



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:29 AM UTC

PDB ID : 6MSH / pdb_00006msh
EMDB ID : EMD-9220
Title : Cryo-EM structures and dynamics of substrate-engaged human 26S proteasome
Authors : Mao, Y.D.
Deposited on : 2018-10-16
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

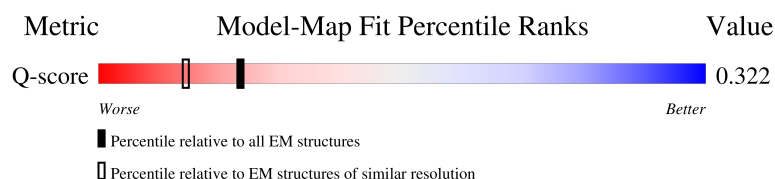
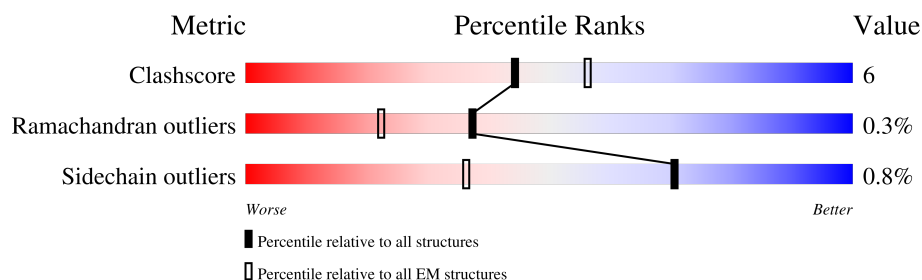
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.60 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	12797 (3.10 - 4.10)

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	U	953	64% 72% 14% 14%
2	V	533	75% 76% 14% 10%
3	W	456	71% 76% 22% .
4	X	422	17% 81% 9% 10%

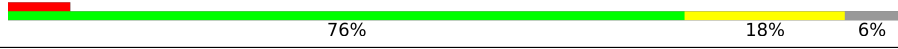
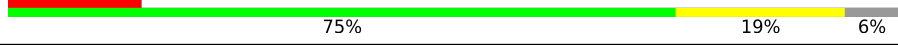
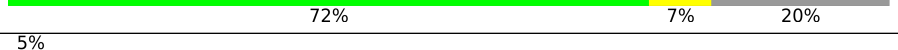
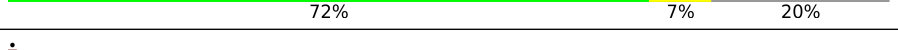
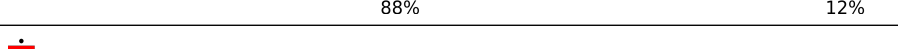
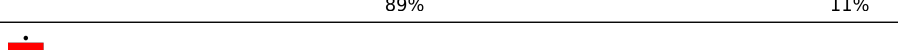
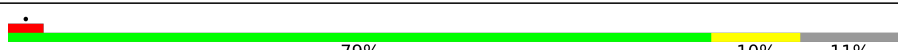
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Mol	Chain	Length	Quality of chain
5	Y	389	
6	Z	324	
7	a	376	
8	b	377	
9	c	309	
10	d	349	
11	e	70	
12	f	892	
13	A	433	
14	B	440	
15	C	398	
16	D	418	
17	E	403	
18	F	439	
19	v	22	
20	G	245	
20	g	245	
21	H	233	
21	h	233	
22	I	260	
22	i	260	
23	J	247	
23	j	247	
24	K	240	
24	k	240	

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Mol	Chain	Length	Quality of chain
25	L	268	
25	l	268	
26	M	254	
26	m	254	
27	N	238	
27	n	238	
28	O	276	
28	o	276	
29	P	204	
29	p	204	
30	Q	201	
30	q	201	
31	R	262	
31	r	262	
32	S	240	
32	s	240	
33	T	263	
33	t	263	

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 103729 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 non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	820	Total	C	N	O	S	0	0
			6398	4062	1086	1206	44		

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	480	Total	C	N	O	S	0	0
			3852	2444	684	710	14		

- Molecule 3 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	456	Total	C	N	O	S	0	0
			3703	2339	635	704	25		

- Molecule 4 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	380	Total	C	N	O	S	0	0
			3009	1918	509	570	12		

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	378	Total	C	N	O	S	0	0
			3115	1987	533	578	17		

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

- Molecule 11 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	e	40	Total	C	N	O	S	0	0
			334	200	55	77	2		

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	f	886	Total	C	N	O	S	0	0
			6840	4300	1171	1324	45		

- Molecule 13 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	356	Total	C	N	O	S	0	0
			2767	1741	488	521	17		

- Molecule 14 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	350	Total	C	N	O	S	0	0
			2706	1703	458	533	12		

- Molecule 15 is a protein called 26S proteasome regulatory subunit 8.

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

- Molecule 16 is a protein called 26S proteasome regulatory subunit 6B.

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

- Molecule 17 is a protein called 26S proteasome regulatory subunit 10B.

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

- Molecule 18 is a protein called 26S proteasome regulatory subunit 6A.

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

- Molecule 19 is a protein called substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	v	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 20 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	G	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		
20	g	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

- Molecule 21 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	H	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		
21	h	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

- Molecule 22 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	I	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		
22	i	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 23 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	J	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		
23	j	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

- Molecule 24 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	K	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		
24	k	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

- Molecule 25 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	L	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		
25	l	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

- Molecule 26 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	m	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

- Molecule 27 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	N	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		
27	n	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		

- Molecule 28 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	O	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		
28	o	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		

- Molecule 29 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	P	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		
29	p	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		

- Molecule 30 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		
30	q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

- Molecule 31 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	R	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		
31	r	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

- Molecule 32 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	S	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		
32	s	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		

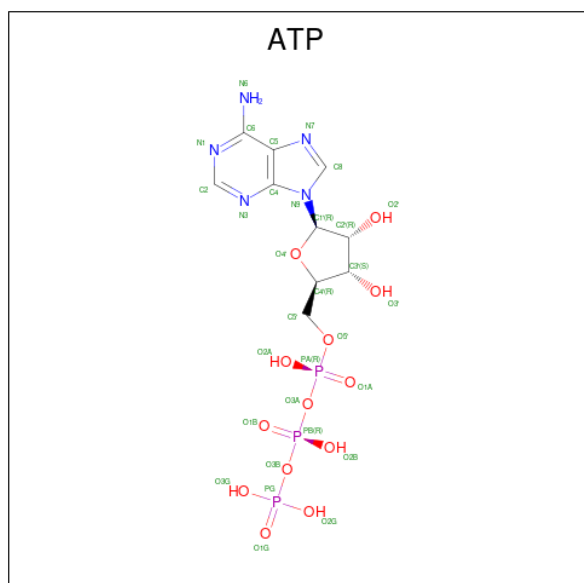
- Molecule 33 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		
33	t	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		

- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

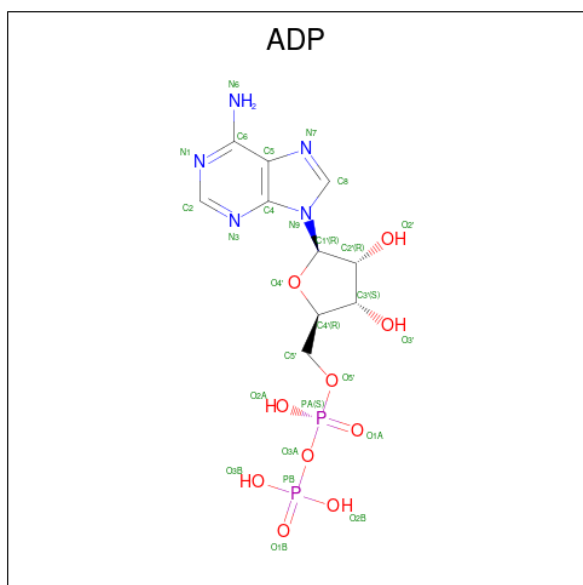
- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

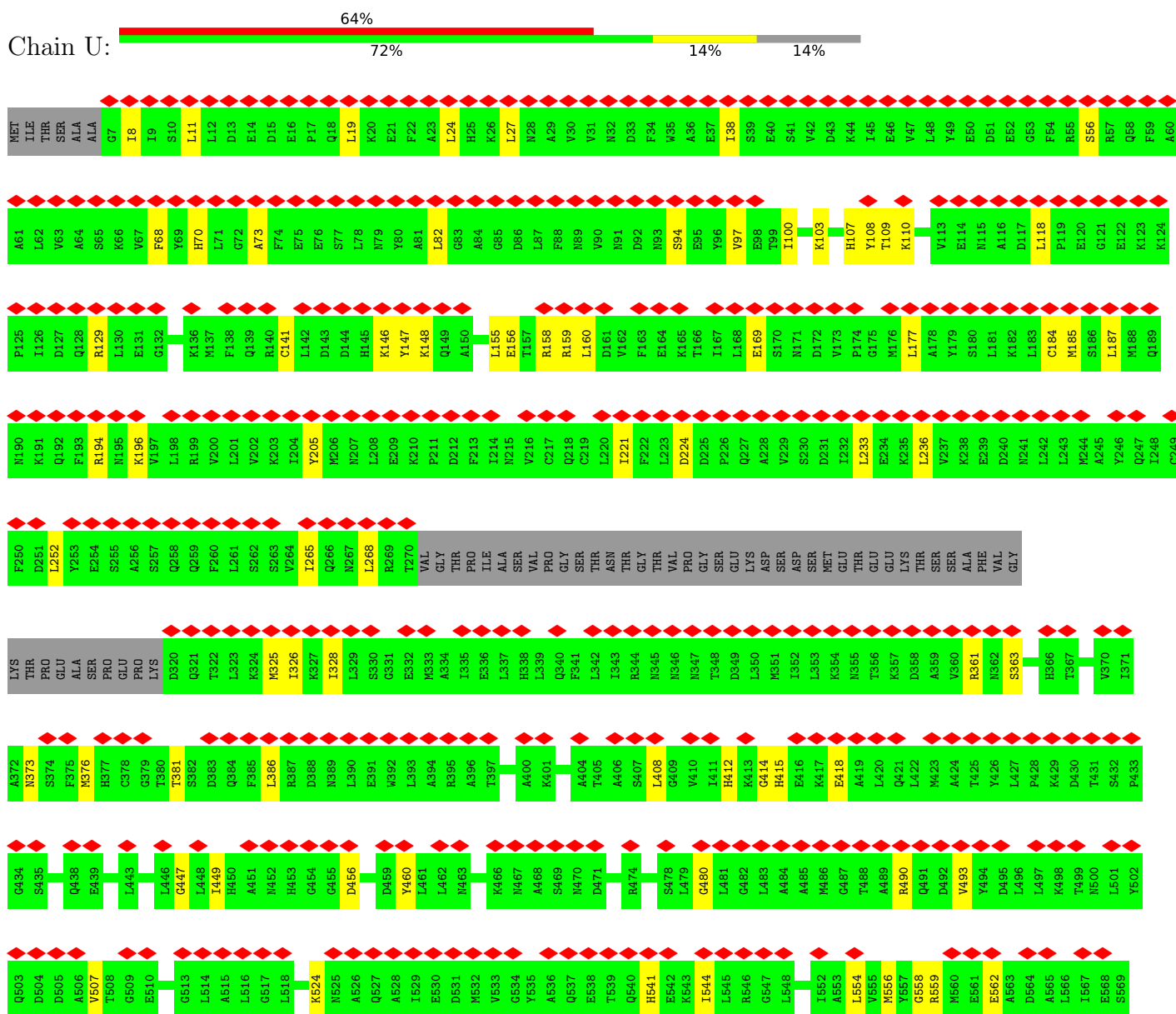


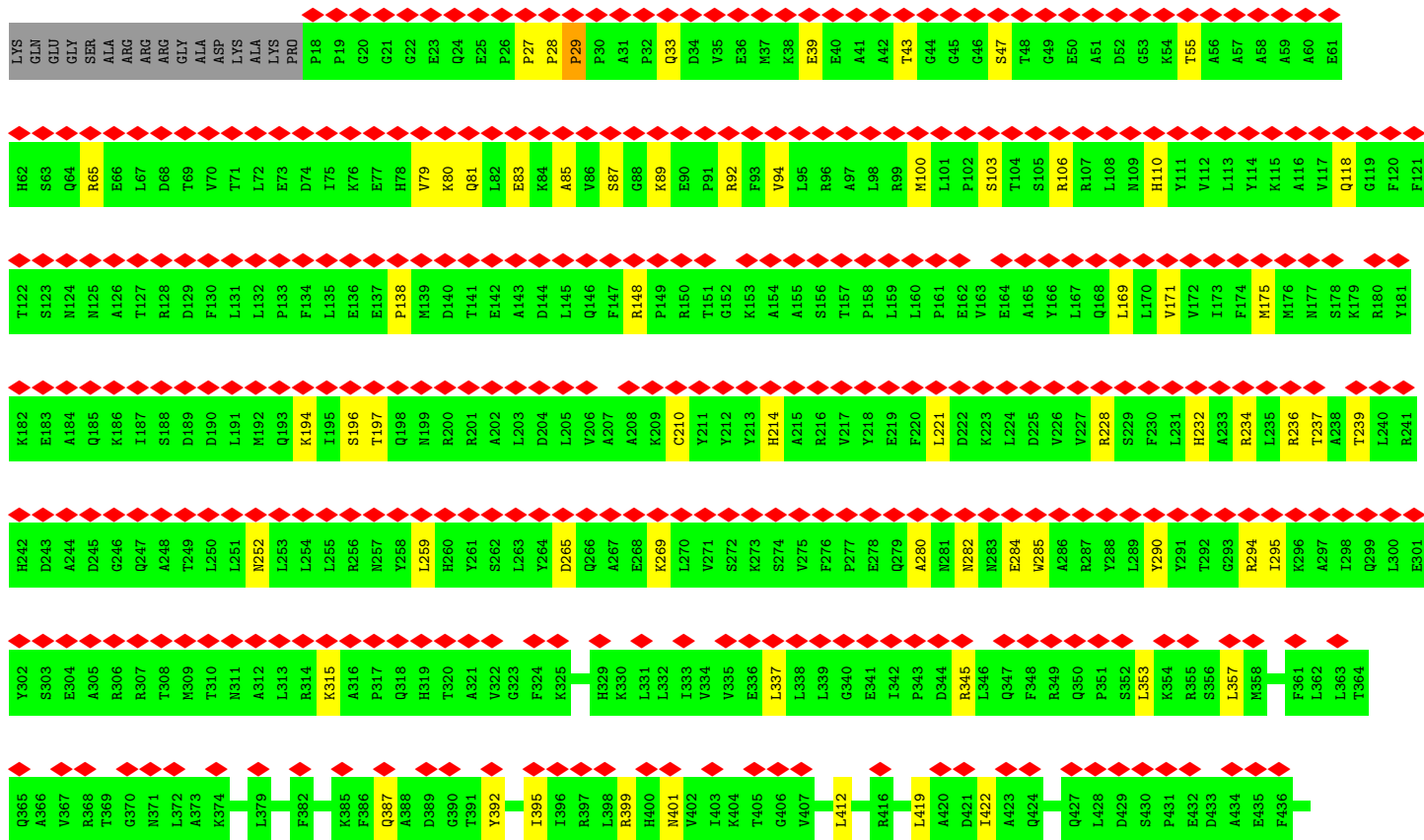
Mol	Chain	Residues	Atoms					AltConf
36	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots

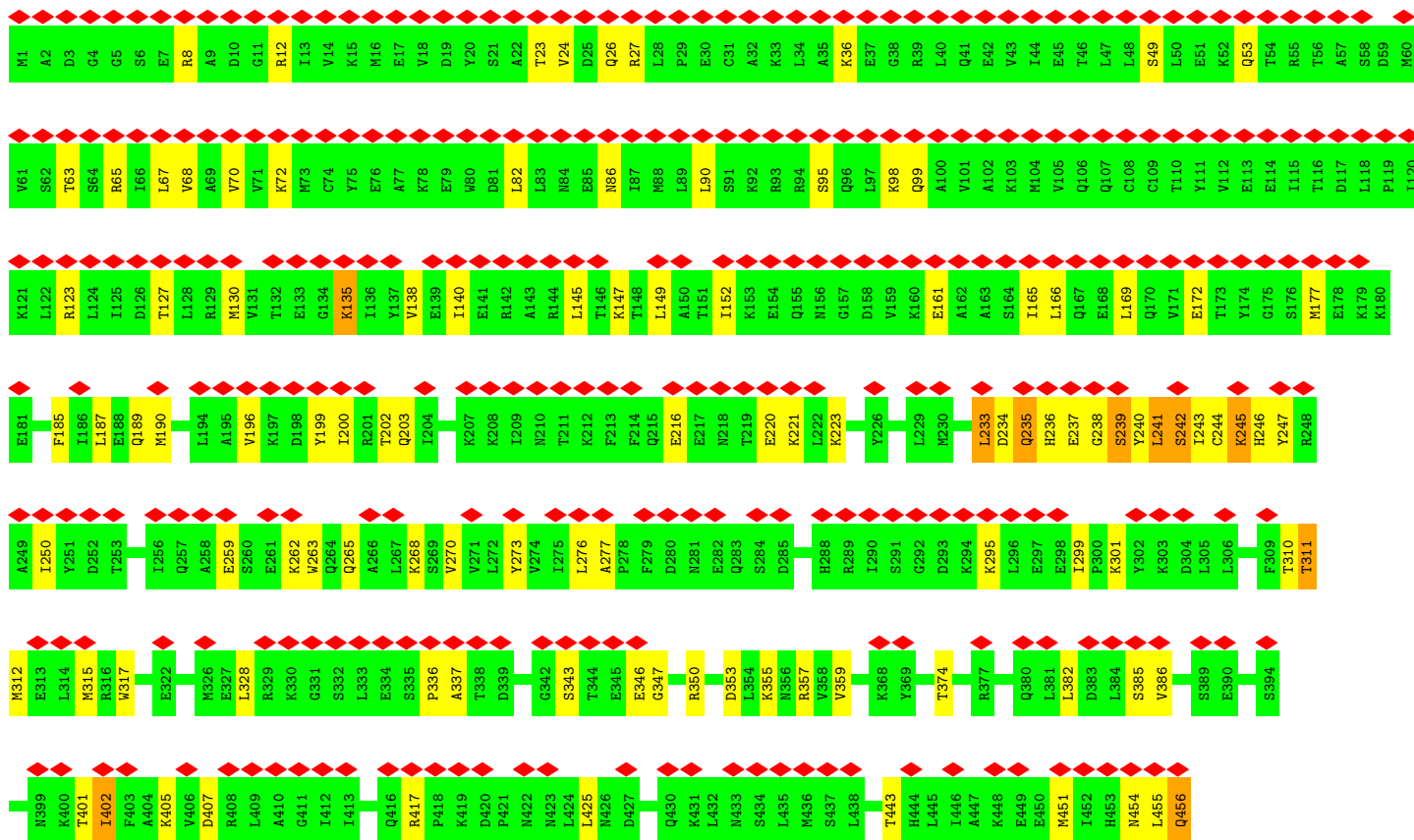
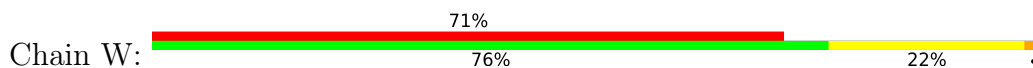
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 non-ATPase regulatory subunit 1

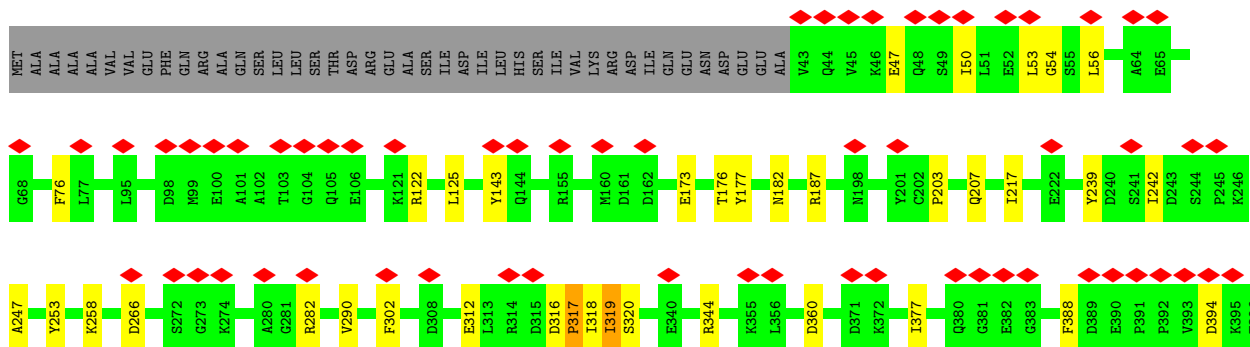
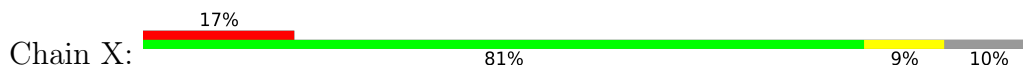


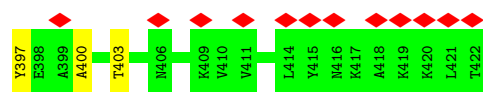


- Molecule 3: 26S proteasome non-ATPase regulatory subunit 12

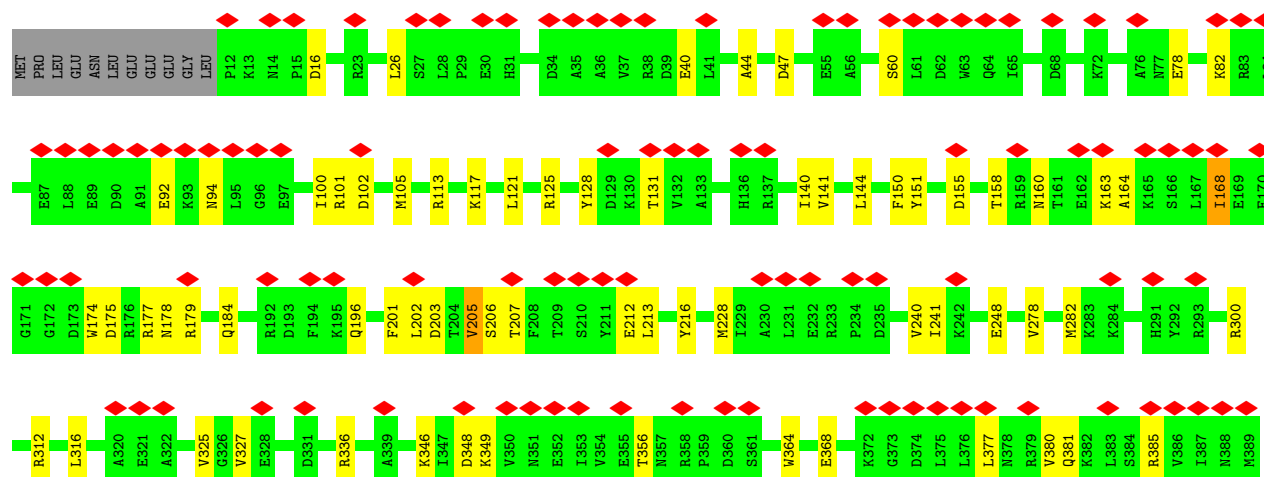
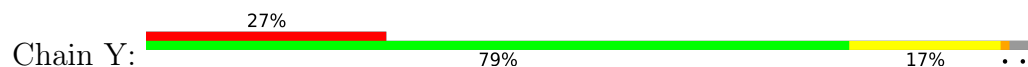


- Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

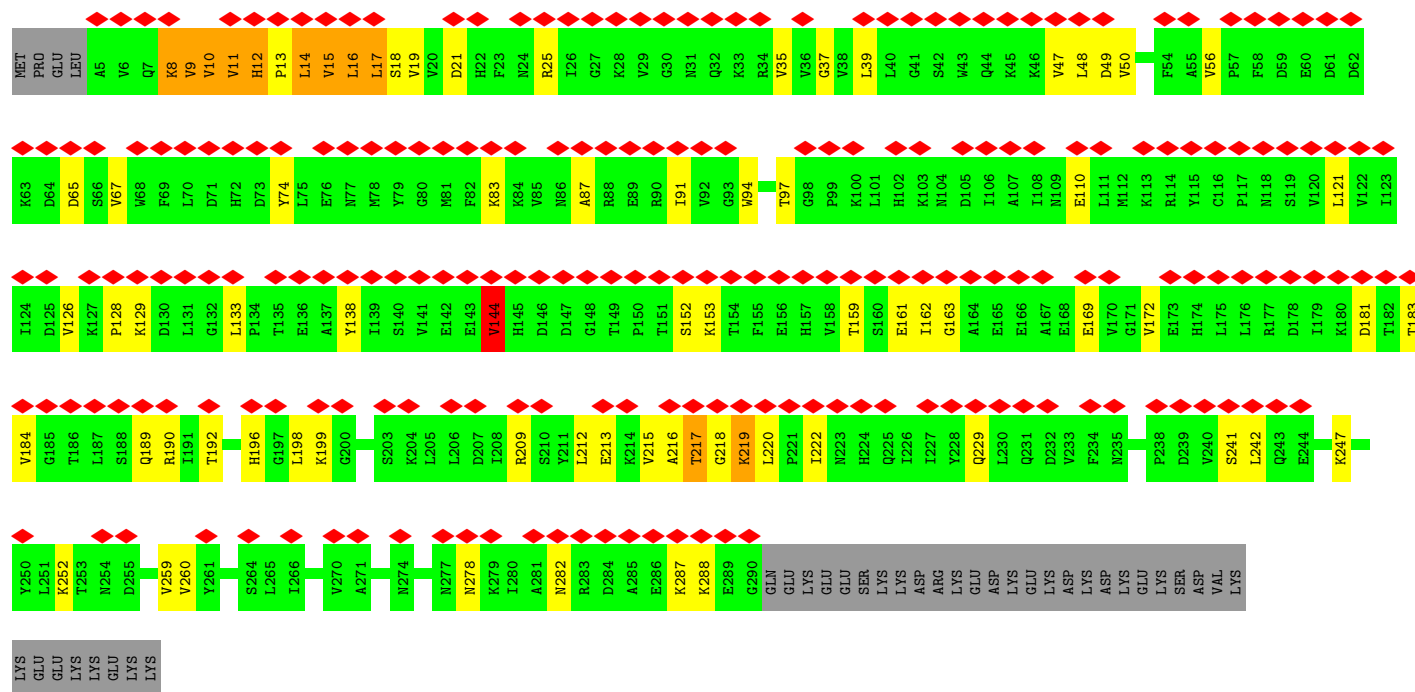




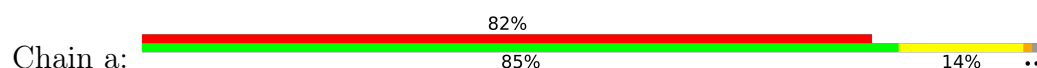
- Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

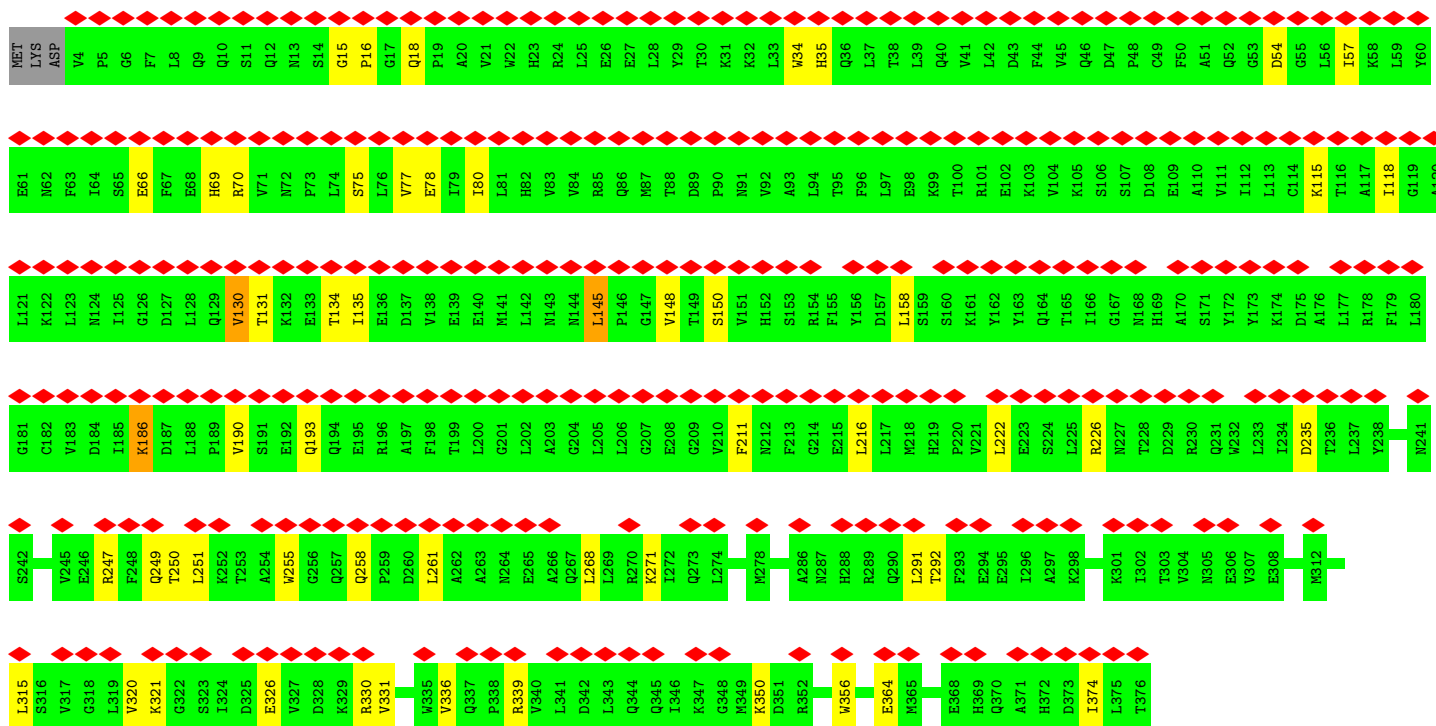


- Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

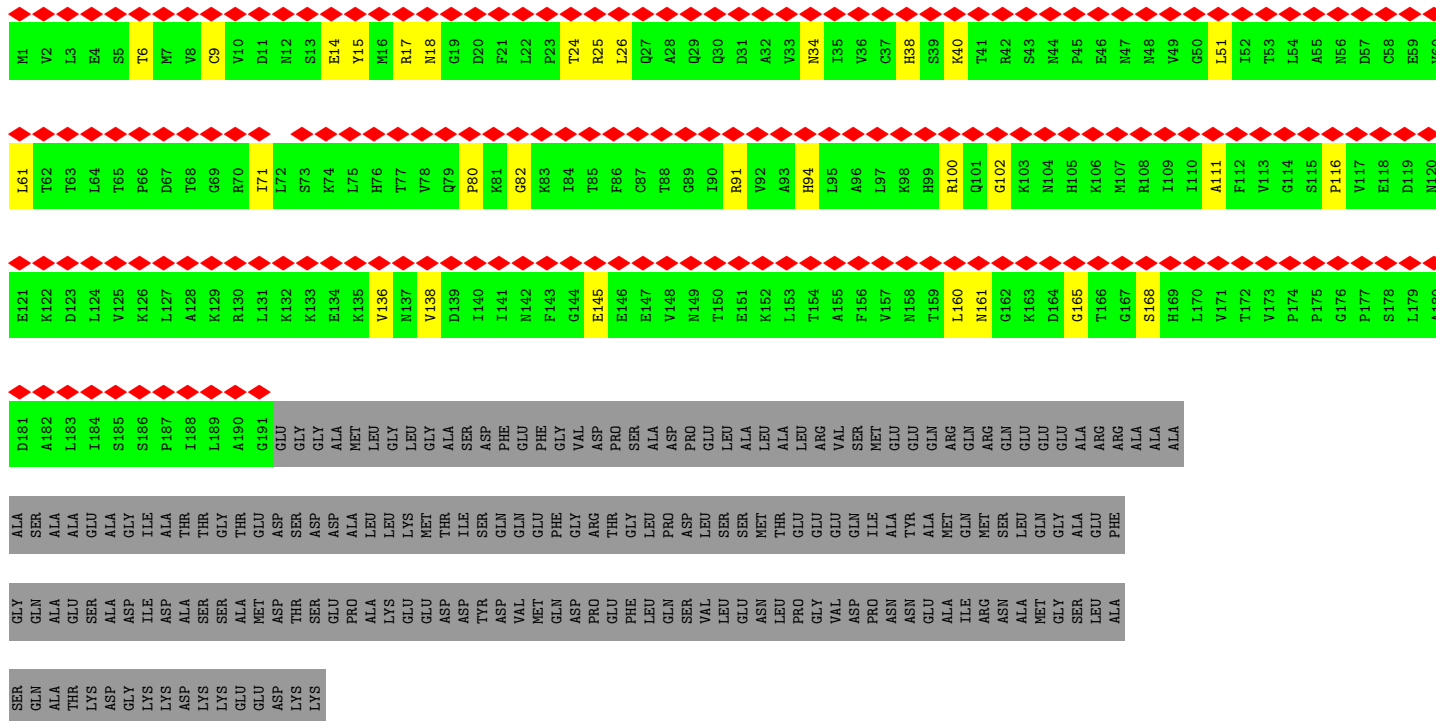
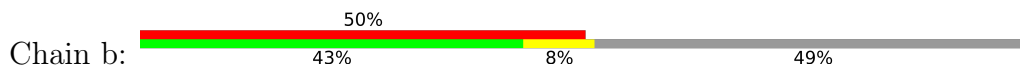


- Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

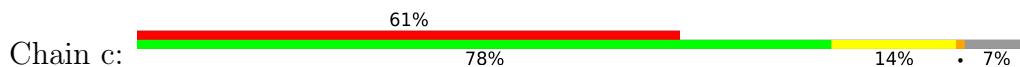


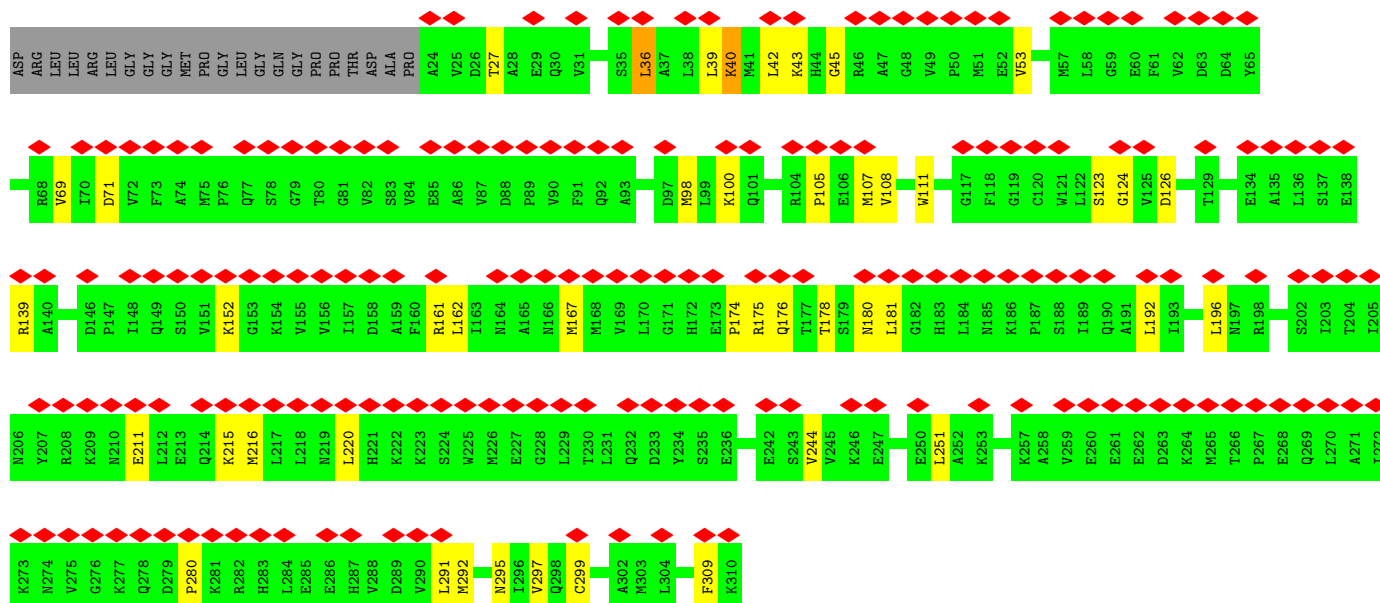


• Molecule 8: 26S proteasome non-ATPase regulatory subunit 4

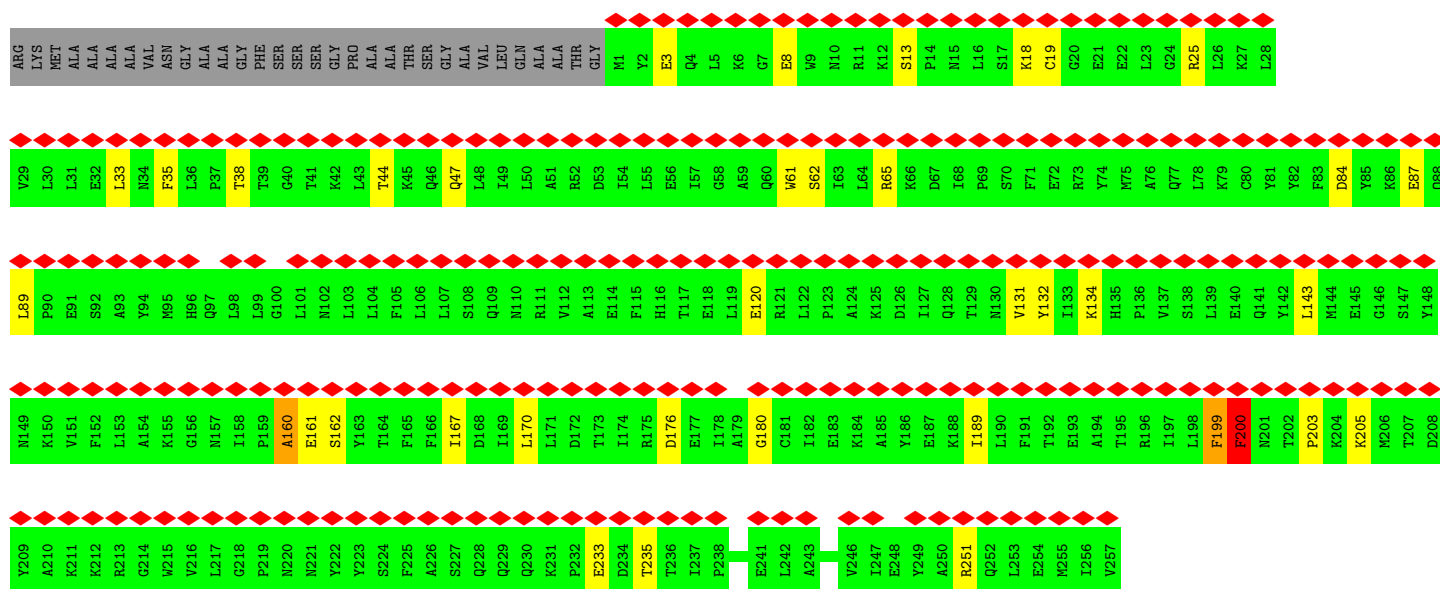


• Molecule 9: 26S proteasome non-ATPase regulatory subunit 14

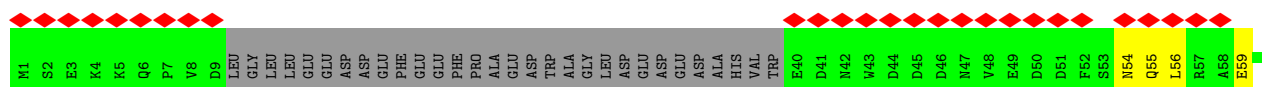
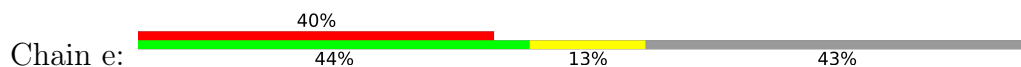




• Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

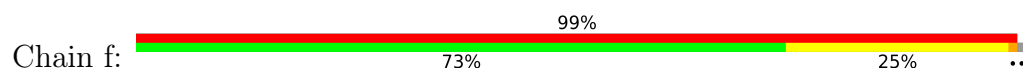


• Molecule 11: 26S proteasome complex subunit SEM1

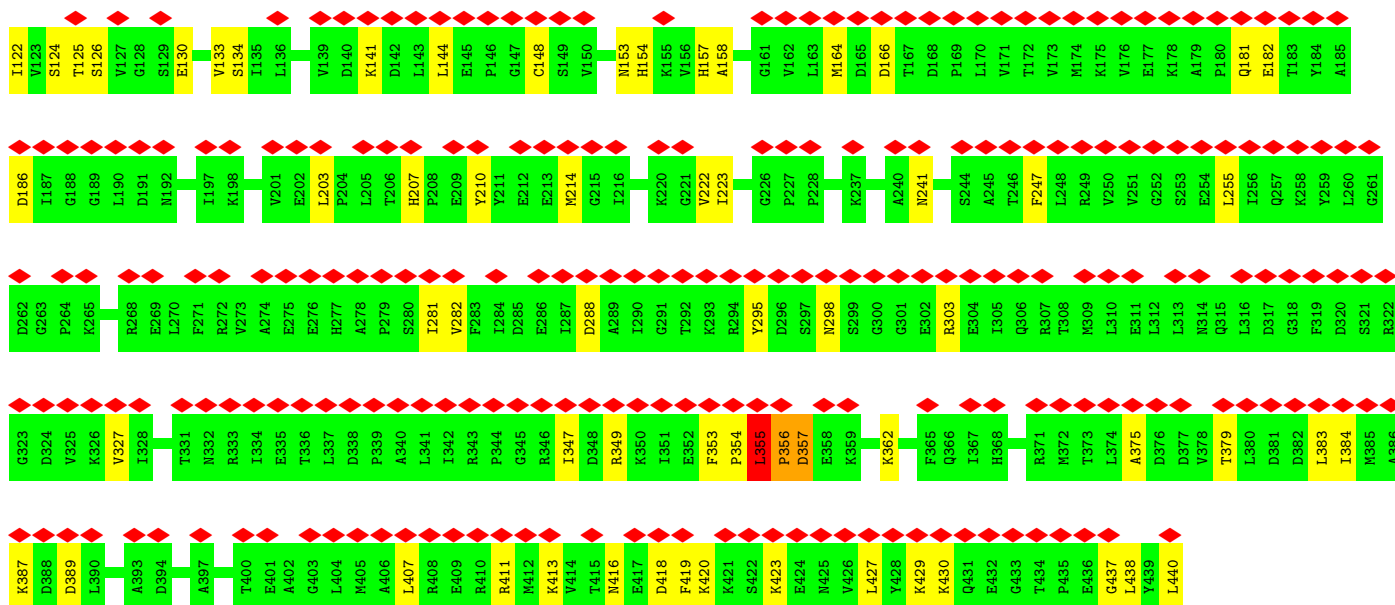




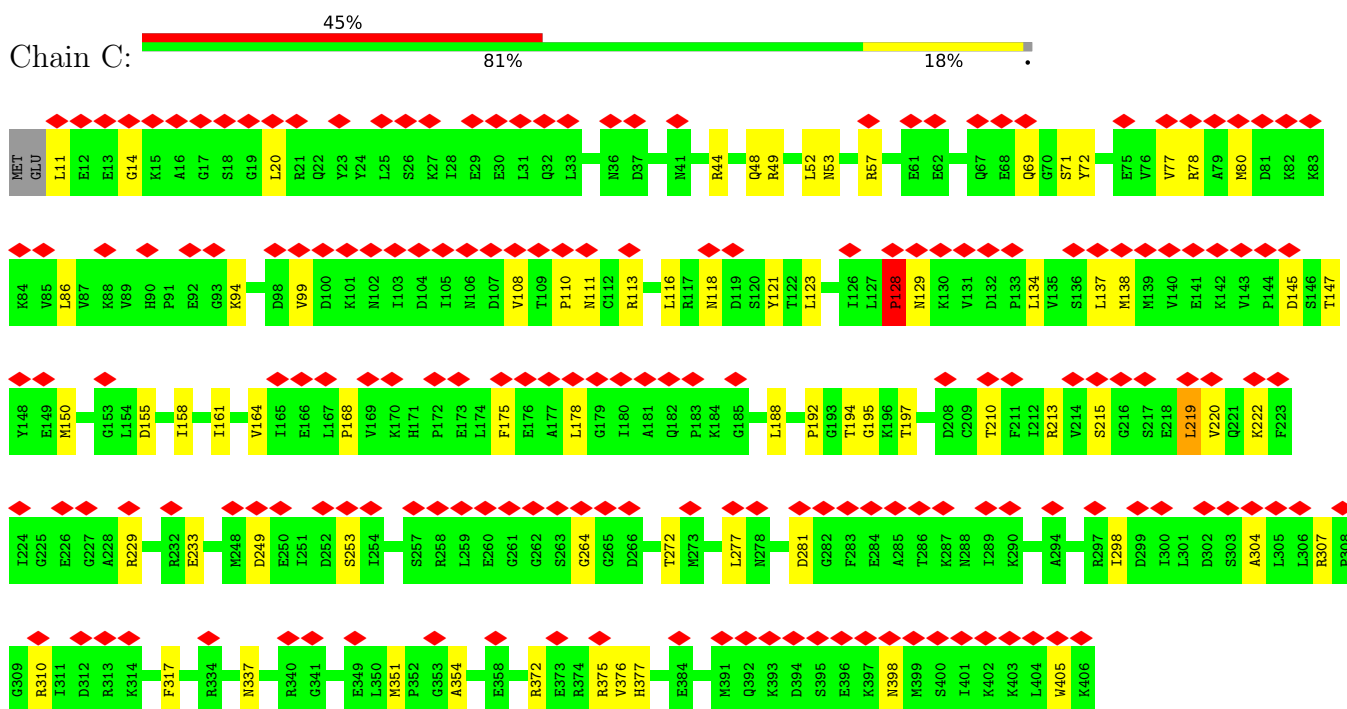
• Molecule 12: 26S proteasome non-ATPase regulatory subunit 2



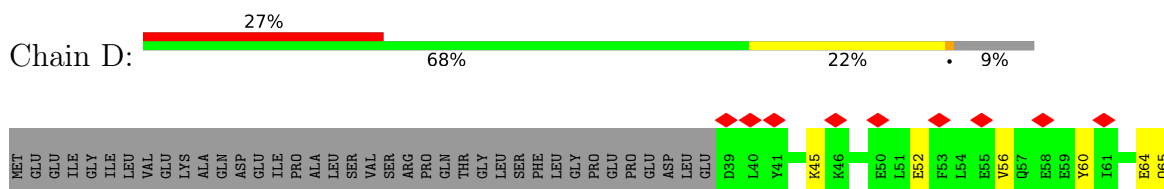
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E61	R62	L63	G64	E65	R66	D67	T68	A69	P70
V71	Q72	P73	Q74	L75	E76	E77	L78	R79	R80
Q81	G82	G83	S84	S85	T86	T87	S88	M89	E90
E91	S92	P93	K94	P95	L96	K97	F98	L99	R100
E101	H102	Y103	G104	K105	L106	K107	E108	I109	Y110
E111	N112	M113	A114	P115	G116	E117	N118	K119	R120
F121	A122	A123	I124	I125	I126	S127	V128	L129	A130
M131	T132	M133	A134	G135	E136	R137	E138	C139	L140
K141	Y142	R143	L144	V145	G146	S147	Q148	E149	E150
L151	E152	S153	V154	G155	H156	E157	Y158	V159	R160
H161	L162	A163	G164	E165	V166	A167	K168	E169	Y170
E171	N172	M173	D174	D175	A176	E177	N178	K179	R180
R181	E182	P183	L184	L185	T186	L187	V188	E189	E190
I191	V192	P193	Y194	N195	M196	A197	H198	N199	A200
E201	H202	E203	A204	C205	D206	L207	L208	M209	E210
I211	E212	Q213	V214	D215	M216	L217	E218	K219	D220
I221	D222	E223	N224	A225	V226	A227	K228	V229	C230
L231	Y232	L233	T234	S235	C236	V237	L238	Y239	V240
P241	E242	P243	E244	N245	S246	A247	L248	L249	R250
C251	A252	L253	G254	V255	P256	R257	K258	F259	S260
R261	P262	P263	E264	A265	L266	E267	L268	A269	L270
E271	L272	N273	D274	M275	E276	L277	V278	E279	D280
I281	P282	T283	S284	C285	K286	D287	V288	V289	V290
Q291	K292	Q293	M294	A295	P296	M297	L298	Q299	R300
H301	G302	V303	F304	L305	E306	L307	S308	E309	D310
V311	E312	E313	Y314	E315	D316	L317	T318	E319	I320
H321	S322	N323	V324	Q325	L326	N327	S328	N329	F330
L331	A332	L333	A334	R335	E336	L337	D338	I339	K340
E341	P342	K343	V344	P345	D346	D347	L348	S349	A350
A351	H352	L353	E354	N355	N356	R357	F358	G359	C360
S361	G362	S363	Q364	V365	D366	S367	A368	R369	I370
H371	L372	A373	S374	S375	F376	V377	N378	G379	F380
V381	N382	A383	A384	F385	G386	Q387	D388	K389	L390
F391	T392	D393	D394	G395	N396	K397	L398	L399	Y400
K401	A402	L403	D404	H405	C406	M407	L408	S409	A410
A411	A412	S413	L414	G415	M416	L417	L418	L419	W420
D421	V422	D423	G424	G425	L426	T427	Q428	I429	D430
K431	Y432	L433	Y434	S435	S436	E437	L438	Y439	L440
K441	S442	G443	A444	L445	L446	A447	D448	Y449	L450
L501	L502	P503	V504	M505	G506	D507	S508	K509	S510
S511	S512	M513	V514	A515	G516	V517	T518	A519	L520
A521	C522	G523	M524	I525	A526	V527	G528	S529	C530
N531	G532	D533	V534	T535	S536	T537	F538	S539	A540
H471	H472	M473	S474	N475	T476	M477	R478	L479	G480
T541	F542	M543	F544	K545	G546	E547	T548	E549	L550
K551	D552	T553	R554	A555	R556	W557	L558	P559	L560
G561	L562	G563	L564	N565	H566	L567	G568	K569	D570
E571	A572	I573	E574	A575	I576	L577	D578	K579	L580
L581	A582	V583	S584	E585	P586	F587	R588	S589	F590
A591	N592	T593	L594	V595	D596	V597	A598	L599	I600
A601	G602	S603	G604	N605	V606	L607	K608	V609	Q610
Q611	L612	L613	H614	L615	C616	S617	E618	H619	F620
D621	K623	E624	K625	E626	E627	D628	K629	D630	K631
K632	E633	K634	K635	D636	K637	D638	K639	K640	E641
A642	P643	A644	D645	M646	G647	D648	H649	Q650	G651
V652	A653	V654	L655	G656	I657	D658	L659	E660	M661
M662	G663	E664	E665	I666	G667	A668	E669	M670	Q671
A671	L672	R673	T674	F675	G676	H677	L678	L679	R680
Y681	G682	E683	P684	T685	L686	R687	R688	A689	V690
P691	L692	A693	L694	A695	L696	I697	S698	V699	S700
N701	P702	R703	L704	N705	T706	L707	D708	T709	L710
S711	K712	F713	S714	H715	D716	A717	D718	F719	E720

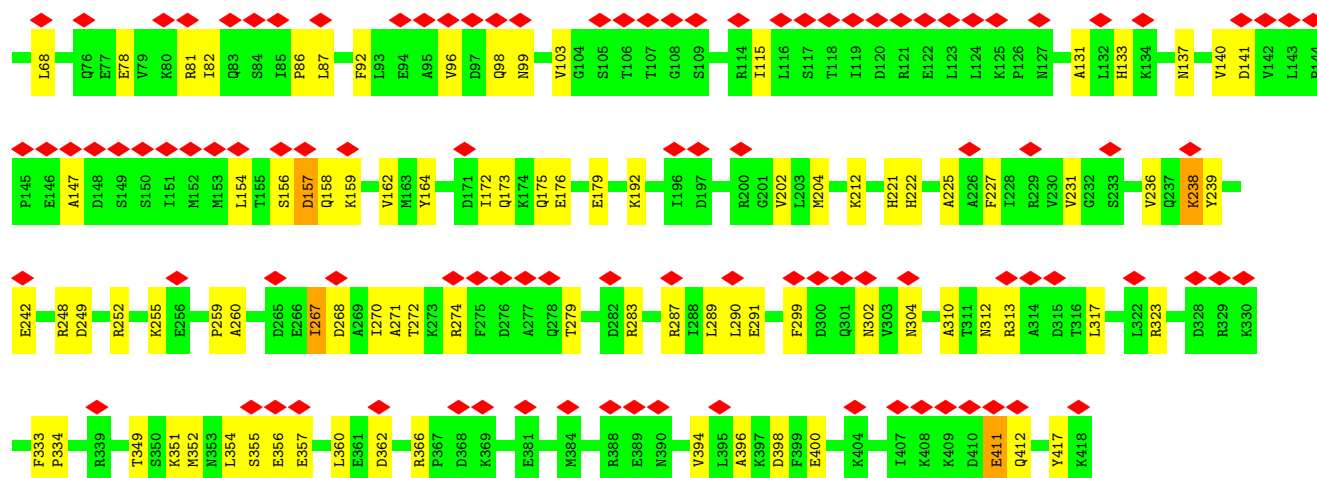


• Molecule 15: 26S proteasome regulatory subunit 8

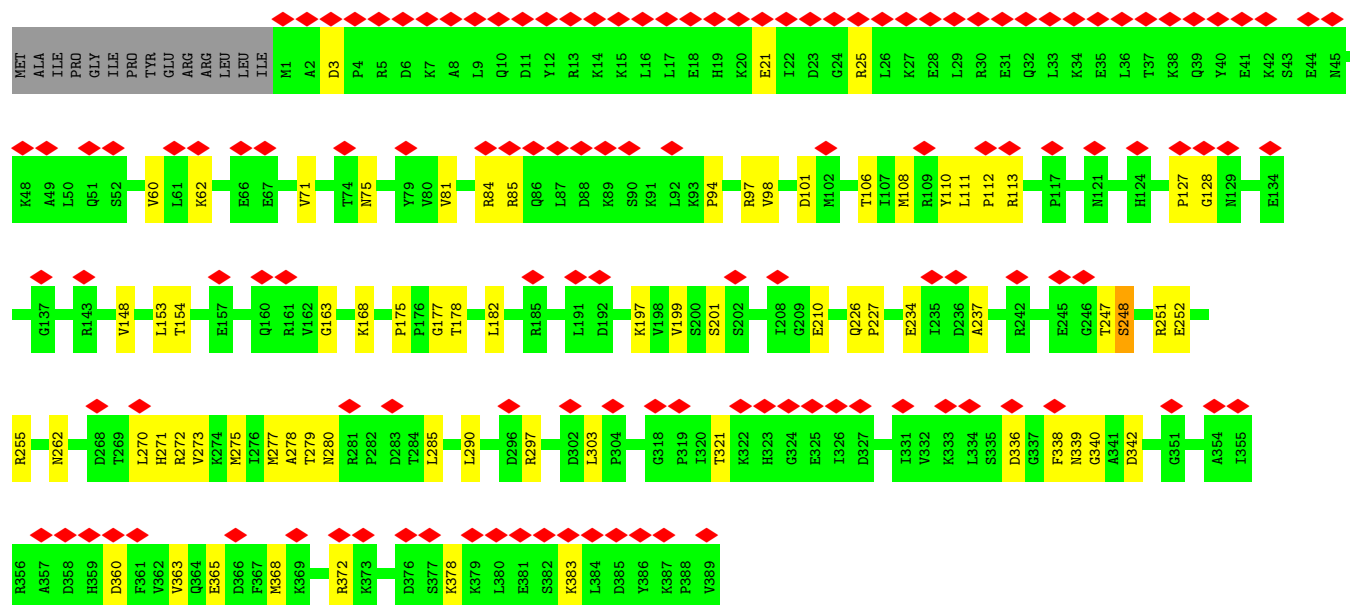
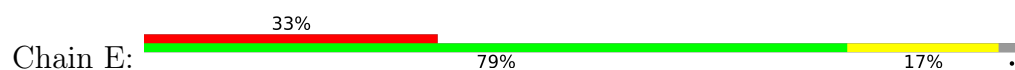


• Molecule 16: 26S proteasome regulatory subunit 6B

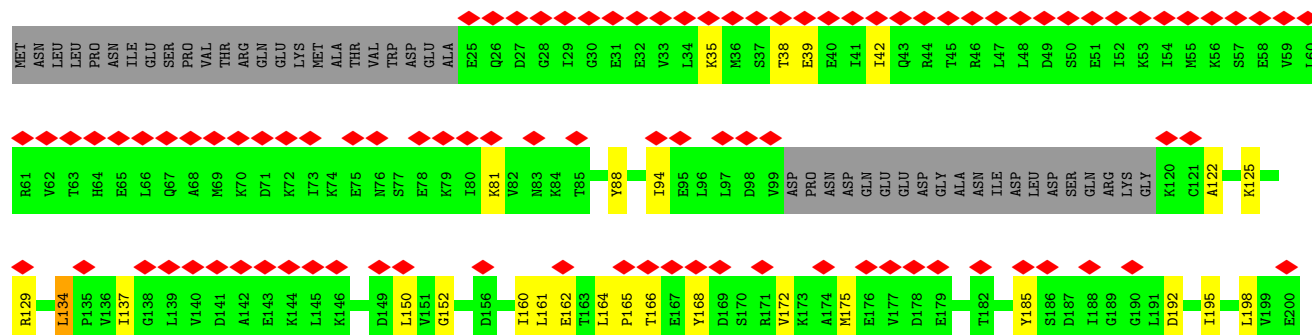


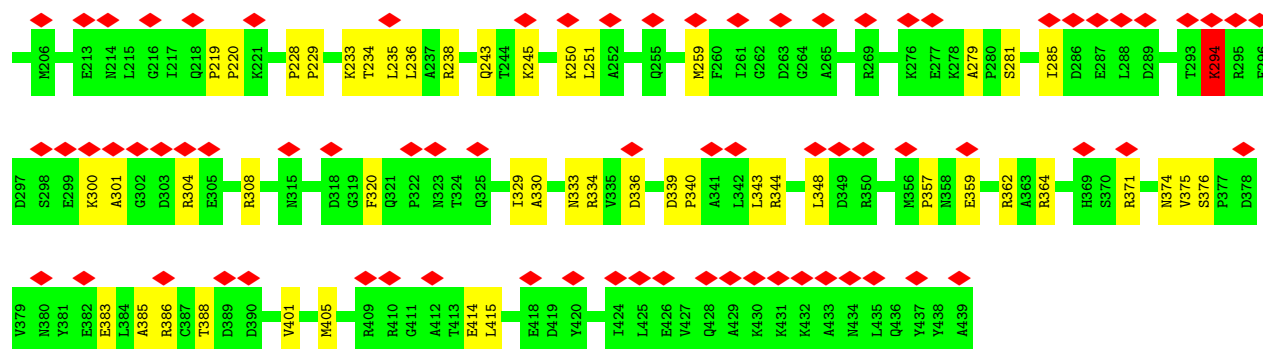


• Molecule 17: 26S proteasome regulatory subunit 10B

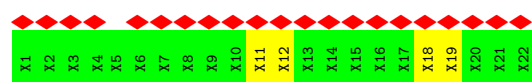
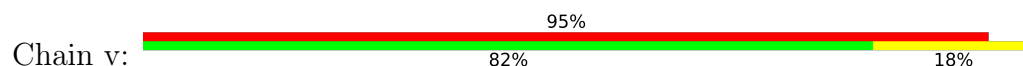


• Molecule 18: 26S proteasome regulatory subunit 6A

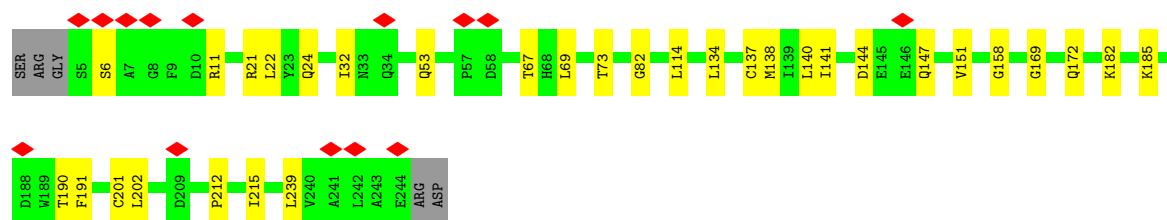
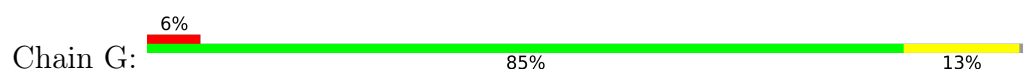




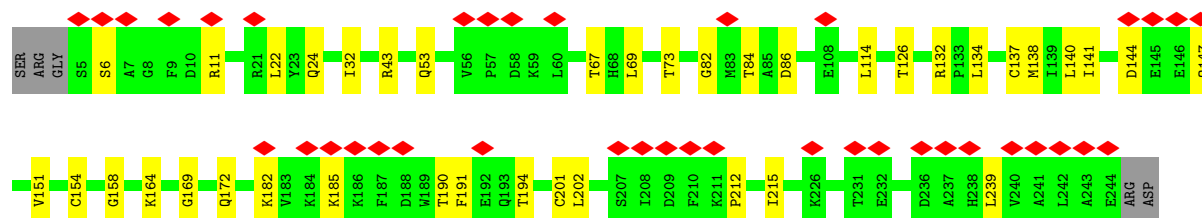
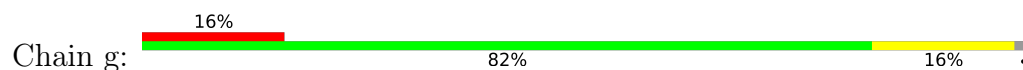
- Molecule 19: substrate



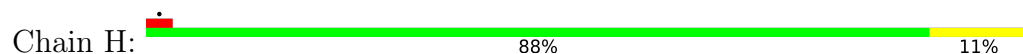
- Molecule 20: Proteasome subunit alpha type-6



- Molecule 20: Proteasome subunit alpha type-6

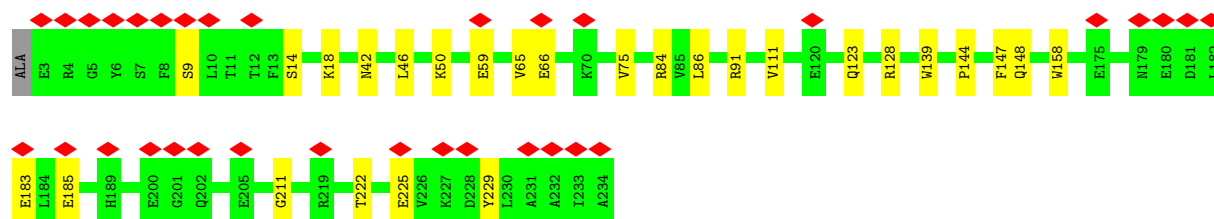
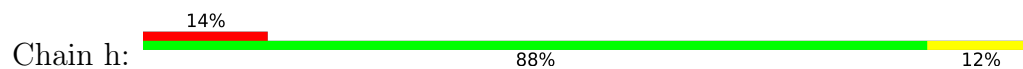


- Molecule 21: Proteasome subunit alpha type-2

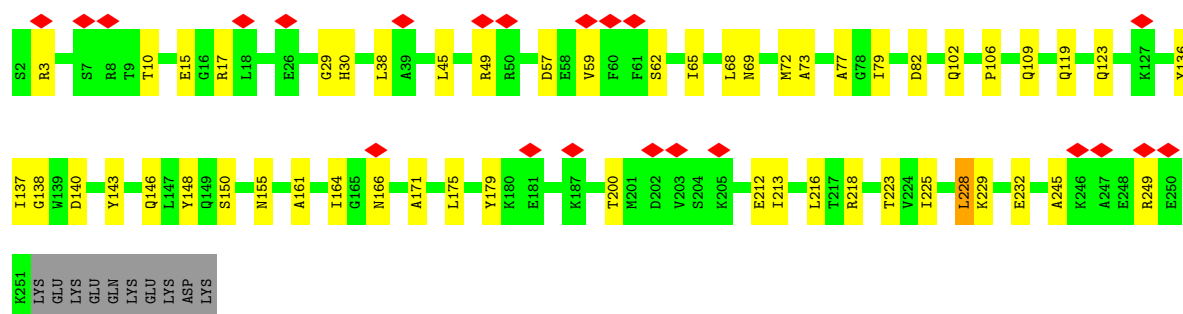
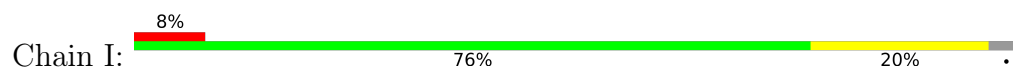




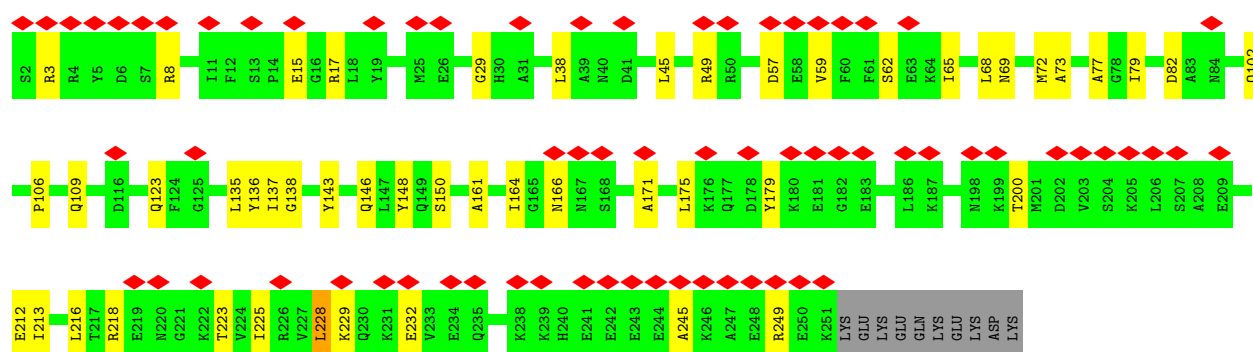
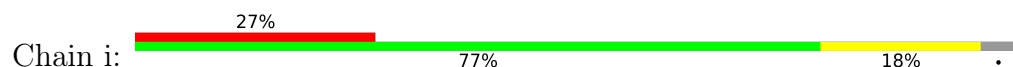
• Molecule 21: Proteasome subunit alpha type-2



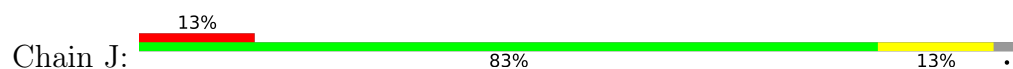
• Molecule 22: Proteasome subunit alpha type-4

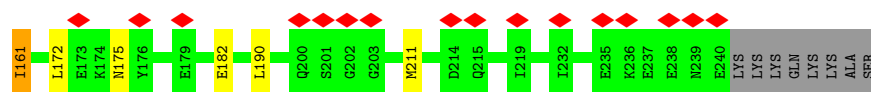


• Molecule 22: Proteasome subunit alpha type-4

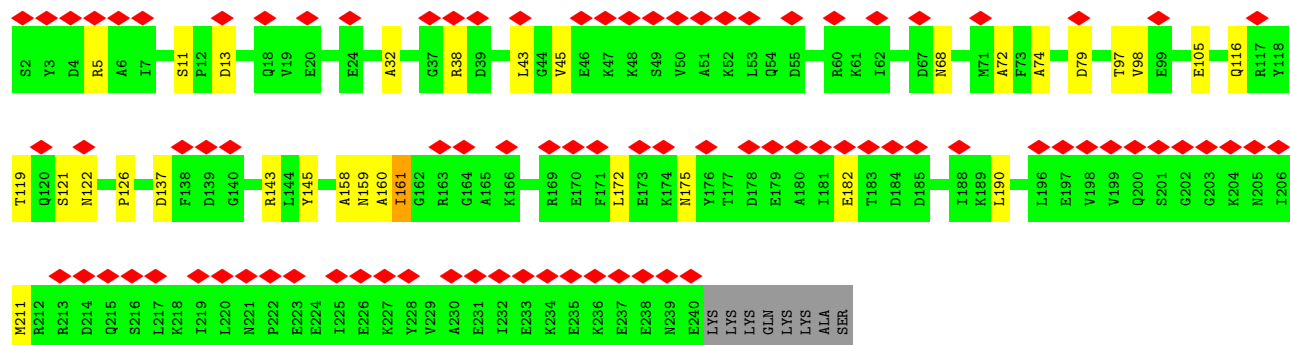
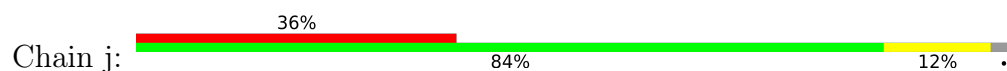


• Molecule 23: Proteasome subunit alpha type-7

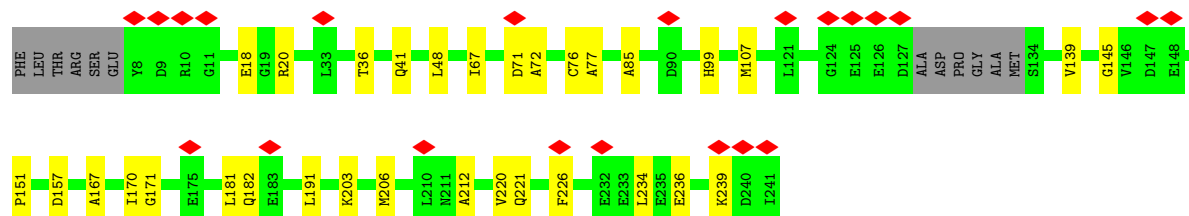
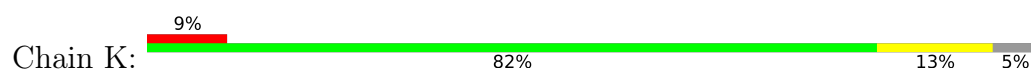




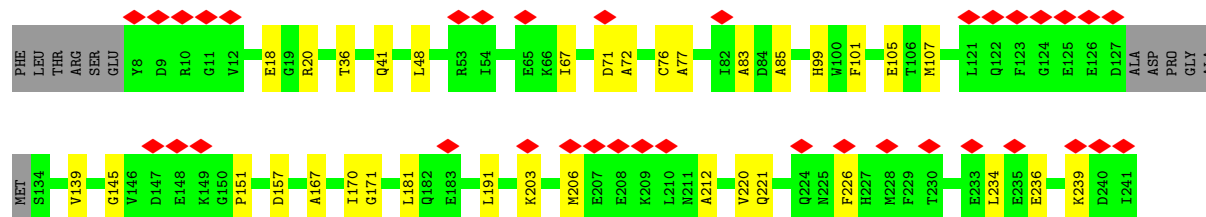
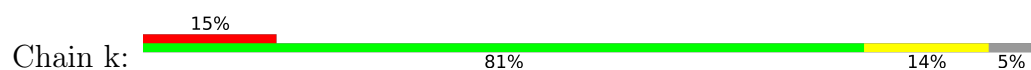
• Molecule 23: Proteasome subunit alpha type-7



• Molecule 24: Proteasome subunit alpha type-5

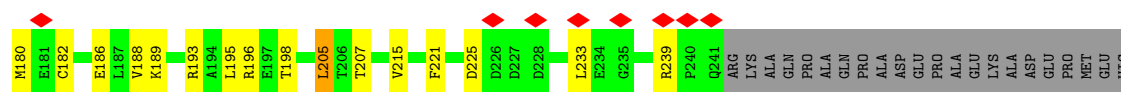


• Molecule 24: Proteasome subunit alpha type-5

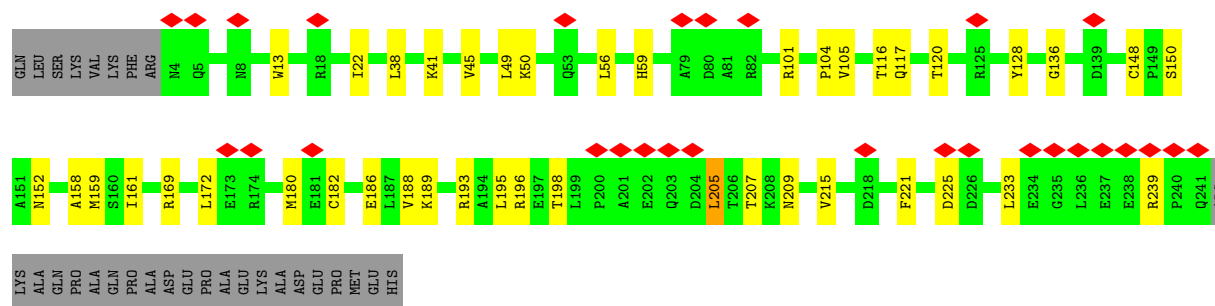
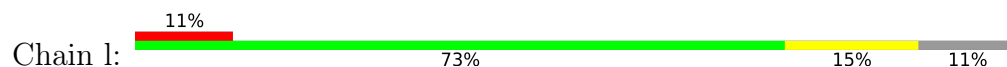


• Molecule 25: Proteasome subunit alpha type-1

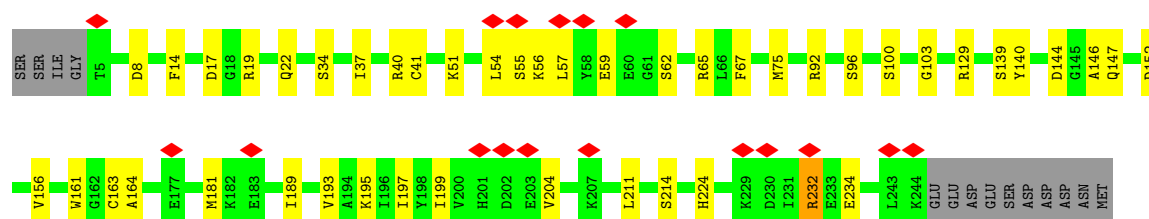
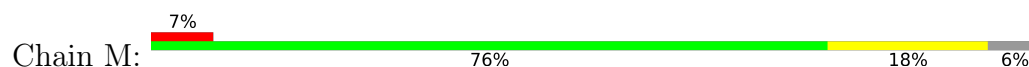




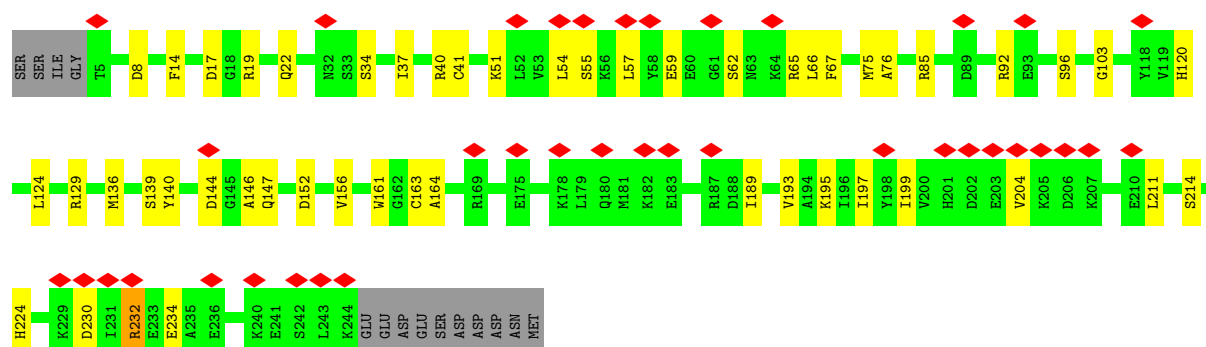
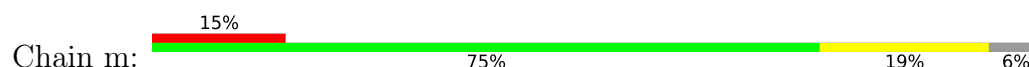
• Molecule 25: Proteasome subunit alpha type-1



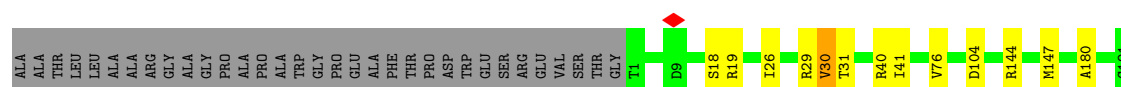
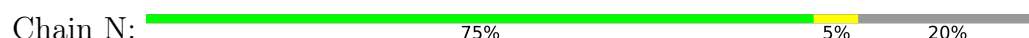
• Molecule 26: Proteasome subunit alpha type-3



• Molecule 26: Proteasome subunit alpha type-3



• Molecule 27: Proteasome subunit beta type-6



ASP
GLN
ILE
PRO
LEU
LYS
PHE
ALA
VAL
THR
LEU
PRO
PRO
ALA

• Molecule 27: Proteasome subunit beta type-6

Chain n:



ALA
ALA
THR
LEU
LEU
ALA
ALA
ARG
GLY
ALA
GLY
GLY
PRO
PRO
ALA
PRO
ALA
ALA
TRP
GLY
PRO
GLU
GLU
ALA
PHE
THR
PRO
ASP
TSP
GLU
SER
ARG
GLU
VAL
SER
THR
GLY
T1
D9
S18
I26
V30
T31
D32
D39
R40
I41
E69
L70
N71
E72
V76
D104
R144

M147
A180
E185
G191
ASP
GLN
ILE
PRO
LYS
PHE
ALA
VAL
ALA
ASP
ASN
THR
LEU
PRO
ALA

• Molecule 28: Proteasome subunit beta type-7

Chain O:



ALA
ALA
VAL
SER
VAL
TYR
ALA
PRO
PRO
VAL
GLY
GLY
PHE
SER
PHE
ASP
ASN
CYS
ARG
ARG
ASN
ALA
VAL
LEU
GLU
ALA
ASP
PHE
ALA
LYS
ARG
GLY
TYR
LYS
LEU
PRO
LYS
VAL
ARG
LYS
THR
GLY
T1
V6
V13
R19
E22
G23
M24
C31
S32
Q57
A96

L100
Y111
P115
Y124
E139
P144
F164
G170
D174
V177
R187
L199
G200
R201
Y202
R203
C204
E205
K206
G207
I216
E220
ILE
GLU
VAL
LEU
GLU
THR
VAL
GLN
THR
MET
ASP
THR
SER

• Molecule 28: Proteasome subunit beta type-7

Chain o:



ALA
ALA
VAL
SER
VAL
TYR
ALA
PRO
PRO
VAL
GLY
GLY
PHE
SER
PHE
ASP
ASN
CYS
ARG
ARG
ASN
ALA
VAL
LEU
GLU
ALA
ASP
PHE
ALA
LYS
ARG
GLY
TYR
LYS
LEU
PRO
LYS
VAL
ARG
LYS
THR
GLY
T1
V6
V13
R19
G23
M24
C31
S32
A96
L100

Y111
P115
Y124
F138
E139
D140
R143
F164
G170
S171
N172
I173
D174
V177
N181
D184
R187
K194
K195
G196
T197
R198
L199
G200
R201
E205
K206
G207
E220
ILE
GLU
VAL
LEU
GLU
THR
VAL
GLN
THR
MET
ASP
THR
SER

• Molecule 29: Proteasome subunit beta type-3

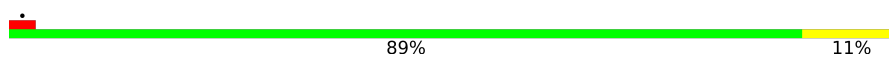
Chain P:

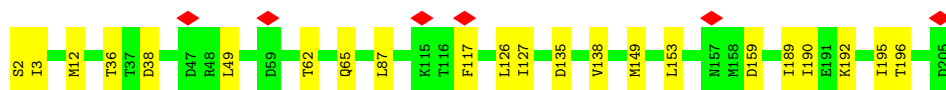


S2
I3
M12
T36
T37
D38
L49
L56
A57
T58
D59
T62
Q65
L87
F117
L126
I127
D135
V138
D159
I189
I190
E191
K192
K194
I195
T196
D205

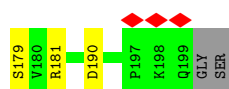
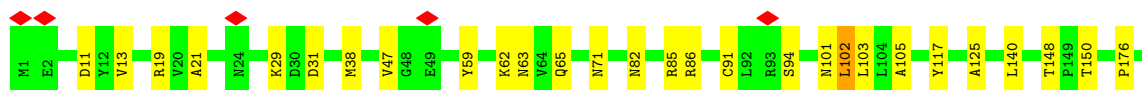
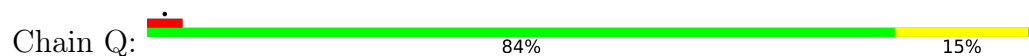
• Molecule 29: Proteasome subunit beta type-3

Chain p:

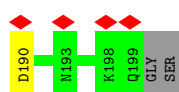
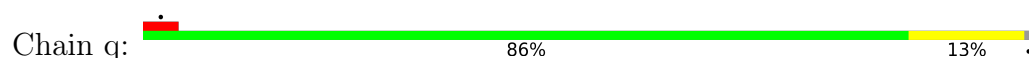




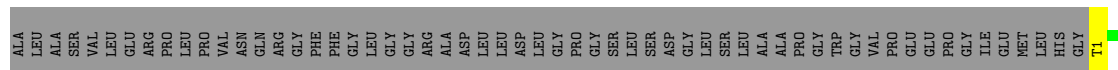
- Molecule 30: Proteasome subunit beta type-2



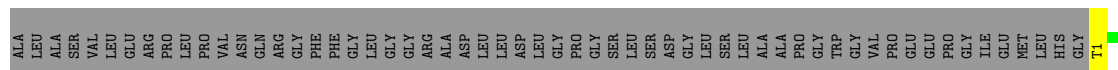
- Molecule 30: Proteasome subunit beta type-2



- Molecule 31: Proteasome subunit beta type-5

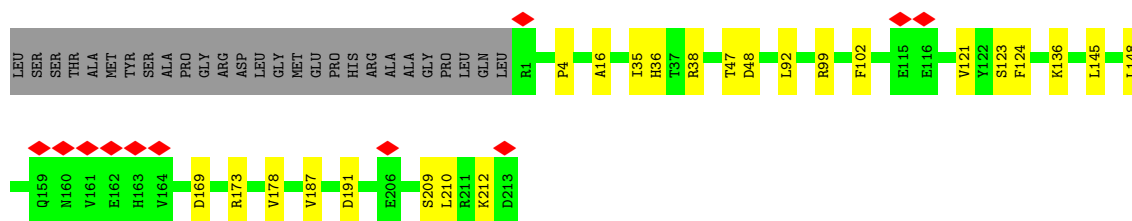


- Molecule 31: Proteasome subunit beta type-5



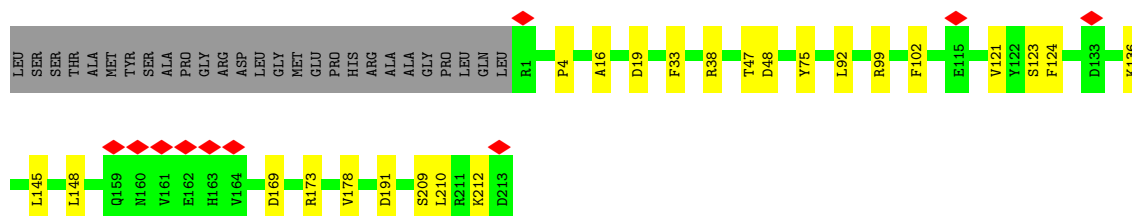
- Molecule 32: Proteasome subunit beta type-1

Chain S: 



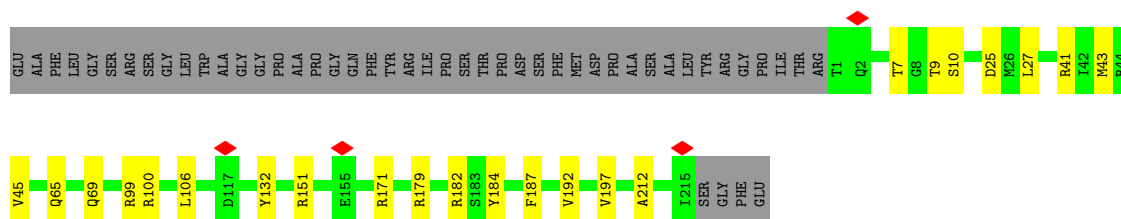
• Molecule 32: Proteasome subunit beta type-1

Chain s: 



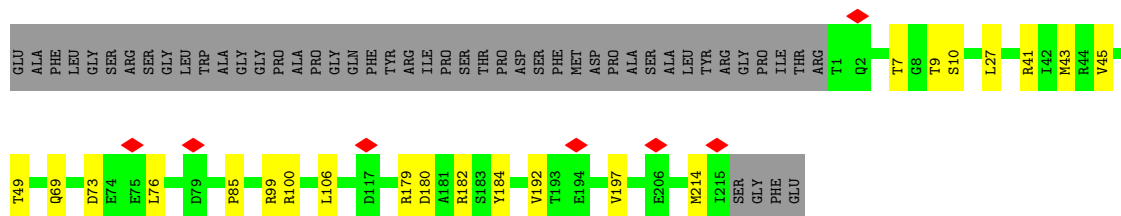
• Molecule 33: Proteasome subunit beta type-4

Chain T: 



• Molecule 33: Proteasome subunit beta type-4

Chain t: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	71651	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.016	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size ($\text{\AA}$)	411.0, 411.0, 411.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.685, 0.685, 0.685	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ZN, 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	U	0.26	0/6513	0.62	2/8816 (0.0%)
2	V	0.31	0/3929	0.71	3/5309 (0.1%)
3	W	0.27	0/3751	0.66	3/5042 (0.1%)
4	X	0.35	0/3053	0.61	1/4115 (0.0%)
5	Y	0.34	0/3173	0.71	1/4273 (0.0%)
6	Z	0.27	0/2324	0.68	0/3150
7	a	0.26	0/3053	0.67	4/4133 (0.1%)
8	b	0.25	0/1478	0.62	0/2001
9	c	0.29	0/2302	0.67	0/3110
10	d	0.27	0/2162	0.70	6/2919 (0.2%)
11	e	0.30	0/338	0.76	1/450 (0.2%)
12	f	0.30	0/6954	0.80	11/9399 (0.1%)
13	A	0.30	0/2814	0.62	2/3801 (0.1%)
14	B	0.27	0/2745	0.66	4/3709 (0.1%)
15	C	0.33	0/3146	0.69	2/4226 (0.0%)
16	D	0.38	0/3090	0.73	4/4168 (0.1%)
17	E	0.35	0/3145	0.71	1/4233 (0.0%)
18	F	0.35	0/3137	0.69	2/4223 (0.0%)
20	G	0.40	0/1859	0.63	1/2523 (0.0%)
20	g	0.40	0/1859	0.63	1/2523 (0.0%)
21	H	0.43	0/1743	0.62	0/2372
21	h	0.43	0/1743	0.62	0/2372
22	I	0.39	0/1942	0.67	0/2628
22	i	0.39	0/1942	0.67	0/2628
23	J	0.36	0/1728	0.58	0/2358
23	j	0.36	0/1728	0.58	0/2358
24	K	0.35	0/1747	0.58	0/2364
24	k	0.35	0/1747	0.58	0/2364
25	L	0.42	0/1885	0.63	0/2552
25	l	0.42	0/1885	0.63	0/2552
26	M	0.41	1/1891 (0.1%)	0.70	3/2552 (0.1%)
26	m	0.41	1/1891 (0.1%)	0.70	3/2552 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	N	0.40	0/1454	0.52	0/1967
27	n	0.40	0/1454	0.52	0/1967
28	O	0.38	0/1670	0.59	0/2265
28	o	0.38	0/1670	0.59	0/2265
29	P	0.40	0/1614	0.56	0/2177
29	p	0.40	0/1614	0.56	0/2177
30	Q	0.45	0/1603	0.67	2/2174 (0.1%)
30	q	0.45	0/1603	0.67	2/2174 (0.1%)
31	R	0.39	0/1579	0.50	0/2134
31	r	0.39	0/1579	0.50	0/2134
32	S	0.39	0/1671	0.54	0/2253
32	s	0.39	0/1671	0.54	0/2253
33	T	0.39	0/1700	0.56	0/2305
33	t	0.39	0/1700	0.56	0/2305
All	All	0.35	2/105279 (0.0%)	0.65	59/142325 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	V	0	1
6	Z	0	2
7	a	0	1
10	d	0	1
12	f	0	12
13	A	0	2
15	C	0	2
16	D	0	2
17	E	0	1
18	F	0	1
All	All	0	25

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	m	14	PHE	C-N	-5.18	1.23	1.33
26	M	14	PHE	C-N	-5.16	1.23	1.33

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	353	PHE	CA-C-N	8.03	129.87	119.84
14	B	353	PHE	C-N-CA	8.03	129.87	119.84
7	a	130	VAL	N-CA-C	-7.68	105.83	113.20
18	F	294	LYS	CA-C-N	7.21	135.30	121.54
18	F	294	LYS	C-N-CA	7.21	135.30	121.54
3	W	70	VAL	N-CA-C	-7.16	105.96	111.62
26	M	204	VAL	N-CA-C	-6.82	106.38	111.90
26	m	204	VAL	N-CA-C	-6.77	106.42	111.90
1	U	38	ILE	N-CA-C	-6.18	106.41	111.91
10	d	160	ALA	CA-C-N	-6.09	114.23	121.90
10	d	160	ALA	C-N-CA	-6.09	114.23	121.90
1	U	507	VAL	N-CA-C	-6.04	107.97	113.71
12	f	875	ALA	CA-C-N	6.02	133.03	121.54
12	f	875	ALA	C-N-CA	6.02	133.03	121.54
16	D	98	GLN	CA-C-N	5.97	130.86	122.08
16	D	98	GLN	C-N-CA	5.97	130.86	122.08
16	D	411	GLU	CA-C-N	5.91	132.84	121.54
16	D	411	GLU	C-N-CA	5.91	132.84	121.54
11	e	62	LYS	N-CA-C	-5.78	106.88	114.04
12	f	868	HIS	CA-C-N	5.68	132.40	121.54
12	f	868	HIS	C-N-CA	5.68	132.40	121.54
7	a	261	LEU	N-CA-C	-5.68	107.60	114.75
13	A	115	VAL	CA-C-N	5.56	132.16	121.54
13	A	115	VAL	C-N-CA	5.56	132.16	121.54
4	X	242	ILE	N-CA-C	-5.50	108.49	113.71
30	q	102	LEU	CA-C-N	5.49	132.03	121.54
30	q	102	LEU	C-N-CA	5.49	132.03	121.54
30	Q	102	LEU	CA-C-N	5.48	132.01	121.54
30	Q	102	LEU	C-N-CA	5.48	132.01	121.54
14	B	255	LEU	N-CA-C	-5.41	107.93	114.75
17	E	210	GLU	N-CA-C	-5.40	108.47	114.62
12	f	822	VAL	CA-C-N	5.34	131.75	121.54
12	f	822	VAL	C-N-CA	5.34	131.75	121.54
7	a	186	LYS	CA-C-N	5.33	131.72	121.54
7	a	186	LYS	C-N-CA	5.33	131.72	121.54
15	C	128	PRO	CA-C-N	5.32	131.70	121.54
15	C	128	PRO	C-N-CA	5.32	131.70	121.54
20	G	134	LEU	N-CA-C	5.29	117.10	110.91
20	g	134	LEU	N-CA-C	5.29	117.10	110.91
10	d	200	PHE	N-CA-C	5.26	122.00	110.80
12	f	619	HIS	CA-C-N	5.23	131.53	121.54
12	f	619	HIS	C-N-CA	5.23	131.53	121.54
5	Y	168	ILE	N-CA-C	-5.20	107.75	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	f	254	GLY	N-CA-C	5.19	118.53	112.50
10	d	120	GLU	N-CA-C	-5.17	107.99	114.56
12	f	858	LYS	CA-C-N	-5.15	113.40	119.84
12	f	858	LYS	C-N-CA	-5.15	113.40	119.84
14	B	438	LEU	N-CA-C	-5.14	107.07	113.55
26	m	232	ARG	CA-C-N	5.11	131.31	121.54
26	m	232	ARG	C-N-CA	5.11	131.31	121.54
26	M	232	ARG	CA-C-N	5.10	131.29	121.54
26	M	232	ARG	C-N-CA	5.10	131.29	121.54
3	W	311	THR	CA-C-N	5.09	131.25	121.54
3	W	311	THR	C-N-CA	5.09	131.25	121.54
2	V	28	PRO	N-CA-C	5.08	116.89	110.70
2	V	239	THR	N-CA-CB	-5.07	108.39	114.17
10	d	199	PHE	CA-C-N	5.06	131.20	121.54
10	d	199	PHE	C-N-CA	5.06	131.20	121.54
2	V	27	PRO	N-CA-C	5.00	116.81	110.70

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	A	157	ILE	Peptide
13	A	284	ARG	Peptide
15	C	128	PRO	Peptide
15	C	220	VAL	Peptide
16	D	157	ASP	Peptide
16	D	411	GLU	Peptide
17	E	226	GLN	Peptide
18	F	294	LYS	Peptide
2	V	29	PRO	Peptide
6	Z	144	VAL	Peptide
6	Z	183	THR	Peptide
7	a	18	GLN	Peptide
10	d	199	PHE	Peptide
12	f	340	MET	Peptide
12	f	642	ALA	Peptide
12	f	737	ASN	Peptide
12	f	755	ASP	Peptide
12	f	807	ARG	Peptide
12	f	809	ILE	Peptide
12	f	816	TYR	Peptide
12	f	822	VAL	Peptide

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Mol	Chain	Res	Type	Group
12	f	823	ALA	Peptide
12	f	854	GLY	Peptide
12	f	870	THR	Peptide
12	f	875	ALA	Peptide

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	U	6398	0	6422	82	0
2	V	3852	0	3893	44	0
3	W	3703	0	3822	103	0
4	X	3009	0	3113	24	0
5	Y	3115	0	3120	44	0
6	Z	2281	0	2312	105	0
7	a	2995	0	3012	35	0
8	b	1458	0	1505	21	0
9	c	2260	0	2276	41	0
10	d	2116	0	2146	21	0
11	e	334	0	294	6	0
12	f	6840	0	6842	142	0
13	A	2767	0	2787	41	0
14	B	2706	0	2731	61	0
15	C	3105	0	3219	53	0
16	D	3040	0	3076	63	0
17	E	3097	0	3174	42	0
18	F	3098	0	3187	44	0
19	v	110	0	32	7	0
20	G	1826	0	1796	16	0
20	g	1826	0	1796	22	0
21	H	1708	0	1594	16	0
21	h	1708	0	1594	14	0
22	I	1912	0	1851	34	0
22	i	1912	0	1851	29	0
23	J	1704	0	1517	22	0
23	j	1704	0	1517	19	0
24	K	1722	0	1673	18	0
24	k	1722	0	1673	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	L	1850	0	1822	23	0
25	l	1850	0	1822	24	0
26	M	1856	0	1814	29	0
26	m	1856	0	1814	32	0
27	N	1430	0	1398	10	0
27	n	1430	0	1398	8	0
28	O	1643	0	1644	15	0
28	o	1643	0	1644	13	0
29	P	1585	0	1598	17	0
29	p	1585	0	1598	13	0
30	Q	1570	0	1547	19	0
30	q	1570	0	1547	16	0
31	R	1548	0	1499	7	0
31	r	1548	0	1499	11	0
32	S	1641	0	1618	18	0
32	s	1641	0	1618	15	0
33	T	1667	0	1628	18	0
33	t	1667	0	1628	17	0
34	c	1	0	0	0	0
35	C	31	0	12	3	0
35	D	31	0	12	0	0
35	E	31	0	12	2	0
36	F	27	0	12	0	0
All	All	103729	0	103009	1327	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 (1327) 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)
14:B:355:LEU:CD2	14:B:356:PRO:HD3	1.51	1.40
6:Z:10:VAL:HG22	6:Z:161:GLU:CG	1.73	1.17
12:f:657:ILE:O	12:f:661:ALA:HB3	1.44	1.16
14:B:355:LEU:HD22	14:B:356:PRO:CD	1.77	1.14
3:W:202:THR:CG2	3:W:233:LEU:HD21	1.77	1.13
14:B:355:LEU:HD13	14:B:356:PRO:CD	1.76	1.12
6:Z:9:VAL:HG12	6:Z:48:LEU:HD22	1.31	1.10
14:B:355:LEU:CD1	14:B:356:PRO:HD2	1.81	1.10
6:Z:9:VAL:CG1	6:Z:48:LEU:HD22	1.89	1.01
14:B:355:LEU:HD13	14:B:356:PRO:HD2	1.02	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:202:THR:HG21	3:W:233:LEU:HD21	1.40	1.00
6:Z:10:VAL:HG22	6:Z:161:GLU:HG2	1.44	0.99
6:Z:17:LEU:CD1	9:c:36:LEU:HB3	1.93	0.98
13:A:144:ARG:HD2	19:v:19:UNK:CB	1.94	0.97
3:W:234:ASP:OD2	3:W:242:SER:HB3	1.65	0.96
6:Z:13:PRO:O	6:Z:17:LEU:HD23	1.65	0.96
14:B:355:LEU:CG	14:B:356:PRO:HD3	1.94	0.96
3:W:456:GLN:OXT	3:W:456:GLN:NE2	1.98	0.94
3:W:243:ILE:HG21	3:W:273:TYR:OH	1.68	0.93
6:Z:12:HIS:HB3	6:Z:13:PRO:HD2	1.52	0.91
6:Z:10:VAL:HG21	6:Z:161:GLU:OE2	1.70	0.90
6:Z:17:LEU:HD12	9:c:36:LEU:HB3	1.54	0.90
3:W:234:ASP:HB2	3:W:243:ILE:HG13	1.51	0.89
3:W:202:THR:HG22	3:W:233:LEU:HD21	1.52	0.89
3:W:234:ASP:CB	3:W:243:ILE:HG13	2.02	0.88
9:c:111:TRP:HH2	9:c:126:ASP:OD1	1.57	0.87
14:B:355:LEU:CD1	14:B:356:PRO:CD	2.46	0.87
14:B:355:LEU:CG	14:B:356:PRO:CD	2.52	0.87
6:Z:10:VAL:HG22	6:Z:161:GLU:HG3	1.59	0.84
6:Z:219:LYS:HZ3	6:Z:219:LYS:C	1.84	0.84
6:Z:9:VAL:HG12	6:Z:48:LEU:CD2	2.07	0.83
14:B:355:LEU:HD22	14:B:356:PRO:HD3	0.83	0.83
3:W:234:ASP:HB2	3:W:243:ILE:CG1	2.08	0.82
3:W:456:GLN:OXT	3:W:456:GLN:CD	2.23	0.82
6:Z:12:HIS:HB3	6:Z:13:PRO:CD	2.09	0.81
6:Z:10:VAL:CG2	6:Z:161:GLU:OE2	2.29	0.81
14:B:355:LEU:CB	14:B:356:PRO:CD	2.59	0.80
12:f:657:ILE:O	12:f:661:ALA:CB	2.29	0.79
6:Z:212:LEU:HA	6:Z:215:VAL:HG12	1.64	0.78
3:W:202:THR:HG21	3:W:233:LEU:CD2	2.13	0.78
13:A:144:ARG:CD	19:v:19:UNK:CB	2.62	0.78
6:Z:17:LEU:HD11	9:c:36:LEU:CB	2.16	0.76
3:W:456:GLN:OXT	3:W:456:GLN:CG	2.33	0.76
6:Z:216:ALA:C	6:Z:218:GLY:H	1.94	0.76
6:Z:17:LEU:HD11	9:c:36:LEU:HB3	1.68	0.75
3:W:455:LEU:HD23	3:W:455:LEU:O	1.87	0.75
3:W:244:CYS:O	3:W:247:TYR:HB2	1.86	0.74
12:f:828:ARG:CZ	12:f:843:SER:OG	2.37	0.73
3:W:202:THR:CG2	3:W:233:LEU:CD2	2.64	0.73
6:Z:10:VAL:HG13	6:Z:163:GLY:H	1.55	0.72
17:E:248:SER:HA	17:E:251:ARG:HD3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:220:LEU:C	6:Z:220:LEU:HD12	2.16	0.71
6:Z:222:ILE:C	6:Z:222:ILE:HD12	2.16	0.71
6:Z:222:ILE:HD12	6:Z:222:ILE:O	1.90	0.71
23:J:175:ASN:HD21	23:J:190:LEU:HD11	1.56	0.71
29:P:58:THR:HG23	29:P:59:ASP:N	2.07	0.70
18:F:376:SER:HB3	18:F:414:GLU:HB2	1.74	0.70
23:j:175:ASN:HD21	23:j:190:LEU:HD11	1.56	0.70
12:f:828:ARG:NE	12:f:843:SER:OG	2.26	0.69
9:c:111:TRP:CH2	9:c:126:ASP:OD1	2.44	0.69
2:V:79:VAL:HG13	2:V:81:GLN:H	1.58	0.68
2:V:345:ARG:HH12	2:V:357:LEU:HA	1.57	0.68
13:A:165:GLN:NE2	13:A:236:CYS:SG	2.66	0.68
1:U:559:ARG:HB3	1:U:562:GLU:HB2	1.74	0.68
6:Z:212:LEU:HA	6:Z:215:VAL:CG1	2.22	0.68
29:P:56:LEU:HG	29:P:58:THR:HG22	1.76	0.67
6:Z:216:ALA:O	6:Z:218:GLY:N	2.27	0.67
15:C:48:GLN:HB3	16:D:65:GLN:HE22	1.60	0.66
15:C:138:MET:SD	15:C:138:MET:N	2.68	0.66
3:W:98:LYS:HD2	3:W:140:ILE:H	1.61	0.66
6:Z:14:LEU:HD12	9:c:43:LYS:NZ	2.11	0.66
9:c:139:ARG:HB2	9:c:161:ARG:HE	1.60	0.66
13:A:140:VAL:HG12	13:A:152:PRO:HB3	1.77	0.66
17:E:275:MET:HB3	17:E:277:MET:HE2	1.76	0.65
23:j:38:ARG:HH12	23:j:182:GLU:HA	1.61	0.65
3:W:276:LEU:HA	3:W:357:ARG:HG3	1.79	0.65
16:D:274:ARG:HH22	16:D:290:LEU:HD21	1.62	0.65
17:E:177:GLY:O	17:E:339:ASN:ND2	2.30	0.65
12:f:660:ILE:HG13	12:f:660:ILE:O	1.95	0.65
26:M:55:SER:H	26:M:57:LEU:HD23	1.62	0.65
26:m:55:SER:H	26:m:57:LEU:HD23	1.62	0.65
6:Z:8:LYS:HB3	6:Z:159:THR:HG23	1.77	0.65
6:Z:13:PRO:O	6:Z:17:LEU:CD2	2.42	0.65
32:S:38:ARG:NH2	28:o:164:PHE:O	2.29	0.65
26:m:51:LYS:NZ	26:m:62:SER:O	2.30	0.65
3:W:8:ARG:HB3	3:W:27:ARG:HD3	1.77	0.64
12:f:61:GLU:OE2	12:f:62:ARG:NH1	2.30	0.64
1:U:524:LYS:HG3	1:U:556:MET:HE2	1.80	0.64
6:Z:11:VAL:HB	6:Z:50:VAL:HB	1.79	0.64
3:W:199:TYR:CE2	3:W:236:HIS:NE2	2.65	0.64
12:f:125:ILE:HD13	12:f:129:LEU:HB2	1.80	0.64
14:B:429:LYS:HG2	14:B:430:LYS:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:128:PRO:HG2	16:D:96:VAL:HG13	1.79	0.64
24:K:71:ASP:O	31:R:64:ARG:NH2	2.28	0.64
26:M:51:LYS:NZ	26:M:62:SER:O	2.30	0.64
5:Y:336:ARG:NH1	11:e:55:GLN:OE1	2.30	0.64
3:W:235:GLN:N	3:W:243:ILE:HD11	2.13	0.63
23:J:38:ARG:HH12	23:J:182:GLU:HA	1.61	0.63
2:V:452:ASN:HB3	2:V:457:TYR:HB2	1.81	0.63
6:Z:8:LYS:HE3	6:Z:47:VAL:HG23	1.81	0.63
33:T:27:LEU:HD22	33:T:184:TYR:HB2	1.80	0.63
33:T:192:VAL:HG12	33:T:197:VAL:HG22	1.79	0.63
33:t:27:LEU:HD22	33:t:184:TYR:HB2	1.80	0.63
8:b:161:ASN:HB2	8:b:165:GLY:HA3	1.79	0.63
33:t:192:VAL:HG12	33:t:197:VAL:HG22	1.79	0.63
24:K:36:THR:HA	24:K:171:GLY:HA3	1.81	0.62
12:f:673:ARG:HH22	12:f:709:THR:HA	1.63	0.62
33:T:9:THR:O	33:T:41:ARG:NH2	2.33	0.62
14:B:429:LYS:HE2	14:B:430:LYS:HE2	1.80	0.62
22:I:213:ILE:HB	22:I:228:LEU:HD11	1.81	0.62
1:U:599:ILE:HG23	16:D:56:VAL:HG11	1.81	0.62
14:B:141:LYS:HG3	14:B:144:LEU:HD12	1.81	0.62
6:Z:217:THR:O	6:Z:217:THR:HG22	2.00	0.62
22:i:213:ILE:HB	22:i:228:LEU:HD11	1.81	0.62
24:k:36:THR:HA	24:k:171:GLY:HA3	1.81	0.62
6:Z:11:VAL:HG23	6:Z:12:HIS:O	2.00	0.62
5:Y:92:GLU:OE2	5:Y:94:ASN:ND2	2.32	0.61
13:A:144:ARG:HD3	19:v:18:UNK:O	2.00	0.61
1:U:155:LEU:O	1:U:158:ARG:NH1	2.33	0.61
33:t:9:THR:O	33:t:41:ARG:NH2	2.33	0.61
2:V:81:GLN:HB3	2:V:85:ALA:HB3	1.82	0.61
3:W:235:GLN:HG2	3:W:350:ARG:NH2	2.15	0.61
22:I:143:TYR:HB2	22:I:146:GLN:HE21	1.65	0.61
14:B:355:LEU:CD2	14:B:356:PRO:CD	2.46	0.61
24:k:48:LEU:HD21	24:k:77:ALA:HB2	1.82	0.61
2:V:148:ARG:HD2	2:V:197:THR:HG21	1.80	0.61
14:B:379:THR:OG1	14:B:416:ASN:ND2	2.33	0.61
12:f:125:ILE:HD11	12:f:128:VAL:HB	1.81	0.61
20:g:137:CYS:SG	20:g:138:MET:N	2.73	0.61
3:W:234:ASP:HB3	3:W:239:SER:HB2	1.83	0.61
9:c:152:LYS:HG2	16:D:82:ILE:HD12	1.83	0.61
22:I:218:ARG:NH1	22:I:223:THR:OG1	2.32	0.61
24:K:48:LEU:HD21	24:K:77:ALA:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:381:THR:HG22	1:U:412:HIS:HA	1.83	0.60
6:Z:18:SER:O	6:Z:21:ASP:HB3	2.00	0.60
12:f:704:LEU:HA	12:f:707:LEU:HB2	1.83	0.60
4:X:203:PRO:HB2	4:X:207:GLN:HB2	1.81	0.60
10:d:61:TRP:HB3	10:d:65:ARG:HH11	1.66	0.60
12:f:672:LEU:HD21	12:f:690:VAL:HG22	1.83	0.60
6:Z:18:SER:O	6:Z:21:ASP:N	2.34	0.60
6:Z:209:ARG:HD2	6:Z:212:LEU:HD11	1.83	0.60
17:E:101:ASP:HB2	17:E:108:MET:HE3	1.83	0.60
5:Y:240:VAL:HG23	5:Y:241:ILE:HG13	1.83	0.60
22:i:8:ARG:HE	23:j:5:ARG:HH21	1.48	0.60
22:i:229:LYS:N	22:i:232:GLU:OE2	2.35	0.60
12:f:586:PRO:HA	12:f:589:SER:HB2	1.83	0.60
29:P:117:PHE:HB3	29:P:192:LYS:HD3	1.82	0.60
12:f:127:SER:HA	12:f:131:MET:HB2	1.82	0.60
12:f:811:LEU:HD11	12:f:862:ILE:HB	1.84	0.60
3:W:299:ILE:HG22	3:W:301:LYS:H	1.66	0.60
29:p:117:PHE:HB3	29:p:192:LYS:HD3	1.82	0.60
3:W:235:GLN:HG2	3:W:350:ARG:HH22	1.67	0.59
6:Z:10:VAL:CG2	6:Z:161:GLU:CG	2.65	0.59
17:E:21:GLU:OE2	17:E:25:ARG:NH2	2.35	0.59
22:i:143:TYR:HB2	22:i:146:GLN:HE21	1.65	0.59
1:U:160:LEU:HD21	1:U:196:LYS:HB3	1.84	0.59
3:W:49:SER:HB3	3:W:95:SER:HB2	1.84	0.59
6:Z:10:VAL:O	6:Z:10:VAL:HG12	2.01	0.59
12:f:99:LEU:HG	12:f:101:PRO:HD2	1.83	0.59
13:A:307:ASP:OD2	13:A:333:ARG:NH2	2.35	0.59
17:E:368:MET:HB3	17:E:372:ARG:HH12	1.66	0.59
3:W:199:TYR:CE2	3:W:236:HIS:CD2	2.91	0.59
25:L:186:GLU:HA	25:L:189:LYS:HG2	1.84	0.59
10:d:84:ASP:HB3	10:d:87:GLU:HB2	1.85	0.59
22:I:229:LYS:N	22:I:232:GLU:OE2	2.35	0.59
6:Z:10:VAL:HG22	6:Z:161:GLU:CD	2.26	0.59
12:f:872:VAL:HG21	12:f:881:GLU:H	1.67	0.59
15:C:78:ARG:HA	15:C:108:VAL:HG13	1.84	0.59
6:Z:212:LEU:HD12	6:Z:213:GLU:HG3	1.84	0.59
14:B:362:LYS:HG2	14:B:384:ILE:HD13	1.85	0.59
23:J:96:LEU:HD12	30:Q:62:LYS:HG3	1.85	0.59
25:l:186:GLU:HA	25:l:189:LYS:HG2	1.84	0.59
1:U:798:PRO:O	1:U:880:ASN:ND2	2.36	0.59
2:V:480:ILE:HD11	6:Z:260:VAL:HA	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:425:LEU:HB2	6:Z:247:LYS:HD3	1.85	0.59
6:Z:10:VAL:HG13	6:Z:163:GLY:N	2.17	0.59
14:B:440:LEU:HG	23:J:61:LYS:HE2	1.84	0.59
15:C:219:LEU:HD13	15:C:272:THR:HG21	1.85	0.59
16:D:92:PHE:HA	16:D:103:VAL:HG12	1.85	0.59
5:Y:178:ASN:ND2	5:Y:212:GLU:OE1	2.36	0.59
16:D:99:ASN:HA	16:D:115:ILE:HG12	1.84	0.59
27:N:144:ARG:H	27:N:147:MET:HE3	1.68	0.59
29:P:65:GLN:OE1	30:Q:86:ARG:NH2	2.35	0.59
1:U:803:LYS:HD2	1:U:875:PHE:HB2	1.85	0.58
8:b:25:ARG:NH1	8:b:145:GLU:OE1	2.33	0.58
35:C:501:ATP:O2B	16:D:323:ARG:NH2	2.36	0.58
16:D:417:TYR:OH	20:G:21:ARG:NH2	2.36	0.58
18:F:359:GLU:HB3	18:F:385:ALA:HB1	1.84	0.58
1:U:184:CYS:O	1:U:194:ARG:NH2	2.29	0.58
2:V:337:LEU:O	2:V:401:ASN:ND2	2.37	0.58
27:n:144:ARG:H	27:n:147:MET:HE3	1.68	0.58
2:V:494:MET:O	6:Z:278:ASN:ND2	2.36	0.58
22:i:171:ALA:HB2	22:i:200:THR:HG21	1.85	0.58
22:i:218:ARG:NH1	22:i:223:THR:OG1	2.32	0.58
2:V:395:ILE:O	2:V:399:ARG:NH1	2.37	0.58
12:f:302:GLY:HA2	12:f:317:LEU:HD11	1.84	0.58
20:G:201:CYS:SG	20:G:202:LEU:N	2.76	0.58
8:b:51:LEU:HD23	8:b:71:ILE:HG23	1.84	0.58
26:m:37:ILE:HD11	26:m:193:VAL:HG13	1.86	0.58
6:Z:9:VAL:CG1	6:Z:48:LEU:HB3	2.33	0.58
33:T:99:ARG:HG2	33:T:106:LEU:HG	1.85	0.58
24:k:71:ASP:O	31:r:64:ARG:NH2	2.33	0.58
6:Z:17:LEU:CD1	9:c:36:LEU:CB	2.72	0.58
24:K:167:ALA:H	25:L:56:LEU:HD13	1.68	0.58
26:M:37:ILE:HD11	26:M:193:VAL:HG13	1.86	0.58
20:g:201:CYS:SG	20:g:202:LEU:N	2.76	0.58
1:U:625:ILE:HG13	1:U:626:LEU:HG	1.85	0.58
7:a:135:ILE:HG12	7:a:158:LEU:HD13	1.86	0.58
29:P:62:THR:OG1	30:Q:85:ARG:NH2	2.37	0.58
33:T:179:ARG:NH1	27:n:26:ILE:O	2.33	0.58
28:o:31:CYS:SG	28:o:32:SER:N	2.77	0.58
1:U:558:GLY:H	1:U:589:ALA:HA	1.69	0.57
9:c:39:LEU:HD23	9:c:42:LEU:HD21	1.86	0.57
16:D:394:VAL:HG12	16:D:396:ALA:H	1.69	0.57
29:P:189:ILE:HG23	29:P:196:THR:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:t:99:ARG:HG2	33:t:106:LEU:HG	1.85	0.57
1:U:689:ILE:HG12	1:U:732:LEU:HD22	1.87	0.57
28:O:32:SER:OG	28:O:187:ARG:NH2	2.38	0.57
17:E:339:ASN:HB3	17:E:342:ASP:HB2	1.87	0.57
27:N:40:ARG:NH1	27:N:180:ALA:O	2.37	0.57
24:k:76:CYS:SG	24:k:77:ALA:N	2.78	0.57
3:W:240:TYR:HD2	3:W:276:LEU:O	1.87	0.57
10:d:161:GLU:HG2	10:d:162:SER:H	1.70	0.57
12:f:198:HIS:O	12:f:202:HIS:N	2.36	0.57
15:C:264:GLY:HA3	16:D:279:THR:HA	1.87	0.57
12:f:150:GLU:O	12:f:156:HIS:ND1	2.37	0.57
24:k:18:GLU:OE1	24:k:20:ARG:NH2	2.38	0.57
1:U:82:LEU:O	1:U:129:ARG:NE	2.38	0.57
6:Z:14:LEU:HD12	9:c:43:LYS:HZ3	1.70	0.57
6:Z:287:LYS:HG3	6:Z:288:LYS:HG2	1.87	0.57
9:c:178:THR:OG1	9:c:180:ASN:OD1	2.23	0.57
2:V:100:MET:H	2:V:103:SER:HB2	1.69	0.57
12:f:691:PRO:HA	12:f:694:LEU:HB2	1.87	0.57
14:B:182:GLU:HB2	14:B:186:ASP:HB2	1.87	0.57
15:C:77:VAL:HG22	15:C:111:ASN:H	1.70	0.57
27:n:40:ARG:NH1	27:n:180:ALA:O	2.37	0.57
6:Z:129:LYS:O	9:c:215:LYS:NZ	2.38	0.56
3:W:187:LEU:HA	3:W:190:MET:HE3	1.87	0.56
7:a:255:TRP:O	7:a:258:GLN:NE2	2.36	0.56
28:o:32:SER:OG	28:o:187:ARG:NH2	2.38	0.56
3:W:456:GLN:OXT	3:W:456:GLN:HG3	2.04	0.56
7:a:35:HIS:NE2	8:b:14:GLU:O	2.38	0.56
9:c:161:ARG:NH1	9:c:162:LEU:O	2.38	0.56
12:f:77:GLU:OE1	12:f:79:ARG:NH1	2.39	0.56
12:f:556:ARG:HD3	12:f:786:GLN:HB2	1.86	0.56
12:f:591:ALA:HA	12:f:594:LEU:HD23	1.87	0.56
12:f:790:GLN:HG2	12:f:794:ALA:HB3	1.87	0.56
24:K:18:GLU:OE1	24:K:20:ARG:NH2	2.38	0.56
24:K:76:CYS:SG	24:K:77:ALA:N	2.78	0.56
30:Q:181:ARG:NH1	30:Q:190:ASP:OD1	2.38	0.56
1:U:803:LYS:HB3	1:U:877:LEU:HD23	1.88	0.56
10:d:132:TYR:HE1	10:d:160:ALA:HB2	1.70	0.56
15:C:99:VAL:HA	15:C:123:LEU:HD12	1.88	0.56
22:I:171:ALA:HB2	22:I:200:THR:HG21	1.85	0.56
29:P:58:THR:CG2	29:P:59:ASP:N	2.67	0.56
4:X:316:ASP:OD1	4:X:320:SER:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:552:ASP:HB3	12:f:556:ARG:HG3	1.88	0.56
12:f:875:ALA:O	12:f:876:HIS:ND1	2.38	0.56
14:B:181:GLN:O	14:B:241:ASN:ND2	2.38	0.56
18:F:383:GLU:HG2	18:F:386:ARG:HH22	1.70	0.56
3:W:199:TYR:CZ	3:W:236:HIS:CD2	2.94	0.56
12:f:378:ASN:HD21	12:f:392:THR:HG22	1.70	0.56
30:Q:140:LEU:HD13	31:r:166:ARG:HH11	1.70	0.56
20:g:144:ASP:HB3	20:g:147:GLN:HB2	1.88	0.56
1:U:221:ILE:HD11	1:U:252:LEU:HA	1.87	0.56
2:V:285:TRP:HD1	2:V:315:LYS:HE2	1.69	0.56
29:p:189:ILE:HG23	29:p:196:THR:HB	1.86	0.56
2:V:228:ARG:O	2:V:232:HIS:ND1	2.39	0.56
14:B:355:LEU:HB3	14:B:356:PRO:CD	2.32	0.56
30:q:181:ARG:NH1	30:q:190:ASP:OD1	2.38	0.56
1:U:600:ARG:HE	16:D:56:VAL:HG13	1.70	0.56
5:Y:78:GLU:O	5:Y:82:LYS:N	2.39	0.56
6:Z:181:ASP:OD1	6:Z:189:GLN:NE2	2.39	0.56
13:A:114:ASN:HB3	13:A:120:LYS:HG2	1.88	0.56
20:G:144:ASP:HB3	20:G:147:GLN:HB2	1.88	0.56
1:U:376:MET:HA	1:U:739:ALA:HA	1.88	0.56
6:Z:220:LEU:HD12	6:Z:220:LEU:O	2.05	0.56
18:F:161:LEU:HG	18:F:162:GLU:HG2	1.86	0.56
18:F:401:VAL:HG12	18:F:405:MET:HE2	1.87	0.56
26:M:40:ARG:NH1	26:M:146:ALA:O	2.39	0.56
12:f:663:GLY:O	12:f:664:GLU:HG3	2.06	0.55
26:m:40:ARG:NH1	26:m:146:ALA:O	2.39	0.55
23:J:119:THR:HG22	23:J:126:PRO:HB3	1.88	0.55
26:M:34:SER:OG	26:M:65:ARG:NH2	2.32	0.55
1:U:889:LEU:HD13	1:U:909:GLY:H	1.70	0.55
3:W:456:GLN:HE21	3:W:456:GLN:C	2.13	0.55
9:c:192:LEU:HA	9:c:196:LEU:HB2	1.88	0.55
12:f:441:LYS:HB2	12:f:477:MET:HE1	1.88	0.55
9:c:45:GLY:HA2	9:c:53:VAL:HG21	1.89	0.55
12:f:465:LEU:O	12:f:481:SER:OG	2.25	0.55
13:A:125:LEU:HA	13:A:149:ILE:HB	1.88	0.55
23:j:119:THR:HG22	23:j:126:PRO:HB3	1.88	0.55
2:V:85:ALA:O	2:V:89:LYS:NZ	2.39	0.55
12:f:378:ASN:OD1	12:f:382:ASN:ND2	2.40	0.55
12:f:828:ARG:CD	12:f:843:SER:OG	2.54	0.55
5:Y:144:LEU:HB3	5:Y:160:ASN:HD22	1.72	0.55
17:E:97:ARG:NH2	17:E:113:ARG:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:594:LEU:O	12:f:635:LYS:NZ	2.40	0.55
15:C:195:GLY:N	35:C:501:ATP:O2A	2.36	0.55
12:f:378:ASN:O	12:f:382:ASN:ND2	2.39	0.55
17:E:168:LYS:NZ	17:E:270:LEU:O	2.40	0.55
20:g:11:ARG:O	20:g:24:GLN:NE2	2.40	0.55
3:W:273:TYR:HB2	3:W:276:LEU:HB2	1.88	0.55
4:X:377:ILE:HB	4:X:388:PHE:HE1	1.72	0.55
17:E:98:VAL:HA	17:E:110:TYR:HA	1.88	0.54
18:F:150:LEU:HD12	18:F:166:THR:HA	1.89	0.54
33:T:171:ARG:NH2	28:o:140:ASP:OD2	2.40	0.54
3:W:346:GLU:O	3:W:350:ARG:HG2	2.07	0.54
20:g:114:LEU:HD22	20:g:140:LEU:HD21	1.89	0.54
6:Z:74:TYR:HE1	9:c:98:MET:HB3	1.71	0.54
8:b:161:ASN:HD21	8:b:168:SER:H	1.56	0.54
18:F:229:PRO:HB3	18:F:333:ASN:HD22	1.71	0.54
20:G:212:PRO:HG3	20:G:239:LEU:HD23	1.90	0.54
12:f:673:ARG:NH1	12:f:708:ASP:OD2	2.41	0.54
20:G:114:LEU:HD22	20:G:140:LEU:HD21	1.89	0.54
3:W:234:ASP:CB	3:W:239:SER:HB2	2.38	0.54
13:A:165:GLN:NE2	13:A:167:GLU:OE2	2.41	0.54
18:F:228:PRO:O	18:F:233:LYS:NZ	2.40	0.54
1:U:885:MET:H	1:U:888:GLN:HE21	1.55	0.54
2:V:440:LYS:NZ	10:d:143:LEU:O	2.40	0.54
10:d:131:VAL:HA	10:d:134:LYS:HB3	1.88	0.54
12:f:585:GLU:HG3	12:f:588:ARG:HE	1.73	0.54
16:D:231:VAL:HG13	17:E:262:ASN:HD22	1.72	0.54
1:U:107:HIS:HA	1:U:110:LYS:HE3	1.89	0.54
2:V:476:PHE:HB3	6:Z:260:VAL:HG21	1.90	0.54
6:Z:259:VAL:HG13	9:c:292:MET:HG3	1.89	0.54
12:f:634:LYS:HD2	12:f:637:LYS:HD2	1.90	0.54
14:B:223:ILE:HG13	14:B:347:ILE:HG21	1.88	0.54
17:E:175:PRO:O	17:E:178:THR:OG1	2.24	0.54
17:E:303:LEU:HD23	17:E:338:PHE:HB3	1.90	0.54
29:p:135:ASP:OD1	29:p:135:ASP:N	2.41	0.54
1:U:70:HIS:HD2	2:V:236:ARG:HH22	1.55	0.54
1:U:792:ASN:HB3	1:U:914:LEU:H	1.73	0.54
3:W:407:ASP:OD2	4:X:344:ARG:NH2	2.41	0.54
6:Z:9:VAL:HG12	6:Z:48:LEU:HB3	1.88	0.54
12:f:758:ASN:HB2	12:f:809:ILE:HG21	1.88	0.54
20:G:11:ARG:O	20:G:24:GLN:NE2	2.40	0.54
2:V:315:LYS:HE3	5:Y:385:ARG:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:467:TYR:OH	4:X:397:TYR:OH	2.22	0.54
12:f:139:CYS:O	12:f:143:ARG:NH1	2.41	0.54
12:f:202:HIS:ND1	12:f:242:GLU:OE2	2.41	0.54
12:f:447:ALA:HA	12:f:450:ILE:HD12	1.90	0.54
3:W:343:SER:HB3	3:W:347:GLY:H	1.73	0.53
12:f:680:ARG:HB2	12:f:763:ARG:HE	1.72	0.53
24:K:41:GLN:NE2	24:K:151:PRO:O	2.41	0.53
10:d:233:GLU:OE1	10:d:235:THR:OG1	2.26	0.53
17:E:75:ASN:ND2	18:F:129:ARG:O	2.41	0.53
18:F:192:ASP:HA	18:F:195:ILE:HD12	1.89	0.53
29:P:135:ASP:OD1	29:P:135:ASP:N	2.41	0.53
26:m:54:LEU:HB2	26:m:57:LEU:HG	1.90	0.53
10:d:19:CYS:SG	10:d:65:ARG:NH2	2.79	0.53
14:B:122:ILE:HD11	14:B:130:GLU:HB3	1.90	0.53
23:J:68:ASN:HA	23:J:211:MET:HE1	1.89	0.53
26:M:92:ARG:NH2	33:T:69:GLN:OE1	2.38	0.53
32:S:92:LEU:HD23	32:S:124:PHE:HE2	1.73	0.53
32:s:92:LEU:HD23	32:s:124:PHE:HE2	1.73	0.53
1:U:24:LEU:HD21	1:U:56:SER:HB3	1.91	0.53
1:U:642:GLU:O	15:C:53:ASN:ND2	2.42	0.53
12:f:828:ARG:HD2	12:f:843:SER:OG	2.07	0.53
14:B:111:THR:HB	14:B:124:SER:HB2	1.89	0.53
26:M:232:ARG:HG2	26:M:234:GLU:HG2	1.90	0.53
11:e:56:LEU:HG	11:e:63:HIS:HE1	1.72	0.53
20:g:212:PRO:HG3	20:g:239:LEU:HD23	1.90	0.53
26:m:232:ARG:HG2	26:m:234:GLU:HG2	1.90	0.53
2:V:282:ASN:ND2	5:Y:385:ARG:O	2.41	0.53
3:W:199:TYR:HD1	3:W:233:LEU:CD1	2.22	0.53
6:Z:128:PRO:HB2	6:Z:133:LEU:HD11	1.90	0.53
30:Q:117:TYR:HB3	30:Q:125:ALA:HB3	1.91	0.53
12:f:209:MET:HG3	12:f:211:ILE:H	1.72	0.53
14:B:383:LEU:HD11	14:B:419:PHE:HB3	1.91	0.53
20:G:6:SER:HB2	20:G:11:ARG:HE	1.73	0.53
20:g:6:SER:HB2	20:g:11:ARG:HE	1.74	0.53
24:k:41:GLN:NE2	24:k:151:PRO:O	2.41	0.53
1:U:185:MET:HA	1:U:194:ARG:HH12	1.74	0.53
3:W:245:LYS:NZ	3:W:245:LYS:HB3	2.21	0.53
4:X:177:TYR:HB3	4:X:182:ASN:HB3	1.91	0.53
12:f:240:VAL:HG13	12:f:257:ARG:HE	1.74	0.53
15:C:372:ARG:HH22	16:D:175:GLN:HE22	1.57	0.53
23:j:68:ASN:HA	23:j:211:MET:HE1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:n:18:SER:HB2	27:n:31:THR:H	1.74	0.53
1:U:68:PHE:HB3	1:U:73:ALA:HB3	1.91	0.53
3:W:405:LYS:HB2	3:W:417:ARG:HH12	1.74	0.53
6:Z:35:VAL:H	6:Z:97:THR:HG22	1.73	0.53
15:C:155:ASP:HA	15:C:158:ILE:HD12	1.91	0.53
32:S:35:ILE:HB	33:T:151:ARG:HH12	1.74	0.53
30:q:117:TYR:HB3	30:q:125:ALA:HB3	1.91	0.53
3:W:12:ARG:HD2	3:W:24:VAL:HG22	1.90	0.53
6:Z:10:VAL:CG2	6:Z:161:GLU:HG2	2.28	0.53
7:a:268:LEU:HD23	7:a:271:LYS:HD3	1.91	0.53
12:f:221:ILE:HA	12:f:224:ASN:HB2	1.90	0.53
12:f:497:VAL:HA	12:f:500:LEU:HB2	1.91	0.53
23:J:137:ASP:OD2	23:J:143:ARG:NH1	2.42	0.53
26:m:163:CYS:SG	26:m:164:ALA:N	2.82	0.53
15:C:351:MET:HB3	15:C:354:ALA:HB2	1.89	0.52
18:F:251:LEU:HD23	18:F:285:ILE:HG12	1.91	0.52
1:U:233:LEU:HD23	1:U:236:LEU:HD12	1.91	0.52
6:Z:37:GLY:HA2	6:Z:56:VAL:HG12	1.91	0.52
12:f:110:TYR:OH	12:f:118:ASN:ND2	2.43	0.52
14:B:355:LEU:HB3	14:B:356:PRO:HD2	1.90	0.52
14:B:411:ARG:NH2	14:B:418:ASP:OD2	2.42	0.52
16:D:154:LEU:HD12	16:D:227:PHE:HD2	1.73	0.52
18:F:340:PRO:HA	18:F:343:LEU:HB3	1.90	0.52
22:I:109:GLN:OE1	30:Q:71:ASN:ND2	2.42	0.52
27:N:18:SER:HB2	27:N:31:THR:H	1.74	0.52
28:O:31:CYS:SG	28:O:32:SER:N	2.77	0.52
12:f:873:LEU:HG	12:f:875:ALA:H	1.73	0.52
13:A:212:VAL:HG22	13:A:339:ARG:HB3	1.92	0.52
14:B:355:LEU:CG	14:B:356:PRO:HD2	2.29	0.52
3:W:63:THR:HB	3:W:68:VAL:HA	1.92	0.52
3:W:247:TYR:HB3	3:W:270:VAL:HG22	1.91	0.52
6:Z:39:LEU:H	6:Z:94:TRP:HA	1.74	0.52
12:f:291:GLN:HE21	12:f:879:ARG:HH21	1.56	0.52
12:f:836:GLU:H	12:f:840:LEU:HD21	1.73	0.52
15:C:192:PRO:HG2	15:C:194:THR:HG23	1.91	0.52
26:M:54:LEU:HB2	26:M:57:LEU:HG	1.90	0.52
32:S:123:SER:HB3	32:S:136:LYS:HG3	1.92	0.52
22:i:15:GLU:OE1	22:i:17:ARG:NE	2.39	0.52
26:m:34:SER:OG	26:m:65:ARG:NH2	2.32	0.52
2:V:92:ARG:NH2	2:V:118:GLN:OE1	2.43	0.52
12:f:816:TYR:HB3	12:f:821:LEU:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:189:GLU:O	13:A:193:THR:OG1	2.24	0.52
22:I:106:PRO:HD2	22:I:109:GLN:HE21	1.75	0.52
26:M:8:ASP:O	26:M:22:GLN:NE2	2.43	0.52
32:S:145:LEU:HD22	32:S:178:VAL:HB	1.92	0.52
4:X:253:TYR:OH	4:X:317:PRO:O	2.28	0.52
9:c:27:THR:HG23	9:c:176:GLN:H	1.74	0.52
3:W:165:ILE:HD13	3:W:189:GLN:HB3	1.92	0.52
3:W:220:GLU:OE2	3:W:221:LYS:NZ	2.42	0.52
12:f:94:LYS:HA	12:f:97:LYS:HB2	1.92	0.52
12:f:809:ILE:HG23	12:f:810:ILE:HG12	1.91	0.52
20:G:67:THR:HG22	20:G:69:LEU:H	1.75	0.52
24:k:99:HIS:HB2	24:k:107:MET:HE3	1.92	0.52
28:o:100:LEU:HB3	28:o:111:TYR:HB2	1.91	0.52
18:F:175:MET:HA	18:F:250:LYS:HE3	1.92	0.52
22:I:15:GLU:OE1	22:I:17:ARG:NE	2.39	0.52
23:j:137:ASP:OD2	23:j:143:ARG:NH1	2.42	0.52
3:W:65:ARG:HG3	3:W:67:LEU:H	1.76	0.51
6:Z:259:VAL:HG22	9:c:292:MET:HA	1.92	0.51
21:h:148:GLN:OE1	21:h:158:TRP:NE1	2.43	0.51
26:m:214:SER:OG	26:m:224:HIS:NE2	2.35	0.51
1:U:265:ILE:HD11	1:U:326:ILE:HG23	1.92	0.51
3:W:177:MET:SD	3:W:177:MET:N	2.82	0.51
13:A:363:SER:HB2	14:B:214:MET:HG2	1.91	0.51
15:C:375:ARG:HG2	15:C:377:HIS:H	1.74	0.51
32:S:35:ILE:O	33:T:151:ARG:NH2	2.37	0.51
22:i:161:ALA:HB1	22:i:175:LEU:HD13	1.92	0.51
29:p:126:LEU:HD12	29:p:127:ILE:HG23	1.92	0.51
32:s:145:LEU:HD22	32:s:178:VAL:HB	1.92	0.51
3:W:451:MET:O	3:W:455:LEU:O	2.29	0.51
12:f:571:GLU:HG3	12:f:573:ILE:H	1.73	0.51
20:G:137:CYS:SG	20:G:138:MET:N	2.73	0.51
28:O:100:LEU:HB3	28:O:111:TYR:HB2	1.91	0.51
6:Z:216:ALA:C	6:Z:218:GLY:N	2.60	0.51
7:a:247:ARG:HH21	7:a:250:THR:HG23	1.76	0.51
22:I:29:GLY:HA3	22:I:166:ASN:HB2	1.93	0.51
25:l:41:LYS:NZ	25:l:180:MET:O	2.44	0.51
28:o:174:ASP:OD2	28:o:187:ARG:NH1	2.44	0.51
13:A:181:LYS:HD2	13:A:184:ILE:HD12	1.92	0.51
5:Y:141:VAL:HG11	5:Y:164:ALA:HB2	1.91	0.51
5:Y:155:ASP:O	5:Y:158:THR:OG1	2.27	0.51
12:f:812:GLY:HA3	12:f:853:VAL:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:407:LEU:HD21	15:C:178:LEU:HB2	1.93	0.51
29:P:126:LEU:HD12	29:P:127:ILE:HG23	1.92	0.51
24:k:191:LEU:HD21	24:k:221:GLN:HE21	1.75	0.51
1:U:637:VAL:HG13	1:U:652:ALA:HB1	1.93	0.51
3:W:455:LEU:HD23	3:W:455:LEU:C	2.34	0.51
16:D:175:GLN:NE2	16:D:179:GLU:OE2	2.44	0.51
21:H:148:GLN:OE1	21:H:158:TRP:NE1	2.43	0.51
21:H:185:GLU:O	21:H:229:TYR:OH	2.28	0.51
24:K:191:LEU:HD21	24:K:221:GLN:HE21	1.75	0.51
26:M:163:CYS:SG	26:M:164:ALA:N	2.82	0.51
1:U:100:ILE:HG22	1:U:103:LYS:HZ1	1.76	0.51
15:C:69:GLN:HG3	15:C:118:ASN:HD21	1.76	0.51
29:p:65:GLN:OE1	30:q:86:ARG:NH2	2.43	0.51
10:d:44:THR:OG1	10:d:47:GLN:NE2	2.42	0.51
12:f:828:ARG:CZ	12:f:843:SER:HG	2.23	0.51
28:O:174:ASP:OD2	28:O:187:ARG:NH1	2.44	0.51
33:T:9:THR:OG1	33:T:10:SER:N	2.44	0.51
7:a:70:ARG:HH21	8:b:17:ARG:HA	1.76	0.51
12:f:149:GLU:HG3	12:f:152:ALA:HB2	1.93	0.51
14:B:164:MET:HG2	14:B:166:ASP:H	1.76	0.51
16:D:283:ARG:HG2	16:D:287:ARG:HH11	1.76	0.51
6:Z:209:ARG:NH2	7:a:350:LYS:O	2.45	0.50
12:f:796:LEU:HA	12:f:799:VAL:HG12	1.93	0.50
13:A:258:ARG:HA	13:A:305:GLN:HE22	1.76	0.50
22:i:106:PRO:HD2	22:i:109:GLN:HE21	1.75	0.50
32:s:47:THR:OG1	32:s:48:ASP:N	2.45	0.50
32:s:123:SER:HB3	32:s:136:LYS:HG3	1.92	0.50
2:V:495:ARG:HB2	15:C:44:ARG:HG3	1.94	0.50
12:f:682:GLY:HA3	12:f:687:ARG:HH11	1.76	0.50
12:f:705:ASN:HB3	12:f:787:LEU:HD21	1.92	0.50
23:J:121:SER:OG	23:J:122:ASN:N	2.44	0.50
22:i:29:GLY:HA3	22:i:166:ASN:HB2	1.93	0.50
29:p:2:SER:OG	29:p:3:ILE:N	2.44	0.50
5:Y:26:LEU:HD21	5:Y:60:SER:HB2	1.93	0.50
32:S:209:SER:OG	32:S:212:LYS:NZ	2.44	0.50
20:g:67:THR:HG22	20:g:69:LEU:H	1.75	0.50
20:g:158:GLY:O	21:h:84:ARG:NH2	2.44	0.50
22:i:216:LEU:HD12	22:i:225:ILE:HG12	1.94	0.50
24:k:101:PHE:HA	31:r:57:ARG:HH21	1.76	0.50
32:s:209:SER:OG	32:s:212:LYS:NZ	2.44	0.50
2:V:412:LEU:O	5:Y:346:LYS:NZ	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:212:GLU:HG3	5:Y:213:LEU:HG	1.94	0.50
10:d:87:GLU:HA	10:d:89:LEU:HD23	1.93	0.50
16:D:173:GLN:HE22	16:D:334:PRO:HD2	1.76	0.50
17:E:153:LEU:HD12	17:E:154:THR:HG23	1.92	0.50
17:E:237:ALA:O	18:F:304:ARG:NH1	2.44	0.50
20:G:158:GLY:O	21:H:84:ARG:NH2	2.43	0.50
30:q:38:MET:O	30:q:65:GLN:NE2	2.44	0.50
17:E:234:GLU:N	17:E:278:ALA:O	2.45	0.50
20:G:32:ILE:HA	20:G:82:GLY:HA2	1.93	0.50
22:I:161:ALA:HB1	22:I:175:LEU:HD13	1.92	0.50
24:K:99:HIS:HB2	24:K:107:MET:HE3	1.92	0.50
25:L:41:LYS:NZ	25:L:180:MET:O	2.44	0.50
21:h:14:SER:HG	21:h:18:LYS:H	1.58	0.50
23:j:121:SER:OG	23:j:122:ASN:N	2.44	0.50
5:Y:102:ASP:HA	5:Y:105:MET:HG2	1.94	0.50
9:c:167:MET:HE1	9:c:174:PRO:HG3	1.92	0.50
12:f:119:LYS:HA	12:f:122:ALA:HB3	1.94	0.50
12:f:252:ALA:O	12:f:257:ARG:NH1	2.45	0.50
16:D:78:GLU:OE1	16:D:81:ARG:NH1	2.44	0.50
16:D:259:PRO:HB3	16:D:304:ASN:HB3	1.93	0.50
17:E:182:LEU:HD22	35:E:401:ATP:H2'	1.94	0.50
1:U:764:LEU:O	1:U:767:THR:OG1	2.28	0.50
6:Z:144:VAL:O	6:Z:152:SER:N	2.39	0.50
9:c:244:VAL:HB	9:c:291:LEU:HD11	1.94	0.50
12:f:612:LEU:HD21	12:f:636:ASP:HA	1.94	0.50
17:E:97:ARG:HH21	17:E:111:LEU:HB3	1.75	0.50
25:l:225:ASP:OD1	25:l:225:ASP:N	2.44	0.50
22:i:245:ALA:O	22:i:249:ARG:NH2	2.45	0.50
3:W:53:GLN:OE1	3:W:99:GLN:NE2	2.44	0.49
3:W:245:LYS:NZ	3:W:245:LYS:CB	2.73	0.49
3:W:401:THR:HG23	3:W:402:ILE:HD12	1.93	0.49
5:Y:177:ARG:NH2	5:Y:206:SER:OG	2.34	0.49
5:Y:184:GLN:NE2	5:Y:196:GLN:O	2.32	0.49
5:Y:300:ARG:NH2	11:e:59:GLU:OE1	2.38	0.49
22:I:57:ASP:HB3	22:I:59:VAL:HG13	1.93	0.49
26:M:214:SER:OG	26:M:224:HIS:NE2	2.36	0.49
27:N:29:ARG:HH21	33:t:179:ARG:HG2	1.77	0.49
32:S:191:ASP:O	32:S:210:LEU:N	2.45	0.49
20:g:32:ILE:HA	20:g:82:GLY:HA2	1.93	0.49
32:s:191:ASP:O	32:s:210:LEU:N	2.45	0.49
2:V:106:ARG:O	2:V:110:HIS:ND1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:373:ALA:HB2	12:f:744:MET:HA	1.94	0.49
16:D:351:LYS:NZ	17:E:163:GLY:O	2.46	0.49
32:S:16:ALA:HB2	32:S:121:VAL:HG23	1.95	0.49
26:m:139:SER:OG	26:m:140:TYR:N	2.45	0.49
30:q:21:ALA:HB3	30:q:29:LYS:HB3	1.94	0.49
1:U:373:ASN:HA	1:U:376:MET:HG2	1.94	0.49
1:U:724:VAL:HG11	9:c:175:ARG:HH11	1.77	0.49
4:X:122:ARG:HD2	4:X:125:LEU:HB2	1.95	0.49
9:c:178:THR:HG23	9:c:181:LEU:HD23	1.93	0.49
12:f:369:ARG:NH2	12:f:791:VAL:O	2.45	0.49
12:f:852:VAL:O	12:f:854:GLY:N	2.43	0.49
7:a:235:ASP:OD2	7:a:249:GLN:NE2	2.45	0.49
12:f:482:ILE:HG22	12:f:501:LEU:HD22	1.95	0.49
16:D:86:PRO:HB3	17:E:81:VAL:HG12	1.94	0.49
28:O:96:ALA:H	28:O:115:PRO:HB3	1.77	0.49
5:Y:160:ASN:HA	5:Y:163:LYS:HB2	1.92	0.49
12:f:469:TYR:O	12:f:472:HIS:ND1	2.32	0.49
18:F:35:LYS:HD3	18:F:38:THR:HB	1.94	0.49
22:I:245:ALA:O	22:I:249:ARG:NH2	2.45	0.49
2:V:210:CYS:O	2:V:214:HIS:N	2.43	0.49
12:f:813:LYS:NZ	12:f:819:TYR:OH	2.34	0.49
17:E:336:ASP:O	17:E:378:LYS:NZ	2.44	0.49
22:I:102:GLN:HG2	30:Q:82:ASN:ND2	2.27	0.49
15:C:277:LEU:O	15:C:310:ARG:NH1	2.36	0.49
22:i:57:ASP:HB3	22:i:59:VAL:HG13	1.93	0.49
29:p:49:LEU:HD21	29:p:87:LEU:HD22	1.94	0.49
3:W:36:LYS:HG3	3:W:86:ASN:HD21	1.78	0.49
3:W:239:SER:O	3:W:243:ILE:HD12	2.12	0.49
5:Y:175:ASP:OD1	5:Y:175:ASP:N	2.44	0.49
6:Z:212:LEU:CA	6:Z:215:VAL:HG12	2.39	0.49
7:a:186:LYS:HB3	7:a:193:GLN:HE22	1.78	0.49
7:a:374:ILE:HG21	10:d:251:ARG:HA	1.94	0.49
14:B:411:ARG:NH1	14:B:413:LYS:O	2.46	0.49
18:F:362:ARG:NH2	18:F:388:THR:O	2.46	0.49
1:U:796:LYS:HA	1:U:924:LEU:HD11	1.93	0.49
3:W:72:LYS:HD3	3:W:123:ARG:HD2	1.95	0.49
3:W:268:LYS:HE2	3:W:299:ILE:HG21	1.93	0.49
3:W:359:VAL:HG23	3:W:382:LEU:HD22	1.95	0.49
6:Z:12:HIS:CB	6:Z:13:PRO:CD	2.83	0.49
22:i:3:ARG:HB2	23:j:5:ARG:HH12	1.78	0.49
9:c:100:LYS:HG2	9:c:105:PRO:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:171:GLN:HG3	12:f:179:VAL:HG22	1.95	0.49
12:f:257:ARG:HG2	12:f:272:LEU:HD13	1.94	0.49
14:B:125:THR:OG1	14:B:126:SER:N	2.46	0.49
22:I:216:LEU:HD12	22:I:225:ILE:HG12	1.94	0.49
1:U:414:GLY:H	1:U:449:ILE:HG23	1.78	0.48
6:Z:190:ARG:HH11	9:c:297:VAL:HG11	1.78	0.48
6:Z:192:THR:O	6:Z:196:HIS:ND1	2.44	0.48
14:B:109:VAL:HG11	15:C:94:LYS:HE2	1.94	0.48
14:B:387:LYS:HG2	14:B:427:LEU:HD13	1.95	0.48
25:L:182:CYS:HB2	25:L:186:GLU:HG3	1.95	0.48
30:Q:38:MET:O	30:Q:65:GLN:NE2	2.44	0.48
32:S:47:THR:OG1	32:S:48:ASP:N	2.45	0.48
23:j:32:ALA:HB2	23:j:45:VAL:HG23	1.95	0.48
26:m:40:ARG:HE	26:m:161:TRP:CD1	2.31	0.48
2:V:290:TYR:OH	2:V:294:ARG:NH2	2.46	0.48
5:Y:364:TRP:NE1	5:Y:368:GLU:OE2	2.46	0.48
7:a:247:ARG:HH12	7:a:251:LEU:HD13	1.78	0.48
12:f:240:VAL:O	12:f:257:ARG:NH2	2.36	0.48
18:F:164:LEU:O	18:F:166:THR:N	2.46	0.48
23:J:32:ALA:HB2	23:J:45:VAL:HG23	1.95	0.48
26:m:92:ARG:NH2	33:t:69:GLN:OE1	2.41	0.48
1:U:646:PRO:O	1:U:650:TYR:N	2.46	0.48
13:A:101:ILE:HB	13:A:137:GLY:H	1.78	0.48
26:M:195:LYS:O	26:M:199:ILE:N	2.43	0.48
29:P:2:SER:OG	29:P:3:ILE:N	2.44	0.48
29:P:49:LEU:HD21	29:P:87:LEU:HD22	1.94	0.48
27:n:76:VAL:HG23	27:n:104:ASP:HB2	1.95	0.48
1:U:363:SER:HB2	9:c:175:ARG:HH12	1.78	0.48
3:W:202:THR:HG22	3:W:233:LEU:CD2	2.33	0.48
3:W:374:THR:HG23	7:a:326:GLU:HB3	1.95	0.48
14:B:423:LYS:HG2	14:B:427:LEU:HD12	1.96	0.48
16:D:271:ALA:HA	16:D:289:LEU:HD21	1.95	0.48
20:g:84:THR:HB	26:m:156:VAL:HG22	1.96	0.48
27:n:18:SER:HB2	27:n:30:VAL:HA	1.96	0.48
28:o:96:ALA:H	28:o:115:PRO:HB3	1.77	0.48
3:W:238:GLY:O	3:W:240:TYR:CD1	2.67	0.48
3:W:240:TYR:CD2	3:W:276:LEU:O	2.66	0.48
12:f:23:GLY:HA3	12:f:34:ARG:HH22	1.78	0.48
12:f:482:ILE:HD11	12:f:517:VAL:HG23	1.95	0.48
13:A:236:CYS:HB3	13:A:270:CYS:HA	1.96	0.48
13:A:365:GLU:HG2	13:A:367:ASP:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:355:LEU:CB	14:B:356:PRO:HD2	2.39	0.48
16:D:248:ARG:NH2	16:D:291:GLU:OE1	2.47	0.48
16:D:255:LYS:HD3	16:D:302:ASN:HB3	1.94	0.48
18:F:94:ILE:HD11	18:F:125:LYS:HE3	1.95	0.48
21:H:222:THR:OG1	21:H:225:GLU:OE1	2.26	0.48
31:R:1:THR:N	31:R:169:TYR:O	2.47	0.48
3:W:268:LYS:HB3	3:W:336:PRO:HG2	1.94	0.48
6:Z:220:LEU:C	6:Z:220:LEU:CD1	2.86	0.48
12:f:487:LEU:HD11	12:f:804:LEU:HD12	1.95	0.48
16:D:398:ASP:OD1	16:D:398:ASP:N	2.44	0.48
32:s:148:LEU:HD23	32:s:178:VAL:HG12	1.95	0.48
4:X:187:ARG:HH21	4:X:217:ILE:HG22	1.78	0.48
12:f:288:VAL:HA	12:f:291:GLN:HG2	1.94	0.48
15:C:80:MET:SD	15:C:80:MET:N	2.83	0.48
25:L:148:CYS:SG	25:L:150:SER:OG	2.64	0.48
25:L:225:ASP:N	25:L:225:ASP:OD1	2.44	0.48
25:l:148:CYS:SG	25:l:150:SER:OG	2.64	0.48
32:s:4:PRO:HB2	33:t:100:ARG:HH21	1.78	0.48
3:W:350:ARG:HA	3:W:353:ASP:HB2	1.95	0.48
6:Z:18:SER:O	6:Z:21:ASP:CB	2.62	0.48
18:F:236:LEU:H	18:F:238:ARG:HH11	1.61	0.48
30:Q:21:ALA:HB3	30:Q:29:LYS:HB3	1.94	0.48
31:R:182:ASP:N	31:R:182:ASP:OD1	2.46	0.48
20:g:190:THR:OG1	20:g:191:PHE:N	2.47	0.48
27:N:19:ARG:NH2	33:t:180:ASP:O	2.43	0.48
32:S:148:LEU:HD23	32:S:178:VAL:HG12	1.95	0.48
32:s:16:ALA:HB2	32:s:121:VAL:HG23	1.94	0.48
33:t:43:MET:HE3	33:t:45:VAL:HG22	1.95	0.48
1:U:415:HIS:HB3	1:U:418:GLU:HB3	1.95	0.48
1:U:456:ASP:O	1:U:460:TYR:N	2.44	0.48
5:Y:40:GLU:O	5:Y:44:ALA:N	2.44	0.48
7:a:131:THR:HA	7:a:134:THR:HG22	1.96	0.48
16:D:147:ALA:HB1	17:E:62:LYS:HD3	1.96	0.48
21:H:50:LYS:HE2	21:H:59:GLU:HG3	1.96	0.48
33:T:43:MET:HE3	33:T:45:VAL:HG22	1.95	0.48
33:T:212:ALA:HA	27:n:30:VAL:HG21	1.95	0.48
31:r:182:ASP:OD1	31:r:182:ASP:N	2.47	0.48
1:U:24:LEU:HA	1:U:27:LEU:HB2	1.96	0.47
2:V:55:THR:HG21	2:V:196:SER:HB3	1.95	0.47
3:W:72:LYS:HD3	3:W:123:ARG:HA	1.96	0.47
3:W:216:GLU:OE1	3:W:223:LYS:NZ	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:437:GLY:O	22:I:155:ASN:ND2	2.47	0.47
17:E:270:LEU:HG	17:E:273:VAL:HB	1.96	0.47
26:M:40:ARG:HE	26:M:161:TRP:CD1	2.31	0.47
26:M:139:SER:OG	26:M:140:TYR:N	2.46	0.47
21:h:185:GLU:O	21:h:229:TYR:OH	2.28	0.47
21:h:222:THR:OG1	21:h:225:GLU:OE1	2.26	0.47
25:l:182:CYS:HB2	25:l:186:GLU:HG3	1.95	0.47
29:p:62:THR:OG1	30:q:85:ARG:NH2	2.44	0.47
6:Z:16:LEU:HD11	9:c:216:MET:HE2	1.96	0.47
7:a:70:ARG:O	8:b:17:ARG:NH1	2.47	0.47
12:f:612:LEU:HA	12:f:632:LYS:HD2	1.96	0.47
13:A:204:LEU:HD23	18:F:374:ASN:HB3	1.96	0.47
15:C:168:PRO:HG3	15:C:175:PHE:HE2	1.79	0.47
21:H:66:GLU:OE2	21:H:91:ARG:NH2	2.47	0.47
21:h:50:LYS:HE2	21:h:59:GLU:HG3	1.96	0.47
24:k:167:ALA:H	25:l:56:LEU:HD13	1.79	0.47
26:m:17:ASP:OD2	26:m:19:ARG:NH2	2.47	0.47
1:U:141:CYS:HA	15:C:20:LEU:HD13	1.95	0.47
1:U:187:LEU:HB2	16:D:45:LYS:HG2	1.95	0.47
4:X:173:GLU:HA	4:X:176:THR:HG22	1.95	0.47
15:C:337:ASN:ND2	15:C:376:VAL:O	2.47	0.47
16:D:249:ASP:OD1	16:D:252:ARG:NH2	2.47	0.47
17:E:60:VAL:HA	17:E:71:VAL:HG12	1.95	0.47
17:E:197:LYS:HE2	18:F:320:PHE:HB2	1.97	0.47
22:i:62:SER:OG	22:i:65:ILE:O	2.33	0.47
1:U:643:SER:O	15:C:57:ARG:NH2	2.32	0.47
6:Z:278:ASN:O	6:Z:282:ASN:N	2.45	0.47
12:f:243:PRO:HD2	12:f:257:ARG:HH22	1.79	0.47
12:f:742:ALA:O	12:f:746:ARG:NE	2.40	0.47
18:F:168:TYR:HE2	18:F:172:VAL:HB	1.79	0.47
20:g:141:ILE:HG22	20:g:151:VAL:HG22	1.96	0.47
3:W:23:THR:HA	3:W:26:GLN:HB2	1.95	0.47
5:Y:128:TYR:O	5:Y:131:THR:OG1	2.28	0.47
6:Z:8:LYS:HE3	6:Z:47:VAL:CG2	2.45	0.47
6:Z:212:LEU:HD13	7:a:350:LYS:HB3	1.95	0.47
10:d:8:GLU:O	10:d:13:SER:OG	2.27	0.47
26:M:17:ASP:OD2	26:M:19:ARG:NH2	2.47	0.47
2:V:94:VAL:HA	2:V:138:PRO:HA	1.96	0.47
3:W:241:LEU:HD23	3:W:277:ALA:CB	2.44	0.47
7:a:148:VAL:HG12	7:a:150:SER:H	1.79	0.47
12:f:93:PRO:HB2	12:f:97:LYS:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:253:LEU:HD11	12:f:272:LEU:HB3	1.95	0.47
12:f:469:TYR:OH	12:f:478:ARG:NH1	2.47	0.47
15:C:253:SER:HB3	16:D:290:LEU:HD12	1.97	0.47
27:N:76:VAL:HG23	27:N:104:ASP:HB2	1.95	0.47
26:m:8:ASP:O	26:m:22:GLN:NE2	2.43	0.47
1:U:802:TYR:O	1:U:878:LEU:N	2.45	0.47
3:W:166:LEU:HD23	3:W:169:LEU:HD12	1.97	0.47
3:W:245:LYS:HB3	3:W:245:LYS:HE2	1.68	0.47
6:Z:10:VAL:CG1	6:Z:163:GLY:HA3	2.44	0.47
8:b:6:THR:HG21	8:b:40:LYS:HG3	1.96	0.47
12:f:168:LYS:HD3	12:f:204:ALA:HB1	1.97	0.47
12:f:281:ILE:HA	12:f:282:PHE:HA	1.54	0.47
14:B:112:LEU:HD12	14:B:148:CYS:HB2	1.97	0.47
15:C:71:SER:OG	15:C:72:TYR:N	2.48	0.47
15:C:405:TRP:HE1	22:I:30:HIS:HB2	1.79	0.47
16:D:133:HIS:HB3	16:D:137:ASN:H	1.79	0.47
16:D:272:THR:HA	16:D:317:LEU:HA	1.95	0.47
22:I:136:TYR:HB2	22:I:148:TYR:HB2	1.96	0.47
27:N:18:SER:HB2	27:N:30:VAL:HA	1.95	0.47
22:i:136:TYR:HE2	22:i:150:SER:HB3	1.80	0.47
22:i:136:TYR:HB2	22:i:148:TYR:HB2	1.96	0.47
24:k:105:GLU:OE2	32:s:75:TYR:OH	2.23	0.47
31:r:1:THR:N	31:r:169:TYR:O	2.47	0.47
1:U:147:TYR:OH	1:U:169:GLU:OE1	2.29	0.47
3:W:12:ARG:HE	3:W:27:ARG:HD2	1.79	0.47
7:a:130:VAL:O	7:a:134:THR:N	2.45	0.47
7:a:291:LEU:O	7:a:331:VAL:N	2.47	0.47
10:d:33:LEU:HD23	10:d:47:GLN:HE22	1.80	0.47
12:f:717:ALA:HB1	12:f:760:PHE:HB2	1.97	0.47
22:I:62:SER:OG	22:I:65:ILE:O	2.33	0.47
2:V:39:GLU:HB3	2:V:65:ARG:HH22	1.80	0.47
4:X:290:VAL:HG13	4:X:302:PHE:HE1	1.80	0.47
12:f:269:ALA:O	12:f:273:ASN:N	2.42	0.47
13:A:346:PRO:HB2	13:A:351:ARG:HG3	1.97	0.47
18:F:330:ALA:HB3	18:F:348:LEU:HD21	1.97	0.47
21:H:65:VAL:HG11	21:H:211:GLY:HA3	1.96	0.47
31:r:18:SER:HB2	31:r:31:VAL:H	1.80	0.47
1:U:554:LEU:HD12	1:U:588:MET:HE1	1.97	0.46
6:Z:259:VAL:HG21	9:c:295:ASN:HB2	1.96	0.46
8:b:24:THR:HG22	8:b:26:LEU:H	1.80	0.46
21:h:66:GLU:OE2	21:h:91:ARG:NH2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:12:ARG:NH2	3:W:23:THR:OG1	2.38	0.46
6:Z:215:VAL:HG22	6:Z:215:VAL:O	2.14	0.46
6:Z:252:LYS:HE2	9:c:299:CYS:HB2	1.98	0.46
13:A:290:GLY:H	14:B:298:ASN:HB3	1.80	0.46
16:D:204:MET:HE3	16:D:310:ALA:HB2	1.97	0.46
17:E:3:ASP:OD1	17:E:3:ASP:N	2.40	0.46
17:E:199:VAL:HG23	17:E:201:SER:H	1.80	0.46
1:U:607:VAL:HG11	16:D:64:GLU:HA	1.98	0.46
3:W:234:ASP:CB	3:W:243:ILE:CG1	2.79	0.46
12:f:637:LYS:HE2	12:f:673:ARG:HB2	1.96	0.46
13:A:144:ARG:HB2	19:v:19:UNK:CB	2.45	0.46
13:A:364:VAL:HA	13:A:404:ALA:HB3	1.97	0.46
16:D:131:ALA:HB3	16:D:141:ASP:H	1.80	0.46
18:F:294:LYS:HA	18:F:339:ASP:HB3	1.98	0.46
25:L:215:VAL:HB	25:L:221:PHE:HD1	1.80	0.46
22:i:228:LEU:H	22:i:228:LEU:HG	1.53	0.46
25:l:117:GLN:O	25:l:120:THR:OG1	2.33	0.46
4:X:394:ASP:N	4:X:394:ASP:OD1	2.46	0.46
6:Z:129:LYS:NZ	9:c:211:GLU:OE2	2.48	0.46
6:Z:219:LYS:HA	6:Z:219:LYS:HD2	1.50	0.46
7:a:34:TRP:HD1	8:b:18:ASN:HA	1.80	0.46
12:f:640:LYS:HD3	12:f:651:GLY:HA3	1.96	0.46
13:A:122:VAL:HB	18:F:88:TYR:HB2	1.97	0.46
20:G:141:ILE:HG22	20:G:151:VAL:HG22	1.96	0.46
4:X:50:ILE:O	4:X:54:GLY:N	2.44	0.46
6:Z:11:VAL:CB	6:Z:50:VAL:HB	2.45	0.46
12:f:202:HIS:CE1	12:f:241:PRO:HB2	2.50	0.46
16:D:225:ALA:HB1	16:D:260:ALA:HA	1.97	0.46
17:E:285:LEU:HD12	17:E:290:LEU:HD11	1.97	0.46
25:l:45:VAL:HG11	25:l:188:VAL:HG22	1.96	0.46
25:l:215:VAL:HB	25:l:221:PHE:HD1	1.80	0.46
6:Z:198:LEU:HD22	7:a:364:GLU:HB2	1.97	0.46
14:B:389:ASP:OD1	14:B:389:ASP:N	2.48	0.46
1:U:900:TYR:HB3	1:U:914:LEU:HD11	1.97	0.46
12:f:505:MET:HE3	12:f:537:THR:HG22	1.98	0.46
22:I:136:TYR:HE2	22:I:150:SER:HB3	1.80	0.46
1:U:700:GLU:OE1	1:U:707:ASN:ND2	2.49	0.46
8:b:14:GLU:N	8:b:82:GLY:O	2.48	0.46
16:D:238:LYS:HZ3	16:D:238:LYS:CB	2.29	0.46
18:F:334:ARG:HH22	18:F:336:ASP:HB2	1.80	0.46
21:H:9:SER:OG	21:H:123:GLN:O	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:146:LYS:HE2	1:U:148:LYS:HB2	1.97	0.46
3:W:200:ILE:HD12	3:W:203:GLN:HE21	1.80	0.46
4:X:400:ALA:O	4:X:403:THR:OG1	2.34	0.46
5:Y:174:TRP:HE1	16:D:192:LYS:HB3	1.80	0.46
6:Z:110:GLU:OE2	6:Z:153:LYS:NZ	2.49	0.46
12:f:626:GLU:OE1	12:f:665:GLU:HB3	2.16	0.46
16:D:162:VAL:O	16:D:221:HIS:ND1	2.48	0.46
25:L:45:VAL:HG11	25:L:188:VAL:HG22	1.96	0.46
33:T:7:THR:OG1	33:T:182:ARG:NH2	2.49	0.46
1:U:108:TYR:OH	1:U:159:ARG:NH1	2.49	0.46
1:U:490:ARG:HB3	1:U:493:VAL:HG12	1.98	0.46
5:Y:312:ARG:HA	5:Y:356:THR:HG22	1.97	0.46
14:B:106:PRO:HB3	15:C:121:TYR:HB2	1.98	0.46
14:B:247:PHE:HD1	14:B:281:ILE:HB	1.81	0.46
16:D:239:TYR:CD1	16:D:239:TYR:N	2.81	0.46
21:h:9:SER:OG	21:h:123:GLN:O	2.25	0.46
21:h:65:VAL:HG11	21:h:211:GLY:HA3	1.96	0.46
8:b:34:ASN:O	8:b:38:HIS:ND1	2.36	0.45
17:E:363:VAL:HG13	17:E:365:GLU:H	1.81	0.45
2:V:353:LEU:HG	2:V:357:LEU:HB3	1.99	0.45
3:W:312:MET:HG3	3:W:315:MET:HG2	1.98	0.45
4:X:282:ARG:NH2	4:X:312:GLU:OE2	2.49	0.45
7:a:145:LEU:HD12	7:a:148:VAL:HG23	1.98	0.45
12:f:778:LEU:HA	12:f:803:PHE:HB3	1.99	0.45
20:G:182:LYS:HD3	20:G:185:LYS:HE2	1.98	0.45
22:I:10:THR:HG23	23:J:125:ARG:HB2	1.98	0.45
25:L:105:VAL:HG21	25:L:136:GLY:HA3	1.98	0.45
1:U:742:HIS:O	1:U:883:ARG:NE	2.47	0.45
4:X:316:ASP:OD1	4:X:319:ILE:N	2.48	0.45
6:Z:25:ARG:HH22	9:c:71:ASP:HB2	1.81	0.45
12:f:75:LEU:HD12	12:f:78:LEU:HD13	1.98	0.45
12:f:417:ILE:HG22	12:f:418:LEU:HD12	1.98	0.45
12:f:827:PRO:HG2	12:f:848:GLN:HB3	1.96	0.45
16:D:268:ASP:OD1	16:D:268:ASP:N	2.49	0.45
27:N:26:ILE:O	33:t:179:ARG:NH1	2.47	0.45
31:R:18:SER:HB2	31:R:31:VAL:H	1.80	0.45
5:Y:207:THR:HG22	5:Y:216:TYR:CZ	2.51	0.45
6:Z:169:GLU:HA	6:Z:172:VAL:HB	1.98	0.45
17:E:279:THR:OG1	17:E:280:ASN:N	2.50	0.45
31:R:44:THR:HG21	31:R:100:MET:HE3	1.98	0.45
33:t:7:THR:OG1	33:t:182:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:33:GLN:NE2	2:V:83:GLU:O	2.50	0.45
5:Y:203:ASP:OD1	5:Y:203:ASP:N	2.35	0.45
7:a:315:LEU:HD23	7:a:320:VAL:HG13	1.99	0.45
8:b:138:VAL:HB	8:b:160:LEU:HD11	1.99	0.45
15:C:298:ILE:H	15:C:298:ILE:HG13	1.66	0.45
19:v:11:UNK:O	19:v:12:UNK:CB	2.64	0.45
32:S:4:PRO:HB2	33:T:100:ARG:HH21	1.80	0.45
20:g:182:LYS:HD3	20:g:185:LYS:HE2	1.99	0.45
3:W:246:HIS:O	3:W:250:ILE:HG12	2.17	0.45
7:a:190:VAL:HA	7:a:193:GLN:HB2	1.99	0.45
8:b:9:CYS:HB3	8:b:111:ALA:HA	1.99	0.45
13:A:102:ILE:HD12	13:A:112:ILE:HG22	1.98	0.45
15:C:113:ARG:NH2	15:C:129:ASN:O	2.39	0.45
16:D:267:ILE:HG22	16:D:270:ILE:HD11	1.98	0.45
30:Q:11:ASP:N	30:Q:11:ASP:OD1	2.49	0.45
32:S:187:VAL:HG21	28:o:24:MET:HE3	1.97	0.45
25:l:189:LYS:O	25:l:193:ARG:NH1	2.50	0.45
31:r:44:THR:HG21	31:r:100:MET:HE3	1.98	0.45
5:Y:117:LYS:HD3	5:Y:151:TYR:HD2	1.81	0.45
5:Y:179:ARG:HA	5:Y:179:ARG:HD3	1.80	0.45
12:f:608:LYS:HE3	12:f:608:LYS:HB3	1.85	0.45
16:D:212:LYS:HG2	16:D:333:PHE:HD2	1.82	0.45
25:L:189:LYS:O	25:L:193:ARG:NH1	2.50	0.45
26:M:41:CYS:HB3	26:M:189:ILE:HG13	1.99	0.45
30:Q:59:TYR:O	30:Q:63:ASN:ND2	2.50	0.45
26:m:195:LYS:O	26:m:199:ILE:N	2.43	0.45
3:W:245:LYS:C	3:W:247:TYR:N	2.74	0.45
5:Y:316:LEU:HD13	5:Y:327:VAL:HG13	1.98	0.45
6:Z:215:VAL:O	6:Z:222:ILE:HG22	2.17	0.45
12:f:24:THR:HG23	12:f:31:LYS:HG3	1.97	0.45
13:A:78:TRP:HZ3	14:B:99:VAL:HG21	1.80	0.45
20:G:190:THR:OG1	20:G:191:PHE:N	2.47	0.45
21:H:111:VAL:HG21	21:H:147:PHE:HD2	1.82	0.45
28:O:144:PRO:HB3	33:t:214:MET:HE1	1.99	0.45
24:k:85:ALA:HB2	24:k:139:VAL:HG21	1.99	0.45
2:V:234:ARG:HA	2:V:237:THR:HG22	1.98	0.45
2:V:387:GLN:HA	2:V:392:TYR:HE1	1.82	0.45
3:W:12:ARG:HD3	3:W:12:ARG:HA	1.79	0.45
3:W:152:ILE:HG13	3:W:161:GLU:HB3	1.99	0.45
6:Z:9:VAL:HG11	6:Z:48:LEU:HD22	1.90	0.45
6:Z:196:HIS:HA	6:Z:199:LYS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:8:GLU:H	10:d:18:LYS:HE3	1.82	0.45
12:f:403:LYS:HG3	12:f:406:GLY:H	1.82	0.45
13:A:167:GLU:HG2	13:A:236:CYS:HA	1.98	0.45
14:B:120:HIS:HA	14:B:134:SER:HA	1.98	0.45
15:C:304:ALA:O	15:C:307:ARG:NH1	2.50	0.45
17:E:81:VAL:HB	17:E:106:THR:HA	1.99	0.45
22:I:123:GLN:OE1	23:J:118:TYR:OH	2.35	0.45
30:Q:91:CYS:O	30:Q:94:SER:OG	2.32	0.45
26:m:41:CYS:HB3	26:m:189:ILE:HG13	1.99	0.45
5:Y:164:ALA:HA	5:Y:168:ILE:HD12	1.99	0.45
12:f:167:ALA:HA	12:f:170:TRP:HD1	1.82	0.45
14:B:295:TYR:OH	18:F:259:MET:SD	2.72	0.45
17:E:62:LYS:HA	17:E:94:PRO:HB3	1.99	0.45
24:K:85:ALA:HB2	24:K:139:VAL:HG21	1.99	0.45
24:K:182:GLN:NE2	25:L:55:GLU:OE1	2.50	0.45
20:g:132:ARG:HD3	26:m:124:LEU:HD23	1.99	0.45
27:n:41:ILE:HG12	27:n:76:VAL:HG22	1.99	0.45
30:q:47:VAL:O	30:q:101:ASN:N	2.45	0.45
1:U:268:LEU:HD21	1:U:325:MET:HG3	1.99	0.44
7:a:66:GLU:HB3	18:F:42:ILE:HG12	1.98	0.44
7:a:292:THR:HA	7:a:330:ARG:HA	1.98	0.44
10:d:35:PHE:O	10:d:38:THR:OG1	2.35	0.44
14:B:356:PRO:O	14:B:357:ASP:HB3	2.18	0.44
14:B:383:LEU:HD21	14:B:420:LYS:HD3	1.99	0.44
17:E:383:LYS:HG3	18:F:294:LYS:HE3	1.98	0.44
22:i:38:LEU:O	22:i:179:TYR:OH	2.35	0.44
2:V:171:VAL:HG12	2:V:175:MET:HE3	1.99	0.44
3:W:241:LEU:HD22	3:W:241:LEU:HA	1.73	0.44
11:e:54:ASN:OD1	11:e:54:ASN:N	2.48	0.44
30:Q:103:LEU:HB3	30:Q:117:TYR:HA	1.99	0.44
26:m:92:ARG:NH1	26:m:96:SER:OG	2.51	0.44
30:q:59:TYR:O	30:q:63:ASN:ND2	2.50	0.44
2:V:33:GLN:HE21	2:V:85:ALA:HB2	1.82	0.44
6:Z:10:VAL:CG2	6:Z:161:GLU:CD	2.84	0.44
9:c:123:SER:OG	9:c:124:GLY:N	2.51	0.44
12:f:564:LEU:HD22	12:f:776:LEU:HG	1.98	0.44
15:C:147:THR:H	15:C:150:MET:HE3	1.81	0.44
16:D:255:LYS:HE3	16:D:302:ASN:HD22	1.83	0.44
22:I:72:MET:HG2	22:I:138:GLY:HA3	1.99	0.44
23:J:43:LEU:HD13	23:J:72:ALA:HB2	2.00	0.44
21:h:111:VAL:HG21	21:h:147:PHE:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:219:LYS:CB	6:Z:219:LYS:NZ	2.80	0.44
12:f:656:GLY:O	12:f:660:ILE:CG2	2.66	0.44
13:A:172:VAL:O	13:A:231:ASN:ND2	2.51	0.44
17:E:252:GLU:HA	17:E:255:ARG:HE	1.82	0.44
18:F:279:ALA:O	18:F:281:SER:N	2.51	0.44
22:I:73:ALA:HB3	22:I:137:ILE:HD11	1.99	0.44
22:I:123:GLN:NE2	23:J:79:ASP:OD1	2.51	0.44
25:L:116:THR:HG22	25:L:128:TYR:HD2	1.83	0.44
25:l:159:MET:HE1	25:l:169:ARG:HE	1.83	0.44
1:U:643:SER:O	1:U:649:ARG:NH1	2.50	0.44
24:K:212:ALA:HA	24:K:234:LEU:HD22	2.00	0.44
26:M:152:ASP:OD1	26:M:156:VAL:N	2.51	0.44
31:R:125:THR:OG1	30:q:170:ARG:NH2	2.51	0.44
20:g:53:GLN:HA	20:g:215:ILE:HA	2.00	0.44
22:i:73:ALA:HB3	22:i:137:ILE:HD11	1.99	0.44
24:k:203:LYS:HA	24:k:206:MET:HG2	1.99	0.44
25:l:105:VAL:HG21	25:l:136:GLY:HA3	1.98	0.44
26:m:144:ASP:HB3	26:m:147:GLN:HE22	1.82	0.44
1:U:640:LEU:HD23	1:U:640:LEU:HA	1.78	0.44
3:W:199:TYR:CZ	3:W:236:HIS:CG	3.06	0.44
3:W:237:GLU:OE2	3:W:237:GLU:HA	2.18	0.44
3:W:454:ASN:ND2	6:Z:220:LEU:HB2	2.32	0.44
10:d:62:SER:HA	10:d:65:ARG:HG2	1.99	0.44
12:f:399:LEU:HD11	12:f:440:ILE:HG12	2.00	0.44
13:A:103:ASN:HA	13:A:136:GLU:HG2	2.00	0.44
13:A:140:VAL:HA	13:A:152:PRO:HA	1.98	0.44
15:C:188:LEU:HB3	15:C:317:PHE:HE2	1.82	0.44
18:F:357:PRO:O	18:F:362:ARG:NH1	2.50	0.44
22:I:38:LEU:O	22:I:179:TYR:OH	2.35	0.44
23:J:97:THR:OG1	23:J:98:VAL:N	2.51	0.44
24:k:72:ALA:HB1	24:k:226:PHE:HE1	1.83	0.44
1:U:643:SER:HA	15:C:53:ASN:HD21	1.82	0.44
1:U:792:ASN:HD21	1:U:796:LYS:NZ	2.15	0.44
7:a:356:TRP:HH2	9:c:309:PHE:HA	1.83	0.44
23:J:74:ALA:HB2	23:J:161:ILE:HD13	1.99	0.44
27:N:41:ILE:HG12	27:N:76:VAL:HG22	1.99	0.44
20:g:191:PHE:O	20:g:194:THR:OG1	2.32	0.44
22:i:45:LEU:HD11	22:i:137:ILE:HG12	2.00	0.44
23:j:97:THR:OG1	23:j:98:VAL:N	2.51	0.44
1:U:109:THR:OG1	1:U:156:GLU:O	2.35	0.44
1:U:686:GLY:HA2	1:U:689:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:145:LEU:HD12	3:W:172:GLU:HG2	1.99	0.44
3:W:239:SER:O	3:W:240:TYR:HD1	2.01	0.44
3:W:245:LYS:C	3:W:247:TYR:H	2.26	0.44
4:X:143:TYR:OH	5:Y:248:GLU:O	2.36	0.44
4:X:316:ASP:C	4:X:318:ILE:HA	2.43	0.44
5:Y:228:MET:HB3	5:Y:228:MET:HE2	1.79	0.44
12:f:43:GLN:HG3	12:f:121:PHE:HB2	2.00	0.44
13:A:277:ILE:HD13	13:A:319:MET:HB3	2.00	0.44
18:F:339:ASP:OD1	18:F:339:ASP:N	2.44	0.44
26:M:144:ASP:HB3	26:M:147:GLN:HE22	1.82	0.44
32:S:169:ASP:OD2	32:S:173:ARG:NH2	2.51	0.44
1:U:609:ASP:O	1:U:615:ARG:NH1	2.43	0.44
4:X:258:LYS:HD3	4:X:266:ASP:HB2	1.99	0.44
5:Y:325:VAL:HG21	11:e:67:MET:HA	2.00	0.44
12:f:130:ALA:O	12:f:134:SER:N	2.49	0.44
13:A:123:VAL:HG11	13:A:147:TYR:HB2	1.99	0.44
14:B:133:VAL:HB	14:B:158:ALA:HA	2.00	0.44
14:B:288:ASP:OD1	14:B:288:ASP:N	2.49	0.44
18:F:152:GLY:HA3	18:F:162:GLU:HB2	1.99	0.44
23:j:74:ALA:HB2	23:j:161:ILE:HD13	1.99	0.44
30:q:13:VAL:HG11	30:q:105:ALA:HB1	2.00	0.44
2:V:43:THR:O	2:V:47:SER:N	2.46	0.43
2:V:259:LEU:HD11	2:V:294:ARG:HG2	2.00	0.43
3:W:234:ASP:HB3	3:W:243:ILE:HG13	1.95	0.43
3:W:454:ASN:ND2	6:Z:220:LEU:CB	2.81	0.43
22:I:119:GLN:NE2	23:J:79:ASP:OD1	2.51	0.43
22:i:72:MET:HG2	22:i:138:GLY:HA3	2.00	0.43
23:j:43:LEU:HD13	23:j:72:ALA:HB2	2.00	0.43
25:l:195:LEU:O	25:l:198:THR:OG1	2.32	0.43
30:q:11:ASP:N	30:q:11:ASP:OD1	2.49	0.43
3:W:149:LEU:HD13	3:W:185:PHE:HD1	1.83	0.43
7:a:321:LYS:HE2	7:a:336:VAL:HG21	2.00	0.43
23:J:105:GLU:HA	23:J:145:TYR:HE2	1.83	0.43
26:M:92:ARG:NH1	26:M:96:SER:OG	2.51	0.43
23:j:159:ASN:OD1	23:j:160:ALA:N	2.51	0.43
25:l:13:TRP:NE1	26:m:129:ARG:HD2	2.33	0.43
25:l:116:THR:HG22	25:l:128:TYR:HD2	1.83	0.43
25:l:158:ALA:HB1	25:l:172:LEU:HD13	2.00	0.43
2:V:259:LEU:HD12	2:V:295:ILE:HD11	2.01	0.43
3:W:310:THR:HG23	3:W:311:THR:HG23	2.01	0.43
5:Y:377:LEU:HA	5:Y:380:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:397:ILE:HG23	14:B:210:TYR:HB3	2.00	0.43
15:C:222:LYS:NZ	16:D:242:GLU:OE2	2.51	0.43
16:D:400:GLU:OE1	16:D:400:GLU:N	2.51	0.43
24:K:157:ASP:OD1	24:K:157:ASP:N	2.52	0.43
32:S:38:ARG:HH12	33:T:151:ARG:HD3	1.84	0.43
24:k:167:ALA:HB3	24:k:181:LEU:HD21	2.00	0.43
26:m:152:ASP:OD1	26:m:156:VAL:N	2.51	0.43
4:X:360:ASP:OD1	4:X:360:ASP:N	2.51	0.43
5:Y:101:ARG:HH22	5:Y:140:ILE:HD11	1.83	0.43
5:Y:348:ASP:OD1	5:Y:349:LYS:N	2.51	0.43
12:f:253:LEU:HA	12:f:257:ARG:HD3	2.01	0.43
12:f:773:LYS:HA	12:f:774:GLY:HA3	1.79	0.43
13:A:165:GLN:HG2	13:A:167:GLU:HG3	1.99	0.43
15:C:77:VAL:HG13	15:C:110:PRO:HA	2.00	0.43
15:C:137:LEU:O	15:C:213:ARG:NH2	2.52	0.43
17:E:360:ASP:OD1	17:E:360:ASP:N	2.52	0.43
23:J:159:ASN:OD1	23:J:160:ALA:N	2.51	0.43
25:L:195:LEU:O	25:L:198:THR:OG1	2.32	0.43
26:M:197:ILE:HG21	26:M:211:LEU:HD13	2.01	0.43
25:l:49:LEU:HB2	25:l:195:LEU:HD23	1.99	0.43
25:l:101:ARG:HH12	25:l:104:PRO:HD3	1.84	0.43
25:l:196:ARG:HH21	25:l:239:ARG:HG3	1.83	0.43
33:t:9:THR:OG1	33:t:10:SER:N	2.44	0.43
1:U:8:ILE:H	1:U:8:ILE:HG13	1.59	0.43
1:U:386:LEU:HD22	1:U:408:LEU:HD13	1.99	0.43
3:W:454:ASN:HD22	6:Z:220:LEU:HB2	1.84	0.43
10:d:200:PHE:O	10:d:203:PRO:HD3	2.18	0.43
16:D:157:ASP:HA	16:D:158:GLN:HA	1.55	0.43
16:D:172:ILE:O	16:D:176:GLU:N	2.51	0.43
26:M:40:ARG:HE	26:M:161:TRP:HD1	1.65	0.43
30:Q:13:VAL:HG11	30:Q:105:ALA:HB1	2.00	0.43
1:U:599:ILE:HD13	1:U:625:ILE:HD11	1.99	0.43
2:V:252:ASN:ND2	2:V:284:GLU:OE2	2.51	0.43
11:e:66:LYS:O	11:e:69:THR:OG1	2.33	0.43
13:A:331:LEU:HB3	13:A:337:LEU:HD12	1.99	0.43
14:B:222:VAL:HA	14:B:349:ARG:HB2	2.00	0.43
16:D:354:LEU:HB2	16:D:355:SER:H	1.73	0.43
23:J:158:ALA:HB1	23:J:172:LEU:HD13	2.01	0.43
32:S:36:HIS:HB3	33:T:132:TYR:CZ	2.54	0.43
2:V:265:ASP:O	2:V:269:LYS:NZ	2.51	0.43
2:V:280:ALA:HB1	2:V:284:GLU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:705:ASN:OD1	12:f:706:ILE:N	2.48	0.43
16:D:238:LYS:H	16:D:238:LYS:HG3	1.52	0.43
18:F:364:ARG:HH12	18:F:371:ARG:NH2	2.16	0.43
24:K:203:LYS:HA	24:K:206:MET:HG2	1.99	0.43
25:L:49:LEU:HB2	25:L:195:LEU:HD23	1.99	0.43
25:L:159:MET:HE1	25:L:169:ARG:HE	1.83	0.43
25:L:196:ARG:HH21	25:L:239:ARG:HG3	1.83	0.43
1:U:637:VAL:HG11	1:U:656:LEU:HB2	2.00	0.43
18:F:375:VAL:HG22	18:F:415:LEU:HD12	2.01	0.43
20:G:53:GLN:HA	20:G:215:ILE:HA	2.00	0.43
24:K:167:ALA:HB3	24:K:181:LEU:HD21	2.00	0.43
29:P:159:ASP:N	29:P:159:ASP:OD1	2.50	0.43
22:i:102:GLN:HG2	30:q:82:ASN:ND2	2.33	0.43
3:W:443:THR:HG22	6:Z:229:GLN:HE22	1.84	0.43
7:a:54:ASP:HA	7:a:57:ILE:HG22	1.99	0.43
12:f:171:GLN:HE21	12:f:179:VAL:HA	1.83	0.43
14:B:375:ALA:HB2	14:B:413:LYS:HB3	2.00	0.43
16:D:349:THR:HA	16:D:352:MET:HB3	2.01	0.43
22:I:79:ILE:HG22	22:I:82:ASP:H	1.84	0.43
25:L:101:ARG:HH12	25:L:104:PRO:HD3	1.84	0.43
27:N:29:ARG:NH1	28:O:139:GLU:OE1	2.40	0.43
22:i:123:GLN:NE2	23:j:79:ASP:OD1	2.52	0.43
25:l:205:LEU:H	25:l:205:LEU:HG	1.36	0.43
25:l:207:THR:HG22	25:l:233:LEU:HD12	2.01	0.43
1:U:224:ASP:OD1	1:U:224:ASP:N	2.50	0.43
1:U:603:LEU:HB3	16:D:60:TYR:CD1	2.54	0.43
1:U:641:SER:HA	1:U:649:ARG:HA	2.00	0.43
3:W:328:LEU:HD13	3:W:328:LEU:HA	1.81	0.43
4:X:53:LEU:HD23	4:X:56:LEU:HD12	2.01	0.43
4:X:377:ILE:HG12	5:Y:312:ARG:HB3	2.01	0.43
8:b:26:LEU:HD11	8:b:80:PRO:HG3	2.01	0.43
24:k:157:ASP:OD1	24:k:157:ASP:N	2.52	0.43
24:k:212:ALA:HA	24:k:234:LEU:HD22	2.00	0.43
28:o:13:VAL:HG22	28:o:177:VAL:HG22	2.01	0.43
30:q:19:ARG:HH11	30:q:179:SER:HB3	1.84	0.43
5:Y:177:ARG:NH1	5:Y:205:VAL:H	2.17	0.42
12:f:438:ASP:HA	12:f:477:MET:HE2	2.00	0.42
12:f:828:ARG:HG2	12:f:845:ARG:C	2.44	0.42
18:F:38:THR:HG22	18:F:39:GLU:HG2	2.00	0.42
24:K:72:ALA:HB1	24:K:226:PHE:HE1	1.83	0.42
28:O:164:PHE:O	32:s:38:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Q:148:THR:HG22	30:Q:150:THR:H	1.84	0.42
30:q:103:LEU:HB3	30:q:117:TYR:HA	1.99	0.42
1:U:649:ARG:HB3	1:U:675:MET:HE1	2.01	0.42
2:V:194:LYS:H	2:V:194:LYS:HD2	1.84	0.42
6:Z:222:ILE:C	6:Z:222:ILE:CD1	2.86	0.42
13:A:274:PHE:HB2	13:A:319:MET:HG2	2.01	0.42
23:j:105:GLU:HA	23:j:145:TYR:HE2	1.83	0.42
25:l:50:LYS:HB3	25:l:59:HIS:HB3	2.01	0.42
1:U:447:GLY:HA3	1:U:480:GLY:HA2	2.00	0.42
10:d:167:ILE:HA	10:d:170:LEU:HB3	2.01	0.42
12:f:265:ALA:HB3	12:f:268:LEU:HB2	2.02	0.42
12:f:478:ARG:HG3	12:f:514:VAL:HG11	2.01	0.42
15:C:215:SER:HA	15:C:249:ASP:HB3	2.01	0.42
18:F:122:ALA:HB3	18:F:134:LEU:HD11	2.01	0.42
22:I:3:ARG:HB2	23:J:5:ARG:HH12	1.84	0.42
22:I:45:LEU:HD11	22:I:137:ILE:HG12	2.00	0.42
29:P:12:MET:HG3	29:P:138:VAL:HG12	2.02	0.42
26:m:40:ARG:HE	26:m:161:TRP:HD1	1.65	0.42
26:m:67:PHE:HB2	26:m:75:MET:HB2	2.01	0.42
29:p:149:MET:O	29:p:153:LEU:N	2.52	0.42
32:s:169:ASP:OD2	32:s:173:ARG:NH2	2.51	0.42
1:U:900:TYR:HB3	1:U:914:LEU:HD21	2.02	0.42
12:f:764:LEU:HD12	12:f:771:LEU:HG	2.02	0.42
18:F:81:LYS:HE2	18:F:81:LYS:HB3	1.87	0.42
28:O:13:VAL:HG22	28:O:177:VAL:HG22	2.01	0.42
29:P:56:LEU:CG	29:P:58:THR:HG22	2.48	0.42
22:i:77:ALA:HB3	22:i:164:ILE:HG21	2.01	0.42
32:s:99:ARG:HH21	32:s:102:PHE:HD2	1.68	0.42
1:U:94:SER:HB3	1:U:97:VAL:HG12	2.01	0.42
12:f:283:THR:O	12:f:287:ASP:N	2.46	0.42
12:f:294:MET:HE1	12:f:456:ARG:HG2	2.02	0.42
12:f:412:ALA:HA	12:f:447:ALA:HB2	2.01	0.42
13:A:144:ARG:CB	19:v:19:UNK:CB	2.97	0.42
15:C:281:ASP:O	15:C:310:ARG:NH2	2.53	0.42
17:E:84:ARG:O	17:E:85:ARG:NE	2.47	0.42
30:Q:47:VAL:O	30:Q:101:ASN:N	2.45	0.42
24:k:236:GLU:HA	24:k:239:LYS:HE3	2.02	0.42
3:W:265:GLN:HG3	3:W:336:PRO:HG3	2.02	0.42
12:f:674:THR:O	12:f:678:LEU:N	2.51	0.42
13:A:181:LYS:HA	13:A:184:ILE:HD12	2.01	0.42
17:E:271:HIS:CD2	17:E:272:ARG:HG2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:m:197:ILE:HG21	26:m:211:LEU:HD13	2.01	0.42
29:p:159:ASP:OD1	29:p:159:ASP:N	2.50	0.42
5:Y:381:GLN:HB3	5:Y:385:ARG:NH1	2.35	0.42
6:Z:17:LEU:HD11	9:c:36:LEU:CA	2.49	0.42
6:Z:152:SER:OG	6:Z:153:LYS:N	2.52	0.42
10:d:3:GLU:HB2	10:d:25:ARG:HD3	2.01	0.42
13:A:236:CYS:SG	13:A:267:LYS:HD2	2.60	0.42
30:Q:19:ARG:HH11	30:Q:179:SER:HB3	1.84	0.42
22:i:79:ILE:HG22	22:i:82:ASP:H	1.84	0.42
28:o:171:SER:HB3	28:o:172:ASN:H	1.70	0.42
30:q:148:THR:HG22	30:q:150:THR:H	1.84	0.42
3:W:317:TRP:CE2	3:W:355:LYS:HD3	2.54	0.42
9:c:36:LEU:O	9:c:40:LYS:HG2	2.19	0.42
12:f:93:PRO:HB2	12:f:97:LYS:HE3	2.00	0.42
12:f:261:ARG:HG2	12:f:266:LEU:HD13	2.02	0.42
14:B:106:PRO:HG2	14:B:154:HIS:CD2	2.54	0.42
15:C:52:LEU:HB3	16:D:68:LEU:HD12	2.01	0.42
16:D:362:ASP:O	16:D:366:ARG:NE	2.53	0.42
17:E:340:GLY:HA3	35:E:401:ATP:C5	2.54	0.42
25:L:158:ALA:HB1	25:L:172:LEU:HD13	2.00	0.42
25:L:205:LEU:H	25:L:205:LEU:HG	1.36	0.42
23:j:158:ALA:HB1	23:j:172:LEU:HD13	2.01	0.42
24:k:145:GLY:HA2	24:k:220:VAL:HG11	2.02	0.42
26:m:92:ARG:NH2	33:t:73:ASP:OD1	2.52	0.42
31:r:83:LEU:HD11	31:r:97:MET:HE1	2.02	0.42
6:Z:67:VAL:HG21	8:b:91:ARG:HD2	2.02	0.42
6:Z:121:LEU:HD11	6:Z:138:TYR:HD2	1.84	0.42
8:b:94:HIS:CD2	8:b:136:VAL:HG21	2.55	0.42
12:f:621:ASP:O	12:f:623:LYS:N	2.51	0.42
21:H:42:ASN:ND2	21:H:183:GLU:OE1	2.53	0.42
22:I:49:ARG:HH22	22:I:212:GLU:HG3	1.85	0.42
22:I:77:ALA:HB3	22:I:164:ILE:HG21	2.01	0.42
22:I:119:GLN:HE22	23:J:79:ASP:HA	1.85	0.42
29:P:36:THR:OG1	29:P:38:ASP:OD1	2.33	0.42
29:P:190:ILE:HG22	29:P:195:ILE:HG23	2.01	0.42
31:R:83:LEU:HD11	31:R:97:MET:HE1	2.02	0.42
20:g:86:ASP:OD1	26:m:120:HIS:NE2	2.30	0.42
3:W:234:ASP:HB2	3:W:243:ILE:CD1	2.48	0.42
3:W:263:TRP:HZ2	3:W:295:LYS:HB3	1.85	0.42
6:Z:83:LYS:HD3	6:Z:87:ALA:HA	2.02	0.42
6:Z:241:SER:OG	6:Z:242:LEU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:355:SER:OG	16:D:356:GLU:N	2.52	0.42
25:L:207:THR:HG22	25:L:233:LEU:HD12	2.01	0.42
26:M:67:PHE:HB2	26:M:75:MET:HB2	2.01	0.42
20:g:126:THR:HG22	21:h:128:ARG:HH12	1.85	0.42
21:h:42:ASN:ND2	21:h:183:GLU:OE1	2.53	0.42
22:i:68:LEU:HD12	22:i:69:ASN:HB2	2.02	0.42
30:q:31:ASP:N	30:q:31:ASP:OD1	2.53	0.42
1:U:639:LEU:HD21	15:C:49:ARG:HD2	2.02	0.41
12:f:663:GLY:C	12:f:664:GLU:HG3	2.45	0.41
17:E:97:ARG:HE	17:E:111:LEU:HB2	1.85	0.41
17:E:148:VAL:HB	17:E:297:ARG:HH22	1.84	0.41
32:S:136:LYS:HA	32:S:136:LYS:HD2	1.90	0.41
3:W:82:LEU:HB3	3:W:90:LEU:HD11	2.02	0.41
5:Y:16:ASP:HB3	5:Y:150:PHE:CZ	2.55	0.41
8:b:100:ARG:NH1	8:b:102:GLY:O	2.53	0.41
18:F:219:PRO:HA	18:F:220:PRO:HD3	1.94	0.41
25:L:50:LYS:HB3	25:L:59:HIS:HB3	2.01	0.41
32:S:99:ARG:HH21	32:S:102:PHE:HD2	1.68	0.41
32:s:19:ASP:OD1	32:s:19:ASP:N	2.53	0.41
3:W:12:ARG:HH12	3:W:23:THR:HB	1.86	0.41
7:a:15:GLY:HA2	7:a:16:PRO:HD3	1.85	0.41
7:a:75:SER:HA	7:a:78:GLU:HB2	2.01	0.41
7:a:216:LEU:HB2	7:a:222:LEU:HD21	2.02	0.41
12:f:276:GLU:O	12:f:286:LYS:NZ	2.39	0.41
12:f:594:LEU:HD13	12:f:594:LEU:HA	1.93	0.41
12:f:665:GLU:HG2	12:f:669:GLU:HG3	2.01	0.41
15:C:219:LEU:H	15:C:219:LEU:HG	1.56	0.41
25:L:14:SER:OG	25:L:18:ARG:O	2.35	0.41
26:M:181:MET:HE3	26:M:181:MET:HB3	2.00	0.41
23:j:11:SER:OG	23:j:13:ASP:OD1	2.29	0.41
23:j:98:VAL:HG13	31:r:78:ALA:HB2	2.02	0.41
26:m:144:ASP:O	26:m:147:GLN:NE2	2.54	0.41
2:V:419:LEU:HA	2:V:422:ILE:HG22	2.02	0.41
3:W:130:MET:HB3	3:W:135:LYS:NZ	2.35	0.41
3:W:259:GLU:HB3	3:W:262:LYS:HB3	2.02	0.41
4:X:47:GLU:HG2	4:X:76:PHE:HZ	1.85	0.41
5:Y:47:ASP:OD1	5:Y:113:ARG:NE	2.37	0.41
6:Z:56:VAL:HG23	6:Z:74:TYR:HD2	1.86	0.41
7:a:77:VAL:HA	7:a:80:ILE:HG22	2.02	0.41
8:b:138:VAL:H	8:b:160:LEU:HD21	1.85	0.41
12:f:248:LEU:HD12	12:f:250:ARG:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:144:ARG:HD2	19:v:19:UNK:CA	2.48	0.41
15:C:197:THR:N	35:C:501:ATP:O1A	2.52	0.41
21:H:118:MET:HE2	21:H:151:PRO:HA	2.03	0.41
31:r:22:ALA:N	31:r:25:TYR:O	2.54	0.41
1:U:361:ARG:CZ	1:U:363:SER:HB3	2.50	0.41
5:Y:201:PHE:HD1	5:Y:201:PHE:HA	1.75	0.41
7:a:115:LYS:HD3	7:a:118:ILE:HD12	2.03	0.41
8:b:15:TYR:HD2	8:b:116:PRO:HD2	1.86	0.41
12:f:762:VAL:HG13	12:f:806:VAL:HG13	2.01	0.41
14:B:153:ASN:H	14:B:157:HIS:HA	1.85	0.41
15:C:145:ASP:OD1	15:C:145:ASP:N	2.53	0.41
16:D:154:LEU:HD23	16:D:154:LEU:HA	1.79	0.41
18:F:137:ILE:HG23	18:F:160:ILE:HD12	2.02	0.41
22:I:68:LEU:HD12	22:I:69:ASN:HB2	2.02	0.41
28:o:19:ARG:CZ	28:o:170:GLY:HA3	2.51	0.41
29:p:190:ILE:HG22	29:p:195:ILE:HG23	2.01	0.41
2:V:80:LYS:O	2:V:87:SER:OG	2.30	0.41
3:W:127:THR:OG1	3:W:147:LYS:NZ	2.50	0.41
12:f:326:LEU:HD22	12:f:329:ASN:HB2	2.02	0.41
12:f:407:MET:HE3	12:f:439:TYR:HB2	2.02	0.41
14:B:298:ASN:HA	14:B:303:ARG:HH21	1.85	0.41
16:D:156:SER:H	16:D:159:LYS:HE2	1.85	0.41
17:E:321:THR:OG1	17:E:360:ASP:O	2.38	0.41
21:H:225:GLU:O	21:H:229:TYR:N	2.44	0.41
24:K:236:GLU:HA	24:K:239:LYS:HE3	2.02	0.41
26:M:56:LYS:HE2	26:M:56:LYS:HB3	1.92	0.41
26:M:100:SER:HA	33:T:65:GLN:HE21	1.85	0.41
30:Q:31:ASP:OD1	30:Q:31:ASP:N	2.53	0.41
26:m:230:ASP:OD1	26:m:230:ASP:N	2.53	0.41
29:p:12:MET:HG3	29:p:138:VAL:HG12	2.02	0.41
33:t:49:THR:HB	33:t:85:PRO:HG3	2.03	0.41
10:d:176:ASP:O	10:d:180:GLY:N	2.45	0.41
12:f:829:MET:H	12:f:845:ARG:HB3	1.86	0.41
21:H:102:GLN:NE2	28:O:57:GLN:OE1	2.54	0.41
25:L:121:GLN:HG3	26:M:129:ARG:HG2	2.03	0.41
22:i:49:ARG:HH22	22:i:212:GLU:HG3	1.85	0.41
28:o:138:PHE:HD1	28:o:138:PHE:HA	1.77	0.41
5:Y:121:LEU:HB2	5:Y:125:ARG:HH12	1.85	0.41
13:A:124:ASP:OD1	13:A:125:LEU:N	2.53	0.41
13:A:347:ASP:OD1	13:A:347:ASP:N	2.53	0.41
14:B:282:VAL:HB	14:B:327:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:11:LEU:HD13	15:C:14:GLY:HA3	2.02	0.41
15:C:86:LEU:HD21	15:C:94:LYS:HB3	2.01	0.41
15:C:161:ILE:HA	15:C:164:VAL:HG12	2.03	0.41
16:D:164:TYR:HB2	16:D:222:HIS:CD2	2.56	0.41
21:H:86:LEU:HD13	21:H:134:LEU:HD11	2.03	0.41
28:O:6:VAL:HG23	28:O:124:TYR:HB3	2.02	0.41
28:O:24:MET:HE1	32:s:33:PHE:HE1	1.86	0.41
20:g:138:MET:HB3	20:g:154:CYS:HB3	2.02	0.41
20:g:169:GLY:O	20:g:172:GLN:NE2	2.53	0.41
26:m:66:LEU:HD13	26:m:214:SER:HB2	2.03	0.41
1:U:177:LEU:HB3	1:U:205:TYR:HE1	1.86	0.41
3:W:328:LEU:HD13	3:W:337:ALA:HB1	2.02	0.41
6:Z:14:LEU:CD1	9:c:43:LYS:NZ	2.83	0.41
6:Z:15:VAL:O	6:Z:19:VAL:HG23	2.21	0.41
6:Z:162:ILE:HG13	9:c:220:LEU:HB3	2.03	0.41
7:a:222:LEU:HB2	7:a:226:ARG:HH11	1.86	0.41
12:f:331:LEU:HD12	12:f:813:LYS:HE2	2.03	0.41
12:f:340:MET:SD	12:f:757:ASN:ND2	2.94	0.41
12:f:663:GLY:O	12:f:664:GLU:CG	2.69	0.41
16:D:87:LEU:HD21	16:D:140:VAL:HG11	2.03	0.41
16:D:312:ASN:O	16:D:313:ARG:NE	2.53	0.41
18:F:236:LEU:N	18:F:238:ARG:HH11	2.19	0.41
21:H:46:LEU:HD13	21:H:75:VAL:HG13	2.03	0.41
22:I:140:ASP:OD1	22:I:140:ASP:N	2.54	0.41
23:J:61:LYS:HD2	23:J:73:PHE:CZ	2.56	0.41
24:K:145:GLY:HA2	24:K:220:VAL:HG11	2.02	0.41
28:O:19:ARG:CZ	28:O:170:GLY:HA3	2.51	0.41
33:T:25:ASP:HA	33:T:187:PHE:HA	2.03	0.41
20:g:43:ARG:NH2	20:g:164:LYS:HG2	2.36	0.41
21:h:46:LEU:HD13	21:h:75:VAL:HG13	2.02	0.41
25:l:152:ASN:HA	26:m:85:ARG:HH22	1.86	0.41
2:V:169:LEU:H	2:V:171:VAL:HG23	1.85	0.41
5:Y:278:VAL:O	5:Y:282:MET:N	2.53	0.41
6:Z:14:LEU:HA	6:Z:14:LEU:HD23	1.77	0.41
12:f:460:ASP:N	12:f:460:ASP:OD1	2.52	0.41
15:C:71:SER:OG	15:C:116:LEU:O	2.32	0.41
26:M:144:ASP:O	26:M:147:GLN:NE2	2.54	0.41
23:j:116:GLN:HE21	24:k:83:ALA:HB3	1.86	0.41
24:k:101:PHE:HA	31:r:57:ARG:NH2	2.36	0.41
26:m:76:ALA:HB3	26:m:136:MET:HB2	2.03	0.41
1:U:885:MET:HB3	1:U:888:GLN:HG2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c:107:MET:HE3	9:c:108:VAL:HG22	2.03	0.40
12:f:180:GLN:HB3	12:f:219:LYS:NZ	2.36	0.40
12:f:205:CYS:SG	12:f:213:GLN:NE2	2.86	0.40
12:f:414:LEU:HD23	12:f:417:ILE:HD12	2.03	0.40
14:B:94:GLU:HG2	14:B:98:LYS:HE3	2.02	0.40
14:B:356:PRO:HB2	14:B:357:ASP:H	1.50	0.40
15:C:197:THR:HG23	16:D:299:PHE:HE1	1.87	0.40
20:G:169:GLY:O	20:G:172:GLN:NE2	2.53	0.40
28:o:6:VAL:HG23	28:o:124:TYR:HB3	2.02	0.40
1:U:11:LEU:HD22	1:U:19:LEU:HD11	2.02	0.40
7:a:211:PHE:HE2	7:a:339:ARG:HH12	1.70	0.40
12:f:269:ALA:HA	12:f:272:LEU:HB2	2.04	0.40
14:B:118:ASP:OD1	14:B:118:ASP:N	2.53	0.40
14:B:356:PRO:O	14:B:357:ASP:CB	2.69	0.40
26:M:92:ARG:NH1	26:M:96:SER:HG	2.19	0.40
21:h:139:TRP:HA	21:h:144:PRO:HA	2.04	0.40
25:l:50:LYS:HB2	25:l:209:ASN:HA	2.03	0.40
33:t:76:LEU:HD23	33:t:76:LEU:HA	1.89	0.40
1:U:588:MET:HE2	1:U:588:MET:HB3	1.91	0.40
8:b:51:LEU:HD11	8:b:61:LEU:HD23	2.03	0.40
10:d:203:PRO:HG2	10:d:205:LYS:HB3	2.02	0.40
12:f:180:GLN:HE22	12:f:835:GLU:HB3	1.85	0.40
12:f:777:THR:HG22	12:f:803:PHE:HA	2.03	0.40
14:B:203:LEU:HD12	14:B:207:HIS:HB3	2.02	0.40
15:C:398:ASN:HA	21:H:167:TYR:HE2	1.85	0.40
26:M:189:ILE:HD13	26:M:189:ILE:HA	1.95	0.40
1:U:541:HIS:HB2	1:U:544:ILE:HG22	2.04	0.40
3:W:385:SER:OG	3:W:386:VAL:N	2.55	0.40
4:X:239:TYR:HB3	4:X:247:ALA:HB2	2.04	0.40
6:Z:129:LYS:HZ3	9:c:215:LYS:HE3	1.86	0.40
12:f:9:ALA:HA	12:f:13:PRO:HD2	2.03	0.40
15:C:123:LEU:HA	15:C:123:LEU:HD23	1.87	0.40
18:F:304:ARG:HG3	18:F:308:ARG:HH12	1.85	0.40
29:p:36:THR:OG1	29:p:38:ASP:OD1	2.33	0.40
1:U:68:PHE:O	1:U:73:ALA:N	2.54	0.40
1:U:325:MET:HA	1:U:328:ILE:HG12	2.03	0.40
1:U:596:ASN:HD21	16:D:52:GLU:HB3	1.86	0.40
12:f:305:LEU:HB2	12:f:317:LEU:HD13	2.04	0.40
15:C:229:ARG:NH1	15:C:233:GLU:OE1	2.54	0.40
16:D:356:GLU:HG2	16:D:357:GLU:HG2	2.04	0.40
18:F:185:TYR:OH	18:F:243:GLN:NE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:F:300:LYS:HA	18:F:301:ALA:HA	1.81	0.40
28:O:124:TYR:OH	28:O:139:GLU:OE1	2.35	0.40
28:O:216:ILE:HG23	29:P:194:LYS:HD2	2.04	0.40
22:i:135:LEU:HG	22:i:164:ILE:HD11	2.03	0.40
33:t:106:LEU:HD23	33:t:106:LEU:HA	1.94	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	U	814/953 (85%)	760 (93%)	53 (6%)	1 (0%)	48	79
2	V	478/533 (90%)	436 (91%)	41 (9%)	1 (0%)	43	72
3	W	454/456 (100%)	420 (92%)	34 (8%)	0	100	100
4	X	378/422 (90%)	355 (94%)	22 (6%)	1 (0%)	36	65
5	Y	376/389 (97%)	340 (90%)	36 (10%)	0	100	100
6	Z	284/324 (88%)	240 (84%)	38 (13%)	6 (2%)	5	31
7	a	371/376 (99%)	338 (91%)	32 (9%)	1 (0%)	36	65
8	b	189/377 (50%)	171 (90%)	18 (10%)	0	100	100
9	c	285/309 (92%)	241 (85%)	43 (15%)	1 (0%)	30	61
10	d	255/349 (73%)	216 (85%)	38 (15%)	1 (0%)	30	61
11	e	36/70 (51%)	31 (86%)	5 (14%)	0	100	100
12	f	884/892 (99%)	709 (80%)	164 (19%)	11 (1%)	10	41
13	A	354/433 (82%)	310 (88%)	42 (12%)	2 (1%)	21	54
14	B	348/440 (79%)	300 (86%)	44 (13%)	4 (1%)	11	43
15	C	394/398 (99%)	342 (87%)	51 (13%)	1 (0%)	36	65
16	D	378/418 (90%)	335 (89%)	42 (11%)	1 (0%)	36	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	E	387/403 (96%)	338 (87%)	43 (11%)	6 (2%)	7	36
18	F	391/439 (89%)	350 (90%)	40 (10%)	1 (0%)	36	65
20	G	238/245 (97%)	228 (96%)	10 (4%)	0	100	100
20	g	238/245 (97%)	228 (96%)	10 (4%)	0	100	100
21	H	230/233 (99%)	216 (94%)	14 (6%)	0	100	100
21	h	230/233 (99%)	216 (94%)	14 (6%)	0	100	100
22	I	248/260 (95%)	230 (93%)	18 (7%)	0	100	100
22	i	248/260 (95%)	230 (93%)	18 (7%)	0	100	100
23	J	237/247 (96%)	223 (94%)	14 (6%)	0	100	100
23	j	237/247 (96%)	223 (94%)	14 (6%)	0	100	100
24	K	224/240 (93%)	212 (95%)	12 (5%)	0	100	100
24	k	224/240 (93%)	212 (95%)	12 (5%)	0	100	100
25	L	236/268 (88%)	223 (94%)	13 (6%)	0	100	100
25	l	236/268 (88%)	223 (94%)	13 (6%)	0	100	100
26	M	238/254 (94%)	216 (91%)	20 (8%)	2 (1%)	16	49
26	m	238/254 (94%)	216 (91%)	20 (8%)	2 (1%)	16	49
27	N	189/238 (79%)	183 (97%)	6 (3%)	0	100	100
27	n	189/238 (79%)	183 (97%)	6 (3%)	0	100	100
28	O	218/276 (79%)	209 (96%)	9 (4%)	0	100	100
28	o	218/276 (79%)	209 (96%)	9 (4%)	0	100	100
29	P	202/204 (99%)	191 (95%)	11 (5%)	0	100	100
29	p	202/204 (99%)	191 (95%)	11 (5%)	0	100	100
30	Q	197/201 (98%)	181 (92%)	15 (8%)	1 (0%)	24	57
30	q	197/201 (98%)	181 (92%)	15 (8%)	1 (0%)	24	57
31	R	199/262 (76%)	190 (96%)	9 (4%)	0	100	100
31	r	199/262 (76%)	190 (96%)	9 (4%)	0	100	100
32	S	211/240 (88%)	202 (96%)	9 (4%)	0	100	100
32	s	211/240 (88%)	202 (96%)	9 (4%)	0	100	100
33	T	213/263 (81%)	198 (93%)	15 (7%)	0	100	100
33	t	213/263 (81%)	198 (93%)	15 (7%)	0	100	100
All	All	13216/14843 (89%)	12036 (91%)	1136 (9%)	44 (0%)	37	65

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	Z	217	THR
10	d	200	PHE
12	f	808	ASN
12	f	853	VAL
14	B	354	PRO
12	f	876	HIS
14	B	356	PRO
14	B	357	ASP
16	D	412	GLN
17	E	127	PRO
17	E	248	SER
7	a	69	HIS
12	f	118	ASN
12	f	476	THR
12	f	664	GLU
12	f	823	ALA
12	f	859	PRO
26	m	59	GLU
4	X	317	PRO
6	Z	10	VAL
12	f	809	ILE
13	A	109	PRO
17	E	247	THR
18	F	165	PRO
26	M	59	GLU
26	M	103	GLY
26	m	103	GLY
6	Z	65	ASP
9	c	280	PRO
12	f	475	ASN
15	C	128	PRO
30	Q	176	PRO
30	q	176	PRO
6	Z	12	HIS
6	Z	184	VAL
12	f	755	ASP
13	A	285	PHE
17	E	112	PRO
6	Z	144	VAL
17	E	227	PRO
1	U	813	TYR
14	B	355	LEU

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Mol	Chain	Res	Type
17	E	128	GLY
2	V	29	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	700/816 (86%)	695 (99%)	5 (1%)	76	78
2	V	414/459 (90%)	412 (100%)	2 (0%)	81	80
3	W	416/416 (100%)	405 (97%)	11 (3%)	40	62
4	X	327/362 (90%)	326 (100%)	1 (0%)	86	83
5	Y	334/344 (97%)	331 (99%)	3 (1%)	70	76
6	Z	257/295 (87%)	246 (96%)	11 (4%)	26	52
7	a	333/336 (99%)	332 (100%)	1 (0%)	86	83
8	b	167/312 (54%)	167 (100%)	0	100	100
9	c	252/267 (94%)	248 (98%)	4 (2%)	55	69
10	d	231/293 (79%)	230 (100%)	1 (0%)	84	81
11	e	38/63 (60%)	38 (100%)	0	100	100
12	f	742/748 (99%)	734 (99%)	8 (1%)	65	74
13	A	298/372 (80%)	296 (99%)	2 (1%)	76	78
14	B	300/385 (78%)	299 (100%)	1 (0%)	86	83
15	C	340/346 (98%)	337 (99%)	3 (1%)	70	76
16	D	333/366 (91%)	328 (98%)	5 (2%)	57	70
17	E	341/353 (97%)	341 (100%)	0	100	100
18	F	340/379 (90%)	333 (98%)	7 (2%)	47	65
20	G	193/209 (92%)	191 (99%)	2 (1%)	68	75
20	g	193/209 (92%)	191 (99%)	2 (1%)	68	75
21	H	164/190 (86%)	163 (99%)	1 (1%)	78	79
21	h	164/190 (86%)	163 (99%)	1 (1%)	78	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	I	193/220 (88%)	192 (100%)	1 (0%)	81	80
22	i	193/220 (88%)	192 (100%)	1 (0%)	81	80
23	J	152/210 (72%)	151 (99%)	1 (1%)	76	78
23	j	152/210 (72%)	151 (99%)	1 (1%)	76	78
24	K	186/202 (92%)	184 (99%)	2 (1%)	65	74
24	k	186/202 (92%)	184 (99%)	2 (1%)	65	74
25	L	198/229 (86%)	194 (98%)	4 (2%)	48	66
25	l	198/229 (86%)	194 (98%)	4 (2%)	48	66
26	M	192/211 (91%)	192 (100%)	0	100	100
26	m	192/211 (91%)	192 (100%)	0	100	100
27	N	148/180 (82%)	147 (99%)	1 (1%)	76	78
27	n	148/180 (82%)	147 (99%)	1 (1%)	76	78
28	O	177/227 (78%)	177 (100%)	0	100	100
28	o	177/227 (78%)	177 (100%)	0	100	100
29	P	172/173 (99%)	172 (100%)	0	100	100
29	p	172/173 (99%)	172 (100%)	0	100	100
30	Q	164/171 (96%)	163 (99%)	1 (1%)	78	79
30	q	164/171 (96%)	163 (99%)	1 (1%)	78	79
31	R	153/201 (76%)	153 (100%)	0	100	100
31	r	153/201 (76%)	153 (100%)	0	100	100
32	S	174/198 (88%)	174 (100%)	0	100	100
32	s	174/198 (88%)	174 (100%)	0	100	100
33	T	175/214 (82%)	175 (100%)	0	100	100
33	t	175/214 (82%)	175 (100%)	0	100	100
All	All	11045/12582 (88%)	10954 (99%)	91 (1%)	70	77

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

Mol	Chain	Res	Type
1	U	118	LEU
1	U	629	THR
1	U	788	VAL
1	U	819	VAL
1	U	912	ILE

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Mol	Chain	Res	Type
2	V	221	LEU
2	V	469	THR
3	W	135	LYS
3	W	138	VAL
3	W	196	VAL
3	W	233	LEU
3	W	235	GLN
3	W	239	SER
3	W	241	LEU
3	W	242	SER
3	W	245	LYS
3	W	402	ILE
3	W	456	GLN
4	X	319	ILE
5	Y	100	ILE
5	Y	202	LEU
5	Y	205	VAL
6	Z	8	LYS
6	Z	9	VAL
6	Z	11	VAL
6	Z	14	LEU
6	Z	15	VAL
6	Z	16	LEU
6	Z	17	LEU
6	Z	49	ASP
6	Z	91	ILE
6	Z	126	VAL
6	Z	219	LYS
7	a	145	LEU
9	c	36	LEU
9	c	40	LYS
9	c	69	VAL
9	c	251	LEU
10	d	189	ILE
12	f	75	LEU
12	f	344	VAL
12	f	457	ASN
12	f	660	ILE
12	f	662	MET
12	f	672	LEU
12	f	806	VAL
12	f	822	VAL

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Mol	Chain	Res	Type
13	A	373	LEU
13	A	403	ILE
14	B	355	LEU
15	C	134	LEU
15	C	210	THR
15	C	219	LEU
16	D	202	VAL
16	D	236	VAL
16	D	238	LYS
16	D	267	ILE
16	D	360	LEU
18	F	134	LEU
18	F	198	LEU
18	F	234	THR
18	F	235	LEU
18	F	245	LYS
18	F	329	ILE
18	F	344	ARG
20	G	22	LEU
20	G	73	THR
21	H	86	LEU
22	I	228	LEU
23	J	161	ILE
24	K	67	ILE
24	K	170	ILE
25	L	22	ILE
25	L	38	LEU
25	L	161	ILE
25	L	205	LEU
27	N	30	VAL
30	Q	102	LEU
20	g	22	LEU
20	g	73	THR
21	h	86	LEU
22	i	228	LEU
23	j	161	ILE
24	k	67	ILE
24	k	170	ILE
25	l	22	ILE
25	l	38	LEU
25	l	161	ILE
25	l	205	LEU

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Mol	Chain	Res	Type
27	n	30	VAL
30	q	102	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (177) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	70	HIS
1	U	111	GLN
1	U	139	GLN
1	U	267	ASN
1	U	412	HIS
1	U	415	HIS
1	U	438	GLN
1	U	450	HIS
1	U	491	GLN
1	U	596	ASN
1	U	707	ASN
1	U	888	GLN
2	V	33	GLN
2	V	281	ASN
2	V	299	GLN
2	V	453	HIS
3	W	84	ASN
3	W	86	ASN
3	W	106	GLN
3	W	203	GLN
3	W	362	ASN
3	W	456	GLN
4	X	148	HIS
4	X	170	GLN
4	X	178	HIS
4	X	213	GLN
4	X	292	GLN
4	X	296	ASN
4	X	322	HIS
5	Y	49	ASN
5	Y	71	ASN
5	Y	136	HIS
5	Y	178	ASN
5	Y	365	GLN
6	Z	72	HIS
6	Z	77	ASN

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Mol	Chain	Res	Type
6	Z	102	HIS
6	Z	109	ASN
6	Z	229	GLN
6	Z	256	GLN
7	a	18	GLN
7	a	46	GLN
7	a	86	GLN
7	a	152	HIS
7	a	193	GLN
7	a	227	ASN
7	a	249	GLN
7	a	264	ASN
7	a	288	HIS
7	a	332	HIS
9	c	130	GLN
9	c	197	ASN
9	c	214	GLN
9	c	237	HIS
9	c	287	HIS
9	c	298	GLN
10	d	47	GLN
10	d	221	ASN
12	f	14	GLN
12	f	43	GLN
12	f	112	ASN
12	f	118	ASN
12	f	213	GLN
12	f	291	GLN
12	f	327	ASN
12	f	378	ASN
12	f	382	ASN
12	f	396	ASN
12	f	457	ASN
12	f	531	ASN
12	f	565	ASN
12	f	614	HIS
12	f	619	HIS
12	f	737	ASN
12	f	747	GLN
12	f	752	HIS
12	f	766	GLN
12	f	786	GLN

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Mol	Chain	Res	Type
12	f	815	HIS
13	A	85	GLN
13	A	117	GLN
13	A	165	GLN
13	A	305	GLN
13	A	358	HIS
13	A	379	ASN
14	B	207	HIS
14	B	257	GLN
14	B	277	HIS
14	B	368	HIS
14	B	416	ASN
15	C	40	GLN
15	C	53	ASN
15	C	111	ASN
15	C	279	GLN
15	C	288	ASN
15	C	332	HIS
15	C	337	ASN
15	C	398	ASN
16	D	65	GLN
16	D	127	ASN
16	D	175	GLN
16	D	187	HIS
16	D	222	HIS
16	D	294	ASN
16	D	302	ASN
16	D	304	ASN
16	D	353	ASN
17	E	39	GLN
17	E	194	ASN
17	E	262	ASN
17	E	263	GLN
17	E	271	HIS
17	E	300	HIS
17	E	339	ASN
17	E	359	HIS
17	E	364	GLN
18	F	184	GLN
18	F	243	GLN
18	F	333	ASN
18	F	417	HIS

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Mol	Chain	Res	Type
20	G	75	ASN
20	G	193	GLN
21	H	102	GLN
22	I	20	GLN
22	I	30	HIS
22	I	53	HIS
22	I	84	ASN
22	I	102	GLN
22	I	109	GLN
22	I	119	GLN
22	I	149	GLN
23	J	92	GLN
23	J	122	ASN
23	J	175	ASN
24	K	98	ASN
24	K	214	ASN
25	L	59	HIS
25	L	60	GLN
25	L	86	ASN
25	L	90	GLN
26	M	32	ASN
26	M	97	ASN
26	M	147	GLN
27	N	158	ASN
29	P	93	ASN
30	Q	71	ASN
30	Q	82	ASN
30	Q	132	HIS
31	R	10	HIS
31	R	38	ASN
33	T	213	HIS
20	g	193	GLN
21	h	166	ASN
22	i	84	ASN
22	i	102	GLN
22	i	109	GLN
22	i	149	GLN
23	j	85	ASN
23	j	175	ASN
24	k	214	ASN
25	l	59	HIS
25	l	60	GLN

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Mol	Chain	Res	Type
25	l	86	ASN
25	l	90	GLN
26	m	32	ASN
26	m	97	ASN
26	m	147	GLN
27	n	158	ASN
28	o	116	HIS
29	p	18	ASN
30	q	63	ASN
30	q	71	ASN
30	q	82	ASN
30	q	132	HIS
31	r	10	HIS
32	s	163	HIS
33	t	213	HIS

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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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
35	ATP	C	501	-	32,33,33	1.30	5 (15%)	48,52,52	1.82	13 (27%)
36	ADP	F	501	-	28,29,29	1.35	5 (17%)	43,45,45	1.86	10 (23%)
35	ATP	E	401	-	32,33,33	1.32	3 (9%)	48,52,52	1.97	11 (22%)
35	ATP	D	501	-	32,33,33	1.31	4 (12%)	48,52,52	1.78	8 (16%)

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
35	ATP	C	501	-	-	2/22/38/38	0/3/3/3
36	ADP	F	501	-	-	7/16/32/32	0/3/3/3
35	ATP	E	401	-	-	1/22/38/38	0/3/3/3
35	ATP	D	501	-	-	6/22/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	E	401	ATP	C5-C4	4.63	1.47	1.39
35	D	501	ATP	C5-C4	4.48	1.47	1.39
35	C	501	ATP	C5-C4	4.25	1.46	1.39
36	F	501	ADP	C5-C4	4.18	1.46	1.39
35	D	501	ATP	C5-N7	-2.77	1.34	1.39
35	E	401	ATP	C5-N7	-2.69	1.34	1.39
35	E	401	ATP	C5-C6	2.60	1.48	1.41
35	C	501	ATP	C5-N7	-2.58	1.34	1.39
36	F	501	ADP	C5-C6	2.53	1.48	1.41
36	F	501	ADP	C4-N9	-2.51	1.32	1.37
35	C	501	ATP	C5-C6	2.41	1.47	1.41
36	F	501	ADP	C5-N7	-2.39	1.34	1.39
35	D	501	ATP	C5-C6	2.38	1.47	1.41
35	C	501	ATP	C4-N9	-2.33	1.32	1.37
35	D	501	ATP	C4-N9	-2.26	1.33	1.37
36	F	501	ADP	C8-N7	2.07	1.35	1.31
35	C	501	ATP	C8-N7	2.03	1.35	1.31

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	E	401	ATP	C5-C4-N3	-6.77	117.39	126.72
35	D	501	ATP	C5-C4-N3	-5.72	118.84	126.72
35	E	401	ATP	N3-C4-N9	5.63	136.74	127.17
35	C	501	ATP	C5-C4-N3	-5.53	119.11	126.72
36	F	501	ADP	C5-C4-N3	-5.16	119.61	126.72
35	D	501	ATP	N3-C4-N9	4.67	135.10	127.17
35	C	501	ATP	N3-C4-N9	4.61	135.00	127.17
36	F	501	ADP	N3-C4-N9	4.33	134.53	127.17
35	E	401	ATP	C2-N3-C4	4.00	121.60	111.83
35	C	501	ATP	C2-N3-C4	3.74	120.98	111.83
35	C	501	ATP	N3-C2-N1	-3.67	123.03	128.58
36	F	501	ADP	C4-N9-C8	3.62	109.54	105.74
36	F	501	ADP	C2-N3-C4	3.56	120.54	111.83
35	D	501	ATP	C2-N3-C4	3.50	120.38	111.83
36	F	501	ADP	N3-C2-N1	-3.41	123.41	128.58
36	F	501	ADP	C4-C5-N7	-3.29	106.82	110.58
35	C	501	ATP	C4-C5-N7	-3.18	106.95	110.58
35	C	501	ATP	C4-N9-C8	3.14	109.04	105.74
35	E	401	ATP	C4-C5-N7	-3.07	107.07	110.58
35	E	401	ATP	N3-C2-N1	-3.01	124.03	128.58
35	D	501	ATP	C4-C5-N7	-2.99	107.16	110.58
35	D	501	ATP	N3-C2-N1	-2.99	124.06	128.58
35	C	501	ATP	C3'-C2'-C1'	2.83	106.81	101.46
35	E	401	ATP	C3'-C2'-C1'	2.82	106.80	101.46
35	D	501	ATP	C3'-C2'-C1'	2.81	106.78	101.46
36	F	501	ADP	N9-C8-N7	-2.57	110.30	113.94
36	F	501	ADP	C5-N7-C8	2.56	107.48	103.45
35	E	401	ATP	C1'-N9-C8	-2.51	121.53	127.09
35	D	501	ATP	C4-N9-C8	2.38	108.24	105.74
35	C	501	ATP	C5-N7-C8	2.37	107.17	103.45
35	E	401	ATP	O2A-PA-O1A	2.34	123.34	112.44
36	F	501	ADP	C6-C5-N7	2.30	136.52	132.09
36	F	501	ADP	O2A-PA-O1A	2.27	122.99	112.44
35	C	501	ATP	O3G-PG-O2G	2.25	116.24	107.80
35	E	401	ATP	C5-N7-C8	2.22	106.94	103.45
35	C	501	ATP	C2-N1-C6	2.21	122.36	118.73
35	E	401	ATP	C5'-C4'-C3'	-2.13	107.56	115.21
35	D	501	ATP	C5-N7-C8	2.12	106.78	103.45
35	C	501	ATP	C2'-C1'-N9	-2.12	108.04	113.30
35	C	501	ATP	C6-C5-N7	2.12	136.17	132.09
35	C	501	ATP	N9-C8-N7	-2.11	110.94	113.94
35	E	401	ATP	C4-N9-C8	2.10	107.94	105.74

There are no chirality outliers.

All (16) torsion outliers are listed below:

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

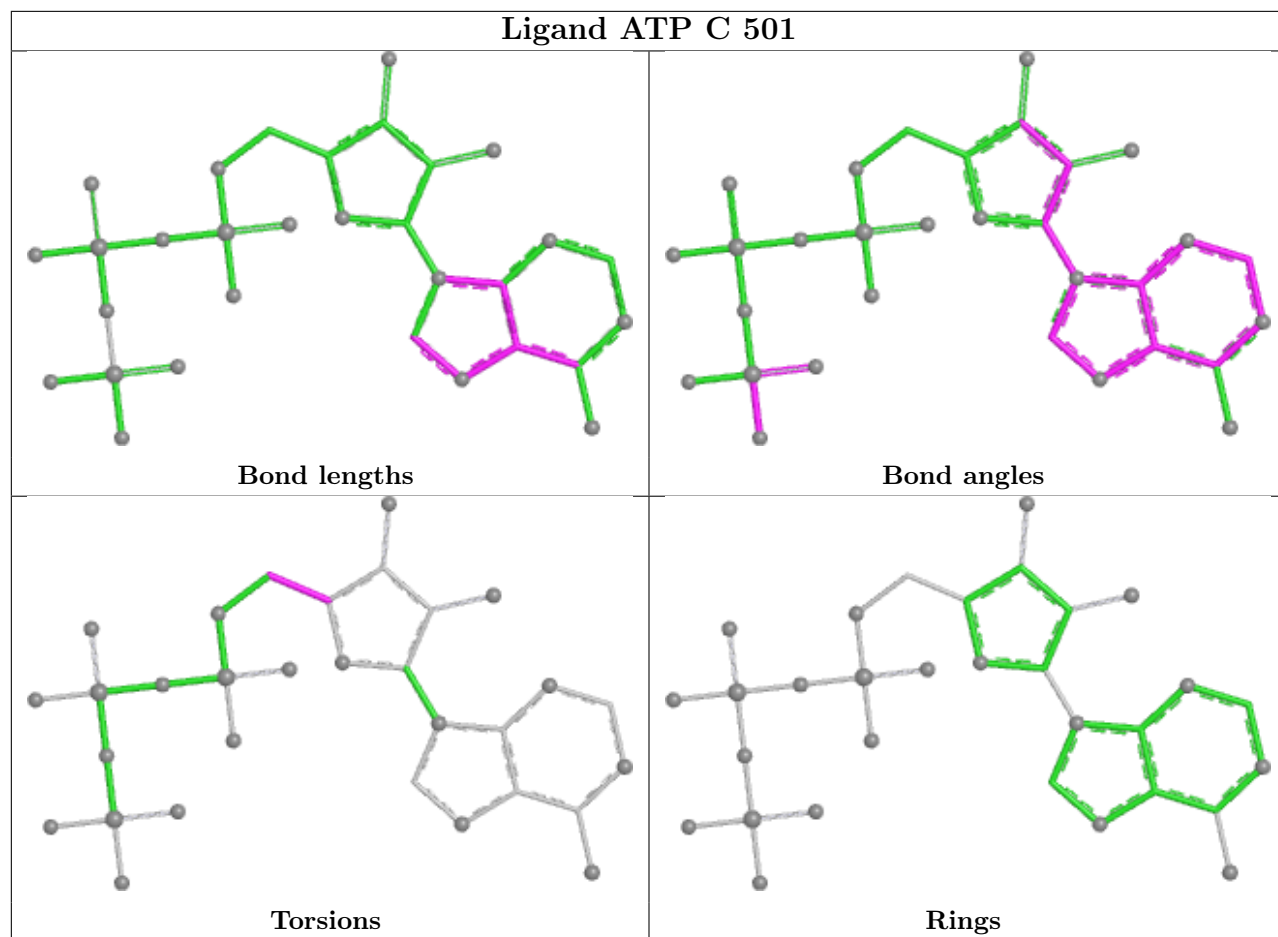
There are no ring outliers.

2 monomers are involved in 5 short contacts:

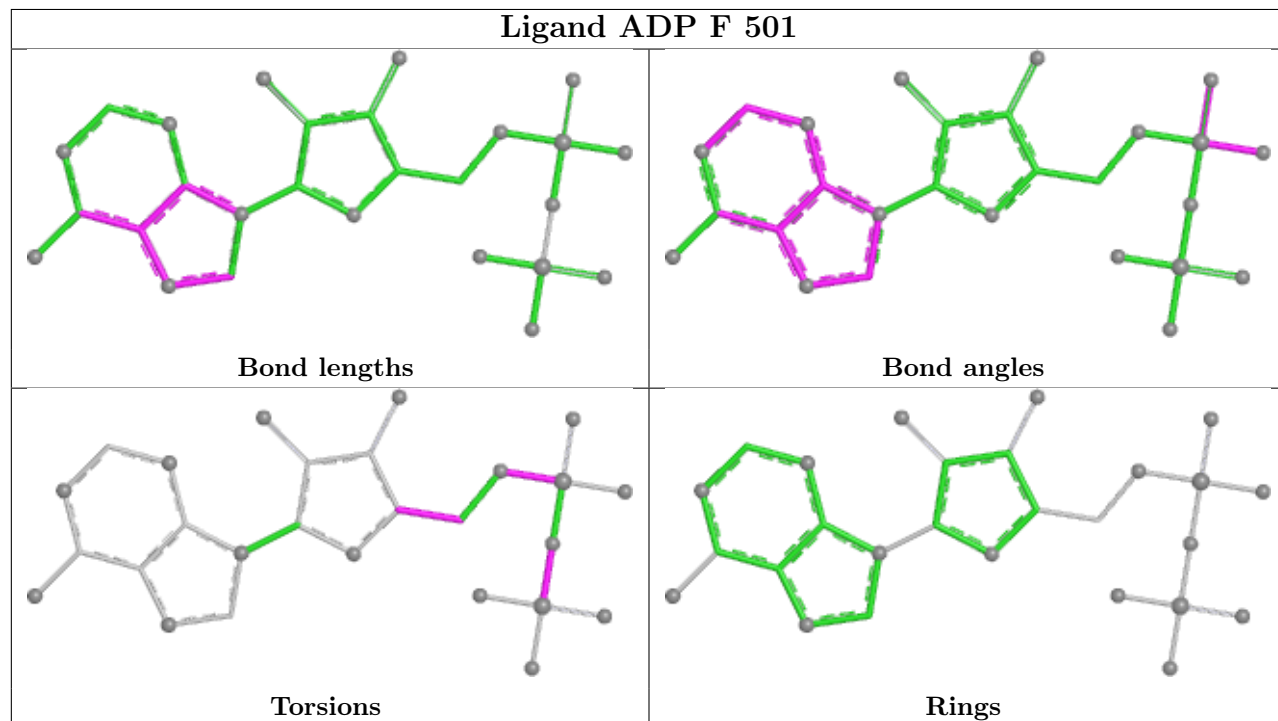
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	C	501	ATP	3	0
35	E	401	ATP	2	0

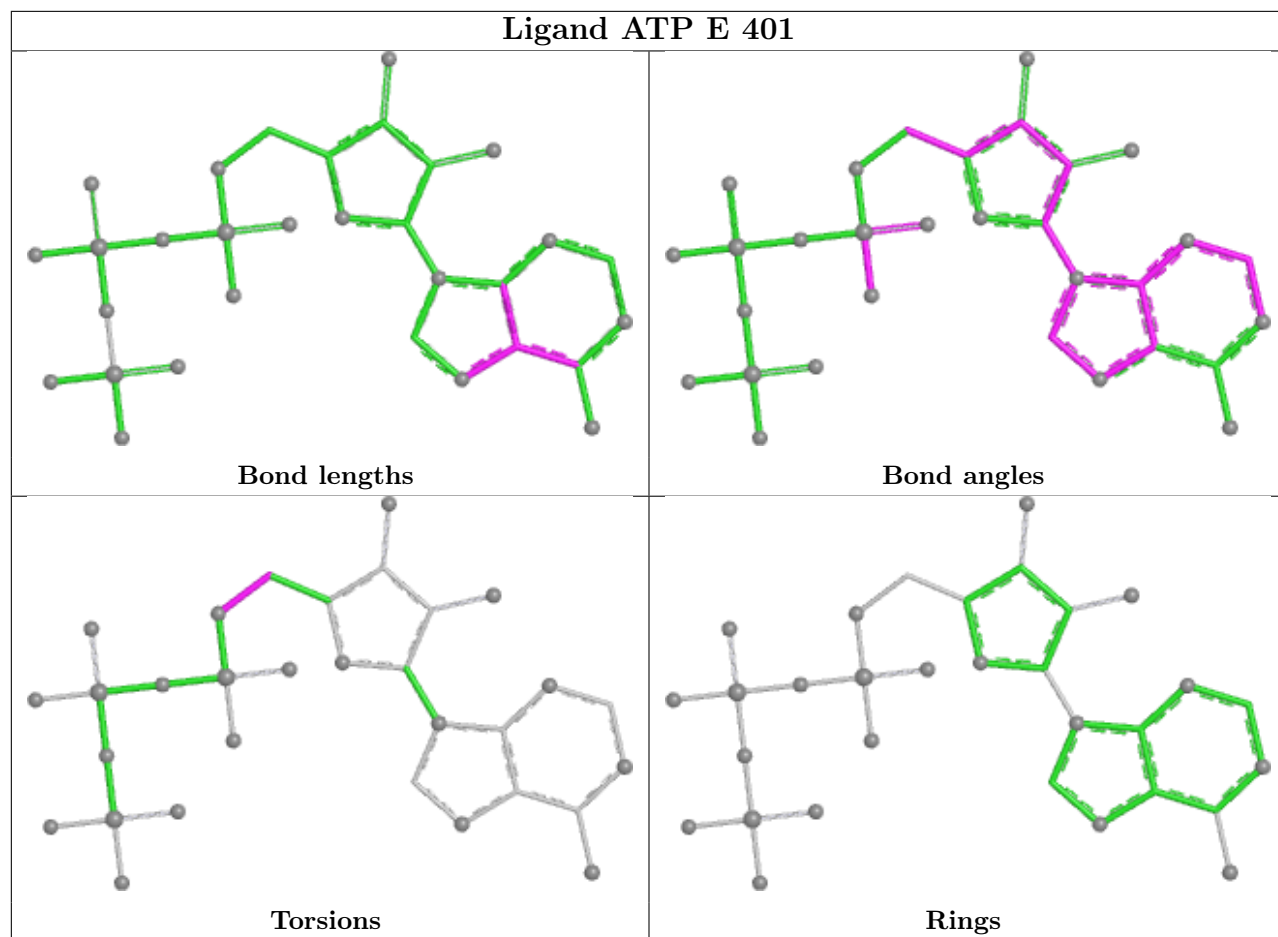
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

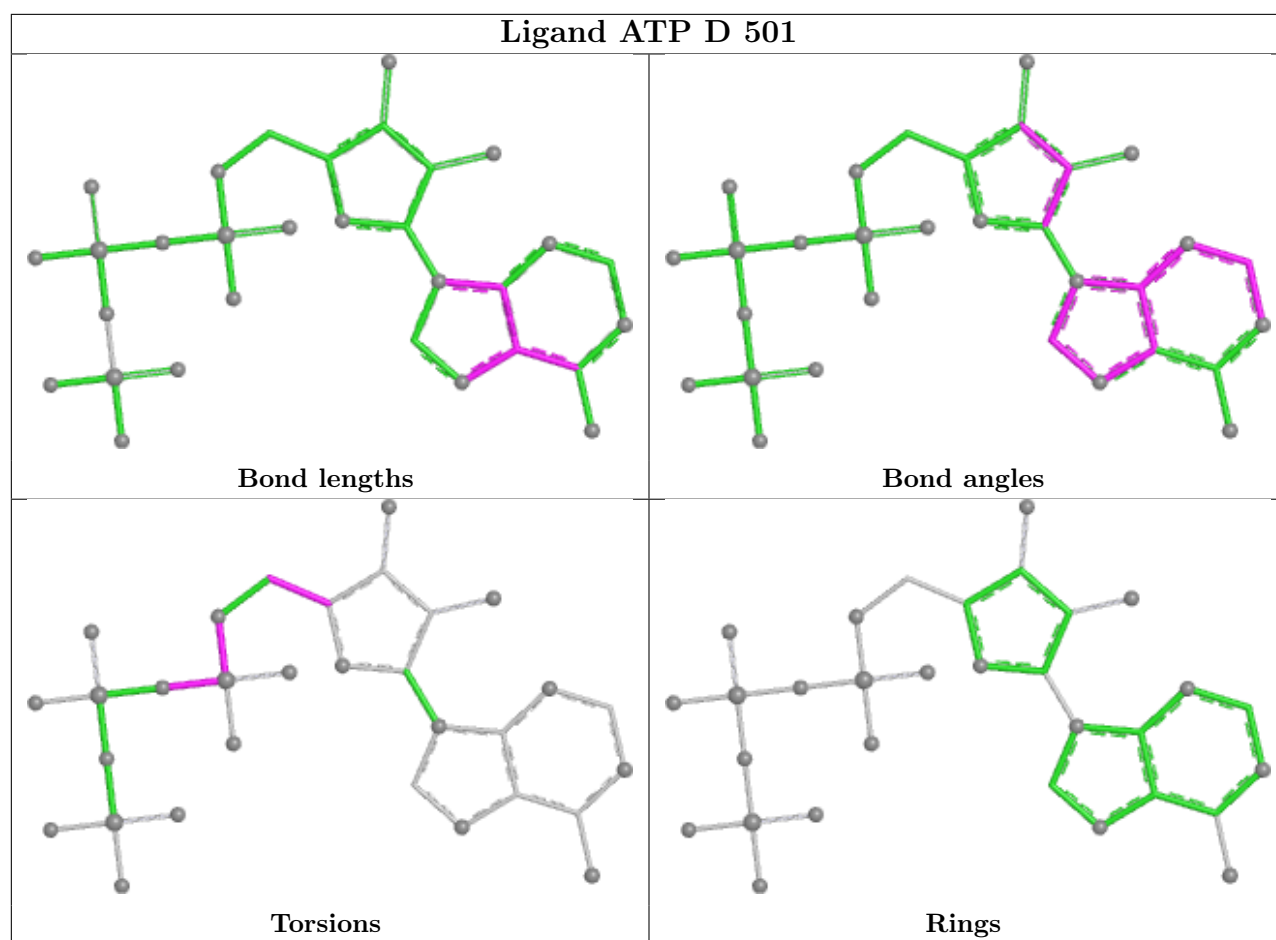
Ligand ATP C 501



Ligand ADP F 501







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.

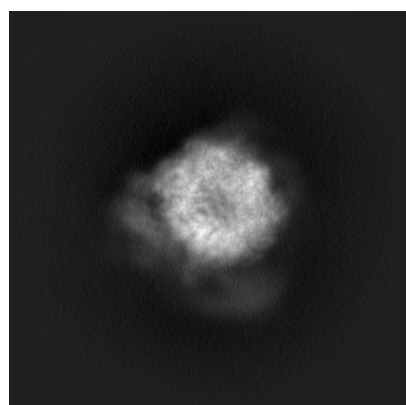
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9220. These allow visual inspection of the internal detail of the map and identification of artifacts.

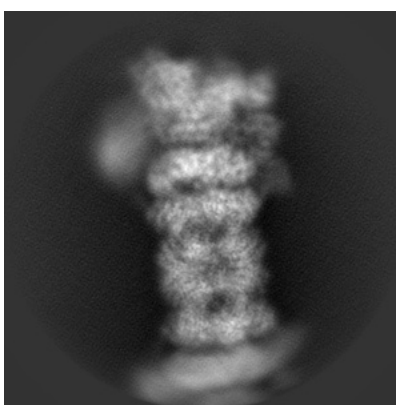
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

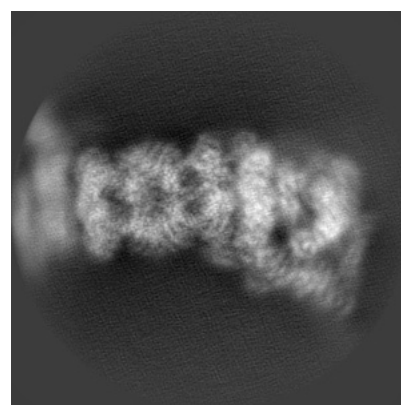
6.1.1 Primary map



X



Y

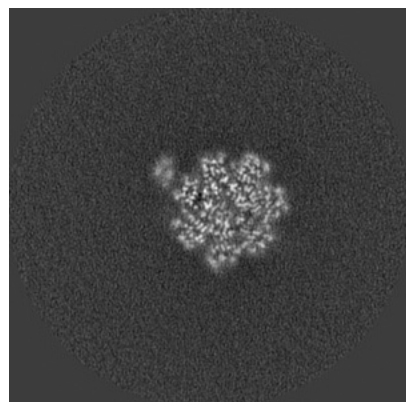


Z

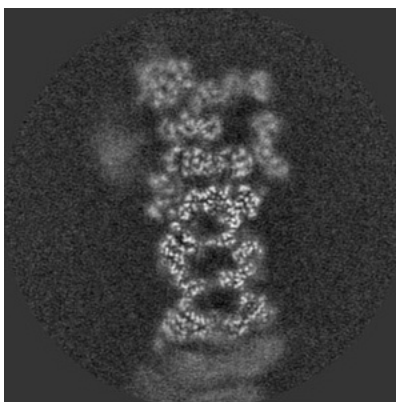
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

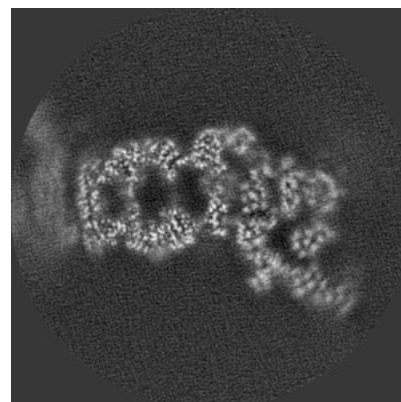
6.2.1 Primary map



X Index: 300



Y Index: 300

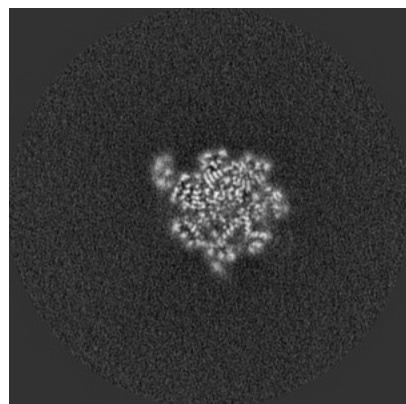


Z Index: 300

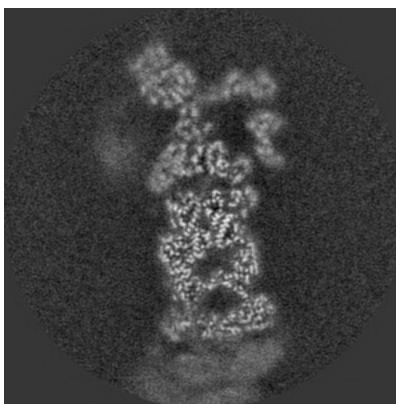
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

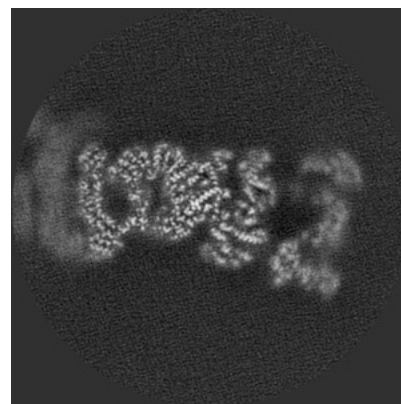
6.3.1 Primary map



X Index: 307



Y Index: 287

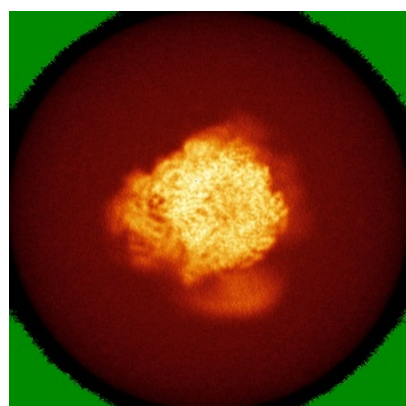


Z Index: 343

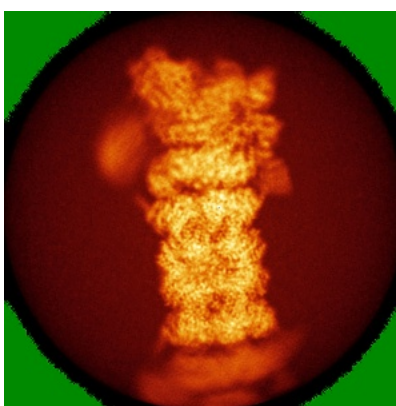
The images above show the largest variance slices of the map in three orthogonal directions.

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

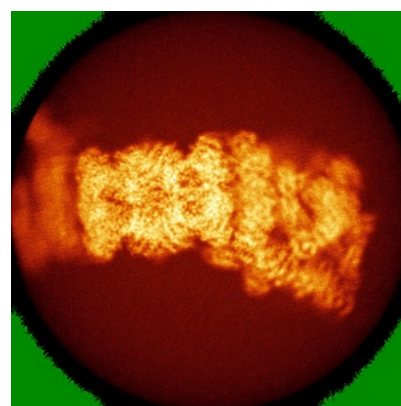
6.4.1 Primary map



X



Y

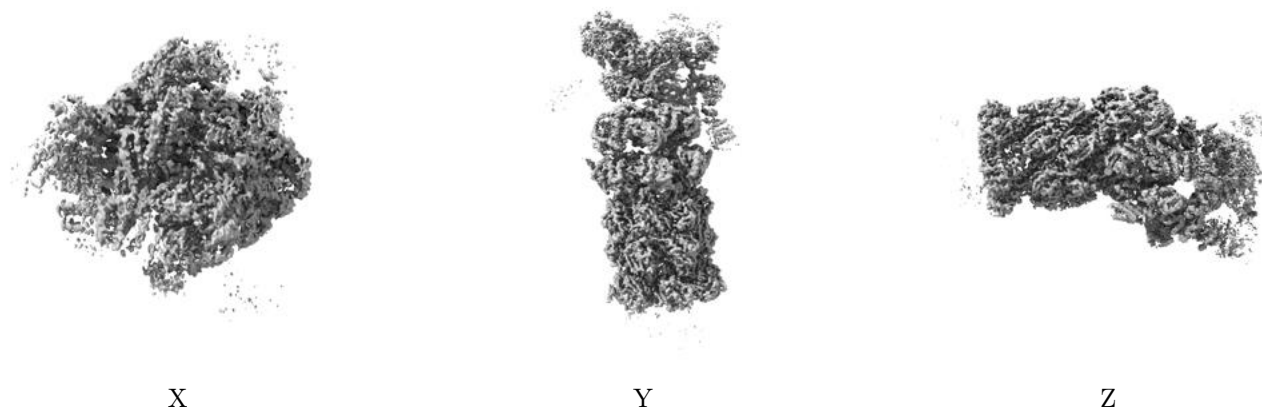


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

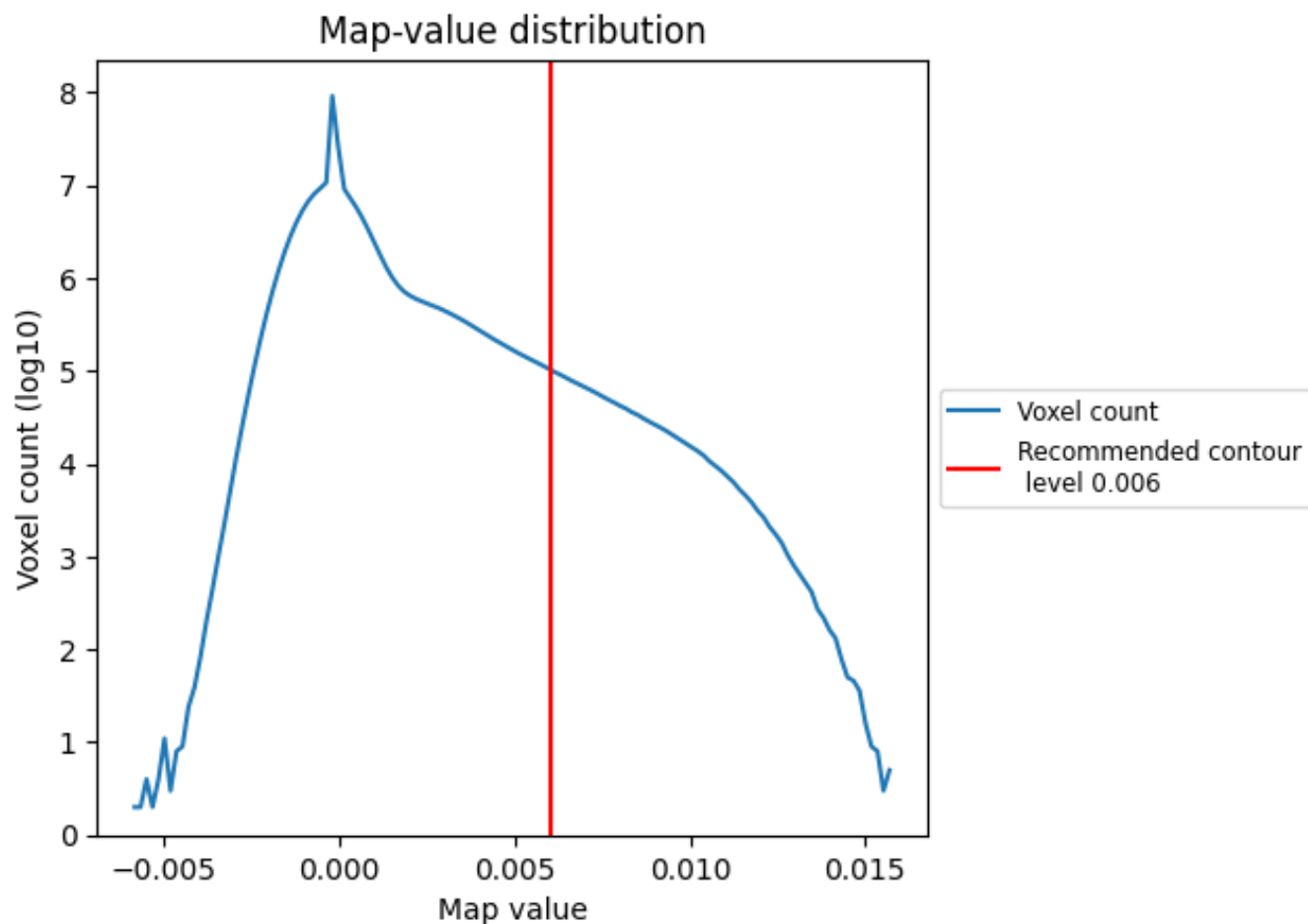
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

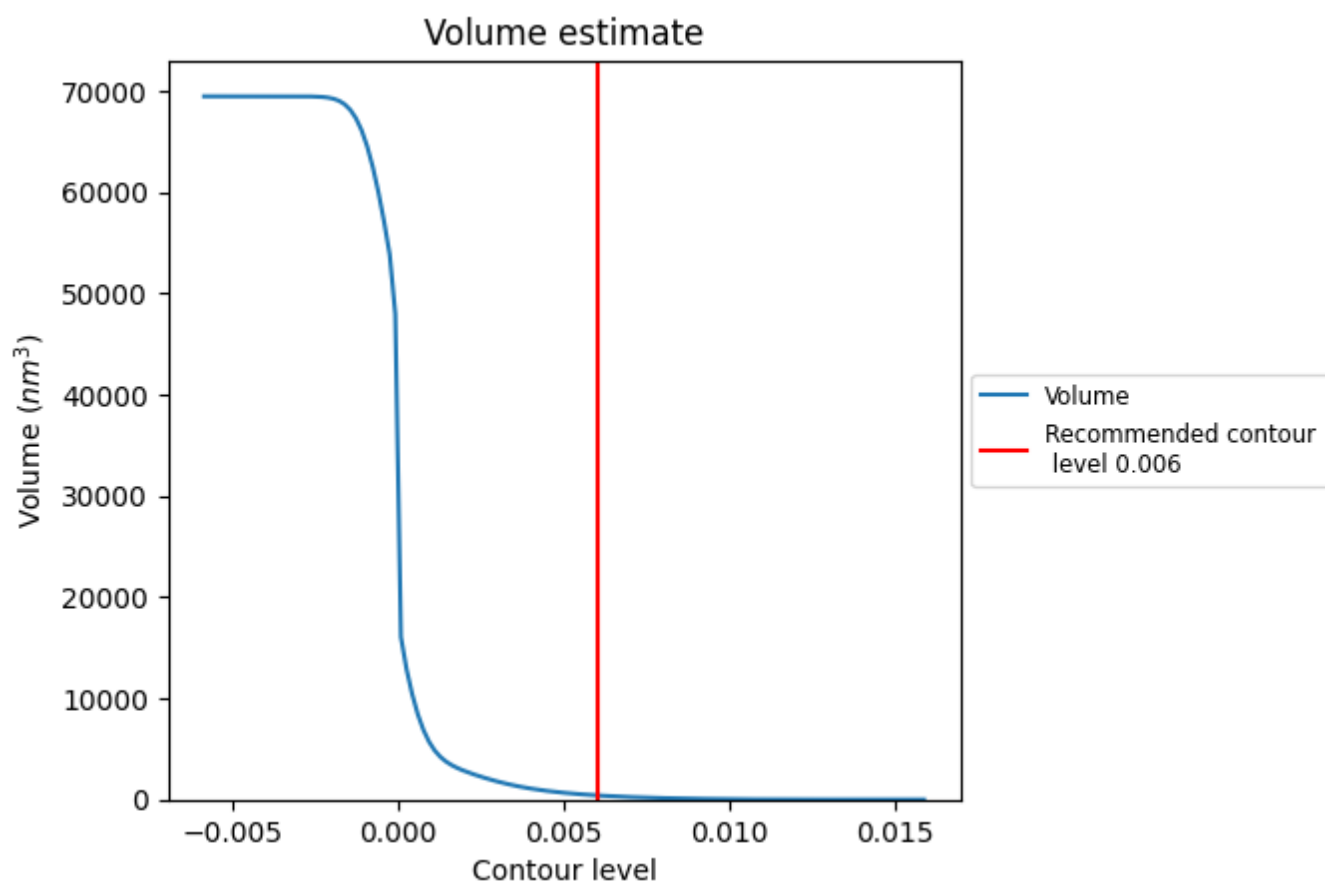
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

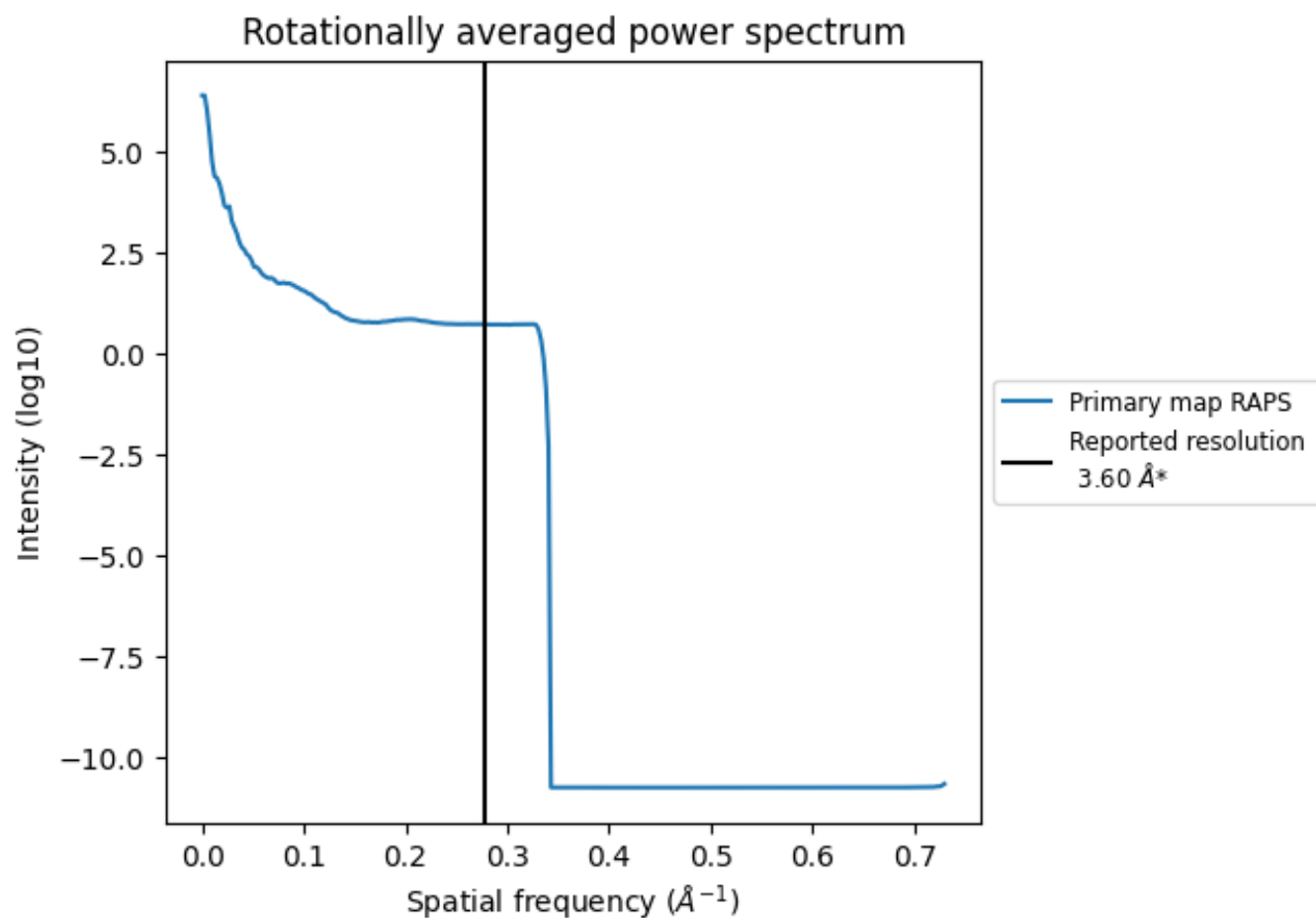
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 414 nm³; this corresponds to an approximate mass of 374 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 0.278 Å⁻¹

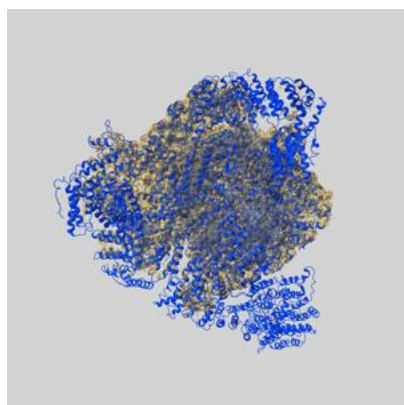
8 Fourier-Shell correlation

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

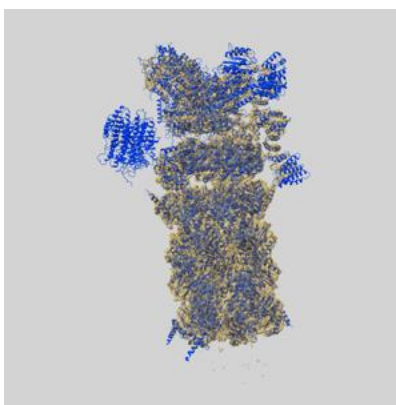
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9220 and PDB model 6MSH. Per-residue inclusion information can be found in section [3](#) on page [12](#).

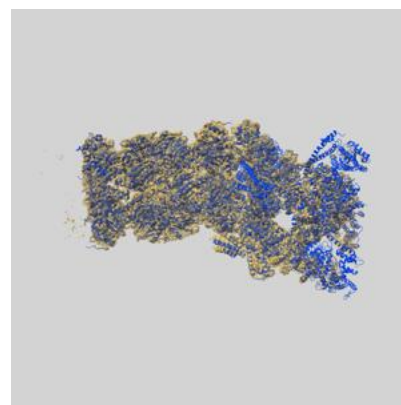
9.1 Map-model overlay [i](#)



X



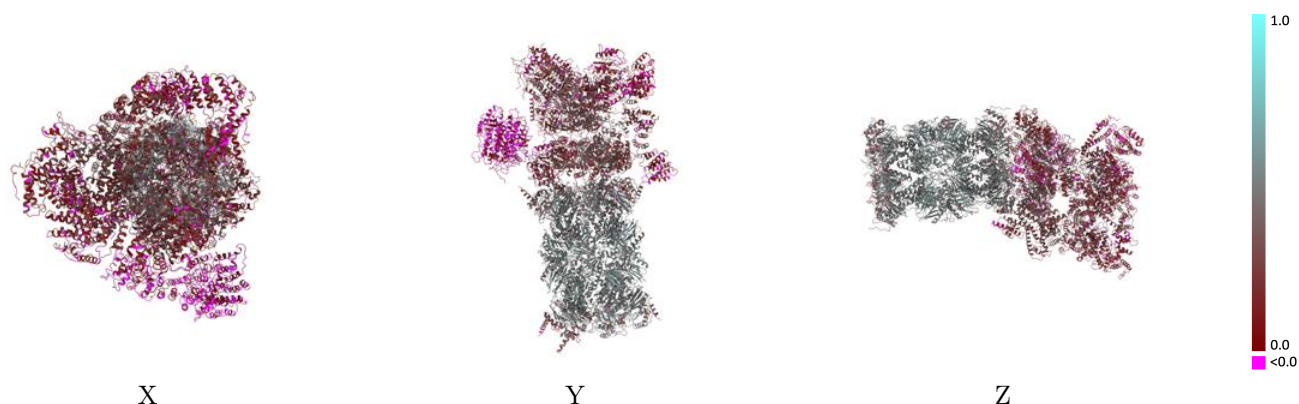
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

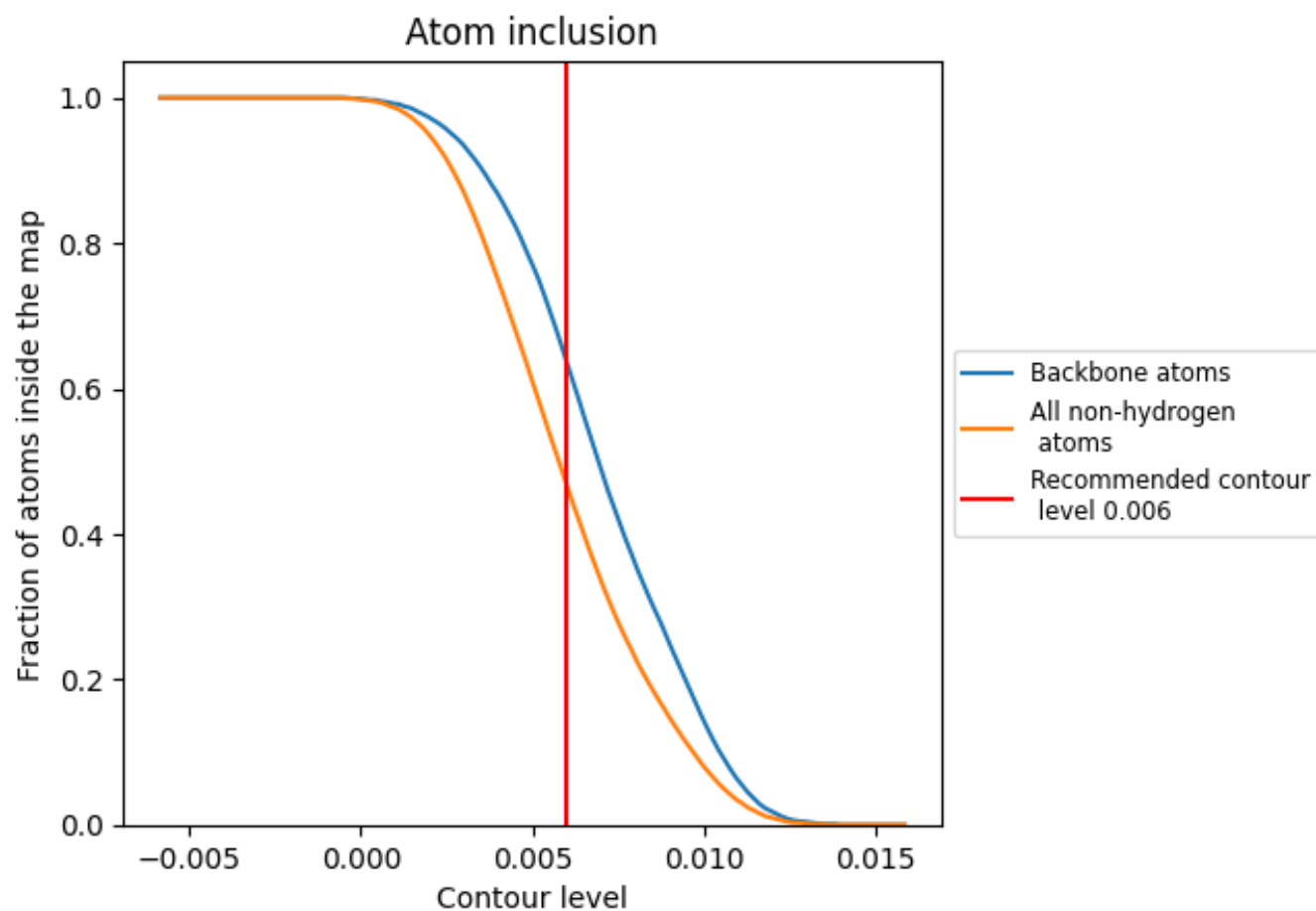


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 47% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4680	 0.3220
A	 0.3550	 0.2230
B	 0.2200	 0.1930
C	 0.4110	 0.2770
D	 0.5110	 0.3430
E	 0.4630	 0.3010
F	 0.4250	 0.2540
G	 0.7230	 0.4480
H	 0.7700	 0.4580
I	 0.6950	 0.4170
J	 0.6640	 0.4090
K	 0.6590	 0.4270
L	 0.7160	 0.4530
M	 0.6960	 0.4230
N	 0.7810	 0.4940
O	 0.7640	 0.4890
P	 0.7680	 0.4970
Q	 0.7500	 0.4730
R	 0.7840	 0.5020
S	 0.7250	 0.4900
T	 0.7680	 0.4990
U	 0.2320	 0.2070
V	 0.1610	 0.1790
W	 0.2420	 0.1690
X	 0.5600	 0.2920
Y	 0.5320	 0.2640
Z	 0.2610	 0.2130
a	 0.1620	 0.1660
b	 0.0210	 0.1490
c	 0.3060	 0.2540
d	 0.0730	 0.1700
e	 0.2580	 0.1920
f	 0.0000	 0.0170
g	 0.6010	 0.4430
h	 0.6160	 0.4520



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Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.5360	 0.4160
j	 0.4980	 0.3920
k	 0.5690	 0.4300
l	 0.6780	 0.4630
m	 0.6230	 0.4350
n	 0.7570	 0.5040
o	 0.7220	 0.4950
p	 0.7370	 0.5030
q	 0.7320	 0.4850
r	 0.7780	 0.5130
s	 0.7450	 0.4980
t	 0.7790	 0.5080
v	 0.0730	 0.2000