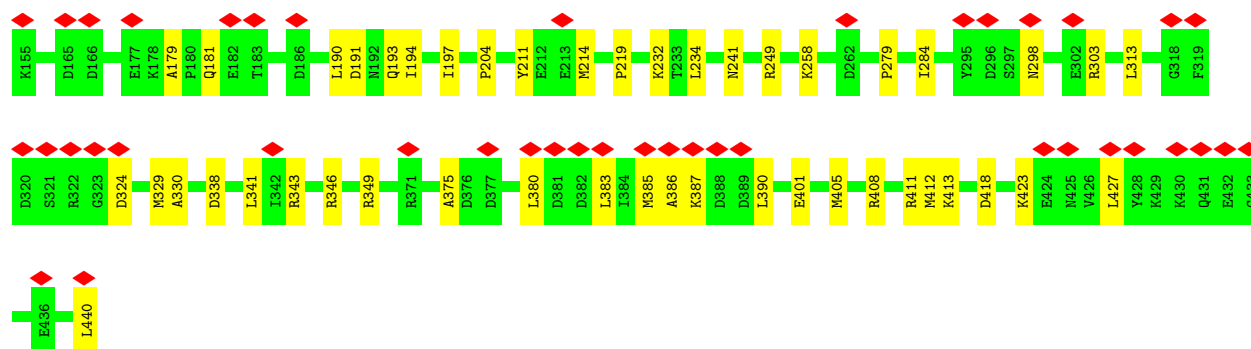
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 26S proteasome regulatory subunit 7



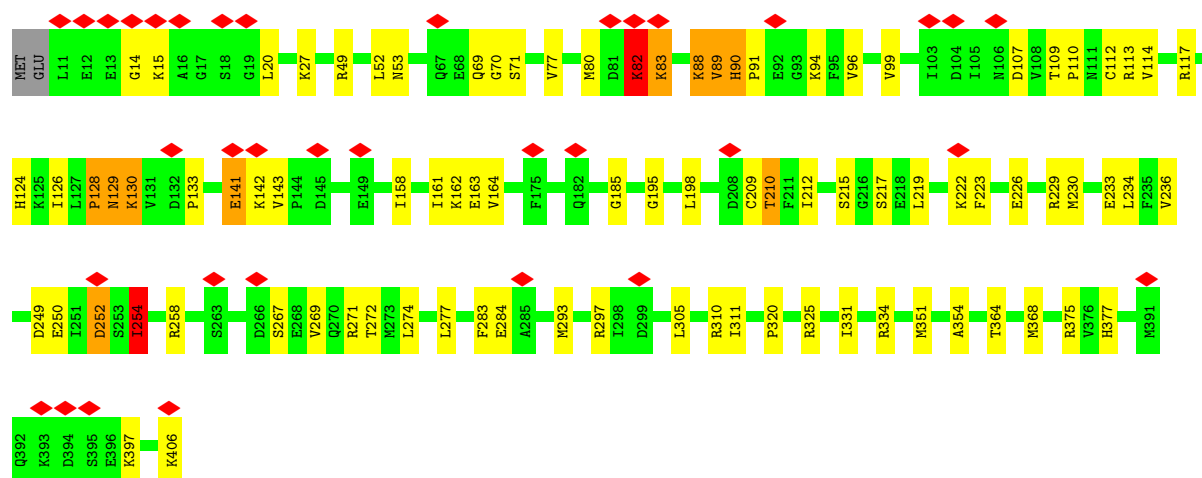
- Molecule 2: 26S proteasome regulatory subunit 4





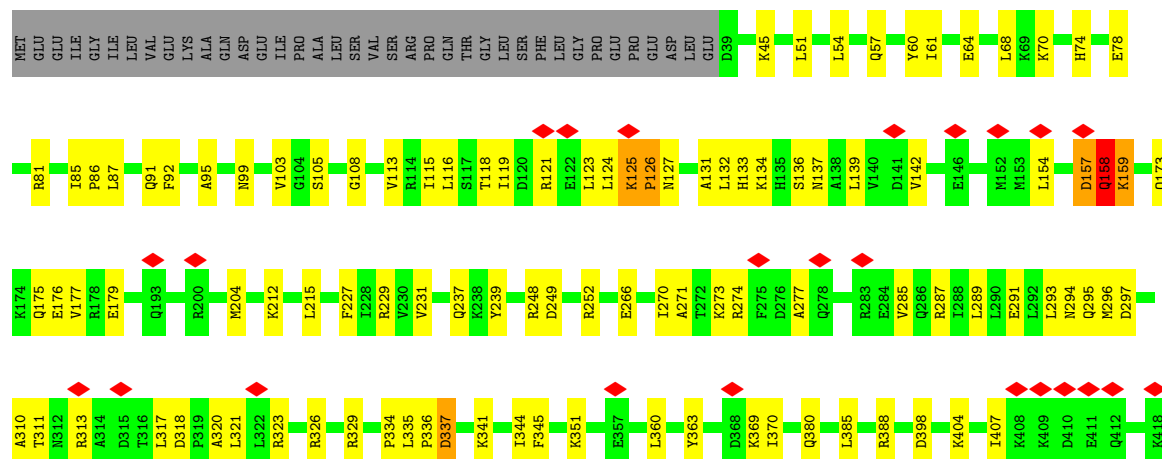
• Molecule 3: 26S proteasome regulatory subunit 8

Chain C: 9% 77% 19% ...



• Molecule 4: 26S proteasome regulatory subunit 6B

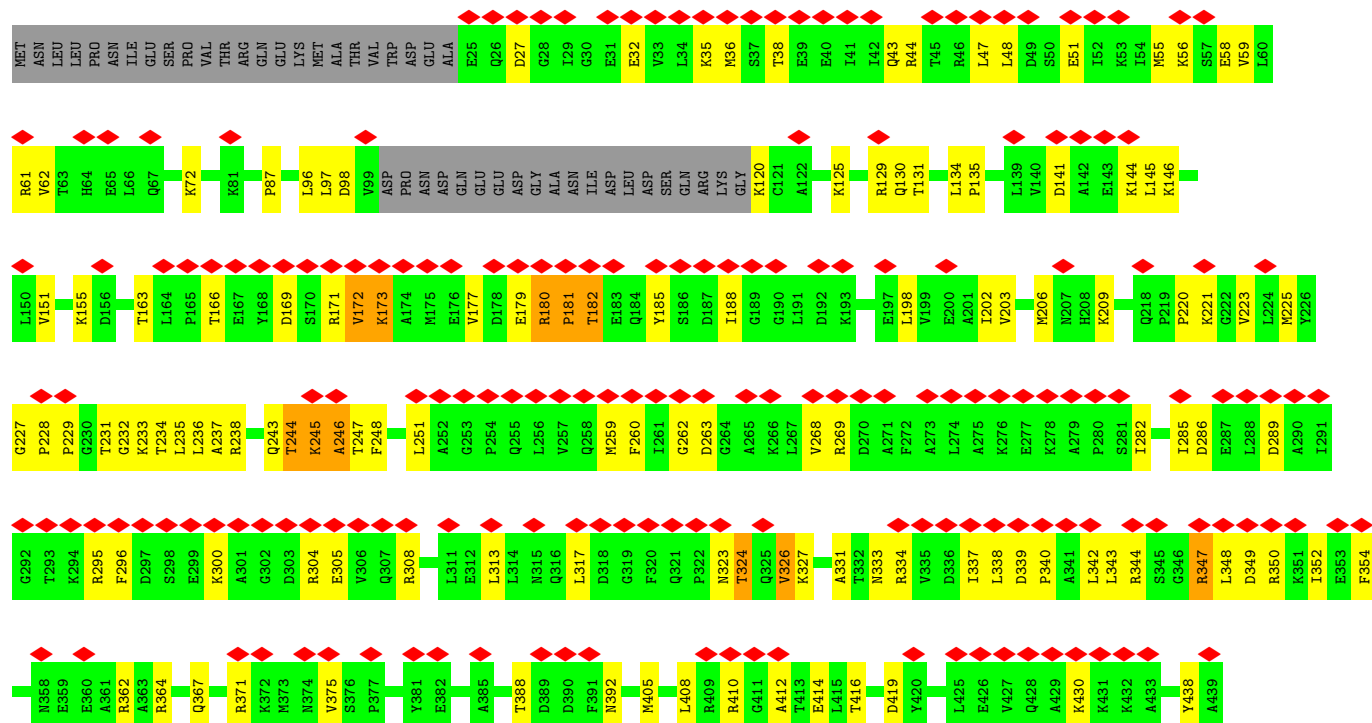
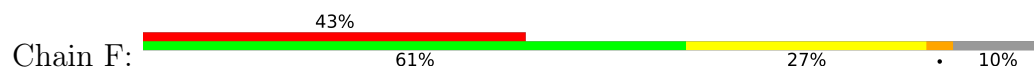
Chain D: 6% 66% 23% 9%



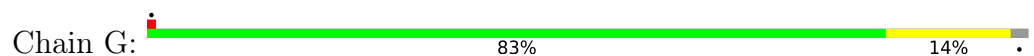
• Molecule 5: Proteasome 26S subunit, ATPase 6

Chain E: 16% 76% 19% ...

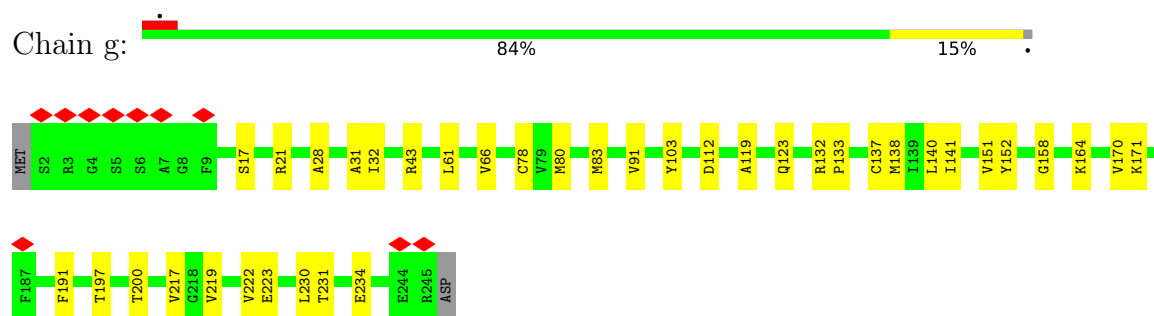
- Molecule 6: 26S proteasome regulatory subunit 6A



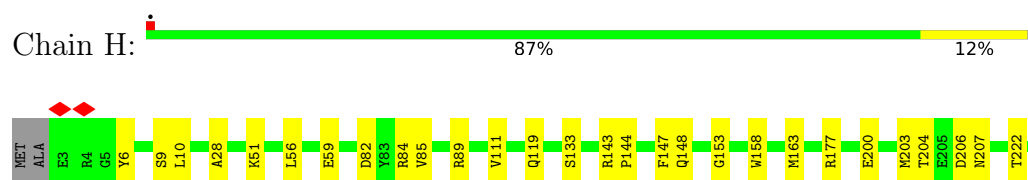
- Molecule 7: Proteasome subunit alpha type-6



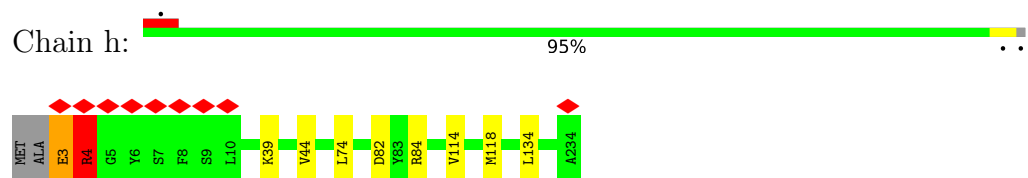
- Molecule 7: Proteasome subunit alpha type-6



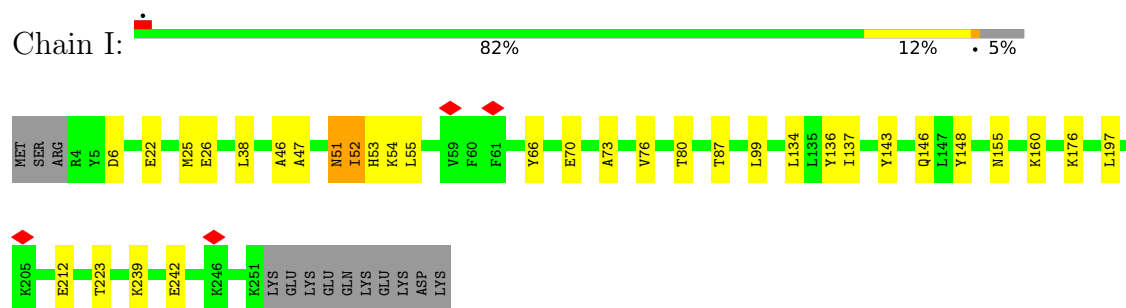
- Molecule 8: Proteasome subunit alpha type-2



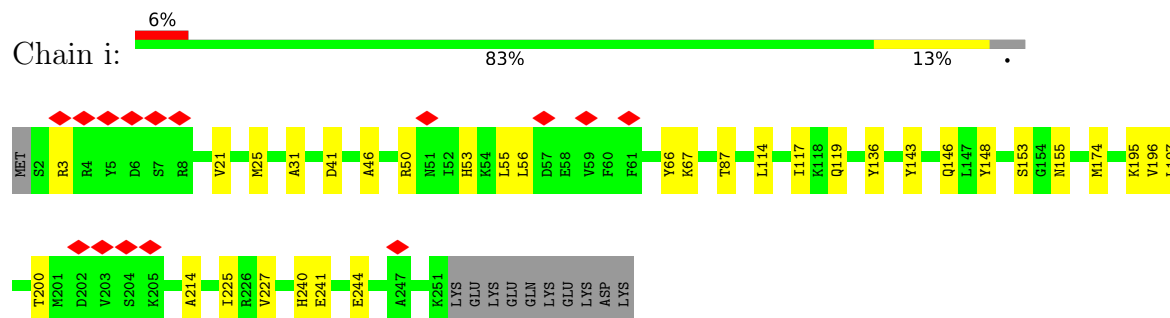
- Molecule 8: Proteasome subunit alpha type-2




- Molecule 9: Proteasome subunit alpha type-4

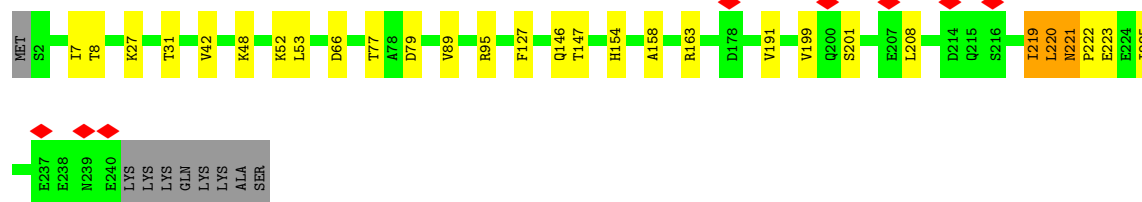


- Molecule 9: Proteasome subunit alpha type-4




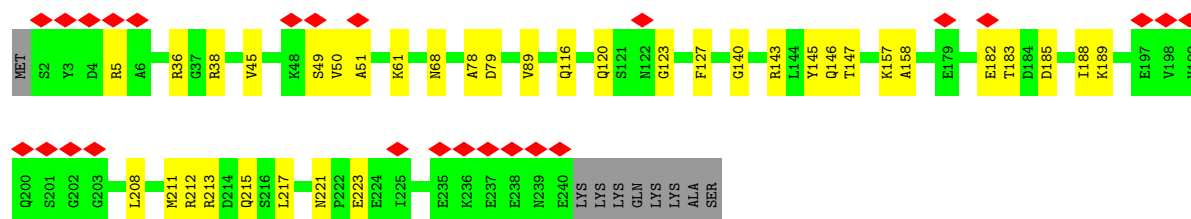
- Molecule 10: Proteasome subunit alpha type-7

Chain J:  85% 10% . .




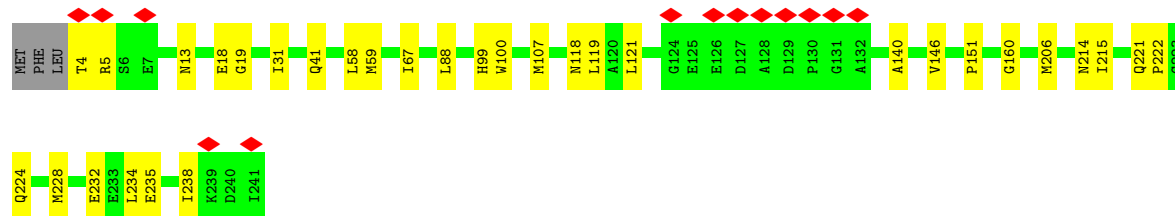
- Molecule 10: Proteasome subunit alpha type-7

Chain j:  10% 82% 15% .




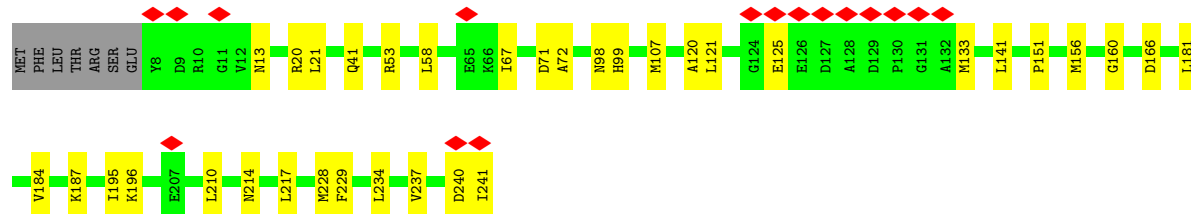
- Molecule 11: Proteasome subunit alpha type-5

Chain K:  5% 85% 13% .




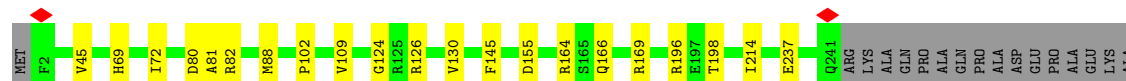
- Molecule 11: Proteasome subunit alpha type-5

Chain k:  7% 83% 15% .



- Molecule 12: Proteasome subunit alpha type-1

Chain L:  83% 8% 9%



ASP
GLU
PRO
MET
GLU
HIS

• Molecule 12: Proteasome subunit alpha type-1

Chain l: 83% 8% 10%

MET PHE ARG N4 D7 H20 Q21 T22 E23 S33 E55 L56 K61 K62 I63 I72 R82 M88 D100 I112 T120 R126 I134 M140 K189 D218 E234 Q241 ARG LYS ALA GLN PRO ALA GLN PRO ALA ASP GLU PRO ALA GLU

LYS
ALA
ASP
GLU
PRO
MET
GLU
HIS

• Molecule 13: Proteasome subunit alpha type-3

Chain M: 83% 12% 5%

MET SER I3 Y7 P16 S34 K42 K51 L52 S62 N63 K64 R65 L66 F67 N68 H72 N105 L108 K109 H120 Y125 V128 L137 Y149 C163 A164 E183 E192 I196 E203 D206 F209 E210 L211 W215

H224 V227 R232 K244 GLU ASP GLU ASP SER ASP ASP ASN MET

• Molecule 13: Proteasome subunit alpha type-3

Chain m: 81% 13% 6%

MET SER ILE GLY T5 D8 S15 R19 Q22 V23 E24 M27 S34 T35 A36 I37 R40 C41 V46 R65 N68 A78 Y125 S126 A127 V128 R129 A146 M150 G166 R169 A172 I176 M181 I189 V193 K205

D206 K207 W215 L219 T220 R223 H224 E225 P228 I231 K244 GLU GLU ASP GLU SER ASP ASP ASN MET

• Molecule 14: Proteasome subunit beta type-6

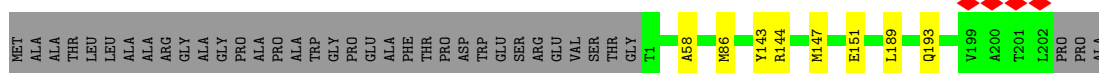
Chain N: 79% 6% 15%

MET ALA THR LEU ALA ARG GLY ALA PRO PRO TRP GLY PRO GLU GLU PHE THR PRO ASP TRP GLU SER ARG GLU VAL SER THR GLY T1 Q7 F8 D9 D32 R45 A58 K84 E85 M86 G109 M120 I179 V184 L190

I194 P195 K196 A200 T201 L202 P203 PRO ALA

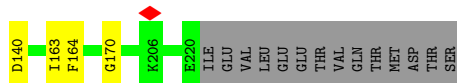
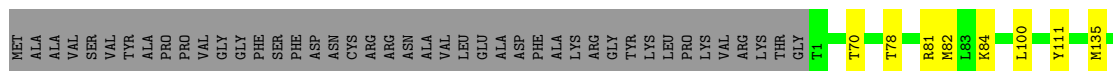
• Molecule 14: Proteasome subunit beta type-6

Chain n: 81% 15%



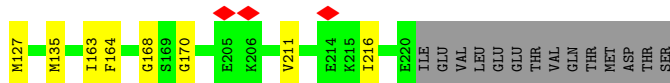
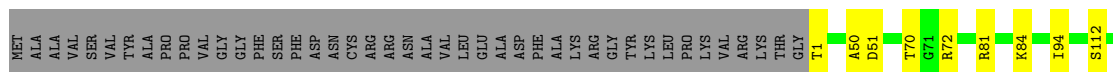
• Molecule 15: Proteasome subunit beta type-7

Chain O: 75% 21%



• Molecule 15: Proteasome subunit beta type-7

Chain o: 73% 6% 21%



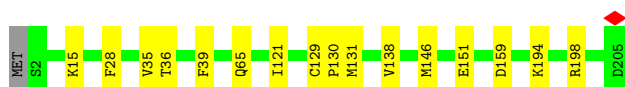
• Molecule 16: Proteasome subunit beta type-3

Chain P: 91% 8%



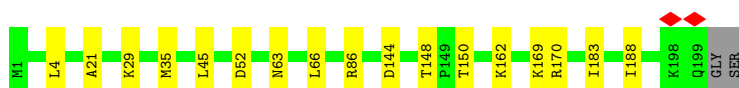
• Molecule 16: Proteasome subunit beta type-3

Chain p: 92% 8%



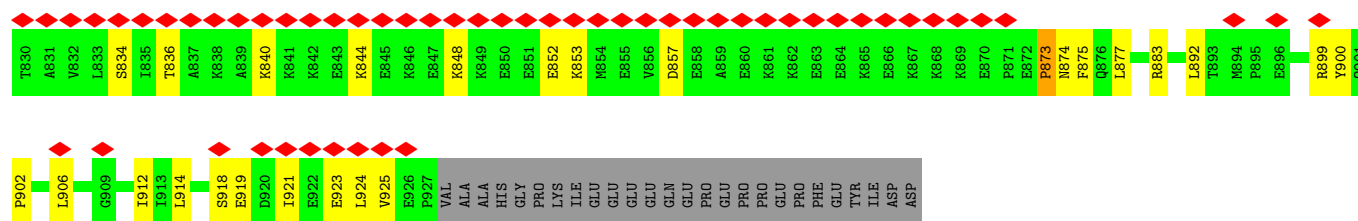
• Molecule 17: Proteasome subunit beta type-2

Chain Q: 91% 8%

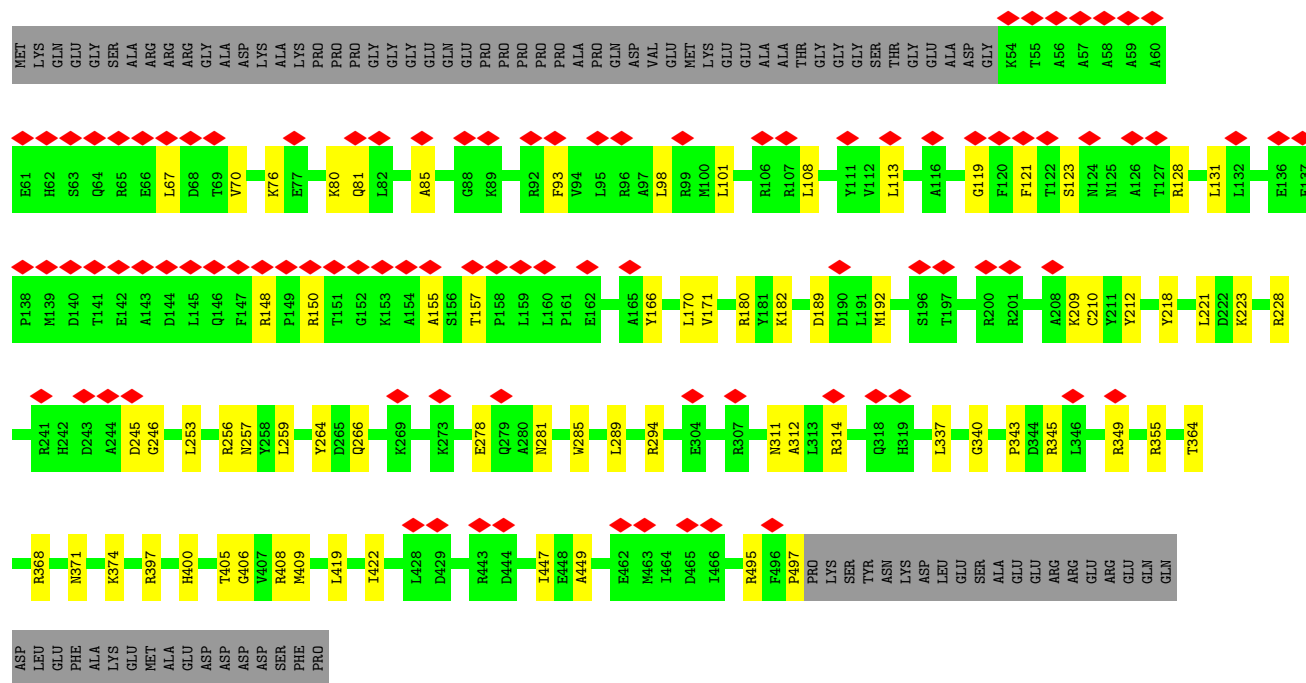


• Molecule 17: Proteasome subunit beta type-2

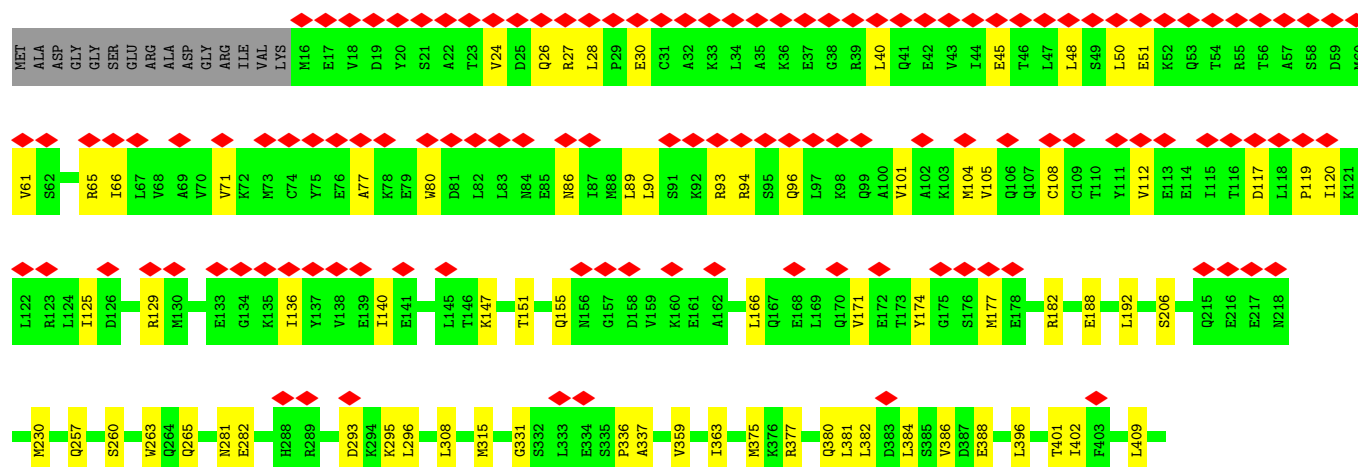
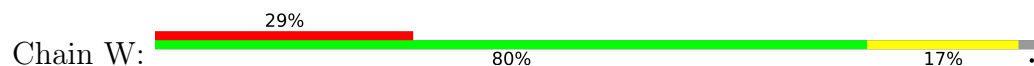


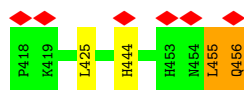


• Molecule 22: 26S proteasome non-ATPase regulatory subunit 3



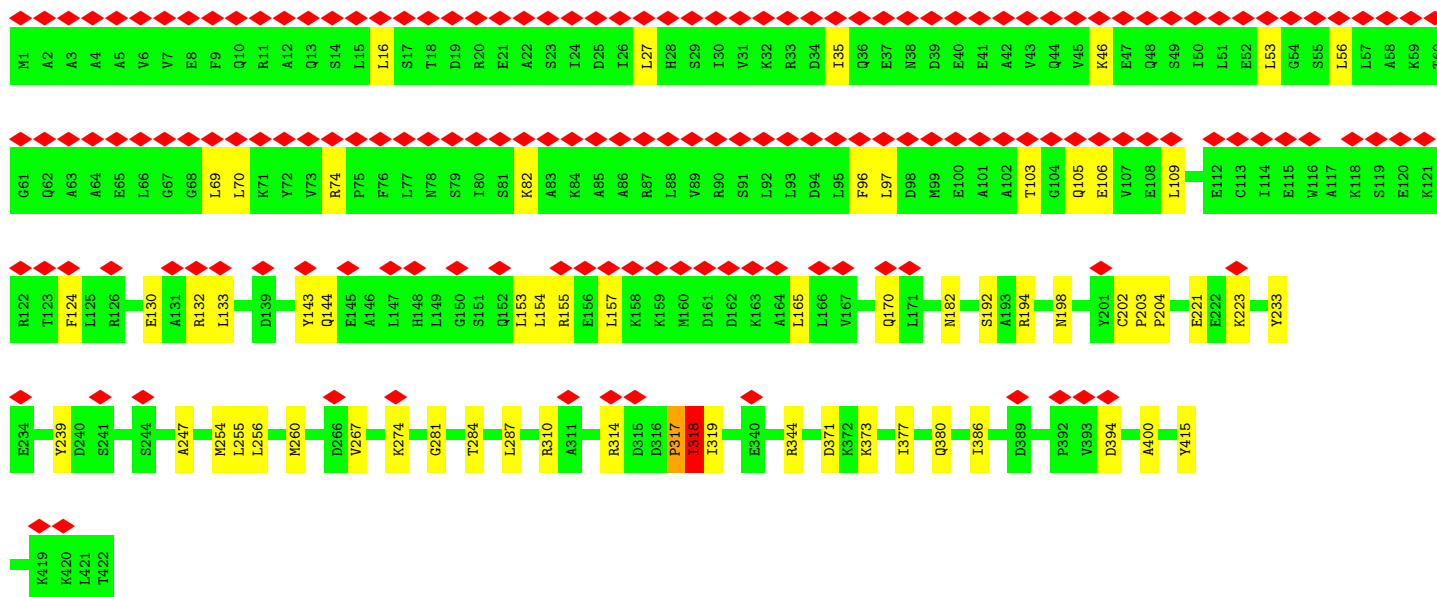
• Molecule 23: 26S proteasome non-ATPase regulatory subunit 12





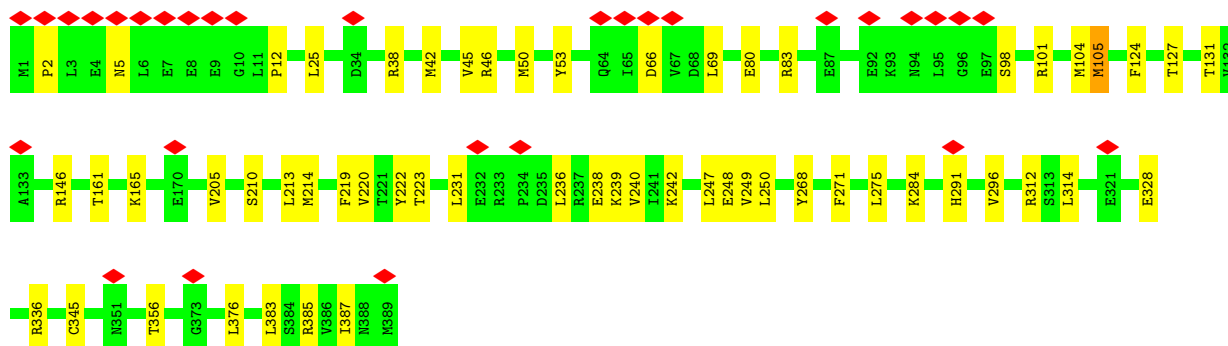
- Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

Chain X: 39% 85% 14%



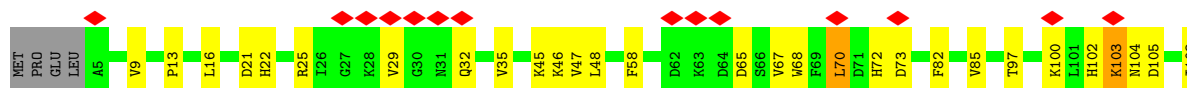
- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6

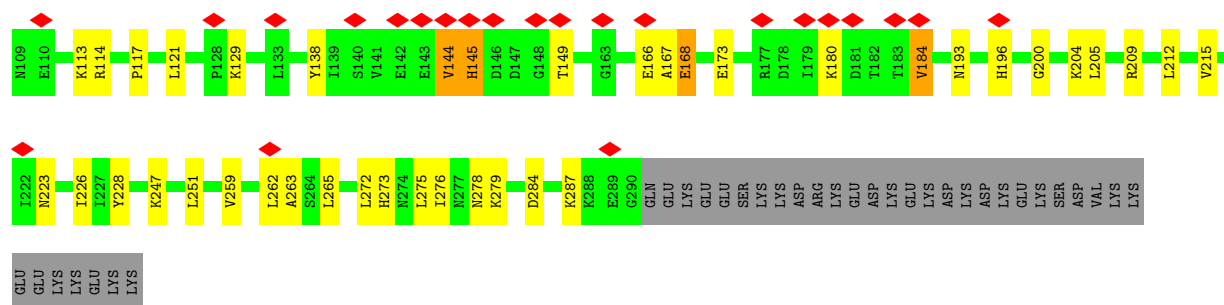
Chain Y: 8% 85% 15%



- Molecule 26: 26S proteasome non-ATPase regulatory subunit 7

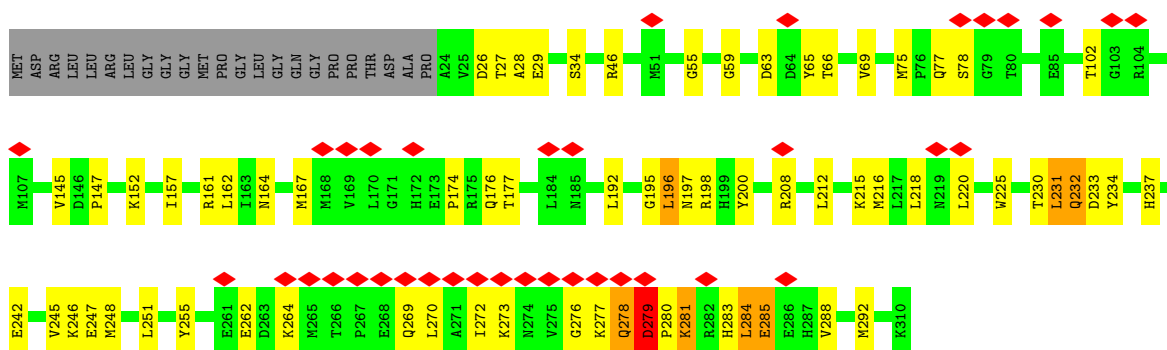
Chain Z: 11% 67% 19% 12%





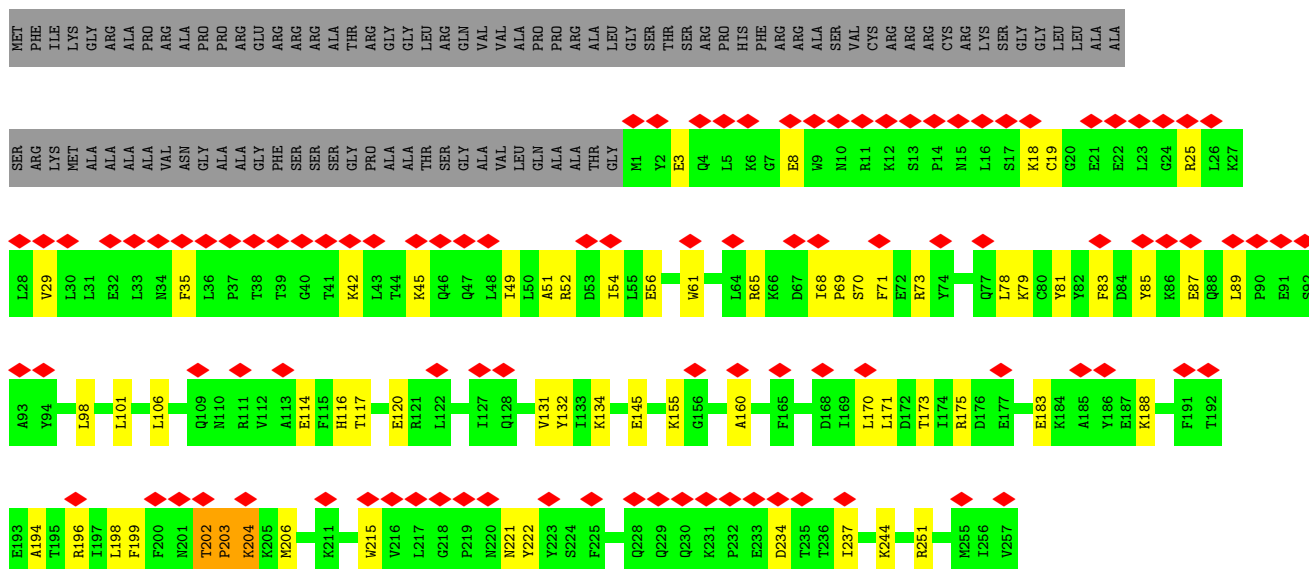
- Molecule 29: 26S proteasome non-ATPase regulatory subunit 14

Chain c: 



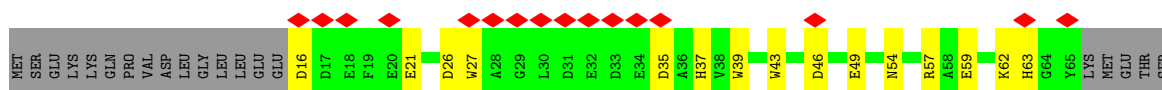
- Molecule 30: 26S proteasome non-ATPase regulatory subunit 8

Chain d: 




- Molecule 31: 26S proteasome complex subunit SEM1

Chain e: 



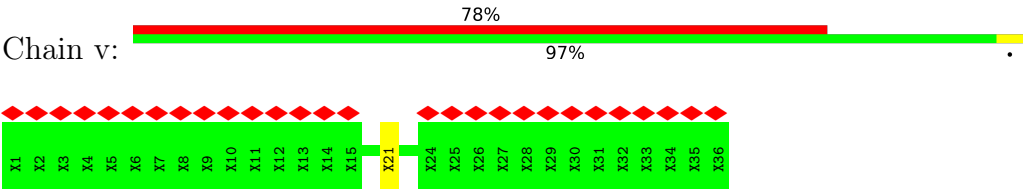
- Molecule 32: 26S proteasome non-ATPase regulatory subunit 2

Chain f: 



T870	P871	V872	L873	L874	A875	H876	Q877	R878	R879	A880	E881	L882	A883	T884	E885	E886	F887	L888	P889	V890	F891	T891	P892	I893	L894	E895	G896	F897	V898	I899	L900	R901	K902	N903	P904	N905	Y906	L908																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
R807		I810	L811	G812	K813	Y816	R817	L818		L821	V822	A823	M825	Q826	R827	E828	R829	L830	V831	T832	F833	D834	E835	E836	L837	R838	P839	L840	R841	V842	S843	L844	R845	V846	G847	Q848	A849	V850	D851	V852	R853	G854	Q855	A856	G857	K858	P859	K860	T861	L862	T863	G864	F865	Q866	T867	H868	T869																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
R740	L741	A742	M743	L744	L745	R746	Q747	L748	A749	Q750	Y751	H752	A753	K754	D755	P756	H757	N758	L759	F760	M761	F762	R763	L764	A765	Q766	H770	K773	G774	T775	L776	T777	L778	C779	F780	Y781	H782	S783	D784	R785	Q786	L787	M788	S789	G790	V791	A794	G795	L796	L797	T798	F803	R804	L805	D806	A739																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
L672	A673	T674	F675	G676	H677	L678	L679	R680	Y681	G682	E683	L686	V690	P691	L692	A693	L694	A695	L696	L697	S698	V699	S700	N701	F702	R703	L704	N705	L706	L707	A648	H649	Q650	C651	V652	A653	V654	L655	L656	L657	A658	L659	L660	A661	M662	G663	E664	E665	L666	G667	A668	E669	M670	A671																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
L612	L613	H614	L615	C616	S617	E618	F620	D621	S621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	A601	G602	S603	G604	N605	V606	L607	K608	V609	Q610	Q611																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
L550	K551	D552	T553	Y554	A555	R556	W557	L558	P559	L560	G561	L562	G563	L564	H565	H566	G570	E571	A572	I573	E574	A575	L576	L577	A578	L579	A580	E581	A582	V583	S584	E585	P586	F587	R588	S589	F590	A591	N592	T593	D596	V597	C598	A599	Y600	E601	G602	S603	G604	N605	V606	L607	K608	V609	Q610	Q611																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
Y489	A490	G491	S492	N493	R494	E495	D496	L497	L498	T499	L500	L501	L502	P503	Y504	M505	D507	S508	K509	S510	S511	N512	E513	V514	A515	G516	V517	T518	A519	L520	A521	C522	G523	M524	L525	S529	C530	N531	D532	D533	V534	T535	S536	T537	L538	L539	Q540	T541	I542	M543	E544	K545	S546	E547	T548	E549																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
G424		T427	Q428	I429	D430	K431	Y432	Y433	Y434	S435	S436	D437	D438	Y439																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		

● Molecule 33: Substrate



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92777	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.021	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00588	Depositor
Map size (Å)	411.0, 411.0, 411.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.685, 0.685, 0.685	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: MG, ZN, ADP, ATP

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	0.27	0/3283	0.62	0/4433
2	B	0.21	0/3254	0.55	0/4388
3	C	0.29	0/3146	0.64	6/4226 (0.1%)
4	D	0.27	0/3090	0.63	1/4168 (0.0%)
5	E	0.26	0/3145	0.62	1/4233 (0.0%)
6	F	0.29	0/3137	0.60	1/4223 (0.0%)
7	G	0.21	0/1901	0.48	0/2572
7	g	0.19	0/1913	0.47	0/2589
8	H	0.17	0/1840	0.46	0/2495
8	h	0.17	0/1844	0.41	0/2497
9	I	0.21	0/1963	0.48	0/2650
9	i	0.18	0/1985	0.47	0/2677
10	J	0.21	0/1887	0.50	0/2553
10	j	0.19	0/1887	0.48	0/2549
11	K	0.16	0/1841	0.40	0/2486
11	k	0.15	0/1809	0.42	1/2444 (0.0%)
12	L	0.15	0/1911	0.40	0/2584
12	l	0.14	0/1896	0.40	0/2565
13	M	0.17	0/1931	0.45	0/2600
13	m	0.15	0/1916	0.43	0/2580
14	N	0.12	0/1548	0.32	0/2097
14	n	0.14	0/1536	0.36	0/2080
15	O	0.17	0/1672	0.47	0/2267
15	o	0.17	0/1686	0.46	0/2282
16	P	0.17	0/1616	0.46	1/2180 (0.0%)
16	p	0.17	0/1620	0.48	0/2184
17	Q	0.16	0/1627	0.42	0/2202
17	q	0.16	0/1611	0.42	0/2182
18	R	0.15	0/1590	0.42	0/2147
18	r	0.14	0/1580	0.38	0/2135
19	S	0.16	0/1671	0.45	0/2252
19	s	0.16	0/1680	0.43	0/2264

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	T	0.15	0/1716	0.43	0/2323
20	t	0.14	0/1720	0.40	0/2328
21	U	0.21	0/6984	0.52	0/9435
22	V	0.21	0/3681	0.51	0/4969
23	W	0.22	0/3644	0.53	0/4901
24	X	0.19	0/3381	0.50	2/4558 (0.0%)
25	Y	0.19	0/3261	0.50	2/4393 (0.0%)
26	Z	0.27	0/2324	0.67	2/3150 (0.1%)
27	a	0.23	0/3053	0.62	0/4133
28	b	0.23	0/1478	0.57	0/2001
29	c	0.27	0/2302	0.69	4/3110 (0.1%)
30	d	0.27	0/2162	0.67	0/2919
31	e	0.25	0/437	0.67	0/595
32	f	0.22	0/6640	0.55	0/8988
All	All	0.21	0/107799	0.52	21/145587 (0.0%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	X	317	PRO	N-CA-C	-12.21	97.03	113.40
26	Z	144	VAL	N-CA-C	-7.19	103.84	110.82
3	C	82	LYS	N-CA-C	-6.89	102.16	111.87
16	P	3	ILE	N-CA-C	-6.44	107.22	113.53
3	C	143	VAL	CA-C-N	-6.21	114.37	120.52
3	C	143	VAL	C-N-CA	-6.21	114.37	120.52
24	X	318	ILE	CB-CA-C	-6.15	101.21	111.29
3	C	397	LYS	CA-C-N	6.01	133.03	121.54
3	C	397	LYS	C-N-CA	6.01	133.03	121.54
5	E	166	PRO	N-CA-C	5.68	117.63	110.70
3	C	252	ASP	N-CA-C	-5.51	106.46	114.12
26	Z	29	VAL	N-CA-C	-5.45	107.17	112.29
29	c	279	ASP	CA-C-N	5.40	126.59	119.84
29	c	279	ASP	C-N-CA	5.40	126.59	119.84
6	F	179	GLU	CA-CB-CG	5.34	124.78	114.10
25	Y	291	HIS	CA-C-N	5.29	131.64	121.54
25	Y	291	HIS	C-N-CA	5.29	131.64	121.54
29	c	230	THR	CA-C-N	-5.13	113.29	121.44
29	c	230	THR	C-N-CA	-5.13	113.29	121.44
4	D	158	GLN	N-CA-C	-5.12	106.87	113.01
11	k	53	ARG	CA-CB-CG	5.02	124.13	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3229	0	3261	81	0
2	B	3207	0	3278	55	0
3	C	3105	0	3219	60	0
4	D	3040	0	3075	82	0
5	E	3097	0	3174	71	0
6	F	3098	0	3187	111	0
7	G	1867	0	1867	23	0
7	g	1879	0	1872	20	0
8	H	1801	0	1773	18	0
8	h	1805	0	1798	10	0
9	I	1933	0	1923	28	0
9	i	1955	0	1955	20	0
10	J	1861	0	1846	24	0
10	j	1861	0	1865	23	0
11	K	1813	0	1796	20	0
11	k	1782	0	1766	21	0
12	L	1876	0	1856	12	0
12	l	1861	0	1839	13	0
13	M	1893	0	1885	17	0
13	m	1881	0	1868	21	0
14	N	1521	0	1494	8	0
14	n	1510	0	1483	5	0
15	O	1645	0	1648	8	0
15	o	1659	0	1681	13	0
16	P	1587	0	1598	10	0
16	p	1591	0	1609	11	0
17	Q	1591	0	1589	14	0
17	q	1578	0	1569	19	0
18	R	1559	0	1523	9	0
18	r	1549	0	1506	12	0
19	S	1641	0	1639	15	0
19	s	1650	0	1645	16	0
20	T	1683	0	1662	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	t	1687	0	1666	17	0
21	U	6867	0	6929	110	0
22	V	3612	0	3682	46	0
23	W	3596	0	3713	49	0
24	X	3335	0	3435	46	0
25	Y	3202	0	3204	38	0
26	Z	2281	0	2312	54	0
27	a	2995	0	3012	47	0
28	b	1458	0	1505	35	0
29	c	2260	0	2276	67	0
30	d	2116	0	2146	49	0
31	e	425	0	328	14	0
32	f	6529	0	6541	93	0
33	v	180	0	50	1	0
34	A	31	0	12	4	0
34	B	31	0	12	1	0
34	C	31	0	12	2	0
34	D	31	0	12	1	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
36	E	27	0	12	3	0
36	F	27	0	12	1	0
37	c	1	0	0	0	0
All	All	106334	0	106620	1368	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 6.

All (1368) 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)
29:c:279:ASP:HA	29:c:283:HIS:HB3	1.13	1.07
5:E:165:ILE:H	5:E:166:PRO:HD2	1.27	0.97
29:c:279:ASP:HA	29:c:283:HIS:CB	1.94	0.96
5:E:165:ILE:C	5:E:167:PRO:HD3	1.91	0.95
30:d:204:LYS:NZ	30:d:204:LYS:HA	1.83	0.94
6:F:245:LYS:HB3	6:F:282:ILE:HD13	1.51	0.92
6:F:181:PRO:HG2	6:F:238:ARG:HH22	1.34	0.91
29:c:279:ASP:CA	29:c:283:HIS:HB3	2.01	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:220:PRO:HA	6:F:348:LEU:HD13	1.53	0.88
30:d:202:THR:HA	30:d:206:MET:HE1	1.55	0.88
6:F:295:ARG:HH12	6:F:340:PRO:HD3	1.39	0.88
29:c:279:ASP:N	29:c:280:PRO:HD2	1.89	0.87
30:d:204:LYS:HA	30:d:204:LYS:CE	2.01	0.87
3:C:83:LYS:HE2	3:C:99:VAL:HG21	1.58	0.85
29:c:281:LYS:O	29:c:284:LEU:HB2	1.77	0.85
6:F:295:ARG:HH22	6:F:340:PRO:HD3	1.46	0.81
29:c:279:ASP:O	29:c:284:LEU:CD2	2.28	0.80
2:B:68:ILE:HA	32:f:670:MET:HE1	1.65	0.79
23:W:425:LEU:HB2	26:Z:247:LYS:HD3	1.65	0.77
32:f:113:MET:HE1	32:f:118:ASN:HB3	1.66	0.77
23:W:48:LEU:HD13	23:W:93:ARG:HH12	1.50	0.77
30:d:188:LYS:HD2	30:d:221:ASN:HD21	1.50	0.76
6:F:317:LEU:HD11	6:F:347:ARG:HG2	1.70	0.73
6:F:295:ARG:NH1	6:F:340:PRO:HD3	2.03	0.73
9:I:99:LEU:HG	17:Q:86:ARG:HH12	1.54	0.73
4:D:380:GLN:HB3	5:E:166:PRO:HG3	1.70	0.73
6:F:181:PRO:HG2	6:F:238:ARG:NH2	2.04	0.73
1:A:55:LEU:HD22	2:B:72:LEU:HB3	1.71	0.72
6:F:260:PHE:HB2	6:F:263:ASP:HB2	1.71	0.72
21:U:773:PHE:HB2	29:c:177:THR:HB	1.72	0.72
30:d:204:LYS:HA	30:d:204:LYS:HZ3	1.55	0.72
29:c:276:GLY:H	29:c:278:GLN:NE2	1.88	0.71
4:D:270:ILE:HG22	4:D:285:VAL:HG13	1.71	0.71
6:F:340:PRO:C	6:F:342:LEU:H	1.99	0.71
9:I:53:HIS:CG	9:I:54:LYS:H	2.08	0.71
5:E:19:HIS:HE1	6:F:48:LEU:HD22	1.56	0.71
29:c:279:ASP:O	29:c:284:LEU:HD23	1.91	0.70
29:c:247:GLU:O	29:c:251:LEU:HB2	1.90	0.70
5:E:165:ILE:N	5:E:166:PRO:HD2	2.04	0.70
3:C:254:ILE:N	3:C:254:ILE:HD12	2.06	0.69
4:D:335:LEU:HB3	4:D:336:PRO:HD2	1.74	0.69
29:c:69:VAL:O	29:c:208:ARG:NH2	2.24	0.69
1:A:167:GLU:HG3	1:A:237:PHE:O	1.92	0.69
27:a:315:LEU:HD23	27:a:320:VAL:HG13	1.73	0.69
22:V:180:ARG:HH12	22:V:182:LYS:HB2	1.58	0.69
10:j:211:MET:HB2	10:j:217:LEU:HD12	1.74	0.69
1:A:155:PRO:HD2	1:A:157:ILE:HD13	1.74	0.68
10:J:154:HIS:HB3	11:K:59:MET:HE1	1.75	0.68
10:J:222:PRO:HA	10:J:225:ILE:HD12	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LYS:O	1:A:62:LEU:HB2	1.94	0.68
3:C:219:LEU:HD13	3:C:272:THR:HG21	1.75	0.68
1:A:157:ILE:O	1:A:159:PRO:HD2	1.93	0.68
6:F:295:ARG:NH2	6:F:340:PRO:HD3	2.07	0.68
9:I:143:TYR:HB2	9:I:146:GLN:HE21	1.57	0.68
1:A:238:ILE:HD12	1:A:272:ILE:HG12	1.75	0.68
9:I:53:HIS:NE2	9:I:55:LEU:HB2	2.08	0.67
29:c:192:LEU:HA	29:c:196:LEU:HB2	1.75	0.67
2:B:401:GLU:HG3	2:B:405:MET:HE2	1.77	0.67
4:D:237:GLN:HA	5:E:209:GLY:HA3	1.76	0.67
4:D:125:LYS:HB2	4:D:126:PRO:HD3	1.77	0.67
19:s:148:LEU:HD23	19:s:178:VAL:HG12	1.76	0.67
7:G:18:PRO:O	7:G:19:GLU:HB2	1.95	0.67
27:a:289:ARG:HB2	27:a:333:MET:HB3	1.76	0.66
3:C:70:GLY:HA3	4:D:113:VAL:HG12	1.77	0.66
10:j:38:ARG:HH12	10:j:182:GLU:HA	1.61	0.66
14:n:144:ARG:HG2	14:n:147:MET:HE3	1.77	0.66
23:W:401:THR:HG23	23:W:402:ILE:HD12	1.77	0.66
21:U:14:GLU:OE2	30:d:73:ARG:NH2	2.28	0.66
21:U:58:GLN:HB2	21:U:87:LEU:HD12	1.76	0.66
19:s:68:ILE:HD11	19:s:92:LEU:HD13	1.76	0.66
24:X:233:TYR:HA	24:X:254:MET:HE1	1.78	0.66
9:i:143:TYR:HB2	9:i:146:GLN:HE21	1.60	0.66
30:d:61:TRP:HB3	30:d:65:ARG:HH21	1.60	0.65
32:f:696:LEU:HD11	32:f:796:LEU:HD13	1.79	0.65
6:F:295:ARG:HH22	6:F:340:PRO:CD	2.10	0.65
23:W:27:ARG:HG3	23:W:50:LEU:HD11	1.77	0.65
4:D:336:PRO:HB3	4:D:344:ILE:HD12	1.79	0.65
5:E:56:ILE:HB	5:E:100:LEU:HB2	1.77	0.65
29:c:251:LEU:HG	29:c:279:ASP:OD1	1.96	0.65
2:B:41:LYS:O	32:f:712:LYS:NZ	2.29	0.65
15:o:163:ILE:HG12	15:o:170:GLY:HA2	1.79	0.65
29:c:279:ASP:O	29:c:284:LEU:HD22	1.96	0.65
30:d:202:THR:HA	30:d:206:MET:CE	2.27	0.65
32:f:271:MET:HE1	32:f:788:MET:HB3	1.78	0.64
16:P:53:LEU:HG	16:P:107:PRO:HB3	1.78	0.64
29:c:231:LEU:O	29:c:232:GLN:HG3	1.97	0.64
23:W:40:LEU:HD21	23:W:77:ALA:HB1	1.79	0.64
32:f:338:ASP:HB3	32:f:340:MET:HG3	1.78	0.64
7:G:202:LEU:HA	7:G:205:VAL:HG12	1.78	0.64
4:D:313:ARG:HH21	5:E:242:ARG:HB3	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:7:MET:HE1	28:b:93:ALA:HA	1.80	0.64
4:D:212:LYS:NZ	4:D:311:THR:O	2.31	0.64
1:A:172:VAL:O	1:A:231:ASN:ND2	2.31	0.64
27:a:223:GLU:O	27:a:227:ASN:HB2	1.97	0.64
5:E:165:ILE:O	5:E:167:PRO:HD3	1.96	0.64
24:X:53:LEU:HD22	24:X:69:LEU:HD22	1.79	0.64
29:c:231:LEU:C	29:c:233:ASP:N	2.55	0.64
31:e:59:GLU:HA	31:e:62:LYS:HG2	1.80	0.64
6:F:340:PRO:CG	6:F:343:LEU:HD13	2.28	0.63
26:Z:259:VAL:HA	29:c:292:MET:HE1	1.79	0.63
10:j:68:ASN:HA	10:j:211:MET:HE1	1.81	0.63
3:C:88:LYS:HA	3:C:94:LYS:HA	1.80	0.63
22:V:221:LEU:HB2	22:V:223:LYS:HZ2	1.63	0.63
22:V:343:PRO:O	31:e:43:TRP:NE1	2.32	0.63
4:D:296:MET:HE3	4:D:326:ARG:HD3	1.80	0.63
29:c:276:GLY:H	29:c:278:GLN:HE21	1.46	0.63
7:G:113:MET:HE3	15:O:70:THR:HA	1.81	0.63
32:f:96:LEU:HD13	32:f:129:LEU:HD13	1.81	0.63
26:Z:212:LEU:HA	26:Z:215:VAL:HG12	1.80	0.63
7:G:203:SER:O	23:W:94:ARG:NH2	2.31	0.63
26:Z:263:ALA:HB1	29:c:288:VAL:HG13	1.81	0.63
2:B:387:LYS:HB3	2:B:390:LEU:HD23	1.80	0.62
10:J:52:LYS:HG3	10:J:53:LEU:HG	1.81	0.62
29:c:34:SER:HB3	29:c:208:ARG:HH21	1.63	0.62
10:j:120:GLN:NE2	11:k:133:MET:SD	2.72	0.62
17:q:44:LEU:HD11	17:q:102:LEU:HD23	1.80	0.62
5:E:165:ILE:O	5:E:167:PRO:CD	2.47	0.62
6:F:305:GLU:OE1	6:F:308:ARG:NH2	2.33	0.62
24:X:103:THR:HA	24:X:106:GLU:HG3	1.81	0.62
26:Z:129:LYS:NZ	29:c:212:LEU:O	2.33	0.62
28:b:22:LEU:HB2	28:b:23:PRO:CD	2.30	0.62
29:c:278:GLN:HB2	29:c:280:PRO:HD2	1.82	0.62
30:d:203:PRO:CD	30:d:206:MET:HE1	2.29	0.62
27:a:120:ALA:O	27:a:161:LYS:NZ	2.33	0.62
29:c:279:ASP:N	29:c:280:PRO:CD	2.62	0.62
13:M:211:LEU:O	13:M:232:ARG:NH2	2.33	0.61
19:S:83:MET:HE1	19:S:91:MET:HE3	1.81	0.61
28:b:21:PHE:CD2	28:b:25:ARG:HG2	2.34	0.61
9:i:53:HIS:HE1	9:i:55:LEU:HD12	1.64	0.61
2:B:122:ILE:HD11	2:B:130:GLU:HB3	1.82	0.61
26:Z:103:LYS:H	26:Z:103:LYS:HZ3	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:153:LEU:HD23	28:b:170:LEU:HD11	1.81	0.61
3:C:14:GLY:O	21:U:93:ASN:ND2	2.34	0.61
23:W:308:LEU:HB3	23:W:315:MET:HE1	1.83	0.61
26:Z:184:VAL:HG13	26:Z:184:VAL:O	2.00	0.61
5:E:75:ASN:ND2	6:F:129:ARG:O	2.33	0.61
21:U:873:PRO:C	21:U:875:PHE:H	2.09	0.61
1:A:212:VAL:HG22	1:A:339:ARG:HB2	1.83	0.61
6:F:206:MET:HB2	6:F:245:LYS:HZ3	1.65	0.61
31:e:35:ASP:HB2	31:e:37:HIS:HD2	1.64	0.61
3:C:297:ARG:NH1	4:D:274:ARG:O	2.33	0.61
6:F:151:VAL:HG12	6:F:163:THR:HG23	1.82	0.61
4:D:119:ILE:O	4:D:121:ARG:NH1	2.34	0.61
21:U:483:LEU:HD11	21:U:781:LEU:HD11	1.81	0.61
27:a:70:ARG:HH21	28:b:17:ARG:HG2	1.66	0.61
12:l:100:ASP:OD1	19:s:66:LYS:NZ	2.34	0.61
6:F:87:PRO:HG2	6:F:155:LYS:HD3	1.82	0.61
3:C:305:LEU:HA	3:C:310:ARG:HD2	1.81	0.60
6:F:43:GLN:HG2	6:F:47:LEU:HD23	1.83	0.60
15:o:112:SER:HB2	15:o:127:MET:HE3	1.83	0.60
4:D:86:PRO:O	4:D:134:LYS:NZ	2.34	0.60
20:t:92:LEU:HD12	20:t:112:ILE:HD11	1.83	0.60
22:V:85:ALA:HB2	22:V:93:PHE:HB2	1.82	0.60
6:F:229:PRO:O	6:F:392:ASN:ND2	2.34	0.60
8:H:59:GLU:HG3	8:H:206:ASP:HB2	1.83	0.60
15:O:163:ILE:HG12	15:O:170:GLY:HA2	1.82	0.60
17:Q:4:LEU:HD22	17:Q:45:LEU:HD23	1.83	0.60
21:U:217:CYS:O	21:U:754:HIS:NE2	2.34	0.60
3:C:267:SER:O	3:C:271:ARG:NH1	2.35	0.60
21:U:148:LYS:HA	21:U:151:ILE:HG22	1.83	0.60
21:U:744:VAL:HA	21:U:785:PRO:HA	1.82	0.60
5:E:84:ARG:HD3	5:E:87:LEU:HD21	1.83	0.60
6:F:35:LYS:HB2	6:F:38:THR:HB	1.83	0.60
8:h:114:VAL:HG12	8:h:118:MET:HE2	1.83	0.60
11:k:210:LEU:HA	11:k:214:ASN:HD21	1.67	0.60
19:S:43:CYS:O	19:S:194:ARG:NH2	2.34	0.60
6:F:430:LYS:NZ	11:K:18:GLU:OE2	2.35	0.60
30:d:3:GLU:O	30:d:25:ARG:NH1	2.35	0.60
1:A:386:ARG:NH1	34:A:501:ATP:O2'	2.34	0.60
4:D:231:VAL:HG13	5:E:262:ASN:HD21	1.66	0.60
6:F:188:ILE:HG12	6:F:235:LEU:HD23	1.84	0.60
26:Z:73:ASP:OD2	28:b:70:ARG:NH1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:9:CYS:HB3	28:b:111:ALA:HA	1.82	0.60
32:f:320:ILE:HA	32:f:325:GLN:HE22	1.66	0.60
2:B:181:GLN:O	2:B:241:ASN:ND2	2.34	0.59
27:a:122:LYS:HD3	27:a:130:VAL:HG13	1.84	0.59
2:B:412:MET:HB2	32:f:90:THR:HG21	1.84	0.59
5:E:230:ILE:HB	5:E:275:MET:HG2	1.83	0.59
8:H:148:GLN:OE1	8:H:158:TRP:NE1	2.34	0.59
25:Y:383:LEU:HD22	26:Z:272:LEU:HD21	1.84	0.59
10:J:220:LEU:HD12	10:J:225:ILE:HG12	1.84	0.59
30:d:234:ASP:HB3	30:d:237:ILE:HG12	1.84	0.59
7:g:61:LEU:HD21	7:g:66:VAL:HG11	1.85	0.59
4:D:99:ASN:HA	4:D:115:ILE:HG12	1.84	0.59
32:f:521:ALA:HA	32:f:524:MET:HE2	1.84	0.59
13:m:34:SER:OG	13:m:65:ARG:NH1	2.35	0.59
13:M:108:LEU:HD11	13:M:137:LEU:HB3	1.84	0.59
2:B:380:LEU:HD23	2:B:383:LEU:HD12	1.84	0.59
7:G:141:ILE:HG22	7:G:151:VAL:HG22	1.85	0.59
25:Y:231:LEU:HD21	25:Y:239:LYS:HZ1	1.67	0.59
19:s:198:VAL:HG22	19:s:203:ILE:HG12	1.85	0.59
29:c:262:GLU:OE2	29:c:264:LYS:NZ	2.36	0.59
23:W:425:LEU:HD23	26:Z:251:LEU:HD23	1.84	0.59
12:l:33:SER:OG	12:l:62:LYS:NZ	2.33	0.59
3:C:49:ARG:NH1	21:U:639:LEU:O	2.36	0.59
23:W:140:ILE:HG12	23:W:177:MET:HB2	1.83	0.59
24:X:182:ASN:ND2	25:Y:248:GLU:OE2	2.35	0.58
32:f:151:LEU:HB3	32:f:159:VAL:HG22	1.84	0.58
12:L:196:ARG:NH1	12:L:237:GLU:O	2.37	0.58
4:D:336:PRO:HB3	4:D:344:ILE:CD1	2.33	0.58
29:c:162:LEU:HD12	29:c:200:TYR:HB3	1.84	0.58
32:f:727:PHE:HA	32:f:761:MET:HE2	1.84	0.58
4:D:115:ILE:HG22	4:D:139:LEU:HD12	1.84	0.58
10:J:208:LEU:HD22	10:J:220:LEU:HG	1.85	0.58
26:Z:70:LEU:HD21	26:Z:108:ILE:HD11	1.84	0.58
10:j:36:ARG:HH21	10:j:157:LYS:HG2	1.69	0.58
4:D:126:PRO:HD2	4:D:127:ASN:H	1.69	0.58
6:F:364:ARG:HA	6:F:367:GLN:HG2	1.86	0.58
16:P:138:VAL:HB	16:P:146:MET:HE2	1.85	0.58
27:a:180:LEU:HD11	27:a:221:VAL:HG11	1.85	0.58
2:B:440:LEU:HA	10:J:48:LYS:HZ1	1.67	0.58
6:F:259:MET:O	6:F:304:ARG:NH2	2.36	0.58
30:d:78:LEU:HD13	30:d:98:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:VAL:O	34:A:501:ATP:N6	2.37	0.58
21:U:3:THR:H	30:d:83:PHE:HE2	1.52	0.58
10:j:158:ALA:HB3	11:k:58:LEU:HD21	1.86	0.58
21:U:399:TRP:HD1	29:c:176:GLN:HG2	1.68	0.57
24:X:130:GLU:HG3	24:X:153:LEU:HG	1.85	0.57
5:E:84:ARG:HD2	5:E:108:MET:HA	1.85	0.57
21:U:252:LEU:HD11	21:U:260:PHE:HE2	1.68	0.57
3:C:53:ASN:ND2	21:U:642:GLU:O	2.36	0.57
4:D:125:LYS:CB	4:D:126:PRO:HD3	2.33	0.57
13:M:68:ASN:OD1	13:M:224:HIS:ND1	2.37	0.57
22:V:349:ARG:HH12	31:e:37:HIS:HE1	1.53	0.57
24:X:255:LEU:HD22	24:X:267:VAL:HG13	1.86	0.57
1:A:287:ASP:O	2:B:298:ASN:HB2	2.05	0.57
2:B:77:GLU:O	2:B:81:ASN:ND2	2.37	0.57
2:B:249:ARG:HH11	3:C:283:PHE:HB3	1.68	0.57
23:W:396:LEU:HD13	23:W:402:ILE:HD13	1.87	0.57
2:B:385:MET:HE1	10:J:201:SER:HA	1.86	0.57
6:F:177:VAL:HA	6:F:180:ARG:HE	1.70	0.57
32:f:779:CYS:HG	32:f:785:ARG:HH12	1.51	0.57
4:D:271:ALA:HB3	4:D:317:LEU:HD22	1.86	0.57
9:I:155:ASN:OD1	10:J:77:THR:OG1	2.22	0.57
30:d:35:PHE:HB2	30:d:81:TYR:HE1	1.70	0.57
3:C:15:LYS:HA	21:U:93:ASN:HD21	1.69	0.57
21:U:235:LYS:HA	21:U:238:LYS:HD2	1.87	0.57
4:D:320:ALA:O	4:D:326:ARG:NH1	2.37	0.57
5:E:130:VAL:HG23	5:E:134:GLU:HB2	1.86	0.57
9:i:119:GLN:NE2	10:j:79:ASP:OD1	2.38	0.57
4:D:91:GLN:NE2	4:D:127:ASN:OD1	2.37	0.57
6:F:97:LEU:O	6:F:120:LYS:N	2.38	0.57
24:X:105:GLN:HG2	24:X:109:LEU:HB2	1.87	0.57
25:Y:38:ARG:HG2	25:Y:42:MET:HE1	1.86	0.57
32:f:47:GLU:HA	32:f:50:LYS:HE2	1.87	0.57
12:l:72:ILE:HG22	12:l:134:ILE:HG12	1.87	0.57
2:B:408:ARG:NH1	3:C:163:GLU:OE1	2.37	0.56
3:C:215:SER:HA	3:C:249:ASP:HB2	1.87	0.56
5:E:19:HIS:CE1	6:F:48:LEU:HD22	2.37	0.56
27:a:70:ARG:O	28:b:17:ARG:NH1	2.34	0.56
29:c:276:GLY:N	29:c:278:GLN:NE2	2.52	0.56
13:m:68:ASN:OD1	13:m:224:HIS:ND1	2.38	0.56
20:t:25:ASP:OD1	20:t:41:ARG:NH2	2.37	0.56
2:B:194:ILE:HA	2:B:197:ILE:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:107:MET:HB3	28:b:136:VAL:HG13	1.87	0.56
15:o:216:ILE:HD11	16:p:194:LYS:HD2	1.86	0.56
2:B:423:LYS:HG3	2:B:427:LEU:HD12	1.87	0.56
20:T:27:LEU:HD22	20:T:184:TYR:HB2	1.87	0.56
21:U:742:HIS:HB3	21:U:883:ARG:HH21	1.68	0.56
23:W:375:MET:HE2	23:W:386:VAL:HB	1.85	0.56
24:X:27:LEU:HB3	24:X:53:LEU:HD12	1.87	0.56
25:Y:66:ASP:HB3	25:Y:69:LEU:HB3	1.87	0.56
25:Y:239:LYS:HG3	25:Y:240:VAL:HG13	1.86	0.56
27:a:28:LEU:HG	27:a:33:LEU:HD11	1.87	0.56
27:a:81:LEU:HA	27:a:84:VAL:HG12	1.88	0.56
11:k:160:GLY:O	12:l:82:ARG:NH2	2.38	0.56
22:V:81:GLN:HB3	22:V:93:PHE:HB3	1.88	0.56
22:V:278:GLU:HA	22:V:285:TRP:HZ2	1.71	0.56
26:Z:144:VAL:O	26:Z:145:HIS:HB2	2.04	0.56
32:f:560:LEU:O	32:f:564:LEU:N	2.38	0.56
4:D:45:LYS:HG2	21:U:187:LEU:HB2	1.87	0.56
5:E:148:VAL:HB	5:E:297:ARG:HH22	1.71	0.56
8:H:177:ARG:NH1	24:X:202:CYS:SG	2.78	0.56
26:Z:273:HIS:HD1	29:c:255:TYR:HH	1.54	0.56
17:q:168:GLN:NE2	17:q:175:LEU:O	2.37	0.56
6:F:235:LEU:HD21	36:F:501:ADP:H2'	1.87	0.56
20:T:174:ARG:NH1	20:T:206:GLU:O	2.39	0.56
23:W:174:TYR:O	23:W:182:ARG:NH2	2.38	0.56
32:f:822:VAL:HA	32:f:825:MET:HE2	1.87	0.56
12:l:61:LYS:NZ	12:l:63:ILE:O	2.37	0.56
7:G:165:ALA:HB3	8:H:56:LEU:HD22	1.86	0.56
28:b:21:PHE:HD2	28:b:25:ARG:HG2	1.70	0.56
13:m:8:ASP:O	13:m:22:GLN:NE2	2.37	0.56
3:C:112:CYS:HB2	3:C:130:LYS:HZ3	1.70	0.56
26:Z:82:PHE:HA	26:Z:85:VAL:HG12	1.88	0.56
11:k:13:ASN:HB2	12:l:126:ARG:HB3	1.88	0.56
1:A:48:VAL:HG13	2:B:69:LYS:HE2	1.87	0.56
1:A:54:GLN:OE1	1:A:57:LYS:NZ	2.39	0.56
25:Y:231:LEU:HG	25:Y:236:LEU:HD12	1.86	0.56
2:B:125:THR:OG1	2:B:126:SER:N	2.37	0.56
2:B:411:ARG:NH1	2:B:413:LYS:O	2.39	0.56
5:E:9:LEU:HD12	6:F:32:GLU:HG3	1.88	0.56
19:S:38:ARG:NH2	15:o:164:PHE:O	2.39	0.56
27:a:70:ARG:HB3	28:b:17:ARG:HB3	1.87	0.56
29:c:231:LEU:C	29:c:233:ASP:H	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:d:87:GLU:HA	30:d:89:LEU:HD23	1.87	0.56
15:o:70:THR:HG23	15:o:72:ARG:H	1.70	0.56
1:A:164:MET:O	1:A:167:GLU:HG2	2.06	0.55
6:F:348:LEU:HD12	6:F:348:LEU:H	1.70	0.55
22:V:212:TYR:HA	22:V:253:LEU:HD11	1.87	0.55
10:j:212:ARG:HB3	10:j:215:GLN:HG3	1.88	0.55
4:D:154:LEU:HD12	4:D:227:PHE:HD2	1.71	0.55
6:F:340:PRO:C	6:F:342:LEU:N	2.64	0.55
17:q:183:ILE:HG12	17:q:188:ILE:HG12	1.87	0.55
1:A:114:ASN:HB3	1:A:120:LYS:HG2	1.87	0.55
8:H:222:THR:OG1	8:H:225:GLU:OE1	2.20	0.55
26:Z:121:LEU:HD11	26:Z:138:TYR:HD2	1.70	0.55
29:c:242:GLU:OE2	29:c:246:LYS:NZ	2.39	0.55
9:i:136:TYR:HB2	9:i:148:TYR:HB2	1.89	0.55
21:U:801:GLN:HB3	21:U:877:LEU:HB3	1.88	0.55
7:g:43:ARG:HH21	7:g:164:LYS:HG2	1.71	0.55
6:F:362:ARG:NH2	6:F:388:THR:O	2.40	0.55
9:I:51:ASN:ND2	9:I:51:ASN:O	2.39	0.55
20:T:25:ASP:OD1	20:T:41:ARG:NH2	2.36	0.55
9:i:53:HIS:HB3	9:i:56:LEU:HD23	1.89	0.55
6:F:295:ARG:CZ	6:F:340:PRO:HD3	2.36	0.55
8:H:51:LYS:NZ	8:H:200:GLU:O	2.40	0.55
20:t:50:MET:HE2	20:t:192:VAL:HG12	1.87	0.55
9:i:31:ALA:O	9:i:50:ARG:NH2	2.40	0.55
9:I:46:ALA:HB1	9:I:197:LEU:HD11	1.88	0.55
10:J:158:ALA:HB3	11:K:58:LEU:HD21	1.89	0.55
22:V:123:SER:OG	22:V:155:ALA:O	2.23	0.55
26:Z:145:HIS:HB3	26:Z:149:THR:OG1	2.07	0.55
1:A:206:ILE:HD11	6:F:408:LEU:HD13	1.89	0.54
12:l:189:LYS:NZ	12:l:234:GLU:O	2.40	0.54
1:A:397:ILE:O	1:A:400:ARG:NH2	2.40	0.54
6:F:228:PRO:O	6:F:233:LYS:NZ	2.36	0.54
13:M:42:LYS:HD3	13:M:183:GLU:HA	1.88	0.54
15:O:164:PHE:O	19:s:38:ARG:NH2	2.39	0.54
17:Q:162:LYS:HZ2	18:r:141:ARG:HE	1.56	0.54
28:b:21:PHE:O	28:b:23:PRO:HD2	2.07	0.54
30:d:106:LEU:HD21	30:d:114:GLU:HB2	1.88	0.54
10:j:146:GLN:NE2	10:j:147:THR:O	2.41	0.54
3:C:375:ARG:HG2	3:C:377:HIS:H	1.72	0.54
19:S:4:PRO:HB2	20:T:100:ARG:HH21	1.72	0.54
1:A:26:ASP:OD1	32:f:43:GLN:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:70:LYS:O	4:D:74:HIS:ND1	2.35	0.54
21:U:792:ASN:HB3	21:U:914:LEU:H	1.72	0.54
27:a:281:THR:HG21	27:a:333:MET:HE2	1.87	0.54
2:B:107:MET:HB3	3:C:96:VAL:HB	1.88	0.54
2:B:258:LYS:NZ	33:v:21:UNK:O	2.40	0.54
6:F:180:ARG:HB2	6:F:181:PRO:HD3	1.90	0.54
21:U:529:ILE:HD13	21:U:555:VAL:HG11	1.90	0.54
25:Y:50:MET:HB3	25:Y:53:TYR:HB3	1.88	0.54
19:s:145:LEU:HD21	19:s:182:ALA:HB2	1.88	0.54
4:D:85:ILE:HG21	29:c:152:LYS:HE2	1.89	0.54
13:m:223:ARG:NH1	13:m:225:GLU:OE2	2.40	0.54
10:J:146:GLN:NE2	10:J:147:THR:O	2.41	0.54
30:d:203:PRO:HD2	30:d:206:MET:HE1	1.89	0.54
1:A:332:MET:HA	1:A:337:LEU:HB2	1.90	0.54
16:p:35:VAL:HG12	16:p:36:THR:HG23	1.89	0.54
16:p:65:GLN:OE1	17:q:86:ARG:NH2	2.41	0.54
3:C:69:GLN:HA	4:D:136:SER:HA	1.90	0.54
5:E:204:VAL:O	6:F:300:LYS:NZ	2.39	0.54
21:U:325:MET:HA	21:U:328:ILE:HG12	1.90	0.54
32:f:593:THR:OG1	32:f:649:HIS:NE2	2.36	0.54
5:E:97:ARG:NH1	5:E:114:GLU:OE1	2.41	0.54
5:E:144:GLU:OE2	5:E:297:ARG:NE	2.30	0.54
9:I:53:HIS:CG	9:I:54:LYS:N	2.73	0.54
23:W:80:TRP:CD1	23:W:120:ILE:HG21	2.43	0.54
30:d:131:VAL:HA	30:d:134:LYS:HB3	1.90	0.54
20:t:26:MET:HE3	20:t:186:ARG:HG2	1.89	0.54
1:A:241:ILE:HG22	1:A:243:SER:H	1.72	0.53
4:D:103:VAL:HG21	4:D:132:LEU:HD11	1.90	0.53
6:F:268:VAL:HG11	6:F:313:LEU:HD22	1.90	0.53
16:P:145:GLN:NE2	19:s:143:ALA:HB1	2.24	0.53
22:V:289:LEU:HB3	22:V:312:ALA:HB2	1.89	0.53
4:D:173:GLN:HE22	4:D:334:PRO:HD2	1.73	0.53
9:I:53:HIS:CD2	9:I:54:LYS:H	2.26	0.53
20:T:44:ARG:NH2	20:T:47:ASN:OD1	2.41	0.53
23:W:147:LYS:HE3	23:W:188:GLU:HG3	1.89	0.53
25:Y:328:GLU:OE2	31:e:62:LYS:NZ	2.37	0.53
26:Z:129:LYS:HZ1	29:c:216:MET:HB3	1.73	0.53
1:A:300:LEU:HD21	6:F:171:ARG:HH22	1.73	0.53
4:D:229:ARG:NH1	5:E:268:ASP:OD1	2.30	0.53
4:D:249:ASP:OD1	4:D:252:ARG:NH2	2.41	0.53
21:U:902:PRO:HA	21:U:914:LEU:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:46:ARG:NH2	29:c:147:PRO:O	2.41	0.53
6:F:410:ARG:NH2	6:F:419:ASP:OD2	2.41	0.53
14:N:58:ALA:HB3	14:N:86:MET:HE1	1.91	0.53
21:U:446:LEU:O	21:U:450:HIS:ND1	2.41	0.53
3:C:217:SER:OG	4:D:291:GLU:OE1	2.25	0.53
4:D:124:LEU:HD21	4:D:142:VAL:HG21	1.89	0.53
9:I:53:HIS:CE1	9:I:55:LEU:H	2.27	0.53
27:a:34:TRP:HZ3	27:a:64:ILE:HG23	1.74	0.53
4:D:266:GLU:OE1	5:E:262:ASN:ND2	2.41	0.53
5:E:122:MET:HE1	5:E:218:MET:HE1	1.91	0.53
19:S:185:ARG:NE	16:p:151:GLU:OE2	2.41	0.53
21:U:803:LYS:HD2	21:U:875:PHE:HB2	1.90	0.53
11:k:41:GLN:NE2	11:k:151:PRO:O	2.41	0.53
5:E:75:ASN:HD21	6:F:130:GLN:HG2	1.74	0.53
6:F:339:ASP:N	6:F:340:PRO:HD2	2.24	0.53
32:f:253:LEU:HD23	32:f:257:ARG:HD2	1.91	0.53
32:f:845:ARG:HD2	32:f:865:PHE:HB3	1.91	0.53
2:B:279:PRO:HB3	2:B:324:ASP:HB3	1.91	0.53
9:I:70:GLU:O	9:I:223:THR:OG1	2.25	0.53
9:I:136:TYR:HB2	9:I:148:TYR:HB2	1.90	0.53
26:Z:35:VAL:H	26:Z:97:THR:HG22	1.73	0.53
27:a:279:GLU:HG2	27:a:339:ARG:HH22	1.73	0.53
32:f:389:LYS:HB2	32:f:392:THR:HB	1.89	0.53
1:A:165:GLN:HG2	1:A:267:LYS:HE3	1.89	0.53
12:L:80:ASP:OD2	12:L:126:ARG:NH1	2.42	0.53
19:S:99:ARG:HH21	19:S:102:PHE:HD2	1.57	0.53
21:U:85:GLY:O	21:U:129:ARG:NH1	2.39	0.53
22:V:192:MET:HE1	22:V:210:CYS:HB3	1.90	0.53
32:f:556:ARG:NH2	32:f:645:ASP:OD1	2.41	0.53
17:q:19:ARG:HH11	17:q:179:SER:HB3	1.73	0.53
1:A:35:THR:O	1:A:39:SER:OG	2.24	0.53
24:X:255:LEU:HB2	24:X:287:LEU:HD13	1.91	0.53
3:C:250:GLU:OE1	4:D:294:ASN:ND2	2.39	0.52
21:U:470:ASN:OD1	21:U:471:ASP:N	2.41	0.52
27:a:292:THR:HA	27:a:330:ARG:HG2	1.91	0.52
3:C:20:LEU:HD13	21:U:149:GLN:HB3	1.91	0.52
5:E:247:THR:HA	5:E:251:ARG:HD3	1.90	0.52
28:b:161:ASN:HD21	28:b:168:SER:H	1.55	0.52
10:j:116:GLN:NE2	10:j:120:GLN:OE1	2.42	0.52
1:A:173:THR:HG22	1:A:175:SER:H	1.74	0.52
6:F:244:THR:O	6:F:245:LYS:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:387:ILE:HG21	26:Z:276:ILE:HD11	1.92	0.52
8:H:143:ARG:NH1	8:H:144:PRO:O	2.43	0.52
9:I:47:ALA:HB3	9:I:212:GLU:HB3	1.90	0.52
28:b:22:LEU:HB2	28:b:23:PRO:HD3	1.90	0.52
4:D:57:GLN:HA	4:D:60:TYR:CE1	2.45	0.52
4:D:118:THR:HA	29:c:277:LYS:HE3	1.91	0.52
5:E:164:ILE:HG13	5:E:166:PRO:HD2	1.92	0.52
6:F:223:VAL:HG12	6:F:350:ARG:HB2	1.90	0.52
2:B:249:ARG:NH1	3:C:284:GLU:OE1	2.35	0.52
3:C:198:LEU:HD11	34:C:501:ATP:H2'	1.92	0.52
24:X:16:LEU:HD11	24:X:56:LEU:HD21	1.91	0.52
32:f:573:ILE:HG13	32:f:599:ALA:HB2	1.92	0.52
21:U:516:LEU:HG	21:U:532:MET:HE2	1.90	0.52
21:U:804:SER:HA	21:U:892:LEU:HA	1.91	0.52
22:V:355:ARG:NH1	31:e:27:TRP:O	2.43	0.52
26:Z:228:TYR:HB2	27:a:338:PRO:HG2	1.92	0.52
3:C:223:PHE:HB2	3:C:226:GLU:OE1	2.10	0.52
6:F:225:MET:HG3	6:F:236:LEU:HD13	1.92	0.52
10:J:79:ASP:HB3	10:J:127:PHE:HD1	1.74	0.52
15:O:78:THR:HG22	15:O:82:MET:HE2	1.91	0.52
21:U:389:ASN:HB2	21:U:392:TRP:HB3	1.92	0.52
23:W:51:GLU:HB2	23:W:66:ILE:HG21	1.90	0.52
27:a:115:LYS:HD3	27:a:118:ILE:HD12	1.91	0.52
9:i:241:GLU:HA	9:i:244:GLU:HG3	1.92	0.52
3:C:128:PRO:O	3:C:129:ASN:C	2.52	0.52
11:K:121:LEU:HD23	11:K:160:GLY:HA3	1.92	0.52
14:N:7:GLN:NE2	14:N:109:GLY:O	2.43	0.52
17:Q:21:ALA:HB3	17:Q:29:LYS:HB3	1.92	0.52
26:Z:105:ASP:HA	26:Z:108:ILE:HG22	1.90	0.52
27:a:72:ASN:HD21	27:a:74:LEU:HD12	1.75	0.52
27:a:190:VAL:HG13	27:a:225:LEU:HD23	1.91	0.52
20:t:27:LEU:HD11	20:t:34:ALA:HB1	1.91	0.52
4:D:175:GLN:NE2	4:D:179:GLU:OE2	2.43	0.52
10:J:31:THR:OG1	10:J:163:ARG:O	2.28	0.52
32:f:845:ARG:CZ	32:f:867:THR:HG23	2.40	0.52
1:A:394:MET:HE3	2:B:219:PRO:HD3	1.92	0.51
12:L:164:ARG:NH1	12:L:198:THR:O	2.42	0.51
26:Z:45:LYS:HB3	26:Z:47:VAL:HG12	1.91	0.51
31:e:26:ASP:OD1	31:e:26:ASP:N	2.43	0.51
32:f:120:ARG:HH21	32:f:146:GLY:HA2	1.73	0.51
8:h:74:LEU:HD12	8:h:134:LEU:HD22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PRO:HD2	1:A:157:ILE:HG23	1.92	0.51
1:A:167:GLU:O	1:A:168:GLU:C	2.53	0.51
1:A:346:PRO:O	1:A:351:ARG:NH1	2.43	0.51
2:B:204:PRO:HG3	2:B:211:TYR:HE2	1.73	0.51
22:V:256:ARG:NH2	31:e:21:GLU:O	2.42	0.51
10:j:185:ASP:OD1	10:j:189:LYS:NZ	2.40	0.51
13:m:40:ARG:NH2	13:m:146:ALA:O	2.43	0.51
5:E:5:ARG:NH2	6:F:32:GLU:O	2.42	0.51
8:H:203:MET:HA	8:H:207:ASN:HD21	1.75	0.51
29:c:279:ASP:H	29:c:280:PRO:HD2	1.74	0.51
3:C:90:HIS:CG	3:C:91:PRO:HD3	2.46	0.51
4:D:336:PRO:HB2	4:D:341:LYS:HG2	1.92	0.51
22:V:228:ARG:NH2	22:V:257:ASN:OD1	2.44	0.51
5:E:166:PRO:N	5:E:167:PRO:HD3	2.22	0.51
5:E:352:MET:HA	5:E:355:ILE:HD12	1.93	0.51
11:K:99:HIS:HB2	11:K:107:MET:HE3	1.93	0.51
13:M:163:CYS:SG	13:M:164:ALA:N	2.84	0.51
21:U:58:GLN:NE2	21:U:83:GLY:O	2.44	0.51
22:V:98:LEU:HD22	22:V:209:LYS:HE2	1.93	0.51
26:Z:9:VAL:HG12	26:Z:48:LEU:HB3	1.93	0.51
30:d:19:CYS:SG	30:d:65:ARG:NH1	2.81	0.51
32:f:654:VAL:HA	32:f:657:ILE:HD12	1.93	0.51
4:D:293:LEU:HD21	4:D:321:LEU:HD22	1.92	0.51
6:F:146:LYS:HD2	6:F:269:ARG:HH12	1.75	0.51
8:H:133:SER:HB2	8:H:163:MET:HE1	1.93	0.51
21:U:510:GLU:HA	21:U:547:GLY:HA3	1.93	0.51
21:U:697:GLN:NE2	21:U:744:VAL:O	2.43	0.51
24:X:400:ALA:HA	26:Z:262:LEU:HD21	1.92	0.51
29:c:231:LEU:O	29:c:233:ASP:N	2.44	0.51
24:X:154:LEU:HB3	24:X:155:ARG:HH12	1.75	0.51
32:f:659:LEU:HD12	32:f:662:MET:HE3	1.93	0.51
20:t:1:THR:N	20:t:104:ASN:OD1	2.44	0.51
34:A:501:ATP:O1G	2:B:343:ARG:NH1	2.42	0.51
5:E:322:LYS:HD3	5:E:326:ILE:HG13	1.93	0.51
13:M:125:TYR:HB2	13:M:128:VAL:HG22	1.92	0.51
22:V:264:TYR:HE2	30:d:120:GLU:HG2	1.76	0.51
29:c:215:LYS:HA	29:c:218:LEU:HB2	1.93	0.51
32:f:240:VAL:O	32:f:245:ASN:ND2	2.43	0.51
4:D:318:ASP:HB3	4:D:321:LEU:HD23	1.93	0.51
6:F:340:PRO:HG2	6:F:343:LEU:HD13	1.93	0.51
11:K:41:GLN:NE2	11:K:151:PRO:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:149:MET:HG2	16:P:170:ALA:HA	1.92	0.51
22:V:349:ARG:NH2	31:e:39:TRP:O	2.44	0.51
7:g:170:VAL:HG13	7:g:171:LYS:HG2	1.91	0.51
13:m:37:ILE:HD11	13:m:193:VAL:HG13	1.93	0.51
19:s:16:ALA:HB2	19:s:121:VAL:HG23	1.91	0.51
2:B:65:LEU:HD23	2:B:68:ILE:HD12	1.93	0.51
3:C:195:GLY:HA2	3:C:198:LEU:HD13	1.93	0.51
4:D:176:GLU:OE2	4:D:329:ARG:NH1	2.44	0.51
22:V:101:LEU:HD13	22:V:166:TYR:HE2	1.76	0.51
23:W:117:ASP:OD1	23:W:119:PRO:HD2	2.12	0.51
25:Y:336:ARG:NH1	31:e:49:GLU:OE2	2.44	0.51
29:c:285:GLU:H	29:c:285:GLU:CD	2.17	0.51
1:A:179:GLY:C	1:A:181:LYS:N	2.68	0.50
5:E:165:ILE:H	5:E:166:PRO:CD	2.11	0.50
25:Y:376:LEU:HD23	26:Z:265:LEU:HD23	1.93	0.50
29:c:278:GLN:O	29:c:283:HIS:HB2	2.10	0.50
32:f:686:LEU:O	32:f:690:VAL:HG23	2.10	0.50
3:C:351:MET:HB3	3:C:354:ALA:HB2	1.92	0.50
9:I:73:ALA:HB3	9:I:137:ILE:HD11	1.93	0.50
19:S:27:THR:HB	19:S:40:SER:H	1.76	0.50
30:d:29:VAL:HG11	30:d:54:ILE:HD11	1.92	0.50
12:l:55:GLU:HG2	12:l:56:LEU:HG	1.92	0.50
5:E:344:ARG:NH2	36:E:401:ADP:O2'	2.44	0.50
21:U:681:ASN:ND2	21:U:723:ASP:OD2	2.45	0.50
32:f:520:LEU:HD21	32:f:798:THR:HG23	1.93	0.50
1:A:158:ASP:HB3	1:A:159:PRO:CD	2.41	0.50
1:A:217:PRO:O	1:A:220:THR:OG1	2.27	0.50
2:B:405:MET:HA	2:B:408:ARG:HD3	1.93	0.50
4:D:289:LEU:HD11	4:D:321:LEU:HD21	1.93	0.50
11:K:88:LEU:HD23	11:K:119:LEU:HD23	1.93	0.50
20:T:157:GLN:NE2	20:T:164:GLU:OE1	2.37	0.50
30:d:194:ALA:O	30:d:198:LEU:HB2	2.11	0.50
19:s:10:GLY:HA3	19:s:42:LYS:HE2	1.93	0.50
6:F:344:ARG:NH2	6:F:349:ASP:OD1	2.45	0.50
16:P:45:MET:HE1	16:P:68:LYS:HA	1.92	0.50
21:U:8:ILE:HD12	21:U:27:LEU:HD13	1.92	0.50
22:V:397:ARG:HH21	30:d:116:HIS:HB3	1.75	0.50
24:X:70:LEU:O	24:X:74:ARG:HG3	2.11	0.50
25:Y:42:MET:HG2	25:Y:46:ARG:HH12	1.77	0.50
27:a:333:MET:HE3	27:a:335:TRP:HB2	1.92	0.50
32:f:384:ALA:HA	32:f:419:LEU:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:q:53:THR:HG22	17:q:100:VAL:HG12	1.92	0.50
19:s:125:ASP:OD1	19:s:129:SER:N	2.45	0.50
6:F:438:TYR:OH	11:K:19:GLY:O	2.30	0.50
15:O:81:ARG:HA	15:O:84:LYS:HG2	1.94	0.50
15:O:140:ASP:OD2	20:t:171:ARG:NH2	2.40	0.50
24:X:256:LEU:HG	24:X:260:MET:HE1	1.93	0.50
29:c:63:ASP:OD1	29:c:66:THR:OG1	2.28	0.50
32:f:779:CYS:SG	32:f:785:ARG:NH1	2.68	0.50
9:i:66:TYR:HD2	9:i:87:THR:HG21	1.76	0.50
18:R:166:ARG:NH2	17:q:144:ASP:OD2	2.44	0.50
28:b:24:THR:HG22	28:b:26:LEU:H	1.77	0.50
32:f:150:GLU:HG3	32:f:152:ALA:H	1.76	0.50
20:t:43:MET:HE3	20:t:64:LYS:HG3	1.94	0.50
1:A:190:VAL:HG11	1:A:212:VAL:HG21	1.92	0.50
3:C:49:ARG:NH2	4:D:64:GLU:OE2	2.40	0.50
3:C:274:LEU:HD13	3:C:277:LEU:HD12	1.94	0.50
4:D:177:VAL:HG11	4:D:215:LEU:HD21	1.93	0.50
5:E:175:PRO:O	5:E:178:THR:OG1	2.29	0.50
5:E:317:ALA:HA	5:E:320:ILE:HD12	1.94	0.50
24:X:35:ILE:HD12	24:X:46:LYS:HD2	1.93	0.50
27:a:135:ILE:HG12	27:a:158:LEU:HD13	1.93	0.50
2:B:313:LEU:O	2:B:346:ARG:NH1	2.45	0.50
12:L:72:ILE:HD13	12:L:88:MET:HE1	1.93	0.50
14:N:194:ILE:O	14:N:196:LYS:NZ	2.44	0.50
24:X:143:TYR:OH	25:Y:248:GLU:O	2.30	0.50
27:a:99:LYS:HA	27:a:102:GLU:HG2	1.94	0.50
27:a:138:VAL:O	27:a:142:LEU:HB2	2.11	0.50
32:f:127:SER:OG	32:f:139:CYS:O	2.26	0.50
32:f:479:LEU:HD21	32:f:816:TYR:CZ	2.47	0.50
6:F:27:ASP:OD2	6:F:44:ARG:NH2	2.45	0.49
29:c:29:GLU:OE1	29:c:161:ARG:NH1	2.45	0.49
30:d:68:ILE:HG23	30:d:69:PRO:HD3	1.92	0.49
32:f:235:SER:HB3	32:f:853:VAL:HG21	1.94	0.49
3:C:406:LYS:HB2	9:I:80:THR:HG22	1.92	0.49
5:E:305:ASN:HB3	5:E:308:ALA:H	1.77	0.49
6:F:180:ARG:CB	6:F:181:PRO:HD3	2.42	0.49
17:Q:144:ASP:OD2	18:r:166:ARG:NE	2.38	0.49
22:V:337:LEU:HD21	22:V:364:THR:HG23	1.94	0.49
29:c:276:GLY:N	29:c:278:GLN:HE21	2.10	0.49
30:d:49:ILE:HD12	30:d:52:ARG:HH21	1.76	0.49
16:P:45:MET:HE3	16:P:71:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:4:PRO:HB3	20:T:103:MET:HE1	1.94	0.49
19:S:125:ASP:OD1	19:S:129:SER:N	2.45	0.49
21:U:32:ASN:HA	21:U:70:HIS:CE1	2.47	0.49
24:X:170:GLN:OE1	24:X:192:SER:OG	2.30	0.49
32:f:178:LYS:HD2	32:f:181:ARG:HD2	1.94	0.49
10:j:79:ASP:HB3	10:j:127:PHE:HD1	1.77	0.49
11:k:20:ARG:HD2	11:k:21:LEU:H	1.77	0.49
11:k:71:ASP:OD1	11:k:72:ALA:N	2.39	0.49
13:m:65:ARG:HH21	13:m:78:ALA:HA	1.77	0.49
16:p:28:PHE:HB2	16:p:39:PHE:HB2	1.94	0.49
17:q:39:SER:OG	17:q:40:GLU:N	2.45	0.49
1:A:155:PRO:HB2	1:A:255:ARG:HH21	1.77	0.49
1:A:158:ASP:HB3	1:A:159:PRO:HD3	1.93	0.49
14:N:179:ILE:HG12	14:N:184:VAL:HG22	1.94	0.49
21:U:216:VAL:HA	21:U:220:LEU:HD23	1.95	0.49
21:U:505:ASP:HB3	21:U:508:THR:HG22	1.94	0.49
26:Z:65:ASP:HB2	26:Z:102:HIS:CD2	2.48	0.49
26:Z:72:HIS:CD2	26:Z:114:ARG:HH21	2.30	0.49
27:a:370:GLN:OE1	30:d:244:LYS:NZ	2.38	0.49
28:b:8:VAL:HA	28:b:110:ILE:HG13	1.94	0.49
29:c:164:ASN:HB2	29:c:167:MET:HE1	1.94	0.49
3:C:331:ILE:HG23	3:C:334:ARG:HH21	1.78	0.49
4:D:388:ARG:HD2	5:E:143:ARG:HH12	1.78	0.49
13:M:192:GLU:O	13:M:196:ILE:HG12	2.13	0.49
21:U:229:VAL:HA	21:U:232:ILE:HG12	1.95	0.49
22:V:150:ARG:NH1	22:V:157:THR:O	2.45	0.49
32:f:278:VAL:HG12	32:f:305:LEU:HD11	1.94	0.49
32:f:668:ALA:HB1	32:f:697:ILE:HD11	1.94	0.49
32:f:679:LEU:HB3	32:f:690:VAL:HG11	1.93	0.49
18:r:125:THR:HB	18:r:139:MET:HE2	1.95	0.49
1:A:394:MET:HG3	2:B:349:ARG:HH21	1.77	0.49
7:G:205:VAL:HG13	7:G:206:LEU:HD12	1.95	0.49
23:W:166:LEU:HD22	23:W:192:LEU:HD12	1.94	0.49
27:a:100:THR:HA	27:a:103:LYS:HG2	1.95	0.49
30:d:56:GLU:HG2	30:d:98:LEU:HD22	1.94	0.49
9:i:119:GLN:HG3	10:j:78:ALA:HB1	1.94	0.49
5:E:136:GLY:H	36:E:401:ADP:HN62	1.60	0.49
26:Z:173:GLU:O	26:Z:180:LYS:NZ	2.46	0.49
29:c:59:GLY:HA3	29:c:69:VAL:HA	1.94	0.49
7:g:103:TYR:O	15:o:81:ARG:NH2	2.46	0.49
6:F:134:LEU:HD12	6:F:135:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:27:LEU:HD11	20:T:34:ALA:HB1	1.95	0.49
24:X:96:PHE:HD2	24:X:97:LEU:HD22	1.77	0.49
25:Y:220:VAL:HA	25:Y:223:THR:HG22	1.94	0.49
29:c:245:VAL:HA	29:c:248:MET:HG2	1.94	0.49
13:M:34:SER:HG	13:M:65:ARG:HH12	1.56	0.49
17:Q:63:ASN:N	17:Q:63:ASN:HD22	2.11	0.49
18:R:7:LYS:HG2	18:R:12:VAL:HG22	1.94	0.49
23:W:384:LEU:HD13	23:W:388:GLU:HG3	1.93	0.49
31:e:54:ASN:OD1	31:e:57:ARG:NH2	2.44	0.49
12:l:20:HIS:HA	12:l:23:GLU:HG2	1.94	0.49
1:A:347:ASP:N	1:A:347:ASP:OD1	2.46	0.49
3:C:112:CYS:H	3:C:130:LYS:HD3	1.77	0.49
6:F:338:LEU:HD22	6:F:344:ARG:HH12	1.78	0.49
15:O:100:LEU:HB3	15:O:111:TYR:HB2	1.95	0.49
23:W:281:ASN:OD1	23:W:282:GLU:N	2.45	0.49
26:Z:193:ASN:HA	26:Z:196:HIS:CE1	2.47	0.49
18:r:164:THR:HG22	18:r:170:SER:HB3	1.94	0.49
1:A:194:PRO:HA	1:A:198:PRO:HB3	1.95	0.48
5:E:181:THR:OG1	36:E:401:ADP:O2A	2.31	0.48
6:F:347:ARG:NH1	6:F:347:ARG:HA	2.27	0.48
16:P:35:VAL:HG12	16:P:36:THR:HG23	1.95	0.48
21:U:559:ARG:HB3	21:U:562:GLU:HB2	1.95	0.48
21:U:796:LYS:HE3	21:U:921:ILE:HG22	1.95	0.48
21:U:857:ASP:OD1	21:U:857:ASP:N	2.45	0.48
22:V:311:ASN:OD1	22:V:314:ARG:NH2	2.46	0.48
30:d:183:GLU:OE2	30:d:215:TRP:NE1	2.46	0.48
17:q:1:MET:HE2	17:q:133:GLY:HA2	1.94	0.48
10:J:220:LEU:HD12	10:J:225:ILE:CG1	2.42	0.48
20:T:63:LEU:HD21	20:T:106:LEU:HD13	1.94	0.48
24:X:132:ARG:HH11	24:X:132:ARG:HA	1.79	0.48
24:X:318:ILE:O	24:X:318:ILE:HG13	2.13	0.48
25:Y:247:LEU:HD12	25:Y:250:LEU:HD11	1.94	0.48
32:f:285:CYS:O	32:f:291:GLN:NE2	2.46	0.48
9:i:153:SER:OG	9:i:155:ASN:ND2	2.46	0.48
2:B:67:ARG:NH2	32:f:664:GLU:OE2	2.46	0.48
2:B:82:GLN:O	2:B:86:LYS:NZ	2.40	0.48
4:D:248:ARG:HA	4:D:295:GLN:HE22	1.78	0.48
9:I:66:TYR:HD2	9:I:87:THR:HG21	1.77	0.48
19:S:211:ARG:NH2	19:S:213:ASP:OD2	2.44	0.48
28:b:161:ASN:HB2	28:b:165:GLY:HA3	1.94	0.48
4:D:125:LYS:NZ	4:D:125:LYS:H	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:404:LYS:HA	4:D:407:ILE:HG22	1.94	0.48
11:K:13:ASN:ND2	12:L:124:GLY:O	2.46	0.48
23:W:455:LEU:HD12	23:W:456:GLN:NE2	2.29	0.48
29:c:77:GLN:NE2	29:c:78:SER:O	2.46	0.48
32:f:438:ASP:OD1	32:f:438:ASP:N	2.45	0.48
10:j:49:SER:O	10:j:51:ALA:N	2.47	0.48
1:A:221:GLY:N	34:A:501:ATP:O2A	2.34	0.48
2:B:284:ILE:HG23	2:B:329:MET:HG2	1.96	0.48
5:E:171:LEU:HB3	5:E:298:LYS:HG2	1.94	0.48
6:F:405:MET:HE3	6:F:405:MET:HB2	1.65	0.48
7:G:123:GLN:NE2	8:H:82:ASP:OD1	2.46	0.48
9:I:22:GLU:HA	9:I:25:MET:HB2	1.95	0.48
21:U:373:ASN:HD22	21:U:385:PHE:HD2	1.61	0.48
23:W:444:HIS:CD2	26:Z:204:LYS:HB3	2.49	0.48
27:a:13:ASN:HA	27:a:18:GLN:HG2	1.96	0.48
32:f:269:ALA:HA	32:f:272:LEU:HD12	1.95	0.48
5:E:5:ARG:HH22	6:F:36:MET:HE1	1.78	0.48
21:U:439:GLU:HG3	21:U:473:VAL:HG22	1.96	0.48
21:U:643:SER:O	21:U:649:ARG:NH1	2.41	0.48
7:g:137:CYS:SG	7:g:138:MET:N	2.87	0.48
1:A:347:ASP:O	1:A:351:ARG:NH2	2.46	0.48
3:C:80:MET:HG3	3:C:82:LYS:HD2	1.95	0.48
19:S:198:VAL:HG22	19:S:203:ILE:HG12	1.95	0.48
25:Y:238:GLU:HA	25:Y:242:LYS:HB2	1.94	0.48
10:j:140:GLY:O	10:j:213:ARG:NH1	2.46	0.48
4:D:335:LEU:CB	4:D:336:PRO:HD2	2.43	0.48
6:F:295:ARG:HH12	6:F:340:PRO:CD	2.18	0.48
21:U:65:SER:O	21:U:77:SER:OG	2.31	0.48
21:U:177:LEU:HD13	21:U:205:TYR:HE1	1.77	0.48
21:U:900:TYR:OH	21:U:919:GLU:O	2.32	0.48
1:A:78:TRP:HA	1:A:81:ALA:HB3	1.95	0.48
2:B:95:GLU:HA	2:B:98:LYS:HE3	1.95	0.48
3:C:320:PRO:O	3:C:325:ARG:NH1	2.47	0.48
21:U:524:LYS:NZ	21:U:562:GLU:O	2.44	0.48
25:Y:127:THR:O	25:Y:131:THR:OG1	2.27	0.48
29:c:145:VAL:HG22	29:c:157:ILE:HG12	1.96	0.48
7:g:191:PHE:HE1	7:g:219:VAL:HG21	1.79	0.48
10:j:45:VAL:HG21	10:j:61:LYS:HD2	1.96	0.48
19:s:145:LEU:HD22	19:s:178:VAL:HB	1.95	0.48
6:F:375:VAL:HG13	6:F:414:GLU:HA	1.96	0.47
11:K:206:MET:HE1	11:K:214:ASN:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:3:THR:OG1	22:V:266:GLN:NE2	2.37	0.47
24:X:202:CYS:O	24:X:204:PRO:HD3	2.14	0.47
27:a:188:LEU:HG	27:a:193:GLN:HE21	1.79	0.47
9:i:174:MET:HE3	9:i:196:VAL:HG23	1.94	0.47
1:A:358:HIS:CE1	1:A:386:ARG:HB3	2.49	0.47
7:G:110:PRO:HG2	7:G:113:MET:HB2	1.96	0.47
23:W:265:GLN:HE21	23:W:336:PRO:HD2	1.79	0.47
26:Z:16:LEU:HD12	29:c:216:MET:HE2	1.96	0.47
32:f:393:ASP:OD1	32:f:393:ASP:N	2.44	0.47
20:t:25:ASP:HA	20:t:187:PHE:HA	1.95	0.47
20:t:26:MET:HE2	20:t:188:GLN:HG3	1.96	0.47
1:A:273:PHE:HA	1:A:318:LEU:HB2	1.97	0.47
1:A:328:ASP:H	1:A:332:MET:HE1	1.78	0.47
3:C:233:GLU:HA	3:C:236:VAL:HG12	1.94	0.47
3:C:269:VAL:HG11	4:D:287:ARG:HH12	1.79	0.47
6:F:221:LYS:HA	6:F:327:LYS:HZ3	1.78	0.47
14:N:190:LEU:HD13	20:t:209:TRP:HB2	1.96	0.47
20:T:96:MET:HE2	20:T:127:MET:HA	1.95	0.47
21:U:611:ASN:HB3	21:U:614:VAL:HG12	1.97	0.47
7:g:78:CYS:HB3	7:g:140:LEU:HD23	1.95	0.47
12:l:7:ASP:O	12:l:21:GLN:NE2	2.46	0.47
5:E:84:ARG:H	5:E:87:LEU:HD23	1.80	0.47
21:U:340:GLN:HG3	21:U:344:ARG:HE	1.79	0.47
21:U:636:VAL:HG23	21:U:637:VAL:HG23	1.96	0.47
23:W:171:VAL:HG12	23:W:182:ARG:HG3	1.96	0.47
25:Y:205:VAL:HA	25:Y:219:PHE:HE2	1.80	0.47
30:d:8:GLU:HB2	30:d:18:LYS:HE3	1.96	0.47
1:A:112:ILE:HG12	1:A:122:VAL:HG22	1.96	0.47
2:B:49:LEU:HD21	32:f:666:ILE:HG12	1.96	0.47
5:E:285:LEU:HB2	5:E:290:LEU:HD11	1.97	0.47
6:F:251:LEU:HB3	6:F:285:ILE:HG12	1.97	0.47
6:F:410:ARG:HG3	6:F:412:ALA:H	1.79	0.47
23:W:24:VAL:O	23:W:28:LEU:HG	2.14	0.47
25:Y:105:MET:HE1	25:Y:124:PHE:HE1	1.80	0.47
30:d:170:LEU:HA	30:d:173:THR:HG22	1.97	0.47
5:E:153:LEU:HD12	5:E:154:THR:HG23	1.95	0.47
5:E:168:LYS:HB3	5:E:168:LYS:HE2	1.75	0.47
5:E:292:PRO:HA	5:E:296:ASP:HA	1.96	0.47
17:Q:183:ILE:HG12	17:Q:188:ILE:HG12	1.95	0.47
27:a:90:PRO:HA	27:a:93:ALA:HB3	1.96	0.47
30:d:203:PRO:HD2	30:d:206:MET:CE	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:q:81:ALA:HB1	17:q:124:LEU:HD11	1.96	0.47
3:C:77:VAL:HA	3:C:110:PRO:CB	2.45	0.47
5:E:4:PRO:HG2	5:E:8:ALA:HB2	1.97	0.47
6:F:203:VAL:HA	6:F:245:LYS:NZ	2.30	0.47
6:F:228:PRO:HG2	6:F:231:THR:HG21	1.97	0.47
11:K:31:ILE:HD13	11:K:140:ALA:HB2	1.95	0.47
13:M:51:LYS:NZ	13:M:62:SER:O	2.41	0.47
16:P:65:GLN:OE1	17:Q:86:ARG:NH2	2.40	0.47
24:X:103:THR:HA	24:X:106:GLU:CG	2.45	0.47
25:Y:2:PRO:HG2	25:Y:5:ASN:HB2	1.96	0.47
28:b:141:ILE:HA	28:b:171:VAL:HB	1.95	0.47
29:c:195:GLY:O	29:c:196:LEU:C	2.58	0.47
11:k:196:LYS:NZ	11:k:240:ASP:OD2	2.48	0.47
21:U:793:LYS:NZ	21:U:794:ASP:OD1	2.42	0.47
28:b:51:LEU:HD23	28:b:71:ILE:HG23	1.97	0.47
28:b:107:MET:HG3	28:b:136:VAL:HG22	1.95	0.47
28:b:121:GLU:HA	28:b:124:LEU:HG	1.96	0.47
29:c:231:LEU:O	29:c:232:GLN:C	2.58	0.47
13:m:35:THR:HA	13:m:166:GLY:HA3	1.96	0.47
2:B:405:MET:HG2	2:B:408:ARG:HD3	1.97	0.47
8:H:204:THR:OG1	8:H:206:ASP:OD1	2.30	0.47
10:J:208:LEU:O	10:J:220:LEU:HB2	2.15	0.47
21:U:852:GLU:HG3	21:U:853:LYS:HE3	1.96	0.47
23:W:377:ARG:HA	23:W:380:GLN:HG2	1.95	0.47
32:f:659:LEU:HD13	32:f:797:LEU:HD21	1.97	0.47
11:k:195:ILE:HG23	11:k:217:LEU:HD11	1.97	0.47
7:G:199:ILE:HG23	7:G:210:PHE:HZ	1.80	0.47
22:V:345:ARG:NH2	31:e:46:ASP:OD1	2.48	0.47
25:Y:210:SER:HB3	25:Y:213:LEU:HD23	1.97	0.47
11:k:234:LEU:HA	11:k:237:VAL:HG12	1.97	0.47
19:s:92:LEU:HD23	19:s:124:PHE:HE2	1.80	0.47
4:D:61:ILE:HD12	21:U:639:LEU:HD23	1.97	0.46
7:G:20:GLY:CA	8:H:28:ALA:HB2	2.45	0.46
7:G:158:GLY:O	8:H:84:ARG:NH2	2.43	0.46
9:I:239:LYS:O	9:I:242:GLU:N	2.48	0.46
12:L:155:ASP:HB3	13:M:62:SER:HB2	1.96	0.46
23:W:359:VAL:HG23	23:W:382:LEU:HD22	1.97	0.46
27:a:168:ASN:OD1	27:a:171:SER:OG	2.32	0.46
29:c:269:GLN:HA	29:c:272:ILE:HG22	1.97	0.46
1:A:210:LYS:HE2	1:A:316:LYS:HE3	1.95	0.46
4:D:87:LEU:HD13	4:D:131:ALA:HB1	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:155:ASP:OD1	7:G:159:TYR:N	2.41	0.46
17:Q:35:MET:HE2	17:Q:45:LEU:HD21	1.96	0.46
25:Y:98:SER:OG	25:Y:101:ARG:NH2	2.48	0.46
14:n:58:ALA:HB3	14:n:86:MET:HE1	1.97	0.46
1:A:158:ASP:O	1:A:159:PRO:C	2.58	0.46
2:B:58:CYS:SG	2:B:59:ARG:N	2.88	0.46
6:F:367:GLN:O	6:F:371:ARG:NH1	2.48	0.46
7:G:217:VAL:HG12	7:G:230:LEU:HD13	1.96	0.46
9:I:143:TYR:HB2	9:I:146:GLN:NE2	2.29	0.46
21:U:834:SER:HB2	21:U:836:THR:HG23	1.97	0.46
26:Z:58:PHE:HE1	26:Z:68:TRP:HB2	1.81	0.46
27:a:14:SER:OG	27:a:52:GLN:NE2	2.42	0.46
32:f:755:ASP:OD2	32:f:758:ASN:ND2	2.43	0.46
12:L:166:GLN:OE1	12:L:169:ARG:NH2	2.41	0.46
21:U:790:GLY:HA2	21:U:912:ILE:HG13	1.98	0.46
32:f:829:MET:HB3	32:f:873:LEU:HD23	1.98	0.46
30:d:114:GLU:HA	30:d:117:THR:HG22	1.98	0.46
32:f:486:GLY:HA2	32:f:525:ILE:HD11	1.96	0.46
3:C:52:LEU:HB3	4:D:68:LEU:HD11	1.97	0.46
5:E:178:THR:HG23	5:E:303:LEU:HG	1.97	0.46
21:U:161:ASP:OD1	21:U:161:ASP:N	2.47	0.46
21:U:269:ARG:NH1	21:U:270:THR:OG1	2.49	0.46
22:V:245:ASP:OD1	22:V:246:GLY:N	2.49	0.46
32:f:709:THR:HA	32:f:712:LYS:HD2	1.97	0.46
11:k:196:LYS:HG3	11:k:241:ILE:HD11	1.97	0.46
15:o:81:ARG:HD2	15:o:84:LYS:HD3	1.98	0.46
3:C:364:THR:O	3:C:368:MET:HG2	2.15	0.46
4:D:78:GLU:HA	4:D:81:ARG:HG2	1.98	0.46
4:D:385:LEU:HD23	4:D:398:ASP:HB2	1.97	0.46
5:E:109:ARG:HH12	6:F:135:PRO:HB3	1.81	0.46
20:T:50:MET:HE2	20:T:197:VAL:HG13	1.96	0.46
32:f:292:LYS:HZ3	32:f:899:ILE:HD13	1.80	0.46
32:f:752:HIS:CG	32:f:758:ASN:HB3	2.51	0.46
21:U:587:ALA:HB2	21:U:621:SER:HB3	1.97	0.46
26:Z:200:GLY:HA3	29:c:225:TRP:HE1	1.81	0.46
29:c:280:PRO:C	29:c:284:LEU:HD23	2.41	0.46
10:j:143:ARG:NH2	10:j:145:TYR:OH	2.49	0.46
16:p:15:LYS:HE3	16:p:121:ILE:HG12	1.98	0.46
20:t:96:MET:HE1	20:t:106:LEU:HB2	1.98	0.46
5:E:10:GLN:O	5:E:14:LYS:NZ	2.38	0.46
5:E:97:ARG:NH2	5:E:112:PRO:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:347:ARG:HA	6:F:347:ARG:CZ	2.45	0.46
7:G:231:THR:OG1	7:G:234:GLU:OE1	2.25	0.46
10:J:27:LYS:HE3	10:J:163:ARG:HA	1.97	0.46
18:R:59:LEU:HD22	18:R:83:LEU:HB2	1.98	0.46
21:U:415:HIS:CD2	21:U:418:GLU:HB3	2.51	0.46
21:U:681:ASN:OD1	21:U:682:TYR:N	2.49	0.46
25:Y:12:PRO:O	25:Y:146:ARG:NH1	2.48	0.46
26:Z:209:ARG:HH22	27:a:350:LYS:HB3	1.81	0.46
27:a:254:ALA:HA	27:a:261:LEU:HD23	1.97	0.46
30:d:98:LEU:HA	30:d:101:LEU:HD12	1.98	0.46
30:d:155:LYS:HD3	30:d:171:LEU:HD21	1.97	0.46
1:A:313:GLY:O	1:A:316:LYS:NZ	2.48	0.46
2:B:74:MET:HE2	2:B:74:MET:HB2	1.85	0.46
5:E:235:ILE:O	5:E:239:GLY:N	2.45	0.46
6:F:317:LEU:HD11	6:F:347:ARG:CG	2.43	0.46
7:G:18:PRO:O	7:G:19:GLU:CB	2.63	0.46
8:H:111:VAL:HG21	8:H:147:PHE:HD2	1.80	0.46
24:X:373:LYS:HE3	24:X:373:LYS:HB2	1.67	0.46
30:d:42:LYS:HA	30:d:45:LYS:HB2	1.98	0.46
32:f:791:VAL:HG12	32:f:823:ALA:HB1	1.97	0.46
11:k:141:LEU:HB2	11:k:156:MET:HE2	1.96	0.46
1:A:164:MET:HG3	1:A:263:MET:HE3	1.98	0.45
3:C:258:ARG:HE	3:C:274:LEU:HD21	1.80	0.45
4:D:336:PRO:O	4:D:369:LYS:NZ	2.49	0.45
6:F:262:GLY:H	6:F:308:ARG:HH11	1.64	0.45
10:J:199:VAL:HG22	10:J:201:SER:H	1.81	0.45
10:J:221:ASN:OD1	10:J:223:GLU:HB3	2.16	0.45
21:U:796:LYS:HA	21:U:924:LEU:HD11	1.98	0.45
25:Y:25:LEU:HD11	25:Y:284:LYS:HZ2	1.81	0.45
32:f:63:LEU:HD21	32:f:75:LEU:HG	1.97	0.45
32:f:137:ARG:HE	32:f:168:LYS:NZ	2.14	0.45
1:A:178:GLY:HA2	1:A:353:HIS:CD2	2.51	0.45
6:F:141:ASP:OD2	6:F:144:LYS:NZ	2.48	0.45
21:U:1:MET:HA	30:d:85:TYR:HA	1.99	0.45
21:U:344:ARG:HH22	21:U:925:VAL:HG13	1.80	0.45
32:f:589:SER:HB3	32:f:649:HIS:CE1	2.51	0.45
20:t:97:TYR:HA	20:t:100:ARG:HG2	1.98	0.45
3:C:88:LYS:O	3:C:89:VAL:C	2.58	0.45
5:E:246:GLY:HA3	5:E:250:ASP:HB2	1.97	0.45
6:F:225:MET:HA	6:F:352:ILE:HB	1.99	0.45
9:I:38:LEU:HD23	9:I:160:LYS:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:221:GLN:HB2	11:K:224:GLN:HG2	1.97	0.45
26:Z:223:ASN:HB3	26:Z:226:ILE:HG22	1.97	0.45
27:a:35:HIS:NE2	28:b:14:GLU:O	2.49	0.45
30:d:70:SER:HA	30:d:73:ARG:HB2	1.97	0.45
31:e:16:ASP:OD1	31:e:16:ASP:N	2.47	0.45
2:B:46:ALA:HB1	2:B:179:ALA:HB2	1.98	0.45
3:C:88:LYS:HB3	3:C:94:LYS:HG2	1.98	0.45
4:D:388:ARG:HD2	5:E:143:ARG:NH1	2.31	0.45
6:F:181:PRO:O	6:F:182:THR:HB	2.15	0.45
8:H:85:VAL:O	8:H:89:ARG:HG2	2.16	0.45
11:K:232:GLU:HA	11:K:235:GLU:HG2	1.99	0.45
21:U:198:LEU:HD21	21:U:218:GLN:HE21	1.81	0.45
29:c:231:LEU:C	29:c:232:GLN:HG3	2.42	0.45
11:k:166:ASP:OD2	11:k:187:LYS:NZ	2.50	0.45
15:o:50:ALA:HB2	16:p:129:CYS:HB2	1.98	0.45
1:A:43:ARG:HA	1:A:46:LYS:HG2	1.97	0.45
1:A:102:ILE:HD12	1:A:112:ILE:HG22	1.99	0.45
4:D:360:LEU:HA	4:D:363:TYR:HD2	1.80	0.45
6:F:209:LYS:HE2	6:F:324:THR:HG21	1.99	0.45
6:F:221:LYS:HB2	6:F:347:ARG:NH1	2.32	0.45
21:U:900:TYR:HB3	21:U:914:LEU:HD21	1.98	0.45
23:W:456:GLN:NE2	26:Z:100:LYS:HD3	2.32	0.45
32:f:564:LEU:HD12	32:f:567:LEU:HD23	1.98	0.45
7:g:31:ALA:HB1	7:g:83:MET:HE3	1.97	0.45
4:D:51:LEU:HA	4:D:54:LEU:HD23	1.99	0.45
5:E:193:CYS:SG	5:E:194:ASN:N	2.89	0.45
6:F:96:LEU:HD12	6:F:145:LEU:HD23	1.97	0.45
11:K:234:LEU:O	11:K:238:ILE:HG12	2.16	0.45
21:U:103:LYS:HE3	21:U:103:LYS:HB2	1.83	0.45
14:n:189:LEU:HD22	14:n:193:GLN:HB3	1.98	0.45
6:F:173:LYS:HE2	6:F:173:LYS:HB3	1.60	0.45
7:G:43:ARG:HH21	7:G:164:LYS:HG2	1.80	0.45
4:D:103:VAL:HG11	4:D:139:LEU:HD21	1.99	0.45
24:X:310:ARG:O	24:X:314:ARG:NE	2.50	0.45
7:G:93:ARG:HE	7:G:121:ILE:HD13	1.81	0.45
17:Q:169:LYS:O	17:q:27:GLN:NE2	2.49	0.45
26:Z:247:LYS:HB3	26:Z:247:LYS:HE3	1.79	0.45
28:b:174:PRO:HA	28:b:175:PRO:HD3	1.86	0.45
30:d:203:PRO:HB2	30:d:204:LYS:H	1.59	0.45
10:j:188:ILE:HD12	10:j:208:LEU:HD21	1.97	0.45
10:j:221:ASN:ND2	10:j:223:GLU:OE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:s:172:MET:HE3	19:s:172:MET:HB3	1.78	0.45
2:B:232:LYS:HD2	2:B:330:ALA:HB1	1.99	0.45
3:C:406:LYS:HE3	9:I:80:THR:HG22	1.98	0.45
4:D:351:LYS:HE3	4:D:351:LYS:HB2	1.79	0.45
6:F:227:GLY:HA3	6:F:354:PHE:HB2	1.98	0.45
11:K:100:TRP:O	18:R:57:ARG:NH2	2.50	0.45
11:K:146:VAL:HG11	11:K:222:PRO:HA	1.98	0.45
22:V:406:GLY:HA2	22:V:409:MET:SD	2.57	0.45
32:f:405:HIS:CE1	32:f:813:LYS:HD2	2.52	0.45
9:i:197:LEU:HA	9:i:200:THR:HG22	1.99	0.45
2:B:62:LEU:O	2:B:66:GLU:HG2	2.17	0.44
6:F:98:ASP:OD1	6:F:120:LYS:N	2.50	0.44
6:F:232:GLY:HA2	6:F:235:LEU:HB2	1.98	0.44
23:W:363:ILE:HD11	23:W:382:LEU:HD11	1.99	0.44
28:b:6:THR:HG21	28:b:40:LYS:HG3	1.98	0.44
32:f:93:PRO:HB2	32:f:96:LEU:HD23	1.97	0.44
32:f:349:TYR:HA	32:f:352:HIS:HB2	1.99	0.44
8:h:3:GLU:OE2	13:m:127:ALA:HB3	2.17	0.44
13:m:24:GLU:HA	13:m:27:MET:HE3	1.98	0.44
16:p:138:VAL:HB	16:p:146:MET:HE2	1.98	0.44
1:A:310:ASP:OD1	1:A:311:PRO:HD3	2.17	0.44
4:D:337:ASP:HA	4:D:369:LYS:HZ3	1.82	0.44
16:P:190:ILE:HG12	16:P:195:ILE:HD12	1.98	0.44
22:V:447:ILE:HG13	22:V:449:ALA:H	1.82	0.44
22:V:495:ARG:NH1	22:V:497:PRO:O	2.50	0.44
23:W:108:CYS:O	23:W:112:VAL:HG23	2.17	0.44
29:c:234:TYR:HA	29:c:237:HIS:HB3	2.00	0.44
4:D:380:GLN:HA	5:E:164:ILE:HG12	2.00	0.44
6:F:220:PRO:HG3	6:F:348:LEU:HD22	1.99	0.44
13:M:72:HIS:CE1	13:M:105:ASN:HB3	2.52	0.44
19:S:13:LEU:HD12	19:S:145:LEU:HD13	1.99	0.44
21:U:550:VAL:HG21	21:U:768:GLN:HG3	2.00	0.44
24:X:82:LYS:HB3	24:X:124:PHE:HZ	1.82	0.44
4:D:123:LEU:O	4:D:124:LEU:HD13	2.17	0.44
10:J:7:ILE:HG13	10:J:8:THR:HG23	1.98	0.44
10:J:220:LEU:HA	10:J:220:LEU:HD22	1.78	0.44
14:N:9:ASP:N	14:N:9:ASP:OD1	2.50	0.44
22:V:123:SER:H	22:V:150:ARG:HH21	1.65	0.44
24:X:317:PRO:HD2	24:X:319:ILE:HG12	1.98	0.44
7:g:141:ILE:HG22	7:g:151:VAL:HG22	1.99	0.44
12:l:120:THR:O	13:m:129:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:113:ARG:NE	3:C:130:LYS:O	2.49	0.44
4:D:116:LEU:HB2	4:D:119:ILE:HD12	2.00	0.44
21:U:123:LYS:HA	21:U:123:LYS:HD2	1.83	0.44
21:U:557:TYR:HD1	21:U:588:MET:HE3	1.83	0.44
23:W:51:GLU:OE2	23:W:96:GLN:NE2	2.49	0.44
24:X:157:LEU:HD11	24:X:165:LEU:HD23	2.00	0.44
24:X:377:ILE:HG22	24:X:386:ILE:HB	1.99	0.44
25:Y:268:TYR:HA	25:Y:271:PHE:HB3	1.99	0.44
7:g:132:ARG:HA	7:g:133:PRO:HD3	1.78	0.44
10:j:89:VAL:HG22	17:q:66:LEU:HD21	1.99	0.44
11:k:67:ILE:HB	11:k:228:MET:HE1	1.99	0.44
2:B:191:ASP:HA	2:B:194:ILE:HG22	2.00	0.44
6:F:334:ARG:HG3	6:F:337:ILE:HD12	2.00	0.44
24:X:274:LYS:HE2	24:X:274:LYS:HB2	1.78	0.44
26:Z:21:ASP:OD1	26:Z:22:HIS:N	2.50	0.44
26:Z:113:LYS:NZ	26:Z:117:PRO:O	2.45	0.44
30:d:171:LEU:O	30:d:175:ARG:HG2	2.17	0.44
10:j:183:THR:HG22	10:j:185:ASP:H	1.83	0.44
4:D:158:GLN:O	4:D:159:LYS:C	2.61	0.44
6:F:220:PRO:O	6:F:327:LYS:NZ	2.50	0.44
6:F:286:ASP:HA	6:F:331:ALA:HB3	2.00	0.44
28:b:181:ASP:HA	28:b:184:ILE:HG12	1.99	0.44
32:f:398:TRP:HA	32:f:401:LYS:HD3	1.99	0.44
7:g:80:MET:HE3	7:g:91:VAL:HG22	2.00	0.44
1:A:179:GLY:O	1:A:181:LYS:N	2.51	0.44
2:B:51:LEU:HD23	32:f:666:ILE:HD11	1.99	0.44
3:C:222:LYS:HG3	4:D:239:TYR:HB3	2.00	0.44
15:O:135:MET:SD	20:t:179:ARG:NH2	2.91	0.44
23:W:331:GLY:HA3	23:W:337:ALA:HB2	2.00	0.44
25:Y:42:MET:HA	25:Y:45:VAL:HB	1.99	0.44
17:q:2:GLU:HG2	17:q:34:LYS:HE2	1.99	0.44
1:A:274:PHE:HB3	1:A:277:ILE:HG21	2.00	0.44
3:C:117:ARG:NH1	3:C:124:HIS:HA	2.32	0.44
4:D:126:PRO:CD	4:D:127:ASN:H	2.30	0.44
5:E:170:CYS:SG	5:E:171:LEU:N	2.91	0.44
6:F:125:LYS:HA	6:F:131:THR:HA	2.00	0.44
9:I:76:VAL:HG12	9:I:134:LEU:HG	1.99	0.44
21:U:146:LYS:HB3	21:U:149:GLN:HG2	2.00	0.44
24:X:103:THR:C	24:X:105:GLN:H	2.24	0.44
24:X:103:THR:C	24:X:105:GLN:N	2.74	0.44
25:Y:161:THR:HG22	25:Y:165:LYS:NZ	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:13:PRO:HD2	26:Z:168:GLU:OE1	2.18	0.44
13:m:228:PRO:HD2	13:m:231:ILE:HD12	1.99	0.44
19:s:114:ASP:OD1	19:s:118:LYS:N	2.42	0.44
3:C:161:ILE:HA	3:C:164:VAL:HG12	2.00	0.43
5:E:165:ILE:O	5:E:166:PRO:C	2.60	0.43
6:F:198:LEU:HG	6:F:202:ILE:HD12	2.00	0.43
6:F:246:ALA:O	6:F:247:THR:C	2.61	0.43
12:L:45:VAL:HG12	12:L:214:ILE:HG12	1.99	0.43
26:Z:72:HIS:HD2	26:Z:114:ARG:HH21	1.64	0.43
26:Z:103:LYS:HZ3	26:Z:103:LYS:N	2.14	0.43
7:g:158:GLY:O	8:h:84:ARG:NH2	2.51	0.43
1:A:168:GLU:O	1:A:169:LYS:C	2.62	0.43
7:G:40:VAL:HG22	7:G:202:LEU:HD23	2.00	0.43
12:L:81:ALA:HB2	12:L:130:VAL:HG21	2.00	0.43
19:S:145:LEU:HD22	19:S:178:VAL:HB	1.99	0.43
24:X:130:GLU:HA	24:X:133:LEU:HB3	1.98	0.43
27:a:118:ILE:O	27:a:122:LYS:HB2	2.18	0.43
29:c:251:LEU:CG	29:c:279:ASP:OD1	2.65	0.43
30:d:203:PRO:HD3	30:d:206:MET:HE1	1.99	0.43
13:m:15:SER:OG	13:m:19:ARG:N	2.50	0.43
1:A:330:ALA:HA	1:A:333:ARG:HE	1.84	0.43
3:C:195:GLY:N	34:C:501:ATP:O1A	2.51	0.43
4:D:297:ASP:OD2	4:D:323:ARG:NH2	2.52	0.43
20:T:211:ILE:HA	20:T:214:MET:HE3	1.99	0.43
21:U:840:LYS:HB3	21:U:844:LYS:NZ	2.33	0.43
32:f:781:TYR:HB2	32:f:785:ARG:NH1	2.33	0.43
2:B:234:LEU:HD11	34:B:501:ATP:H2'	2.01	0.43
3:C:82:LYS:HB3	3:C:82:LYS:HE3	1.71	0.43
10:J:219:ILE:HD12	10:J:219:ILE:HA	1.81	0.43
21:U:245:ALA:HA	21:U:248:ILE:HG12	1.99	0.43
22:V:368:ARG:HH22	31:e:46:ASP:HB2	1.82	0.43
23:W:206:SER:HB2	23:W:230:MET:HE1	1.99	0.43
11:k:98:ASN:OD1	18:r:61:ARG:NH2	2.51	0.43
17:q:38:MET:HE3	17:q:44:LEU:HB3	2.01	0.43
1:A:346:PRO:HB2	1:A:351:ARG:HG3	2.00	0.43
21:U:899:ARG:NH1	21:U:918:SER:OG	2.51	0.43
23:W:293:ASP:HB2	23:W:296:LEU:HD23	2.00	0.43
32:f:701:ASN:HB2	32:f:876:HIS:CD2	2.53	0.43
9:i:3:ARG:NH2	11:k:125:GLU:OE2	2.51	0.43
1:A:265:ARG:HH21	1:A:309:PHE:HB2	1.82	0.43
5:E:130:VAL:HG13	5:E:186:ALA:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:92:LEU:HD23	19:S:124:PHE:HE2	1.84	0.43
32:f:140:LEU:HD22	32:f:165:GLU:HG3	1.99	0.43
1:A:284:ARG:HA	2:B:303:ARG:HH12	1.83	0.43
3:C:27:LYS:NZ	21:U:106:ASP:OD1	2.42	0.43
4:D:274:ARG:HD3	4:D:277:ALA:HB2	2.00	0.43
6:F:166:THR:HB	6:F:169:ASP:HB3	2.01	0.43
24:X:344:ARG:HG3	24:X:386:ILE:HG12	2.01	0.43
25:Y:312:ARG:HA	25:Y:356:THR:HG22	2.01	0.43
32:f:65:GLU:HG2	32:f:66:LYS:H	1.84	0.43
32:f:331:LEU:HG	32:f:335:ARG:HH21	1.83	0.43
32:f:729:MET:HE1	32:f:744:MET:HE3	2.01	0.43
7:g:119:ALA:HB3	8:h:84:ARG:HH12	1.84	0.43
9:i:195:LYS:HA	9:i:240:HIS:CE1	2.52	0.43
15:o:51:ASP:HB3	15:o:94:ILE:HG23	1.99	0.43
1:A:99:THR:HG22	1:A:115:VAL:HA	2.00	0.43
1:A:113:ILE:N	1:A:121:PHE:O	2.45	0.43
4:D:341:LYS:HZ2	4:D:370:ILE:HB	1.83	0.43
9:I:54:LYS:HG3	9:I:55:LEU:HD12	2.00	0.43
13:M:7:TYR:CD2	13:M:16:PRO:HD3	2.53	0.43
23:W:192:LEU:HD23	23:W:192:LEU:HA	1.88	0.43
24:X:143:TYR:HD2	24:X:144:GLN:HG2	1.84	0.43
24:X:221:GLU:HG2	24:X:223:LYS:HE3	2.01	0.43
25:Y:80:GLU:HA	25:Y:83:ARG:HG2	2.00	0.43
26:Z:16:LEU:HD13	29:c:220:LEU:HD22	2.01	0.43
26:Z:212:LEU:HD21	27:a:353:LEU:HD22	2.00	0.43
27:a:77:VAL:HG21	27:a:110:ALA:HB1	2.00	0.43
27:a:148:VAL:HG12	27:a:150:SER:H	1.84	0.43
27:a:250:THR:HA	27:a:253:THR:HG22	2.01	0.43
7:g:217:VAL:HG12	7:g:230:LEU:HD13	2.01	0.43
19:s:72:LEU:HA	19:s:83:MET:HE3	2.00	0.43
1:A:364:VAL:HG12	1:A:404:ALA:HB3	2.01	0.43
2:B:338:ASP:HB3	2:B:341:LEU:HD23	2.00	0.43
5:E:173:TYR:HB2	5:E:282:PRO:HG3	2.00	0.43
13:M:52:LEU:HA	13:M:209:PHE:HA	2.01	0.43
21:U:799:LYS:HB2	21:U:923:GLU:HB3	2.00	0.43
22:V:259:LEU:HD11	22:V:294:ARG:HD3	2.01	0.43
7:g:112:ASP:HB3	7:g:152:TYR:CZ	2.54	0.43
16:p:159:ASP:OD1	16:p:159:ASP:N	2.51	0.43
6:F:177:VAL:HB	6:F:248:PHE:HD2	1.83	0.43
10:J:89:VAL:HG22	17:Q:66:LEU:HD21	1.99	0.43
18:R:82:LEU:O	18:R:86:MET:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:469:SER:OG	21:U:470:ASN:N	2.49	0.43
21:U:696:ILE:HG22	21:U:737:LEU:HA	2.00	0.43
22:V:419:LEU:HA	22:V:422:ILE:HG22	2.01	0.43
28:b:30:GLN:HG3	28:b:75:LEU:HD22	2.00	0.43
17:q:39:SER:HB3	17:q:42:ILE:HB	2.01	0.43
1:A:397:ILE:HD11	2:B:214:MET:HG3	2.01	0.42
3:C:114:VAL:HG12	3:C:126:ILE:HA	2.00	0.42
3:C:293:MET:HE1	3:C:305:LEU:HD13	2.01	0.42
18:R:58:LEU:HD12	18:R:61:ARG:HD3	2.00	0.42
21:U:465:LEU:HD11	21:U:477:GLY:HA3	2.01	0.42
21:U:740:GLY:HA3	21:U:744:VAL:HG22	2.00	0.42
23:W:71:VAL:HB	23:W:104:MET:HE1	2.00	0.42
27:a:186:LYS:O	27:a:193:GLN:NE2	2.52	0.42
28:b:157:VAL:HG21	28:b:170:LEU:HB2	2.00	0.42
32:f:267:ARG:NH2	32:f:297:MET:SD	2.92	0.42
19:s:4:PRO:O	20:t:100:ARG:NH2	2.52	0.42
1:A:73:ALA:O	1:A:78:TRP:NE1	2.51	0.42
5:E:309:ARG:NH1	5:E:335:SER:O	2.52	0.42
6:F:339:ASP:N	6:F:340:PRO:CD	2.82	0.42
26:Z:45:LYS:HG3	26:Z:46:LYS:H	1.84	0.42
7:g:17:SER:OG	7:g:21:ARG:N	2.45	0.42
11:k:217:LEU:HD22	11:k:229:PHE:CD2	2.54	0.42
1:A:117:GLN:HE22	2:B:128:GLY:HA3	1.85	0.42
1:A:154:PRO:HA	1:A:155:PRO:HD3	1.88	0.42
2:B:375:ALA:HB2	2:B:413:LYS:HD3	2.01	0.42
4:D:92:PHE:HA	4:D:103:VAL:HG12	2.01	0.42
4:D:125:LYS:H	4:D:125:LYS:HZ2	1.67	0.42
6:F:146:LYS:HD2	6:F:269:ARG:HH22	1.85	0.42
28:b:53:THR:HG22	28:b:59:GLU:H	1.84	0.42
28:b:149:ASN:OD1	28:b:154:THR:OG1	2.32	0.42
32:f:744:MET:O	32:f:748:LEU:HG	2.19	0.42
32:f:848:GLN:N	32:f:863:THR:O	2.49	0.42
9:i:67:LYS:HE2	9:i:225:ILE:HD12	2.01	0.42
10:J:66:ASP:OD2	10:J:95:ARG:NH2	2.47	0.42
13:M:109:LYS:HA	13:M:149:TYR:HE2	1.84	0.42
18:R:115:ASP:OD1	18:R:119:ASN:N	2.49	0.42
24:X:194:ARG:O	24:X:198:ASN:ND2	2.52	0.42
27:a:34:TRP:CZ3	27:a:64:ILE:HG23	2.53	0.42
29:c:284:LEU:HB3	29:c:285:GLU:H	1.57	0.42
32:f:83:ARG:NH2	32:f:153:SER:O	2.53	0.42
32:f:347:ASP:OD1	32:f:347:ASP:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:46:ALA:HB1	9:i:197:LEU:HD11	2.00	0.42
20:t:100:ARG:HD2	20:t:128:LEU:HA	2.00	0.42
1:A:230:ALA:HA	1:A:233:THR:HG22	2.02	0.42
6:F:340:PRO:O	6:F:342:LEU:N	2.48	0.42
9:I:51:ASN:C	9:I:51:ASN:HD22	2.24	0.42
21:U:177:LEU:HD13	21:U:205:TYR:CE1	2.54	0.42
21:U:694:ILE:HG23	21:U:695:MET:HB3	2.01	0.42
23:W:380:GLN:HG3	23:W:381:LEU:HD12	2.00	0.42
28:b:1:MET:HG2	28:b:44:ASN:HB2	2.01	0.42
32:f:295:ALA:HB1	32:f:321:MET:HB2	2.01	0.42
32:f:679:LEU:HD12	32:f:680:ARG:HB2	2.01	0.42
2:B:386:ALA:HB1	2:B:423:LYS:HG2	2.01	0.42
3:C:212:ILE:HG21	3:C:234:LEU:HD11	2.02	0.42
5:E:104:THR:HG22	5:E:106:THR:HG23	2.01	0.42
5:E:281:ARG:HD2	5:E:281:ARG:HA	1.58	0.42
7:G:78:CYS:HB3	7:G:140:LEU:HD23	2.00	0.42
9:I:176:LYS:HG2	10:J:52:LYS:HD3	2.02	0.42
20:T:63:LEU:HG	20:T:110:MET:HE1	2.01	0.42
22:V:189:ASP:OD1	22:V:218:TYR:OH	2.37	0.42
13:m:41:CYS:HB3	13:m:189:ILE:HG13	2.01	0.42
13:m:181:MET:H	13:m:181:MET:HG2	1.64	0.42
4:D:105:SER:OG	4:D:108:GLY:O	2.35	0.42
21:U:619:VAL:HG11	21:U:648:VAL:HG13	2.02	0.42
26:Z:275:LEU:HD11	26:Z:279:LYS:HE2	2.02	0.42
29:c:55:GLY:HA2	29:c:75:MET:HB2	2.02	0.42
29:c:281:LYS:HA	29:c:281:LYS:HD3	1.26	0.42
32:f:140:LEU:HD11	32:f:169:GLU:HG2	2.02	0.42
32:f:347:ASP:HA	32:f:350:LYS:HB3	2.02	0.42
7:g:123:GLN:NE2	8:h:82:ASP:OD1	2.53	0.42
8:h:3:GLU:HB2	8:h:4:ARG:H	1.67	0.42
9:i:114:LEU:HA	9:i:117:ILE:HG22	2.02	0.42
12:l:88:MET:HE2	12:l:112:ILE:HG13	2.01	0.42
13:m:46:VAL:HG22	13:m:215:TRP:HB3	2.00	0.42
17:q:22:ALA:HA	17:q:27:GLN:HA	2.02	0.42
17:q:26:VAL:HG11	18:r:136:TYR:HE2	1.83	0.42
17:q:54:VAL:O	17:q:58:GLU:HG2	2.20	0.42
18:r:6:PHE:HB3	18:r:139:MET:HE3	2.02	0.42
1:A:169:LYS:HD3	1:A:234:ASP:HA	2.02	0.42
34:D:501:ATP:O3G	5:E:294:ARG:NH1	2.37	0.42
5:E:322:LYS:NZ	5:E:328:TYR:OH	2.42	0.42
6:F:206:MET:HE2	6:F:245:LYS:HZ2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:86:ASP:OD1	13:M:120:HIS:NE2	2.39	0.42
21:U:367:THR:HA	21:U:370:VAL:HG22	2.01	0.42
22:V:119:GLY:HA2	22:V:148:ARG:HD3	2.02	0.42
23:W:151:THR:HG22	23:W:155:GLN:NE2	2.35	0.42
27:a:373:ASP:HB2	30:d:251:ARG:HH12	1.85	0.42
29:c:27:THR:HG22	29:c:28:ALA:H	1.83	0.42
32:f:670:MET:HG2	32:f:673:ARG:HH21	1.83	0.42
20:t:99:ARG:NH1	20:t:104:ASN:O	2.52	0.42
3:C:209:CYS:SG	3:C:210:THR:N	2.93	0.42
6:F:56:LYS:HA	6:F:59:VAL:HG12	2.01	0.42
9:I:22:GLU:O	9:I:26:GLU:HG2	2.20	0.42
17:Q:52:ASP:OD1	18:R:91:LYS:NZ	2.51	0.42
21:U:703:CYS:HA	21:U:704:PRO:HD3	1.91	0.42
22:V:113:LEU:HD23	22:V:113:LEU:HA	1.87	0.42
24:X:281:GLY:H	24:X:284:THR:HG22	1.85	0.42
27:a:251:LEU:HD12	27:a:255:TRP:CE3	2.55	0.42
28:b:131:LEU:HD22	28:b:136:VAL:HB	2.01	0.42
32:f:94:LYS:HA	32:f:97:LYS:HE2	2.01	0.42
7:g:28:ALA:O	7:g:32:ILE:HG13	2.20	0.42
10:j:38:ARG:NH2	10:j:182:GLU:O	2.50	0.42
15:o:1:THR:N	15:o:168:GLY:O	2.53	0.42
1:A:288:GLY:O	1:A:289:ALA:C	2.63	0.42
20:T:127:MET:HE3	20:T:127:MET:HB2	1.85	0.42
22:V:121:PHE:O	22:V:128:ARG:NH1	2.53	0.42
23:W:260:SER:HA	23:W:263:TRP:NE1	2.35	0.42
32:f:323:ASN:HB3	32:f:326:LEU:HB2	2.02	0.42
14:n:144:ARG:NH2	14:n:151:GLU:OE2	2.52	0.42
6:F:340:PRO:HG3	6:F:343:LEU:HD13	1.98	0.41
27:a:252:LYS:HD2	27:a:252:LYS:HA	1.91	0.41
32:f:67:ASP:OD1	32:f:67:ASP:N	2.52	0.41
32:f:833:PHE:HB3	32:f:837:LEU:HA	2.02	0.41
8:h:3:GLU:HA	13:m:125:TYR:CD1	2.55	0.41
1:A:294:GLU:O	1:A:298:THR:OG1	2.30	0.41
5:E:218:MET:HE2	5:E:218:MET:HB3	1.87	0.41
6:F:51:GLU:O	6:F:55:MET:HB2	2.20	0.41
26:Z:205:LEU:HD23	26:Z:205:LEU:HA	1.83	0.41
29:c:29:GLU:HG2	29:c:65:TYR:HB2	2.01	0.41
9:i:214:ALA:HB2	9:i:227:VAL:HG22	2.02	0.41
13:m:172:ALA:O	13:m:176:ILE:HG13	2.20	0.41
3:C:158:ILE:HG22	3:C:162:LYS:HE2	2.02	0.41
4:D:273:LYS:HB3	4:D:318:ASP:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:345:PHE:HB3	4:D:360:LEU:HD22	2.03	0.41
11:K:4:THR:OG1	11:K:5:ARG:N	2.48	0.41
21:U:333:MET:SD	21:U:333:MET:N	2.91	0.41
32:f:59:LEU:HD22	32:f:78:LEU:HD12	2.03	0.41
11:k:120:ALA:O	11:k:121:LEU:HG	2.20	0.41
11:k:181:LEU:HA	11:k:184:VAL:HG22	2.01	0.41
4:D:204:MET:HE3	4:D:310:ALA:HB2	2.03	0.41
6:F:296:PHE:HD1	6:F:339:ASP:HA	1.86	0.41
7:G:112:ASP:HB3	7:G:152:TYR:CZ	2.55	0.41
13:M:64:LYS:HE2	13:M:66:LEU:H	1.85	0.41
21:U:481:LEU:HD23	21:U:496:LEU:HD11	2.03	0.41
21:U:873:PRO:C	21:U:875:PHE:N	2.72	0.41
22:V:281:ASN:HA	25:Y:385:ARG:NH2	2.35	0.41
22:V:400:HIS:HB3	30:d:145:GLU:OE2	2.20	0.41
23:W:125:ILE:HG23	23:W:129:ARG:HH21	1.84	0.41
25:Y:214:MET:HE1	25:Y:222:TYR:CD2	2.55	0.41
26:Z:25:ARG:CZ	29:c:102:THR:HA	2.50	0.41
18:r:7:LYS:HD2	18:r:109:PRO:HB2	2.02	0.41
1:A:285:PHE:O	1:A:286:ASP:C	2.63	0.41
6:F:185:TYR:CD1	6:F:243:GLN:HG3	2.55	0.41
14:N:32:ASP:O	14:N:45:ARG:NH2	2.54	0.41
17:Q:148:THR:HG22	17:Q:150:THR:H	1.86	0.41
21:U:764:LEU:O	21:U:767:THR:OG1	2.39	0.41
22:V:495:ARG:HB3	26:Z:278:ASN:ND2	2.36	0.41
23:W:140:ILE:H	23:W:140:ILE:HG13	1.75	0.41
26:Z:284:ASP:HA	26:Z:287:LYS:HG2	2.01	0.41
30:d:49:ILE:HD13	30:d:52:ARG:HE	1.84	0.41
30:d:71:PHE:HZ	30:d:101:LEU:HB3	1.85	0.41
7:g:231:THR:OG1	7:g:234:GLU:OE1	2.26	0.41
2:B:95:GLU:HA	2:B:98:LYS:HG2	2.02	0.41
21:U:142:LEU:HD23	21:U:142:LEU:HA	1.92	0.41
21:U:541:HIS:HB2	21:U:544:ILE:HG22	2.02	0.41
22:V:76:LYS:O	22:V:80:LYS:HG2	2.21	0.41
22:V:340:GLY:O	22:V:408:ARG:NE	2.48	0.41
24:X:154:LEU:HB3	24:X:155:ARG:NH1	2.34	0.41
25:Y:275:LEU:HD21	25:Y:296:VAL:HG13	2.02	0.41
26:Z:32:GLN:NE2	26:Z:58:PHE:O	2.54	0.41
32:f:806:VAL:HG23	32:f:810:ILE:HB	2.03	0.41
9:i:21:VAL:O	9:i:25:MET:HG3	2.20	0.41
16:p:130:PRO:O	16:p:131:MET:HE2	2.21	0.41
18:r:52:CYS:SG	18:r:97:MET:HG2	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:GLY:O	1:A:180:CYS:C	2.63	0.41
6:F:289:ASP:OD2	6:F:333:ASN:N	2.49	0.41
21:U:98:GLU:HA	21:U:101:ILE:HG12	2.03	0.41
22:V:67:LEU:HA	22:V:70:VAL:HG22	2.02	0.41
22:V:108:LEU:HD21	22:V:170:LEU:HG	2.02	0.41
28:b:4:GLU:HA	28:b:106:LYS:H	1.86	0.41
29:c:26:ASP:OD2	29:c:161:ARG:NH2	2.54	0.41
29:c:174:PRO:O	29:c:176:GLN:NE2	2.53	0.41
32:f:206:ASP:OD1	32:f:232:TYR:OH	2.38	0.41
9:i:41:ASP:N	9:i:41:ASP:OD2	2.53	0.41
13:m:219:LEU:HD12	13:m:220:THR:HG23	2.03	0.41
1:A:123:VAL:HG12	6:F:87:PRO:HB3	2.03	0.41
8:H:9:SER:OG	8:H:10:LEU:N	2.54	0.41
13:M:215:TRP:CE3	13:M:227:VAL:HG22	2.56	0.41
19:S:16:ALA:HB2	19:S:121:VAL:HG23	2.02	0.41
20:T:70:MET:HE1	20:T:91:TRP:CE2	2.56	0.41
21:U:35:TRP:CD1	21:U:70:HIS:HD1	2.38	0.41
22:V:340:GLY:HA2	22:V:405:THR:HB	2.02	0.41
22:V:371:ASN:HB3	22:V:374:LYS:HD2	2.03	0.41
24:X:371:ASP:HB2	24:X:373:LYS:HE2	2.02	0.41
25:Y:220:VAL:HG21	25:Y:249:VAL:HG21	2.02	0.41
30:d:51:ALA:HA	30:d:54:ILE:HG12	2.02	0.41
30:d:132:TYR:HD1	30:d:160:ALA:HB2	1.86	0.41
18:r:33:LYS:HG2	18:r:45:MET:HE2	2.03	0.41
5:E:198:VAL:HG12	5:E:200:SER:H	1.85	0.41
6:F:58:GLU:OE1	6:F:61:ARG:NH2	2.54	0.41
6:F:338:LEU:HD23	6:F:340:PRO:HD2	2.03	0.41
8:H:119:GLN:HB3	8:H:153:GLY:HA3	2.02	0.41
12:L:69:HIS:CE1	12:L:102:PRO:HB3	2.56	0.41
17:Q:170:ARG:NH2	18:r:140:ASP:OD1	2.45	0.41
21:U:22:PHE:O	21:U:26:LYS:NZ	2.54	0.41
21:U:603:LEU:HD12	21:U:622:LEU:HD21	2.02	0.41
21:U:813:TYR:HB2	21:U:883:ARG:HD2	2.01	0.41
21:U:906:LEU:HD13	21:U:912:ILE:HD13	2.03	0.41
23:W:61:VAL:O	23:W:65:ARG:HG3	2.21	0.41
23:W:101:VAL:O	23:W:105:VAL:HG23	2.21	0.41
28:b:22:LEU:HD11	28:b:177:PRO:HB3	2.02	0.41
28:b:146:GLU:HG2	28:b:148:VAL:HB	2.02	0.41
29:c:27:THR:HG23	29:c:176:GLN:HB2	2.02	0.41
30:d:196:ARG:HD2	30:d:196:ARG:HA	1.82	0.41
32:f:537:THR:HB	32:f:562:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:5:ARG:O	10:j:123:GLY:N	2.54	0.41
15:o:211:VAL:HG21	16:p:198:ARG:HD3	2.03	0.41
2:B:411:ARG:NH2	2:B:418:ASP:OD2	2.46	0.41
4:D:92:PHE:HZ	4:D:95:ALA:HB2	1.86	0.41
5:E:307:GLN:HE22	23:W:136:ILE:HD11	1.86	0.41
7:G:137:CYS:SG	7:G:138:MET:N	2.94	0.41
10:J:42:VAL:HG11	10:J:191:VAL:HG21	2.02	0.41
16:P:12:MET:HB2	16:P:138:VAL:HG12	2.02	0.41
18:R:3:THR:HG23	18:R:16:ALA:HB2	2.02	0.41
21:U:403:THR:HG23	21:U:777:HIS:HE1	1.85	0.41
21:U:821:LYS:HA	21:U:821:LYS:HD3	1.87	0.41
23:W:86:ASN:HA	23:W:89:LEU:HG	2.03	0.41
24:X:415:TYR:CD2	25:Y:383:LEU:HD12	2.55	0.41
32:f:412:ALA:HA	32:f:447:ALA:HB2	2.02	0.41
32:f:470:VAL:HG13	32:f:471:LEU:HG	2.02	0.41
32:f:512:MET:HE1	32:f:554:TYR:HB3	2.02	0.41
8:h:39:LYS:HG3	8:h:44:VAL:HG22	2.03	0.41
12:l:140:MET:HE3	12:l:140:MET:HB3	1.82	0.41
15:o:81:ARG:HA	15:o:84:LYS:HG2	2.02	0.41
1:A:124:ASP:OD1	1:A:125:LEU:N	2.54	0.40
1:A:293:ASN:N	6:F:259:MET:HE1	2.36	0.40
2:B:190:LEU:HG	2:B:193:GLN:HB2	2.03	0.40
4:D:133:HIS:HB3	4:D:137:ASN:H	1.85	0.40
6:F:338:LEU:HD21	6:F:340:PRO:HG2	2.03	0.40
6:F:410:ARG:HE	6:F:412:ALA:HB3	1.86	0.40
8:H:6:TYR:OH	9:I:6:ASP:OD2	2.21	0.40
9:I:52:ILE:O	9:I:53:HIS:C	2.64	0.40
20:T:179:ARG:NH2	15:o:135:MET:SD	2.94	0.40
21:U:374:SER:HB3	21:U:407:SER:HB3	2.03	0.40
21:U:639:LEU:HA	21:U:639:LEU:HD12	1.83	0.40
22:V:131:LEU:HD13	22:V:171:VAL:HG21	2.03	0.40
23:W:26:GLN:NE2	23:W:30:GLU:OE2	2.55	0.40
23:W:89:LEU:HD12	23:W:90:LEU:HG	2.02	0.40
23:W:257:GLN:OE1	23:W:295:LYS:NZ	2.41	0.40
25:Y:345:CYS:HA	25:Y:356:THR:HA	2.03	0.40
26:Z:103:LYS:HZ2	26:Z:103:LYS:HG3	1.60	0.40
26:Z:166:GLU:O	26:Z:167:ALA:HB3	2.21	0.40
29:c:270:LEU:HA	29:c:273:LYS:HZ2	1.86	0.40
17:q:196:PHE:HA	17:q:197:PRO:HD3	1.93	0.40
18:r:127:SER:HB3	18:r:136:TYR:CE1	2.56	0.40
1:A:74:PRO:HA	1:A:75:PRO:HD3	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:GLU:HB2	1:A:138:MET:HE1	2.04	0.40
4:D:123:LEU:C	4:D:124:LEU:HD22	2.46	0.40
5:E:40:TYR:CE1	6:F:72:LYS:HE3	2.56	0.40
6:F:234:THR:O	6:F:238:ARG:HG2	2.22	0.40
21:U:32:ASN:HA	21:U:70:HIS:HE1	1.85	0.40
21:U:844:LYS:O	21:U:848:LYS:HG2	2.21	0.40
24:X:394:ASP:OD1	24:X:394:ASP:N	2.53	0.40
27:a:371:ALA:O	27:a:375:LEU:HG	2.21	0.40
30:d:79:LYS:O	30:d:83:PHE:HB2	2.21	0.40
1:A:100:LYS:HG3	1:A:137:GLY:HA2	2.03	0.40
1:A:143:ASP:HB3	1:A:147:TYR:N	2.37	0.40
11:K:67:ILE:HB	11:K:228:MET:HE1	2.03	0.40
12:L:109:VAL:HG21	12:L:145:PHE:HD2	1.86	0.40
21:U:12:LEU:HD21	21:U:24:LEU:HG	2.03	0.40
21:U:695:MET:HE2	21:U:706:VAL:HG22	2.03	0.40
24:X:377:ILE:HG12	25:Y:312:ARG:HB3	2.03	0.40
32:f:583:VAL:HB	32:f:588:ARG:HD3	2.03	0.40
7:g:197:THR:HA	7:g:200:THR:HG22	2.03	0.40
11:k:99:HIS:HB2	11:k:107:MET:HE3	2.03	0.40
13:m:150:MET:HE3	13:m:150:MET:HB3	1.98	0.40
14:n:143:TYR:HA	14:n:147:MET:HE1	2.03	0.40
1:A:287:ASP:HB2	2:B:298:ASN:ND2	2.37	0.40
3:C:185:GLY:HA3	3:C:311:ILE:HA	2.03	0.40
3:C:226:GLU:HA	3:C:229:ARG:HG3	2.02	0.40
4:D:248:ARG:HG2	4:D:295:GLN:HE22	1.85	0.40
6:F:323:ASN:O	6:F:326:VAL:HG23	2.21	0.40
11:K:118:ASN:OD1	12:L:82:ARG:NH2	2.55	0.40
11:K:215:ILE:HD11	11:K:238:ILE:HD11	2.03	0.40
14:N:84:LYS:HG3	14:N:120:MET:HB2	2.02	0.40
21:U:157:THR:HG23	21:U:159:ARG:HB2	2.03	0.40
24:X:380:GLN:HB2	25:Y:314:LEU:HA	2.02	0.40
27:a:64:ILE:O	27:a:68:GLU:HB2	2.21	0.40
27:a:77:VAL:HA	27:a:80:ILE:HG22	2.02	0.40
1:A:182:GLU:OE2	1:A:183:GLN:NE2	2.55	0.40
3:C:133:PRO:HB2	3:C:230:MET:HE1	2.02	0.40
5:E:30:ARG:HH21	6:F:62:VAL:HG11	1.87	0.40
6:F:237:ALA:HB1	6:F:248:PHE:CZ	2.56	0.40
20:T:25:ASP:HA	20:T:187:PHE:HA	2.04	0.40
21:U:633:CYS:HA	21:U:636:VAL:HG22	2.02	0.40
23:W:45:GLU:HA	23:W:48:LEU:HG	2.02	0.40
23:W:409:LEU:HD11	24:X:344:ARG:HH21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:239:TYR:HB3	24:X:247:ALA:HB2	2.02	0.40
26:Z:67:VAL:HG21	28:b:91:ARG:HD2	2.04	0.40
27:a:245:VAL:HG11	27:a:301:LYS:HD3	2.04	0.40
30:d:215:TRP:HE3	30:d:222:TYR:HB3	1.87	0.40
32:f:182:GLU:HA	32:f:185:LEU:HB2	2.03	0.40
32:f:490:ALA:HA	32:f:525:ILE:HA	2.02	0.40
8:h:3:GLU:N	13:m:125:TYR:HB3	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	411/433 (95%)	354 (86%)	51 (12%)	6 (2%)	8	32
2	B	409/440 (93%)	366 (90%)	43 (10%)	0	100	100
3	C	394/398 (99%)	342 (87%)	45 (11%)	7 (2%)	6	29
4	D	378/418 (90%)	328 (87%)	48 (13%)	2 (0%)	24	55
5	E	387/403 (96%)	348 (90%)	34 (9%)	5 (1%)	9	35
6	F	391/439 (89%)	351 (90%)	33 (8%)	7 (2%)	6	29
7	G	238/246 (97%)	225 (94%)	12 (5%)	1 (0%)	30	60
7	g	242/246 (98%)	226 (93%)	15 (6%)	1 (0%)	30	60
8	H	230/234 (98%)	219 (95%)	11 (5%)	0	100	100
8	h	230/234 (98%)	220 (96%)	9 (4%)	1 (0%)	30	60
9	I	246/261 (94%)	237 (96%)	9 (4%)	0	100	100
9	i	248/261 (95%)	243 (98%)	5 (2%)	0	100	100
10	J	237/248 (96%)	223 (94%)	14 (6%)	0	100	100
10	j	237/248 (96%)	223 (94%)	13 (6%)	1 (0%)	30	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	236/241 (98%)	225 (95%)	11 (5%)	0	100	100
11	k	232/241 (96%)	224 (97%)	8 (3%)	0	100	100
12	L	238/263 (90%)	227 (95%)	11 (5%)	0	100	100
12	l	236/263 (90%)	225 (95%)	11 (5%)	0	100	100
13	M	241/255 (94%)	233 (97%)	8 (3%)	0	100	100
13	m	238/255 (93%)	233 (98%)	5 (2%)	0	100	100
14	N	201/239 (84%)	197 (98%)	4 (2%)	0	100	100
14	n	200/239 (84%)	194 (97%)	6 (3%)	0	100	100
15	O	218/277 (79%)	213 (98%)	5 (2%)	0	100	100
15	o	218/277 (79%)	209 (96%)	9 (4%)	0	100	100
16	P	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
16	p	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
17	Q	198/201 (98%)	190 (96%)	8 (4%)	0	100	100
17	q	197/201 (98%)	192 (98%)	5 (2%)	0	100	100
18	R	199/263 (76%)	194 (98%)	5 (2%)	0	100	100
18	r	199/263 (76%)	195 (98%)	4 (2%)	0	100	100
19	S	211/241 (88%)	203 (96%)	8 (4%)	0	100	100
19	s	211/241 (88%)	203 (96%)	8 (4%)	0	100	100
20	T	214/264 (81%)	210 (98%)	4 (2%)	0	100	100
20	t	214/264 (81%)	208 (97%)	6 (3%)	0	100	100
21	U	874/953 (92%)	804 (92%)	69 (8%)	1 (0%)	48	75
22	V	442/534 (83%)	426 (96%)	16 (4%)	0	100	100
23	W	439/456 (96%)	428 (98%)	11 (2%)	0	100	100
24	X	420/422 (100%)	402 (96%)	16 (4%)	2 (0%)	24	55
25	Y	387/389 (100%)	364 (94%)	23 (6%)	0	100	100
26	Z	284/324 (88%)	250 (88%)	31 (11%)	3 (1%)	11	39
27	a	371/376 (99%)	344 (93%)	25 (7%)	2 (0%)	24	55
28	b	189/377 (50%)	165 (87%)	23 (12%)	1 (0%)	24	55
29	c	285/310 (92%)	241 (85%)	42 (15%)	2 (1%)	18	49
30	d	255/350 (73%)	214 (84%)	38 (15%)	3 (1%)	10	37
31	e	48/70 (69%)	45 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	f	840/908 (92%)	813 (97%)	27 (3%)	0	100	100
All	All	13417/14876 (90%)	12567 (94%)	805 (6%)	45 (0%)	37	65

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	ASP
3	C	90	HIS
3	C	141	GLU
4	D	157	ASP
5	E	166	PRO
5	E	167	PRO
6	F	182	THR
24	X	318	ILE
27	a	342	ASP
27	a	343	LEU
28	b	22	LEU
30	d	203	PRO
1	A	286	ASP
3	C	89	VAL
3	C	129	ASN
3	C	254	ILE
4	D	126	PRO
5	E	165	ILE
5	E	282	PRO
6	F	181	PRO
6	F	244	THR
7	G	19	GLU
21	U	873	PRO
26	Z	104	ASN
26	Z	145	HIS
29	c	232	GLN
10	j	50	VAL
1	A	180	CYS
3	C	130	LYS
5	E	164	ILE
6	F	347	ARG
24	X	203	PRO
29	c	198	ARG
30	d	202	THR
7	g	223	GLU
8	h	4	ARG

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Mol	Chain	Res	Type
1	A	288	GLY
30	d	199	PHE
3	C	128	PRO
6	F	246	ALA
6	F	324	THR
26	Z	184	VAL
1	A	109	PRO
1	A	179	GLY
6	F	172	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	348/372 (94%)	346 (99%)	2 (1%)	78	81
2	B	357/385 (93%)	356 (100%)	1 (0%)	86	86
3	C	340/346 (98%)	329 (97%)	11 (3%)	34	60
4	D	333/366 (91%)	328 (98%)	5 (2%)	57	72
5	E	341/353 (97%)	338 (99%)	3 (1%)	70	78
6	F	340/379 (90%)	334 (98%)	6 (2%)	51	70
7	G	202/210 (96%)	200 (99%)	2 (1%)	68	76
7	g	201/210 (96%)	200 (100%)	1 (0%)	81	83
8	H	187/191 (98%)	187 (100%)	0	100	100
8	h	188/191 (98%)	186 (99%)	2 (1%)	65	76
9	I	202/221 (91%)	200 (99%)	2 (1%)	68	76
9	i	206/221 (93%)	206 (100%)	0	100	100
10	J	197/211 (93%)	194 (98%)	3 (2%)	57	72
10	j	196/211 (93%)	196 (100%)	0	100	100
11	K	197/203 (97%)	197 (100%)	0	100	100
11	k	195/203 (96%)	195 (100%)	0	100	100
12	L	202/224 (90%)	202 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	l	201/224 (90%)	201 (100%)	0	100	100
13	M	199/212 (94%)	199 (100%)	0	100	100
13	m	198/212 (93%)	198 (100%)	0	100	100
14	N	158/181 (87%)	158 (100%)	0	100	100
14	n	156/181 (86%)	156 (100%)	0	100	100
15	O	178/228 (78%)	178 (100%)	0	100	100
15	o	181/228 (79%)	181 (100%)	0	100	100
16	P	172/174 (99%)	172 (100%)	0	100	100
16	p	173/174 (99%)	173 (100%)	0	100	100
17	Q	169/171 (99%)	169 (100%)	0	100	100
17	q	166/171 (97%)	166 (100%)	0	100	100
18	R	156/202 (77%)	156 (100%)	0	100	100
18	r	154/202 (76%)	154 (100%)	0	100	100
19	S	175/199 (88%)	175 (100%)	0	100	100
19	s	177/199 (89%)	177 (100%)	0	100	100
20	T	178/215 (83%)	178 (100%)	0	100	100
20	t	179/215 (83%)	179 (100%)	0	100	100
21	U	752/816 (92%)	751 (100%)	1 (0%)	88	90
22	V	390/460 (85%)	390 (100%)	0	100	100
23	W	406/416 (98%)	404 (100%)	2 (0%)	81	83
24	X	362/362 (100%)	362 (100%)	0	100	100
25	Y	344/344 (100%)	342 (99%)	2 (1%)	78	81
26	Z	257/295 (87%)	254 (99%)	3 (1%)	63	75
27	a	333/336 (99%)	332 (100%)	1 (0%)	86	86
28	b	167/312 (54%)	167 (100%)	0	100	100
29	c	252/268 (94%)	244 (97%)	8 (3%)	34	60
30	d	231/294 (79%)	230 (100%)	1 (0%)	84	84
31	e	44/63 (70%)	43 (98%)	1 (2%)	44	66
32	f	711/763 (93%)	710 (100%)	1 (0%)	88	90
All	All	11451/12614 (91%)	11393 (100%)	58 (0%)	78	83

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	ILE
1	A	403	ILE
2	B	125	THR
3	C	71	SER
3	C	82	LYS
3	C	83	LYS
3	C	88	LYS
3	C	107	ASP
3	C	109	THR
3	C	141	GLU
3	C	142	LYS
3	C	210	THR
3	C	252	ASP
3	C	254	ILE
4	D	125	LYS
4	D	157	ASP
4	D	158	GLN
4	D	159	LYS
4	D	337	ASP
5	E	165	ILE
5	E	168	LYS
5	E	281	ARG
6	F	172	VAL
6	F	173	LYS
6	F	180	ARG
6	F	245	LYS
6	F	326	VAL
6	F	416	THR
7	G	19	GLU
7	G	21	ARG
9	I	51	ASN
9	I	52	ILE
10	J	219	ILE
10	J	220	LEU
10	J	221	ASN
21	U	874	ASN
23	W	455	LEU
23	W	456	GLN
25	Y	104	MET
25	Y	105	MET
26	Z	70	LEU
26	Z	103	LYS
26	Z	168	GLU

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Mol	Chain	Res	Type
27	a	343	LEU
29	c	196	LEU
29	c	197	ASN
29	c	231	LEU
29	c	278	GLN
29	c	279	ASP
29	c	281	LYS
29	c	284	LEU
29	c	285	GLU
30	d	204	LYS
31	e	63	HIS
32	f	87	THR
7	g	222	VAL
8	h	3	GLU
8	h	4	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	314	ASN
2	B	81	ASN
2	B	84	GLN
2	B	193	GLN
2	B	257	GLN
3	C	64	GLN
3	C	221	GLN
4	D	67	ASN
4	D	91	GLN
4	D	187	HIS
4	D	295	GLN
4	D	390	ASN
5	E	19	HIS
5	E	45	ASN
5	E	190	GLN
5	E	225	HIS
5	E	226	GLN
5	E	254	GLN
5	E	262	ASN
5	E	263	GLN
6	F	258	GLN
6	F	315	ASN

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Mol	Chain	Res	Type
6	F	392	ASN
6	F	417	HIS
7	G	33	ASN
7	G	53	GLN
7	G	68	HIS
7	G	224	ASN
8	H	88	HIS
8	H	95	GLN
9	I	40	ASN
9	I	53	HIS
9	I	95	GLN
10	J	92	GLN
12	L	53	GLN
12	L	60	GLN
12	L	69	HIS
15	O	193	ASN
16	P	93	ASN
17	Q	63	ASN
17	Q	101	ASN
18	R	10	HIS
18	R	175	ASN
19	S	58	HIS
20	T	65	GLN
21	U	93	ASN
21	U	115	ASN
21	U	128	GLN
21	U	355	ASN
21	U	398	ASN
21	U	452	ASN
21	U	632	GLN
21	U	647	HIS
21	U	698	GLN
22	V	62	HIS
23	W	453	HIS
23	W	456	GLN
24	X	292	GLN
24	X	296	ASN
24	X	333	GLN
24	X	380	GLN
25	Y	136	HIS
25	Y	160	ASN
25	Y	302	HIS

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Mol	Chain	Res	Type
25	Y	351	ASN
26	Z	145	HIS
26	Z	189	GLN
26	Z	235	ASN
27	a	9	GLN
27	a	18	GLN
27	a	62	ASN
27	a	193	GLN
27	a	194	GLN
27	a	257	GLN
27	a	288	HIS
28	b	158	ASN
29	c	128	ASN
29	c	221	HIS
29	c	278	GLN
30	d	15	ASN
30	d	130	ASN
30	d	245	GLN
31	e	63	HIS
32	f	148	GLN
32	f	325	GLN
32	f	356	ASN
32	f	750	GLN
32	f	758	ASN
7	g	75	ASN
8	h	52	GLN
8	h	71	HIS
8	h	95	GLN
9	i	20	GLN
9	i	53	HIS
9	i	167	ASN
10	j	92	GLN
10	j	122	ASN
10	j	154	HIS
11	k	41	GLN
12	l	60	GLN
13	m	110	HIS
14	n	158	ASN
17	q	8	GLN
17	q	61	GLN
17	q	82	ASN
17	q	101	ASN

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Mol	Chain	Res	Type
18	r	119	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	ATP	C	501	35	29,33,33	0.27	0	44,52,52	0.46	1 (2%)
36	ADP	F	501	-	27,29,29	1.36	4 (14%)	42,45,45	1.99	10 (23%)
36	ADP	E	401	-	27,29,29	1.37	4 (14%)	42,45,45	1.95	10 (23%)
34	ATP	A	501	35	29,33,33	0.26	0	44,52,52	0.49	0
34	ATP	B	501	35	29,33,33	0.27	0	44,52,52	0.54	1 (2%)
34	ATP	D	501	35	29,33,33	0.27	0	44,52,52	0.51	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	ATP	C	501	35	-	7/22/38/38	0/3/3/3
36	ADP	F	501	-	-	5/16/32/32	0/3/3/3
36	ADP	E	401	-	-	3/16/32/32	0/3/3/3
34	ATP	A	501	35	-	3/22/38/38	0/3/3/3
34	ATP	B	501	35	-	5/22/38/38	0/3/3/3
34	ATP	D	501	35	-	4/22/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	E	401	ADP	C5-C4	4.59	1.47	1.39
36	F	501	ADP	C5-C4	4.57	1.47	1.39
36	F	501	ADP	C5-C6	2.70	1.48	1.41
36	E	401	ADP	C5-C6	2.68	1.48	1.41
36	E	401	ADP	C8-N7	2.37	1.36	1.31
36	F	501	ADP	C8-N7	2.33	1.36	1.31
36	F	501	ADP	C5-N7	-2.25	1.34	1.39
36	E	401	ADP	C5-N7	-2.23	1.34	1.39

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	F	501	ADP	C5-C4-N3	-6.55	118.20	126.75
36	E	401	ADP	C5-C4-N3	-6.49	118.28	126.75
36	F	501	ADP	N3-C4-N9	5.17	135.60	127.08
36	E	401	ADP	N3-C4-N9	5.03	135.37	127.08
36	E	401	ADP	C2-N3-C4	3.95	121.09	111.75
36	F	501	ADP	C2-N3-C4	3.93	121.03	111.75
36	E	401	ADP	C4-C5-N7	-3.29	106.62	110.62
36	F	501	ADP	C4-C5-N7	-3.26	106.65	110.62
36	F	501	ADP	PA-O3A-PB	-3.08	122.24	132.83
36	F	501	ADP	N3-C2-N1	-3.06	123.82	128.60
36	E	401	ADP	N3-C2-N1	-3.04	123.84	128.60
36	F	501	ADP	C5-N7-C8	2.89	107.62	103.51
36	E	401	ADP	PA-O3A-PB	-2.83	123.13	132.83
36	E	401	ADP	C5-N7-C8	2.72	107.37	103.51
36	F	501	ADP	C3'-C2'-C1'	2.71	106.58	101.43
36	E	401	ADP	C3'-C2'-C1'	2.46	106.11	101.43
36	F	501	ADP	C4-N9-C8	2.45	108.38	105.73
36	E	401	ADP	C4-N9-C8	2.29	108.21	105.73
34	D	501	ATP	PB-O3B-PG	2.09	139.98	132.83
34	B	501	ATP	PB-O3B-PG	2.08	139.97	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	E	401	ADP	C6-C5-N7	2.06	135.85	132.02
36	F	501	ADP	N9-C8-N7	-2.01	111.16	113.91
34	C	501	ATP	PB-O3B-PG	2.01	139.72	132.83

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	A	501	ATP	C5'-O5'-PA-O3A
34	B	501	ATP	O4'-C4'-C5'-O5'
34	B	501	ATP	C3'-C4'-C5'-O5'
34	C	501	ATP	C5'-O5'-PA-O1A
34	C	501	ATP	C5'-O5'-PA-O2A
34	C	501	ATP	C3'-C4'-C5'-O5'
36	F	501	ADP	C5'-O5'-PA-O1A
36	F	501	ADP	C5'-O5'-PA-O2A
36	F	501	ADP	O4'-C4'-C5'-O5'
36	F	501	ADP	C3'-C4'-C5'-O5'
34	C	501	ATP	O4'-C4'-C5'-O5'
34	C	501	ATP	C5'-O5'-PA-O3A
34	C	501	ATP	PB-O3A-PA-O2A
36	E	401	ADP	PB-O3A-PA-O2A
34	A	501	ATP	C5'-O5'-PA-O1A
34	B	501	ATP	C5'-O5'-PA-O2A
34	D	501	ATP	PA-O3A-PB-O2B
34	B	501	ATP	PG-O3B-PB-O2B
34	D	501	ATP	PA-O3A-PB-O1B
34	A	501	ATP	O4'-C4'-C5'-O5'
34	B	501	ATP	C5'-O5'-PA-O3A
36	F	501	ADP	C5'-O5'-PA-O3A
36	E	401	ADP	O4'-C4'-C5'-O5'
34	C	501	ATP	PB-O3A-PA-O1A
34	D	501	ATP	PG-O3B-PB-O1B
34	D	501	ATP	PG-O3B-PB-O2B
36	E	401	ADP	PB-O3A-PA-O1A

There are no ring outliers.

6 monomers are involved in 12 short contacts:

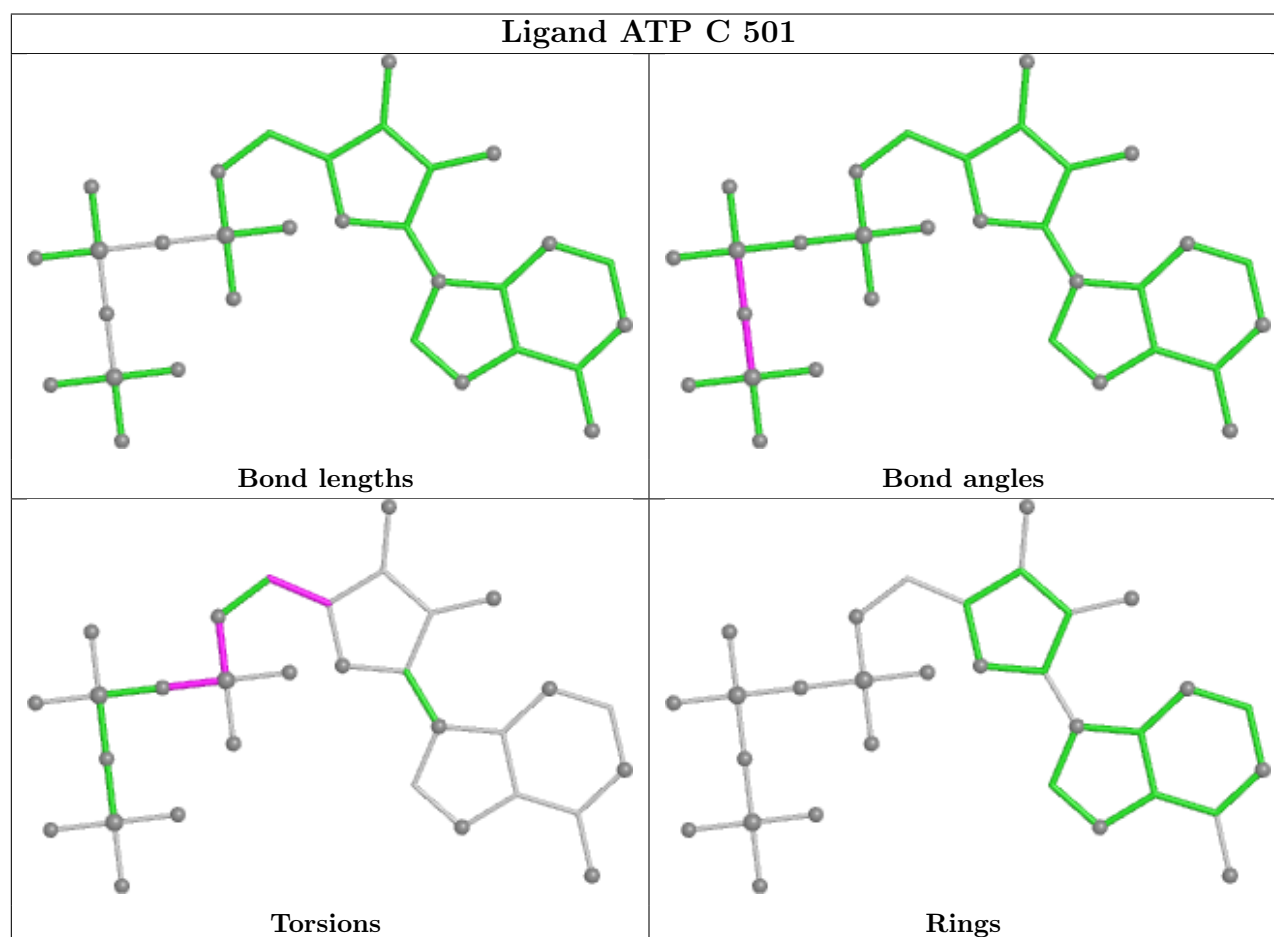
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	C	501	ATP	2	0

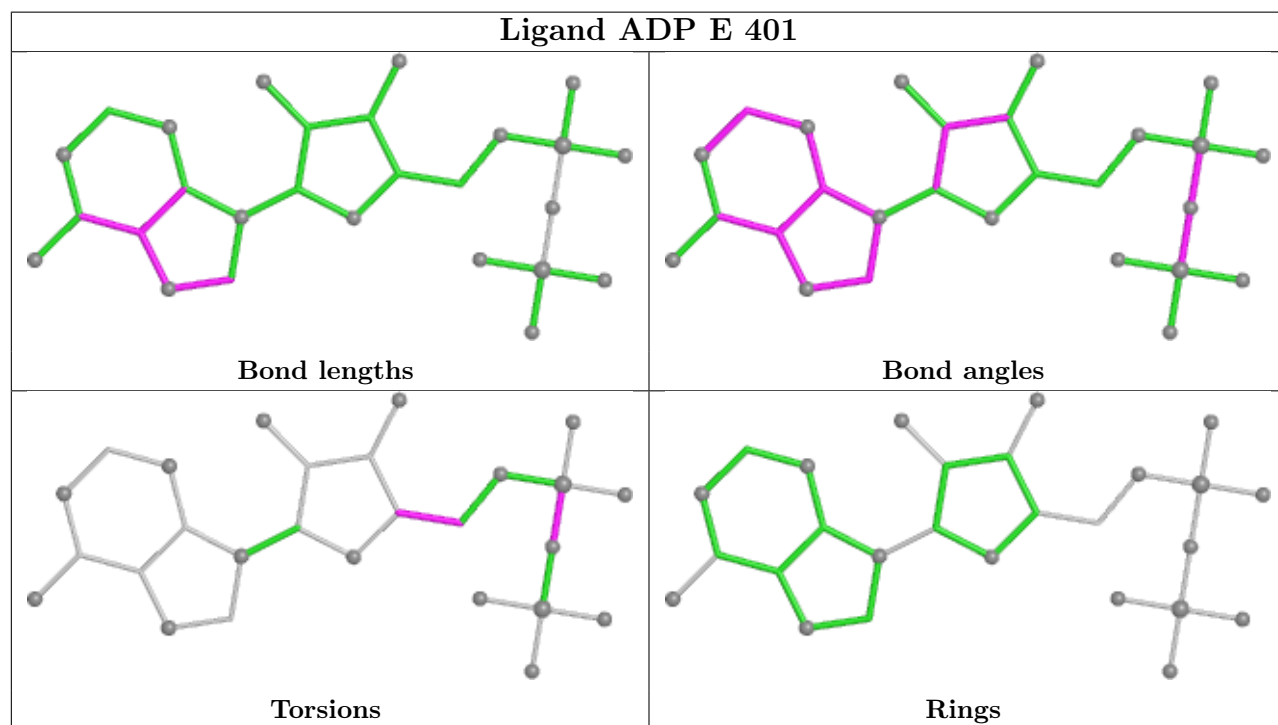
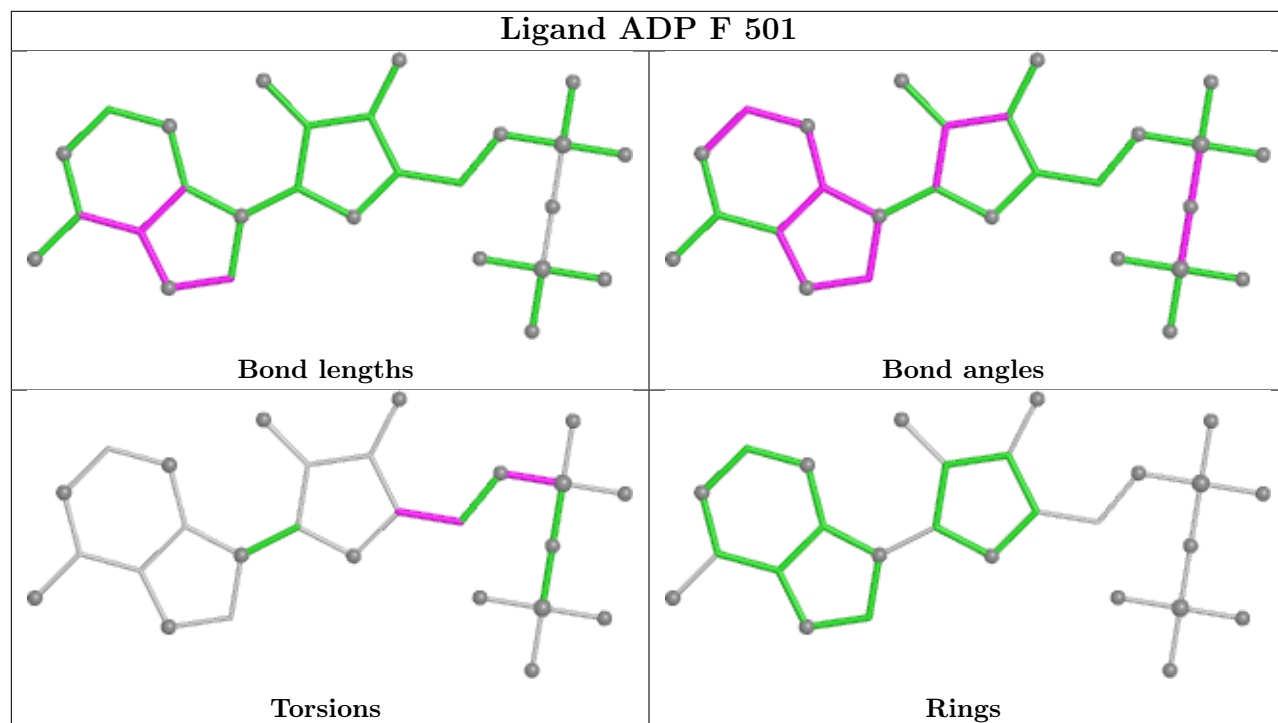
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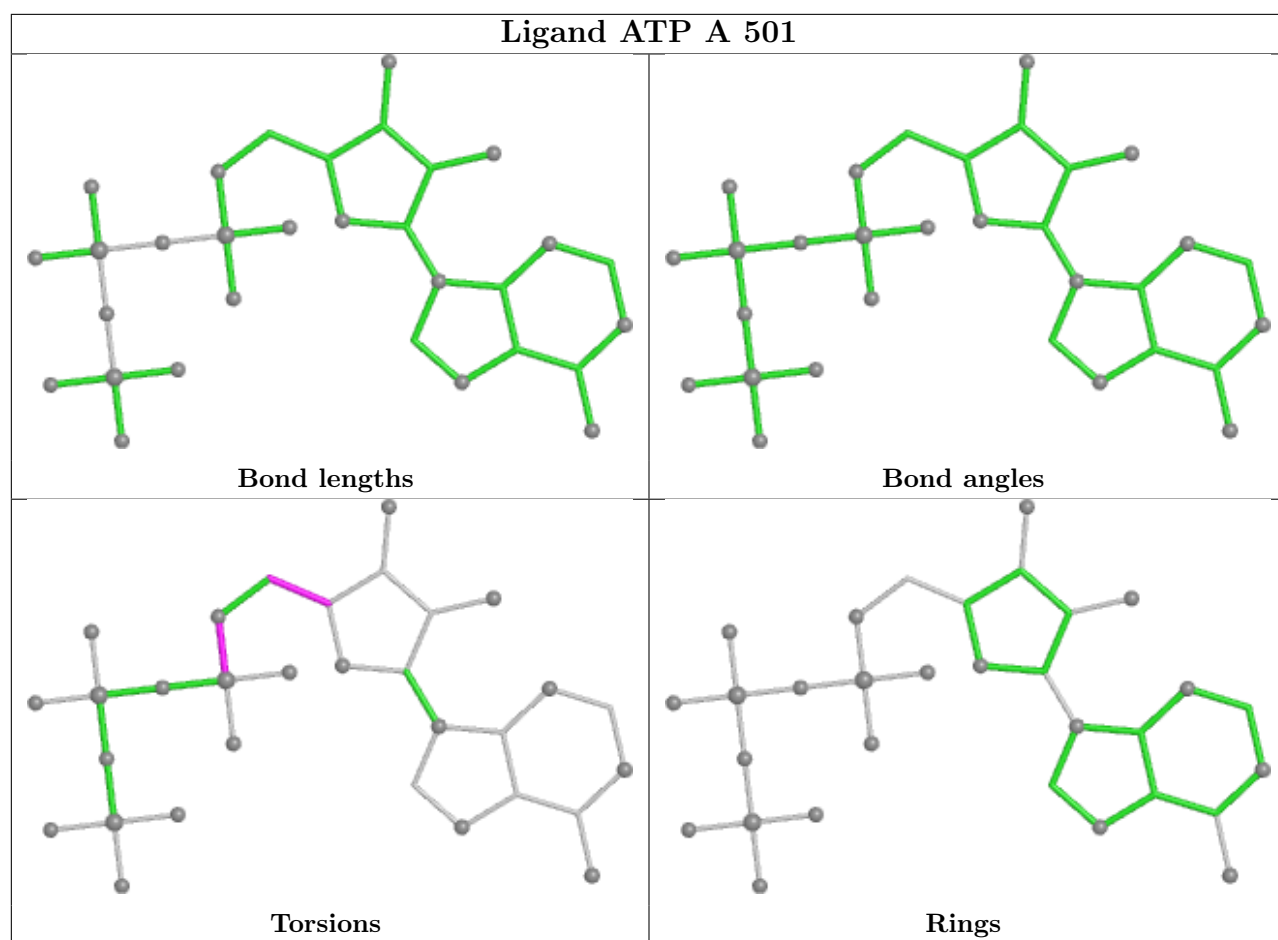
Continued from previous page...

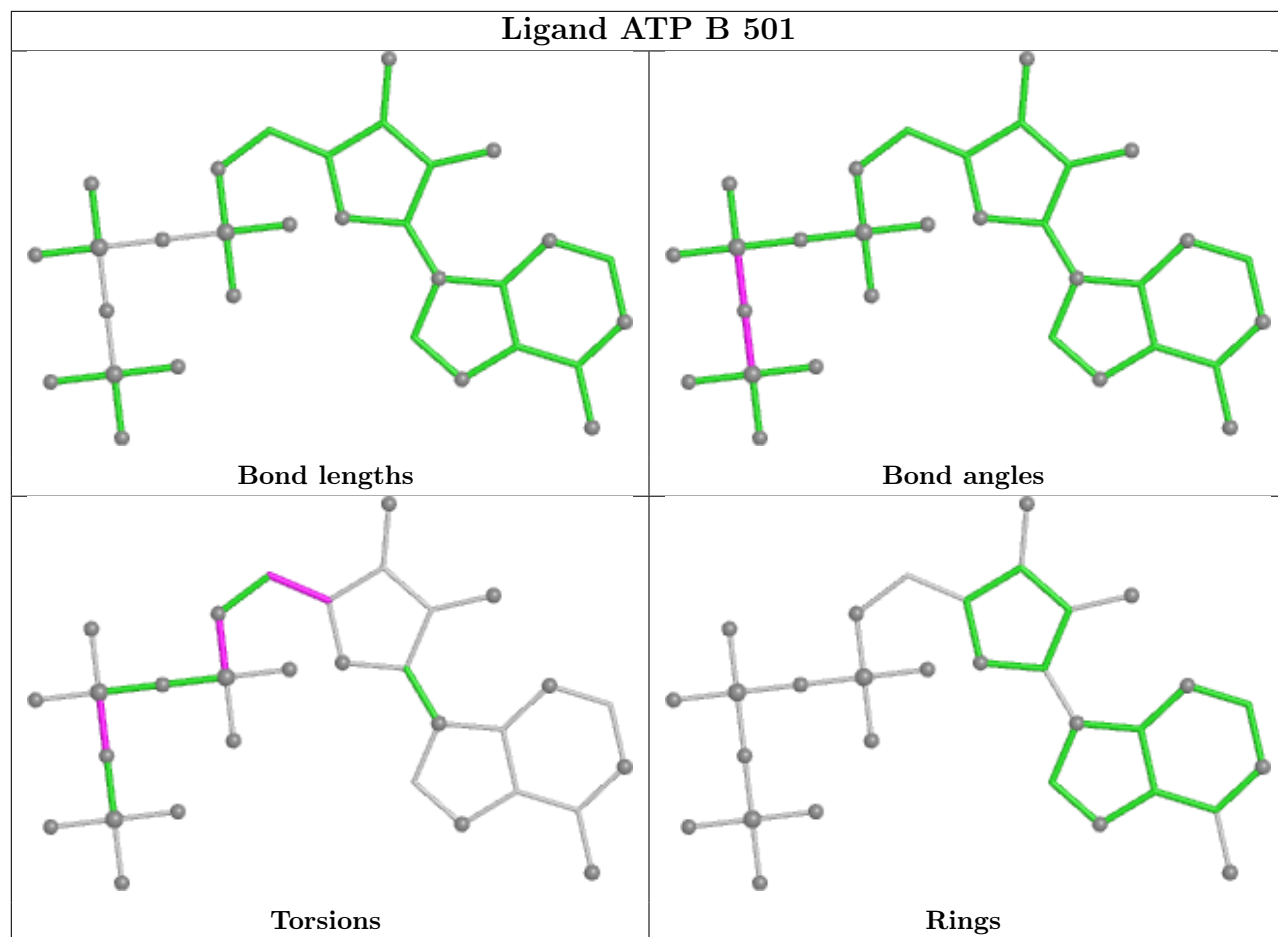
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	F	501	ADP	1	0
36	E	401	ADP	3	0
34	A	501	ATP	4	0
34	B	501	ATP	1	0
34	D	501	ATP	1	0

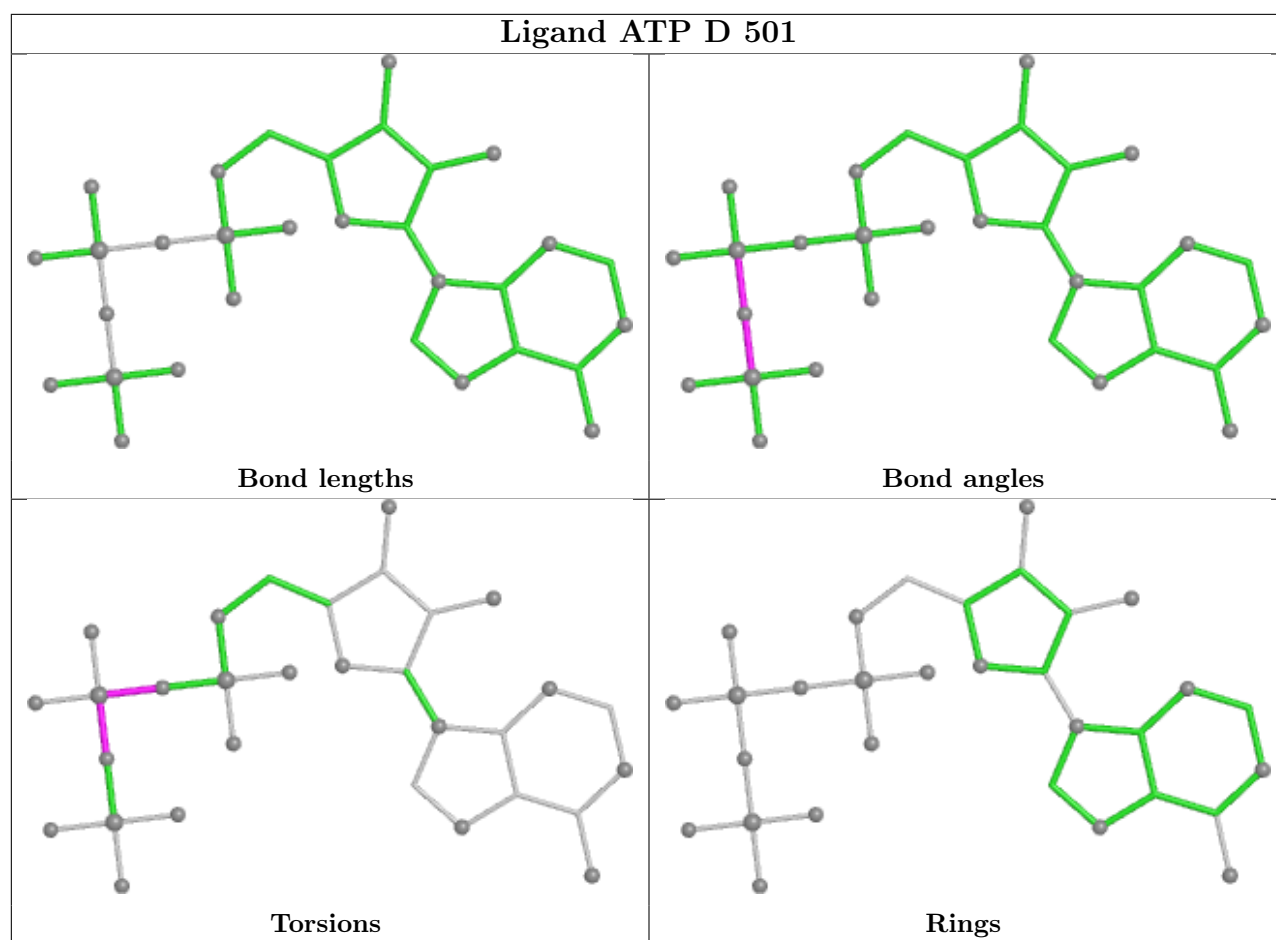
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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.

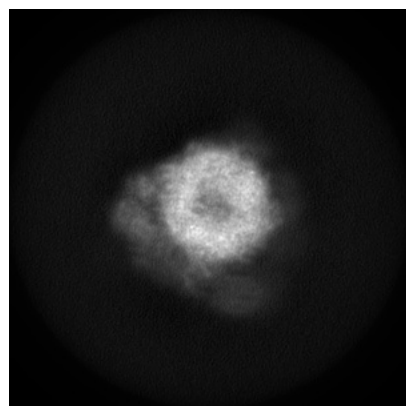
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62075. These allow visual inspection of the internal detail of the map and identification of artifacts.

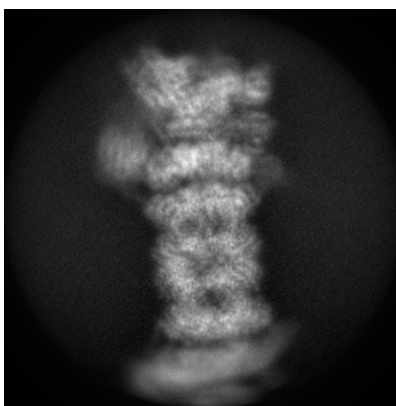
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

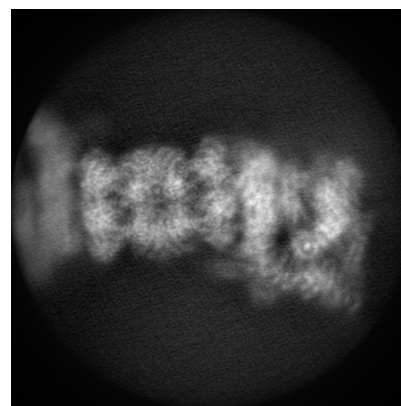
6.1.1 Primary map



X

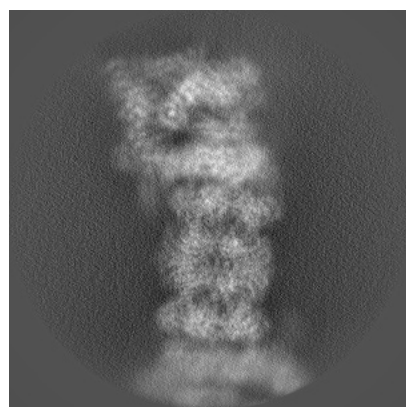


Y

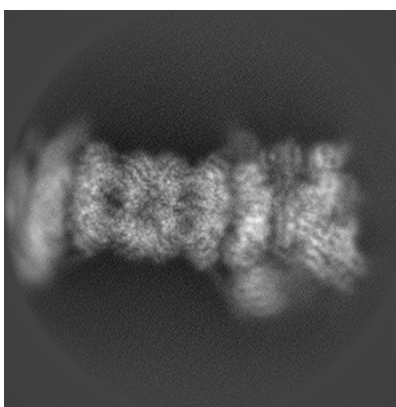


Z

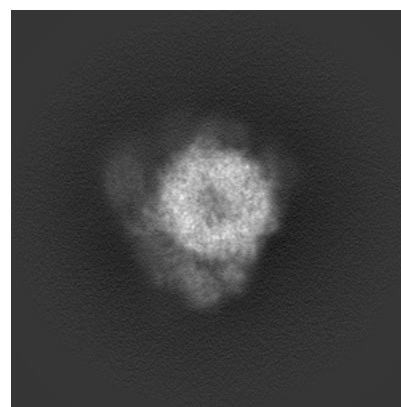
6.1.2 Raw map



X



Y

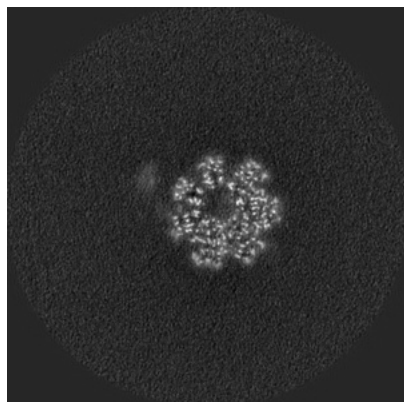


Z

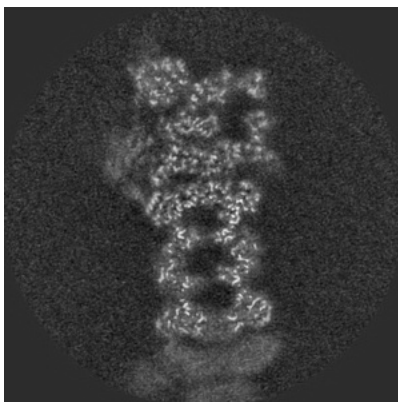
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

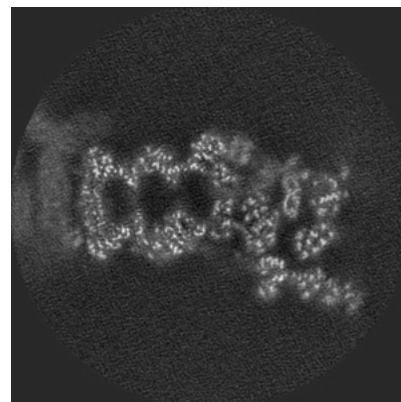
6.2.1 Primary map



X Index: 300

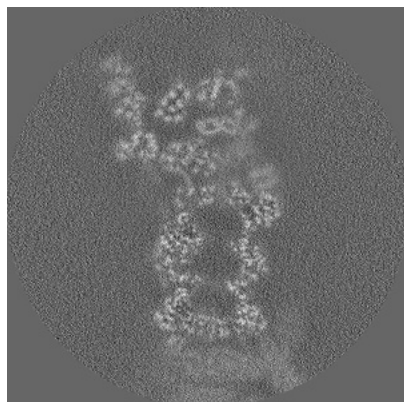


Y Index: 300

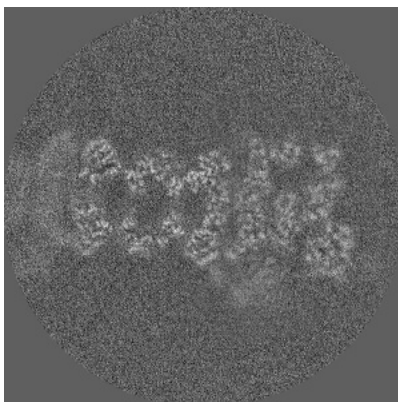


Z Index: 300

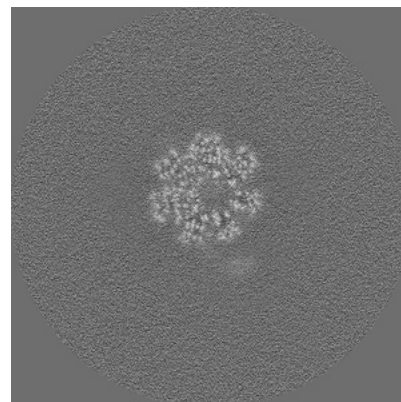
6.2.2 Raw map



X Index: 300



Y Index: 300

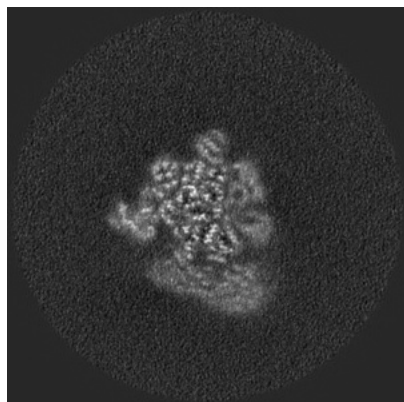


Z Index: 300

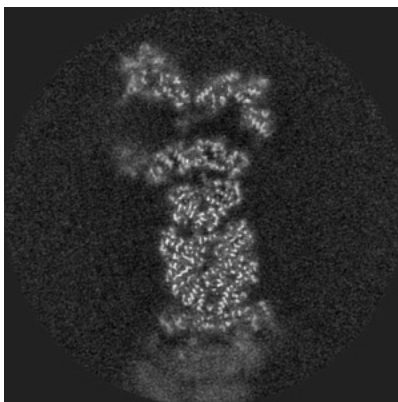
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

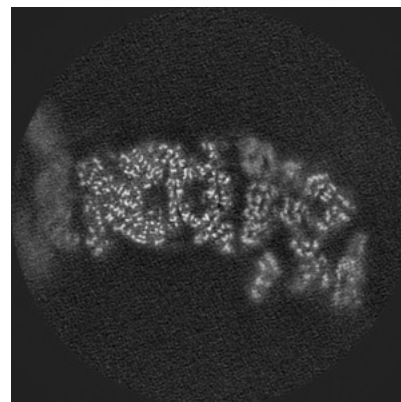
6.3.1 Primary map



X Index: 373

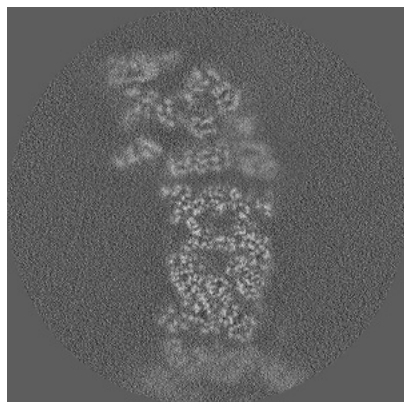


Y Index: 269

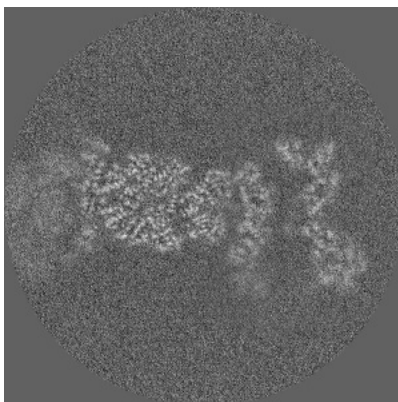


Z Index: 270

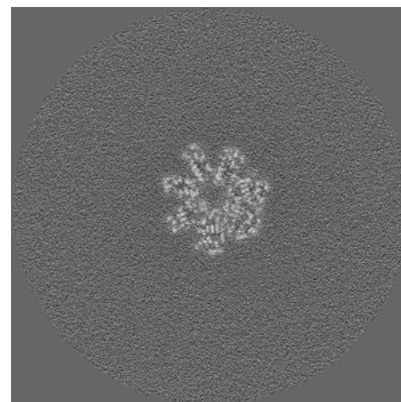
6.3.2 Raw map



X Index: 271



Y Index: 269

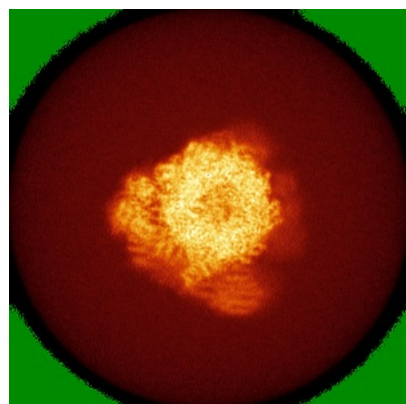


Z Index: 252

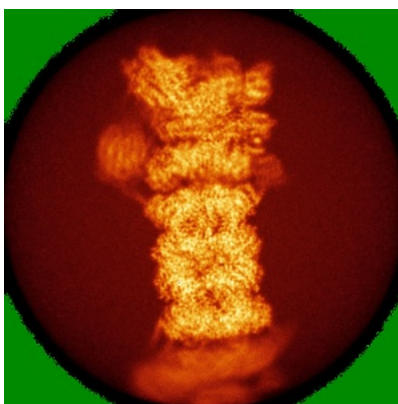
The images above show the largest variance slices of the map in three orthogonal directions.

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

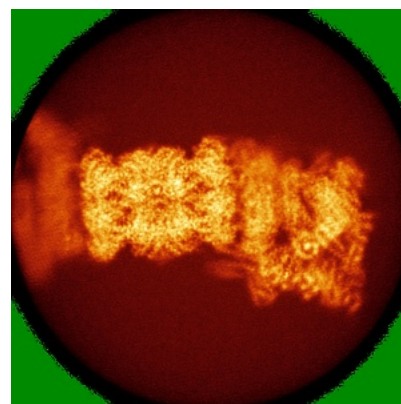
6.4.1 Primary map



X

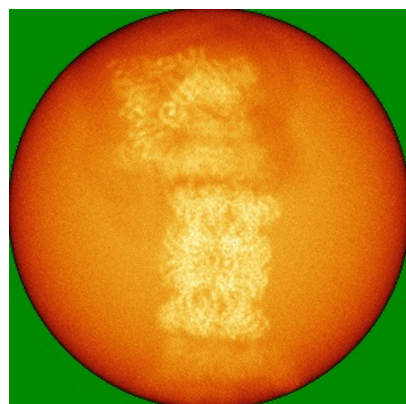


Y

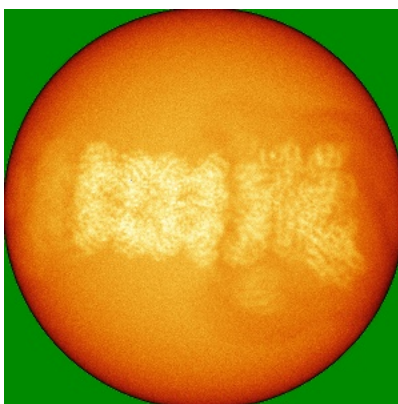


Z

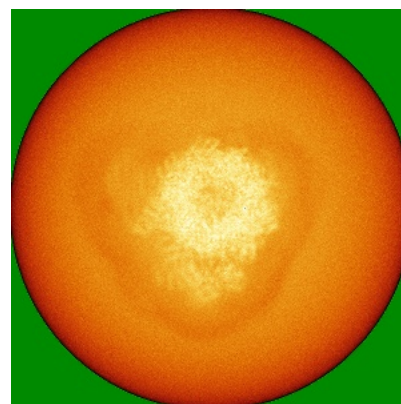
6.4.2 Raw map



X



Y

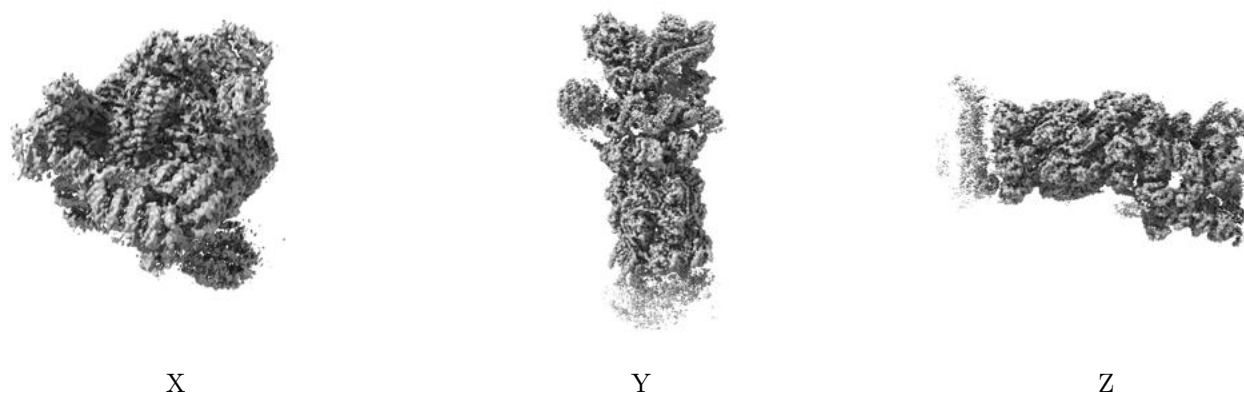


Z

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.

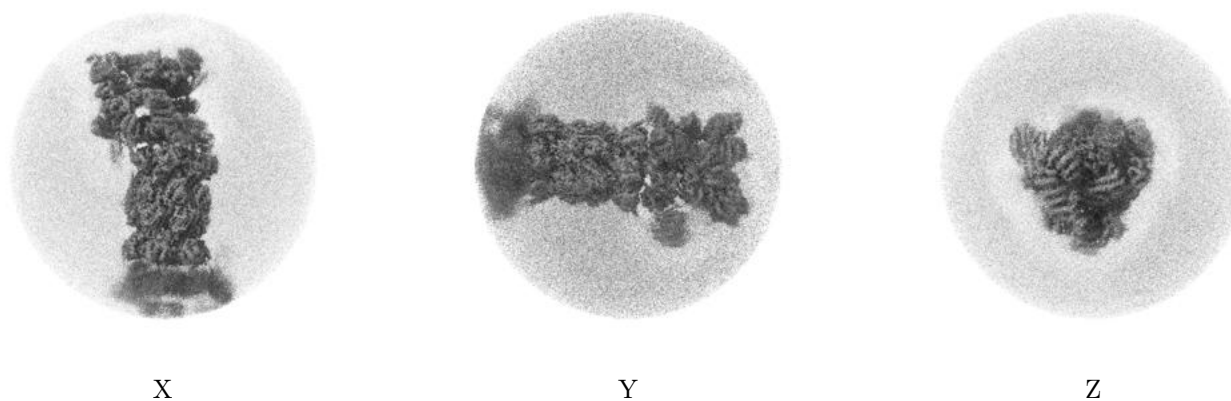
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00588. 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.

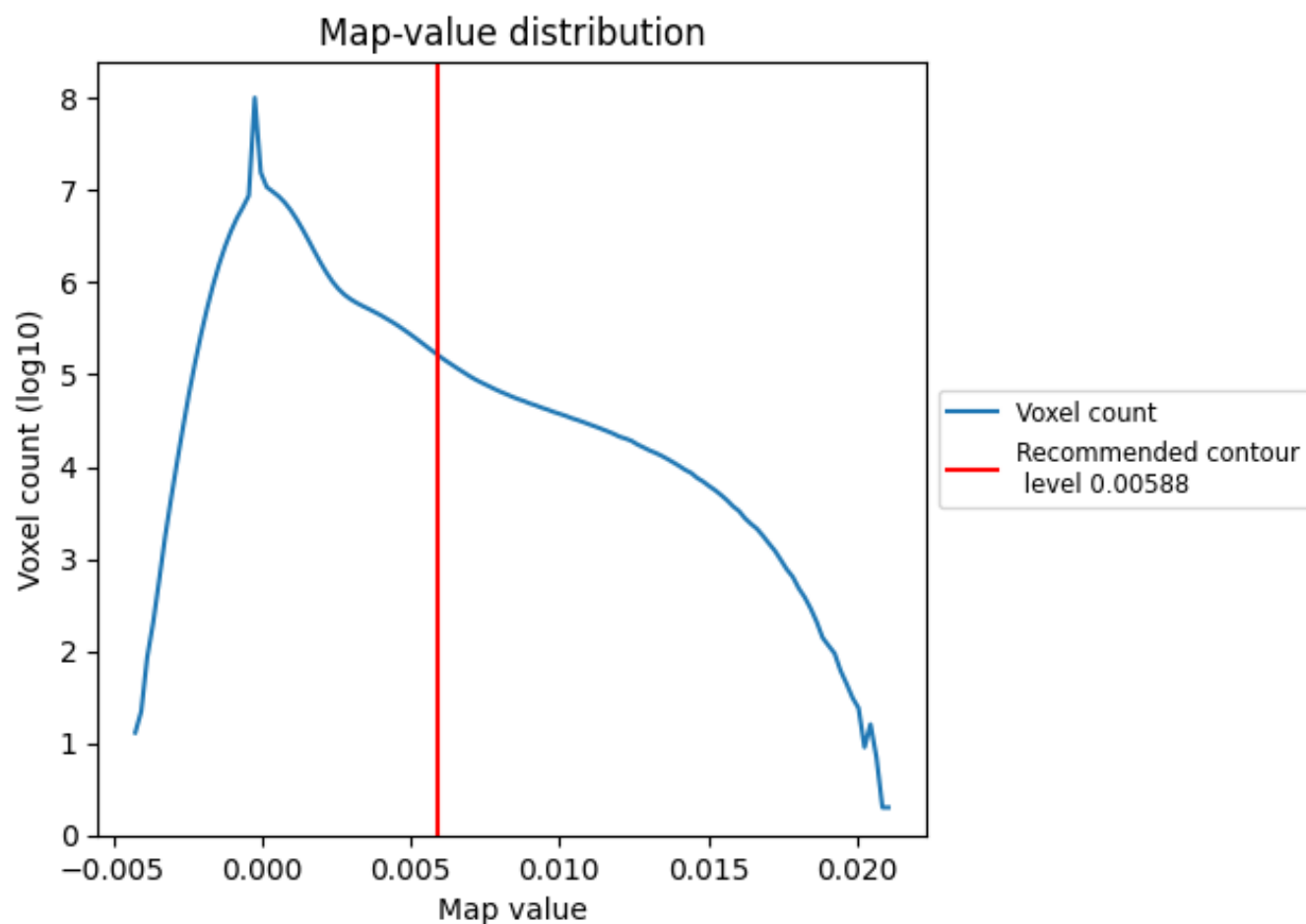
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

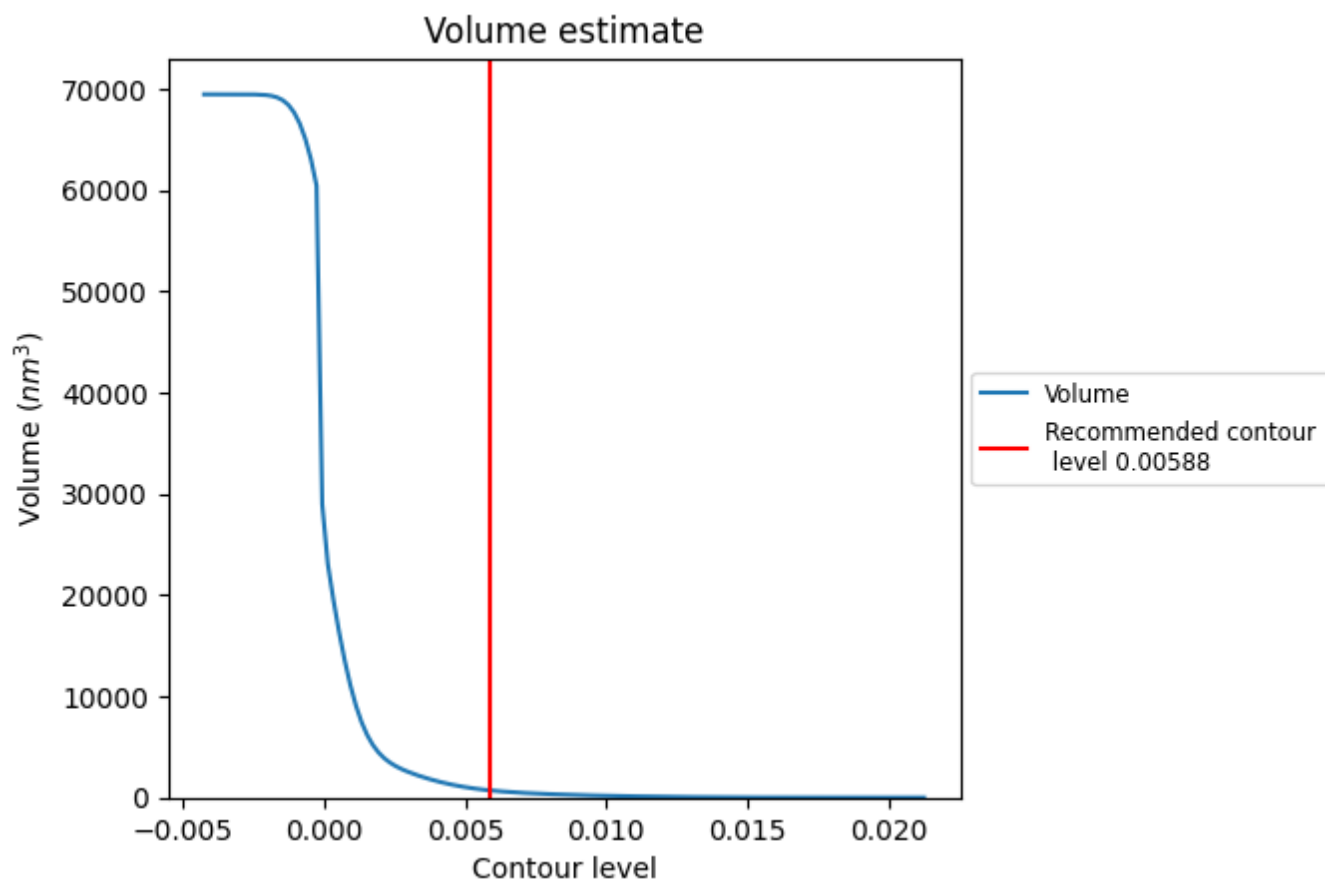
This section contains the results of statistical analysis of the map.

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.

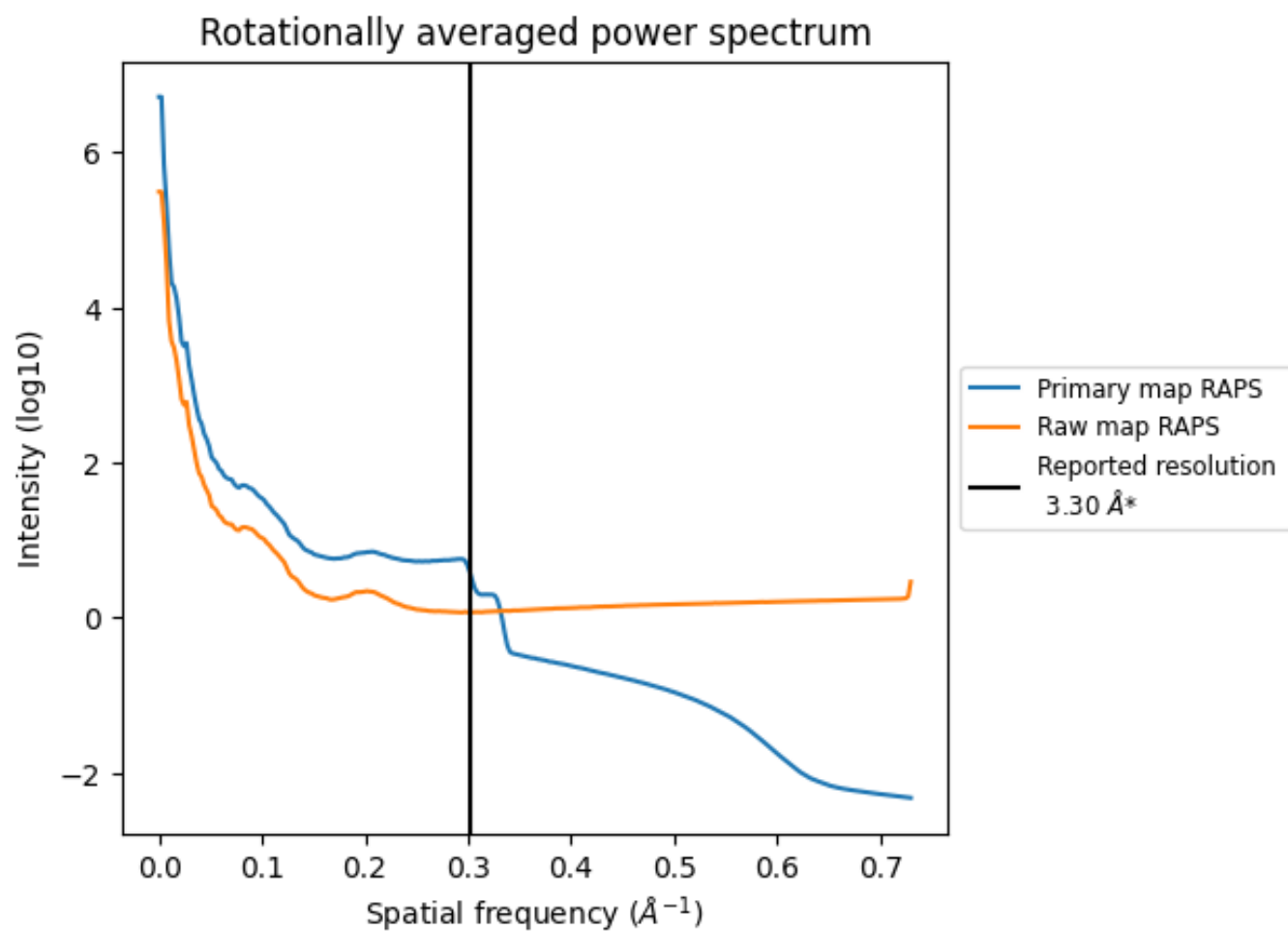
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 709 nm³; this corresponds to an approximate mass of 641 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 ⓘ

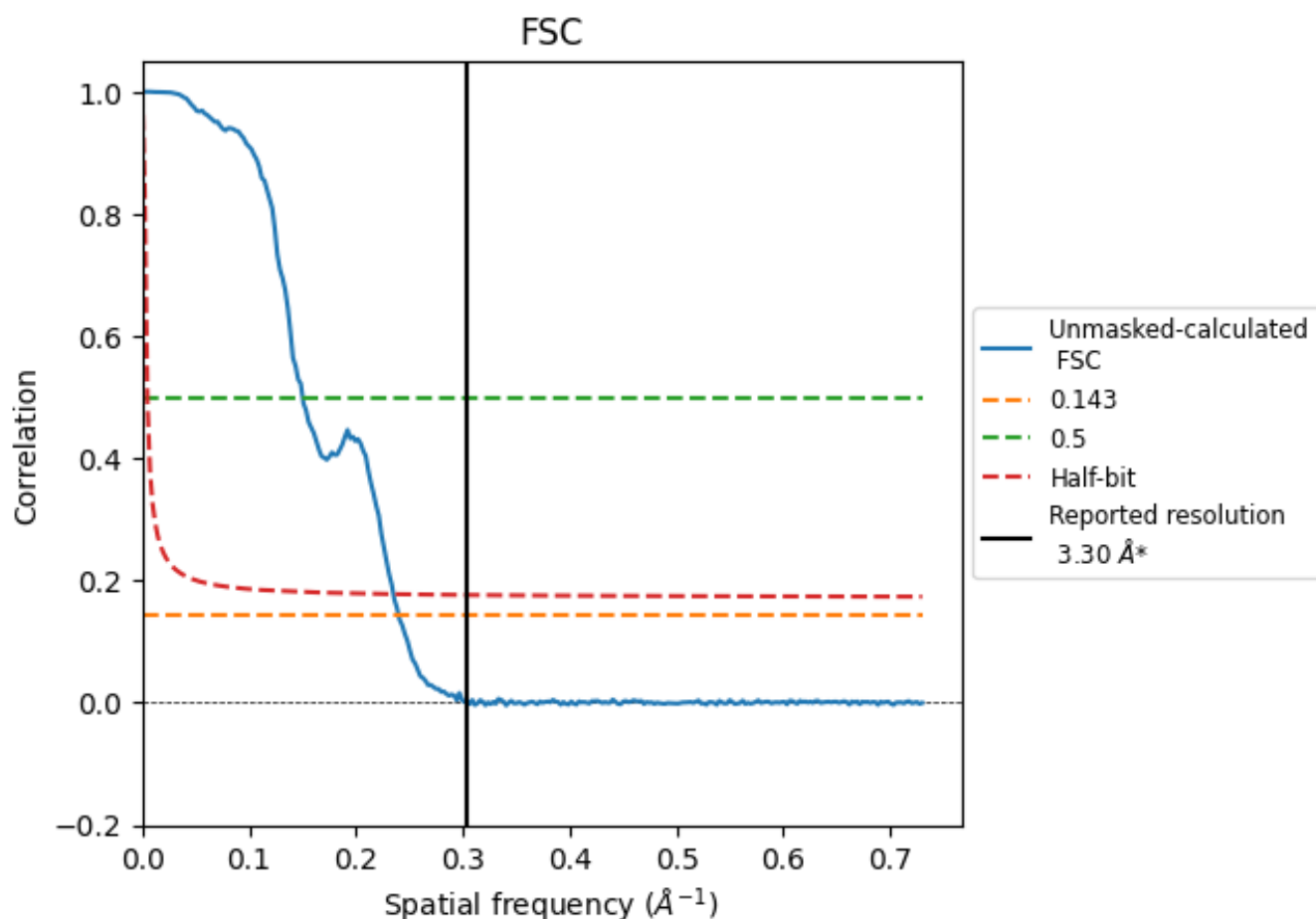


*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

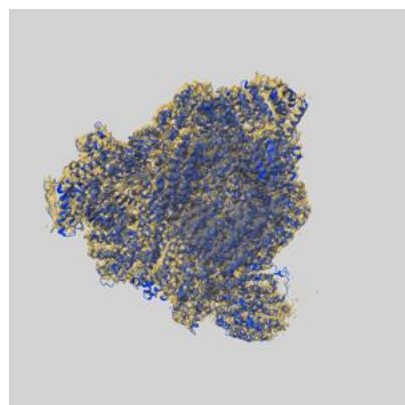
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.17	6.66	4.25

*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 4.17 differs from the reported value 3.3 by more than 10 %

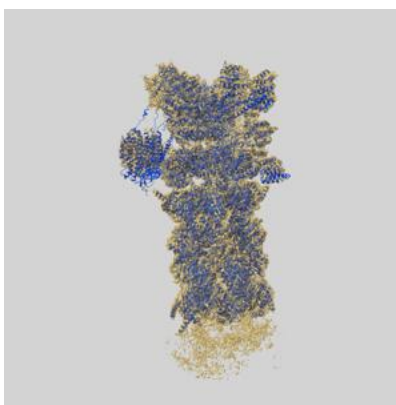
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62075 and PDB model 9K4Z. Per-residue inclusion information can be found in section [3](#) on page [13](#).

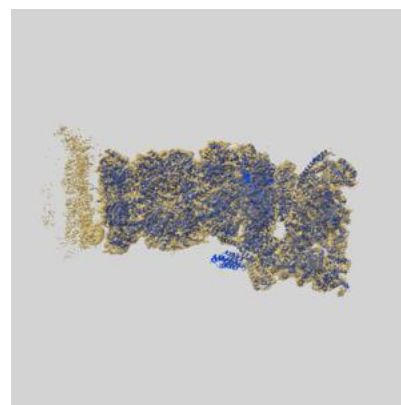
9.1 Map-model overlay [i](#)



X



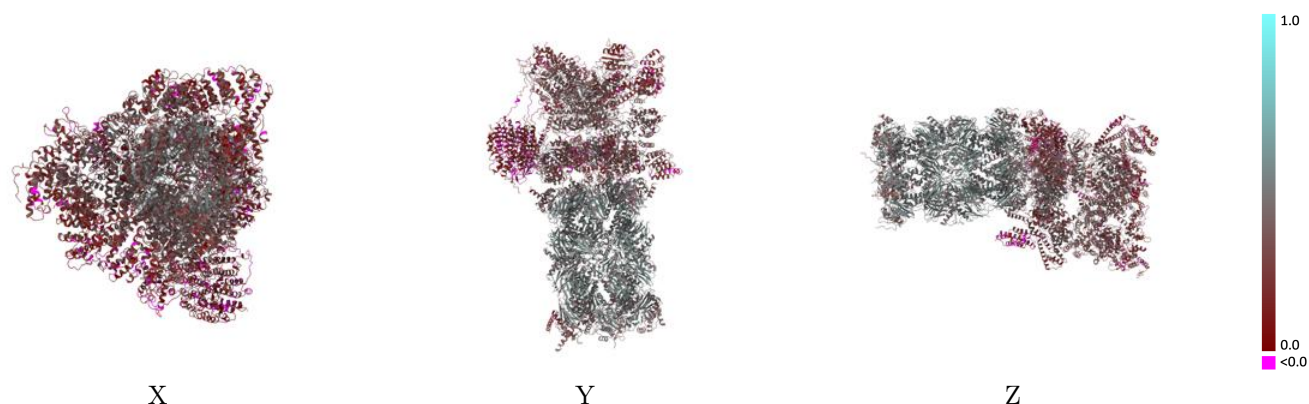
Y



Z

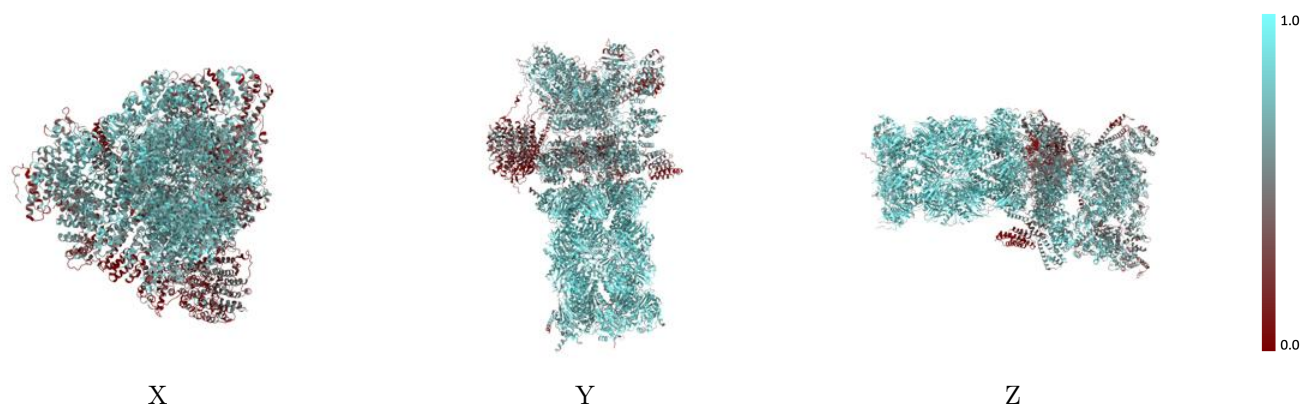
The images above show the 3D surface view of the map at the recommended contour level 0.00588 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



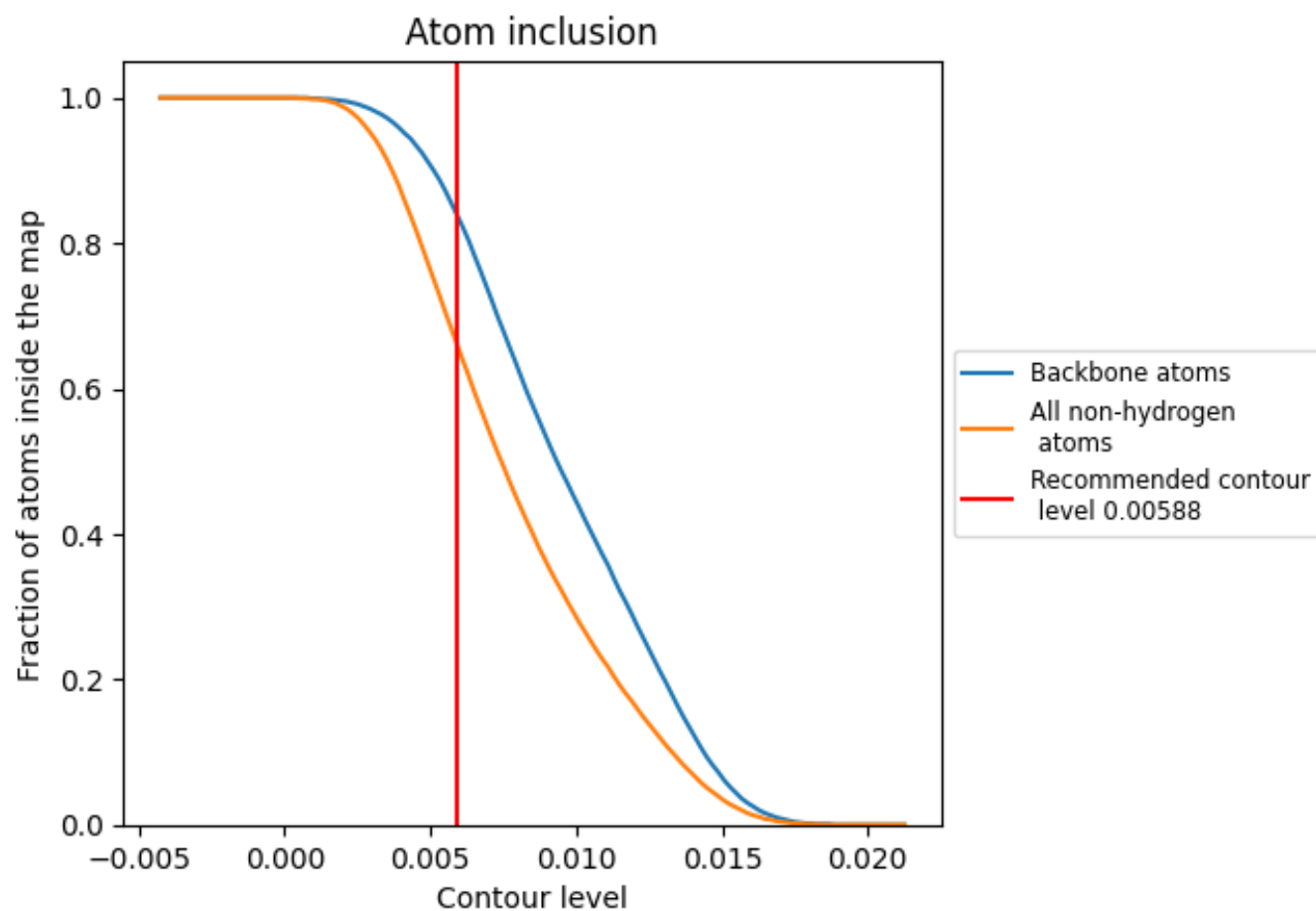
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00588).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 66% 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 (0.00588) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6640	 0.3610
A	 0.4460	 0.2480
B	 0.5460	 0.3270
C	 0.6780	 0.3640
D	 0.6950	 0.3830
E	 0.6030	 0.3290
F	 0.4140	 0.2250
G	 0.8210	 0.4650
H	 0.8210	 0.4700
I	 0.7970	 0.4560
J	 0.7720	 0.4360
K	 0.7660	 0.4560
L	 0.8290	 0.4720
M	 0.8120	 0.4660
N	 0.8550	 0.4990
O	 0.8690	 0.4930
P	 0.8750	 0.5010
Q	 0.8570	 0.4870
R	 0.8690	 0.4930
S	 0.8430	 0.4840
T	 0.8630	 0.5020
U	 0.6030	 0.2540
V	 0.5810	 0.2700
W	 0.5410	 0.2730
X	 0.4750	 0.2510
Y	 0.7210	 0.2970
Z	 0.6520	 0.3260
a	 0.6190	 0.2560
b	 0.5340	 0.2580
c	 0.6700	 0.3400
d	 0.4460	 0.2290
e	 0.5490	 0.2900
f	 0.1980	 0.1370
g	 0.7870	 0.4500
h	 0.7890	 0.4530



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Chain	Atom inclusion	Q-score
i	 0.7420	 0.4340
j	 0.7050	 0.3870
k	 0.7360	 0.4390
l	 0.8200	 0.4650
m	 0.8110	 0.4520
n	 0.8620	 0.4900
o	 0.8490	 0.4850
p	 0.8580	 0.4860
q	 0.8560	 0.4840
r	 0.8630	 0.4930
s	 0.8360	 0.4830
t	 0.8760	 0.4910
v	 0.2330	 0.3070