



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:35 PM UTC

PDB ID : 7W3A / pdb_00007w3a
EMDB ID : EMD-32275
Title : Structure of USP14-bound human 26S proteasome in substrate-engaged state
ED4_USP14
Authors : Zhang, S.; Zou, S.; Yin, D.; Wu, Z.; Mao, Y.
Deposited on : 2021-11-25
Resolution : 3.50 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

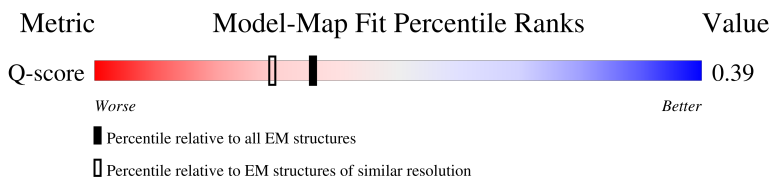
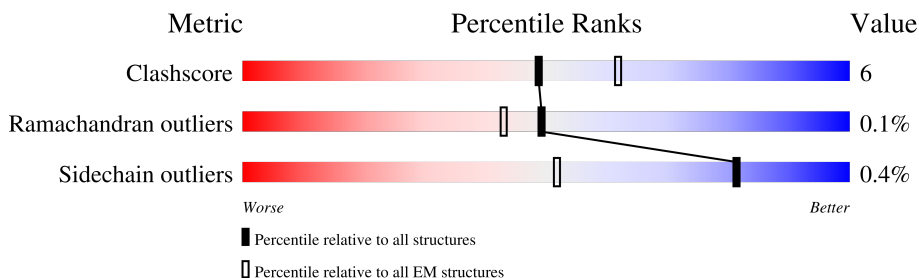
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.



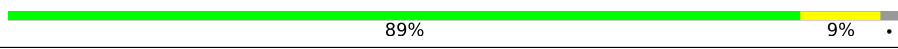
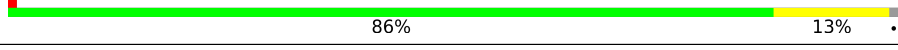
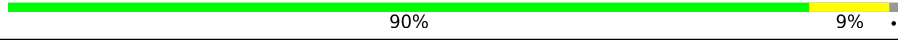
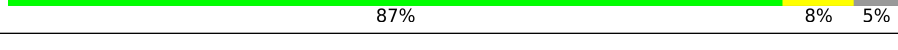
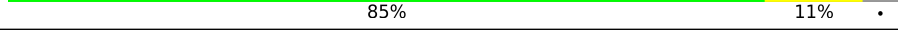
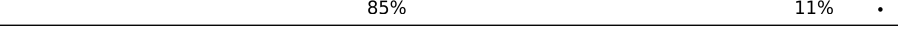
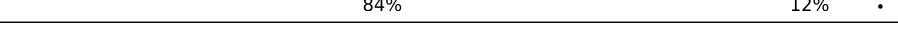
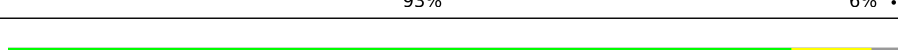
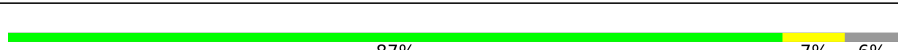
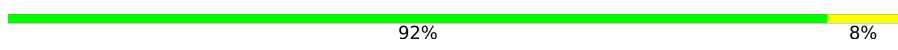
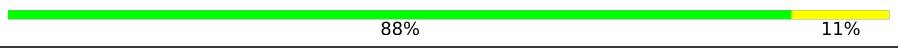
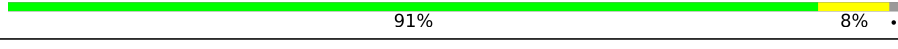
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	A	433	
2	B	440	
3	C	398	
4	D	418	

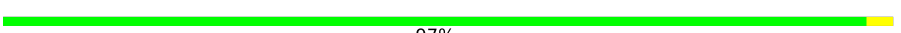
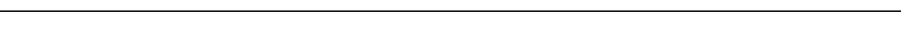
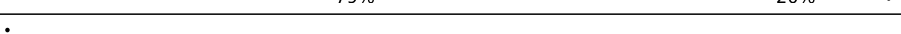
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Mol	Chain	Length	Quality of chain
5	E	403	
6	F	439	
7	G	246	
7	g	246	
8	H	234	
8	h	234	
9	I	261	
9	i	261	
10	J	248	
10	j	248	
11	K	241	
11	k	241	
12	L	269	
12	l	269	
13	M	255	
13	m	255	
14	N	239	
14	n	239	
15	O	277	
15	o	277	
16	P	205	
16	p	205	
17	Q	201	
17	q	201	
18	R	263	

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Mol	Chain	Length	Quality of chain
18	r	263	
19	S	241	
19	s	241	
20	T	264	
20	t	264	
21	v	34	
22	x	494	
23	y	76	
24	U	953	
25	V	534	
26	W	456	
27	X	422	
28	Y	389	
29	Z	324	
30	a	376	
31	b	377	
32	c	310	
33	d	350	
34	f	908	
35	e	70	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 110889 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 protease regulatory subunit 7.

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

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

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

- Molecule 3 is a protein called Isoform 2 of 26S proteasome regulatory subunit 8.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	380	Total	C	N	O	S	0	0
			3039	1923	524	579	13		

- Molecule 5 is a protein called 26S proteasome regulatory subunit 10B.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	400	Total	C	N	O	S	0	0
			3133	1972	540	603	18		

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	242	Total	C	N	O	S	0	0
			1890	1200	323	356	11		
13	m	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	199	Total	C	N	O	S	0	0
			1588	1017	270	292	9		

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

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

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

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

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

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

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

- Molecule 21 is a protein called Substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	v	34	Total	C	N	O	0	0
			170	102	34	34		

- Molecule 22 is a protein called Ubiquitin carboxyl-terminal hydrolase 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	x	494	Total	C	N	O	S	0	0
			3929	2485	647	769	28		

- Molecule 23 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	y	76	Total	C	N	O	S	0	0
			601	378	105	117	1		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	872	Total	C	N	O	S	0	0
			6828	4328	1157	1298	45		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	446	Total	C	N	O	S	0	0
			3635	2302	622	687	24		

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

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

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 31 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 33 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

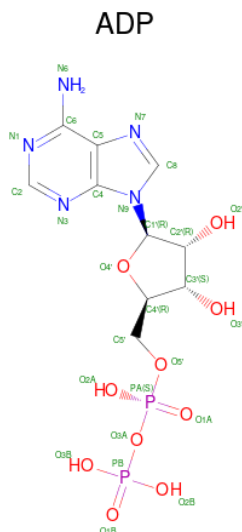
- Molecule 34 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	889	Total	C	N	O	S	0	0
			6866	4315	1174	1331	46		

- Molecule 35 is a protein called 26S proteasome complex subunit DSS1.

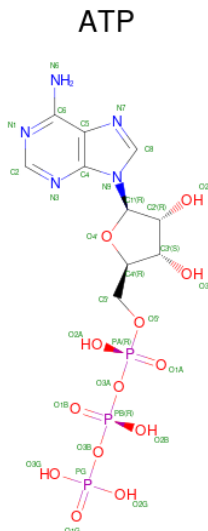
Mol	Chain	Residues	Atoms				AltConf	Trace
35	e	50	Total	C	N	O	0	0
			425	260	65	100		

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



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

- Molecule 37 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



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

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

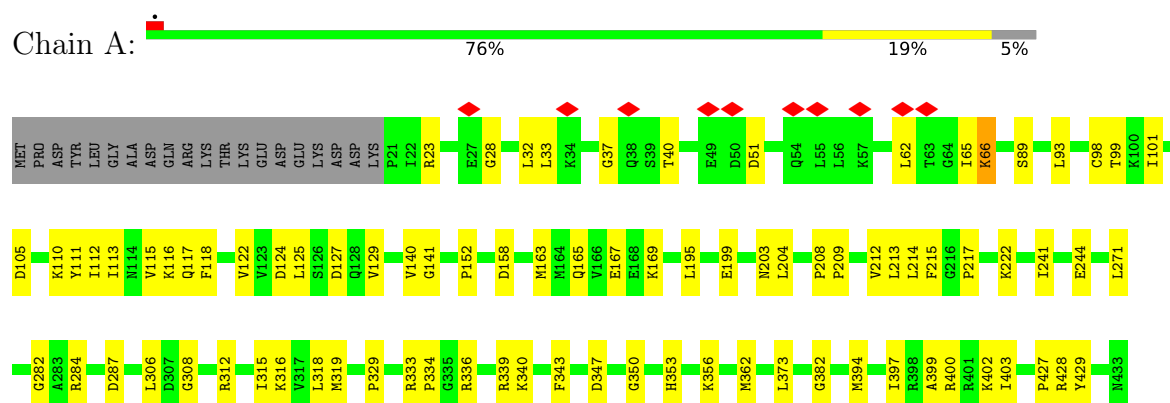
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

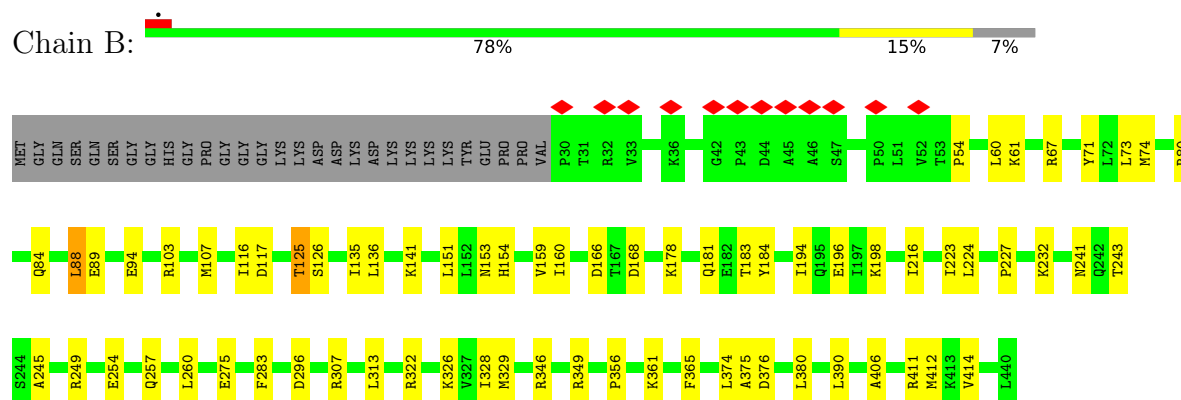
3 Residue-property plots

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

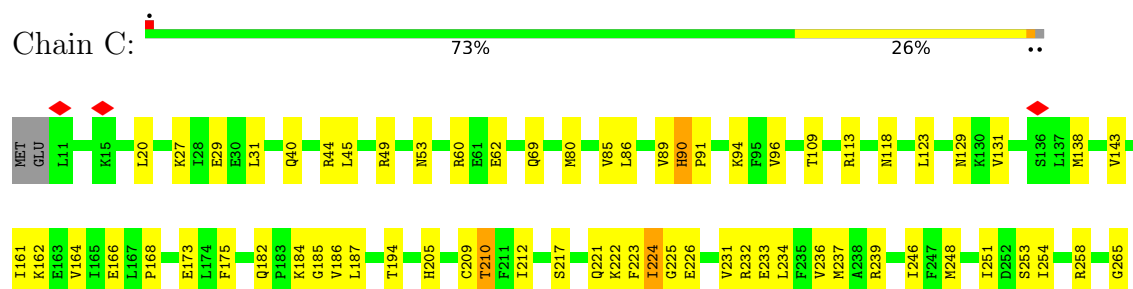
- Molecule 1: 26S protease regulatory subunit 7



- Molecule 2: 26S protease regulatory subunit 4



- Molecule 3: Isoform 2 of 26S proteasome regulatory subunit 8



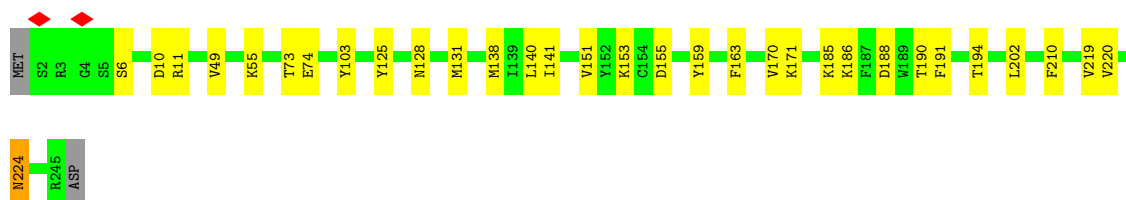
- Molecule 7: Proteasome subunit alpha type-6

Chain G:  89% 9%



- Molecule 7: Proteasome subunit alpha type-6

Chain g:  86% 13%



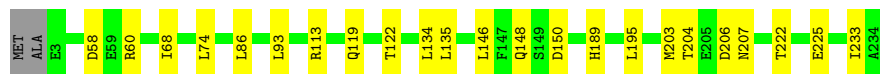
- Molecule 8: Proteasome subunit alpha type-2

Chain H:  90% 9%



- Molecule 8: Proteasome subunit alpha type-2

Chain h:  89% 10%



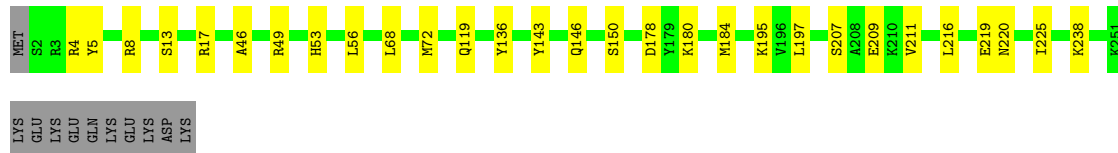
- Molecule 9: Proteasome subunit alpha type-4

Chain I:  87% 8% 5%



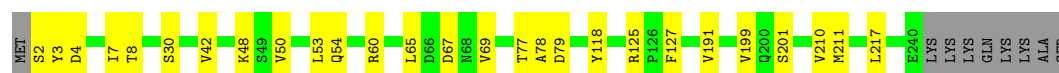
- Molecule 9: Proteasome subunit alpha type-4

Chain i:  85% 11%



- Molecule 10: Proteasome subunit alpha type-7

Chain J:  85% 11% .

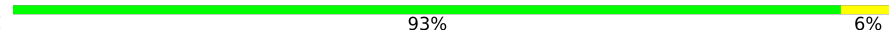


- Molecule 10: Proteasome subunit alpha type-7

Chain j:  84% 12% .



- Molecule 11: Proteasome subunit alpha type-5

Chain K:  93% 6% .



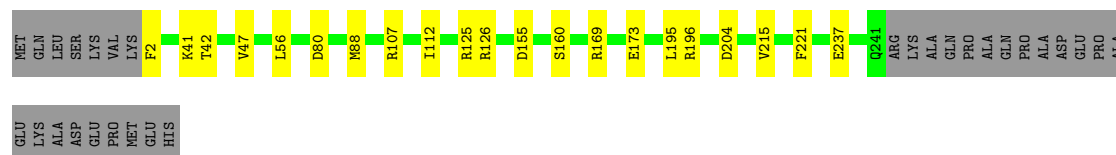
- Molecule 11: Proteasome subunit alpha type-5

Chain k:  88% 9% .



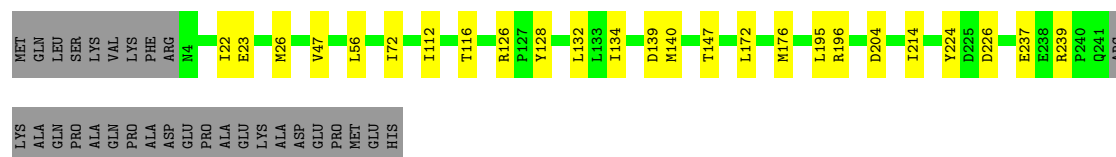
- Molecule 12: Isoform Long of Proteasome subunit alpha type-1

Chain L:  81% 8% 11%



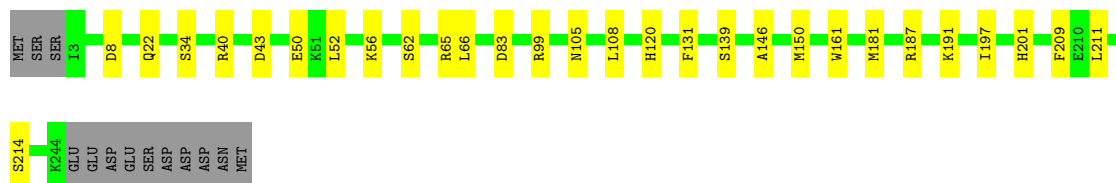
- Molecule 12: Isoform Long of Proteasome subunit alpha type-1

Chain l:  79% 9% 12%



- Molecule 13: Proteasome subunit alpha type-3

Chain M:  84% 11% 5%



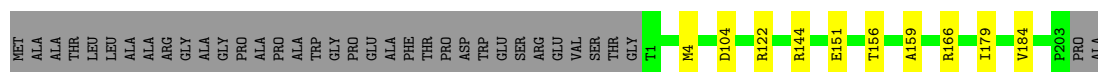
- Molecule 13: Proteasome subunit alpha type-3

Chain m:  87% 7% 6%



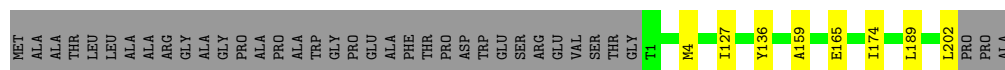
- Molecule 14: Proteasome subunit beta type-6

Chain N:  81% 15%



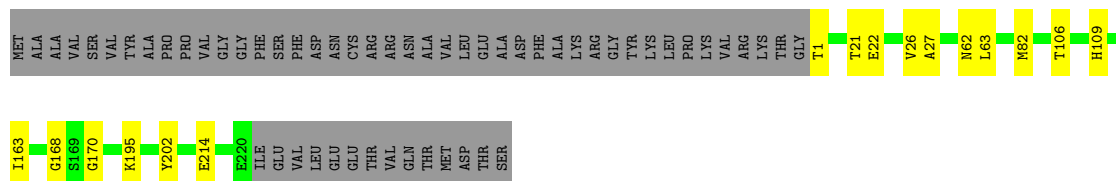
- Molecule 14: Proteasome subunit beta type-6

Chain n:  81% 15%



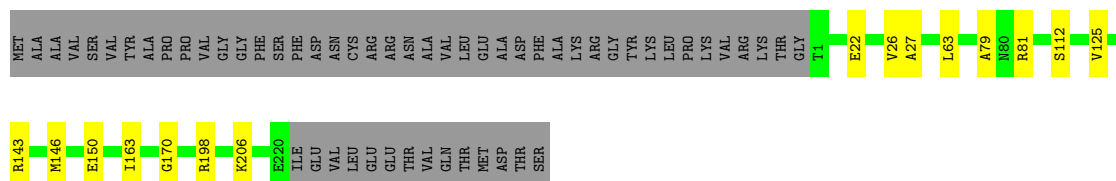
- Molecule 15: Proteasome subunit beta type-7

Chain O:  74% 6% 21%



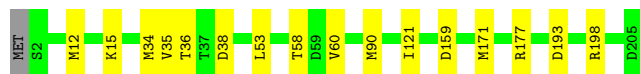
- Molecule 15: Proteasome subunit beta type-7

Chain o:  74% 5% 21%



- Molecule 16: Proteasome subunit beta type-3

Chain P:  92% 8%



- Molecule 16: Proteasome subunit beta type-3

Chain p:  88% 11%



- Molecule 17: Proteasome subunit beta type-2

Chain Q:  88% 11%



- Molecule 17: Proteasome subunit beta type-2

Chain q:  91% 8%



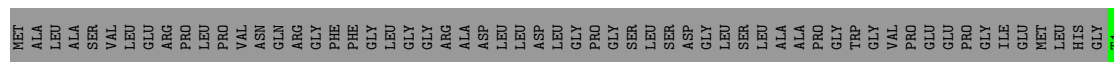
- Molecule 18: Proteasome subunit beta type-5

Chain R:  71% 6% 24%



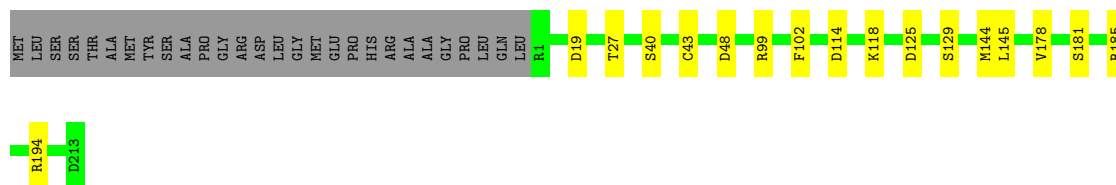
- Molecule 18: Proteasome subunit beta type-5

Chain r:  72% 5% 24%



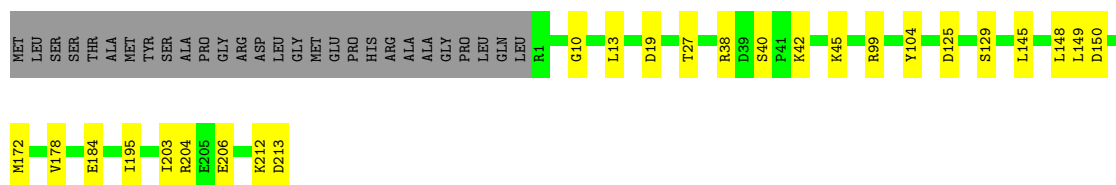
- Molecule 19: Proteasome subunit beta type-1

Chain S:  81% 7% 12%



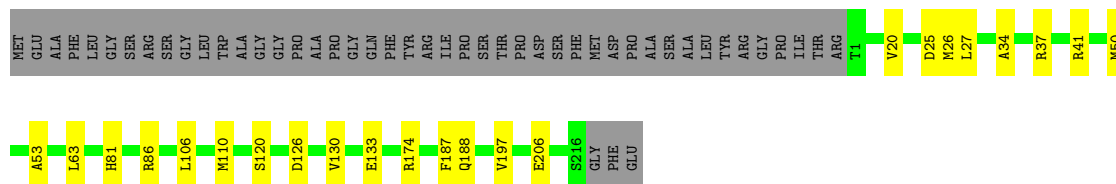
- Molecule 19: Proteasome subunit beta type-1

Chain s:  78% 10% 12%



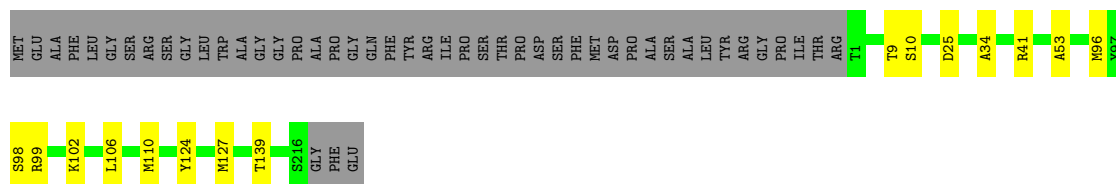
- Molecule 20: Proteasome subunit beta type-4

Chain T:  73% 9% 18%

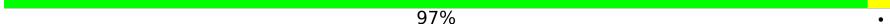


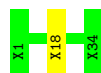
- Molecule 20: Proteasome subunit beta type-4

Chain t:  76% 6% 18%



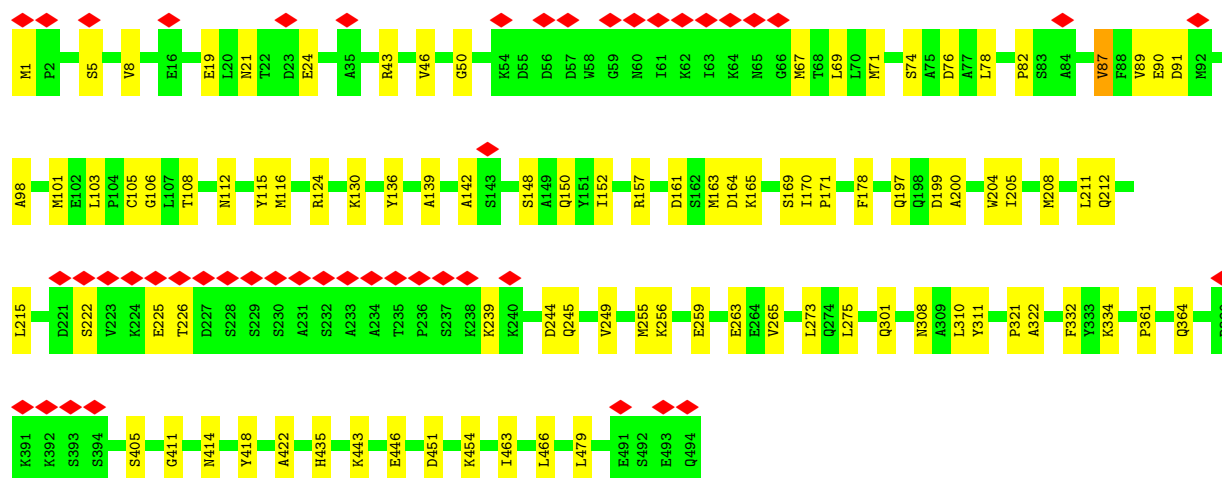
- Molecule 21: Substrate

Chain v:  97% .



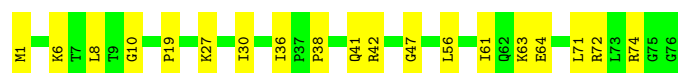
- Molecule 22: Ubiquitin carboxyl-terminal hydrolase 14

Chain x:  10% 81% 18%



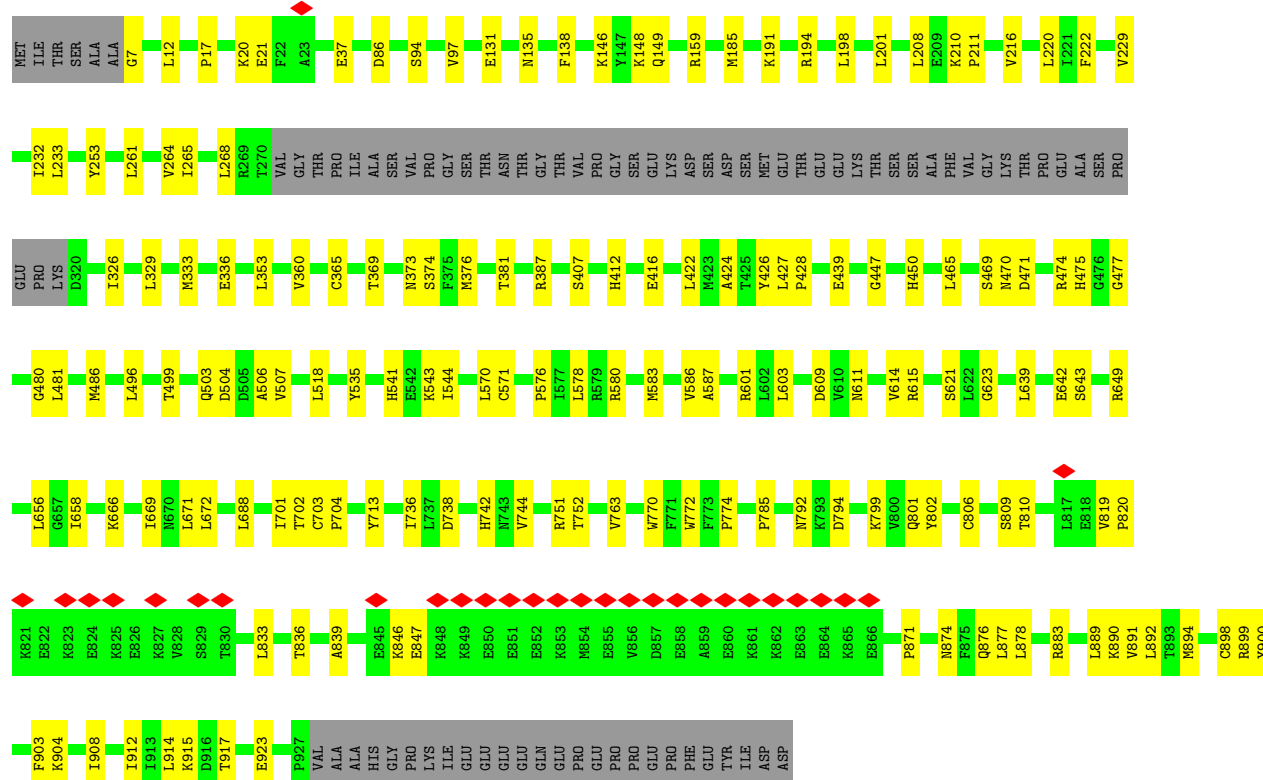
- Molecule 23: Ubiquitin

Chain y: 75% 25%

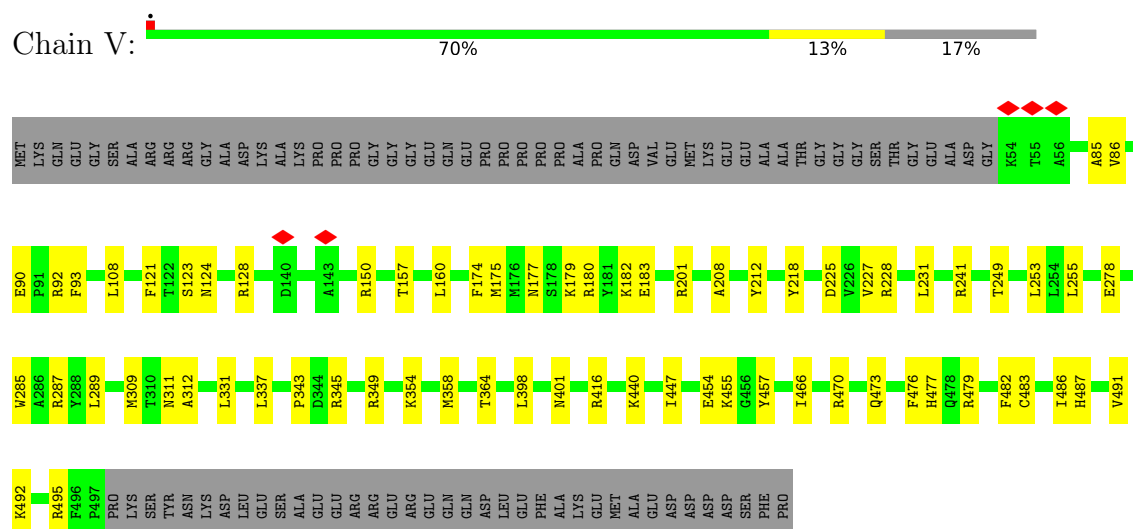


- Molecule 24: 26S proteasome non-ATPase regulatory subunit 1

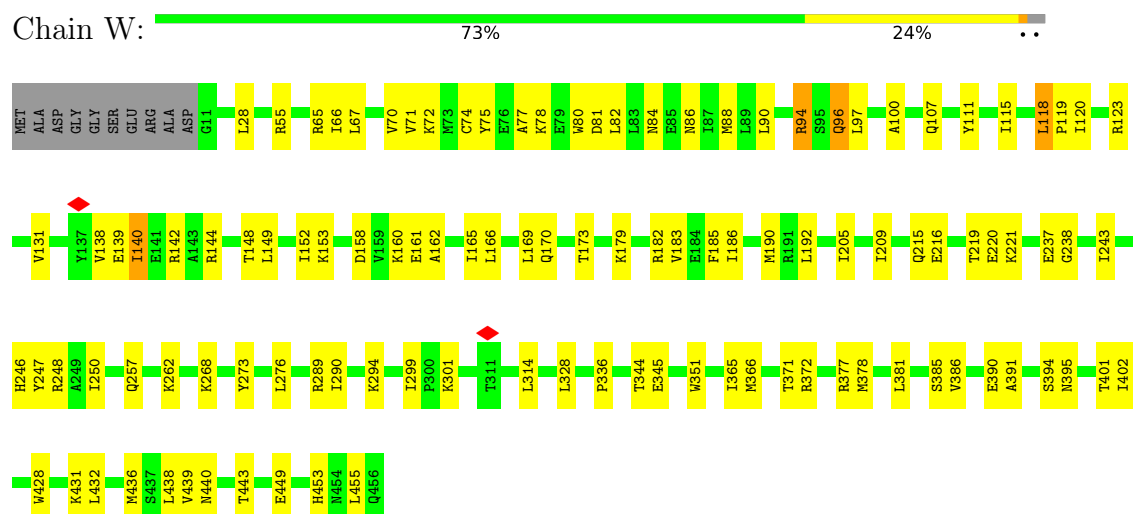
Chain U: 75% 17% 8%



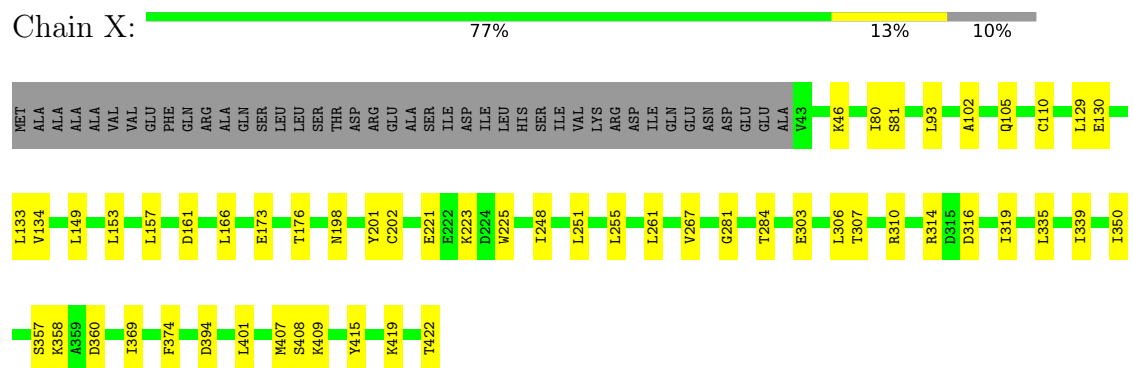
- Molecule 25: 26S proteasome non-ATPase regulatory subunit 3



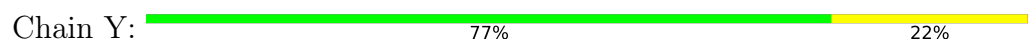
- Molecule 26: 26S proteasome non-ATPase regulatory subunit 12



- Molecule 27: 26S proteasome non-ATPase regulatory subunit 11



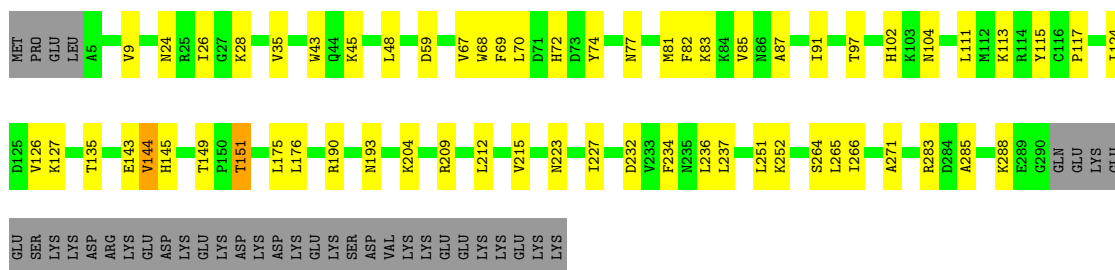
- Molecule 28: 26S proteasome non-ATPase regulatory subunit 6





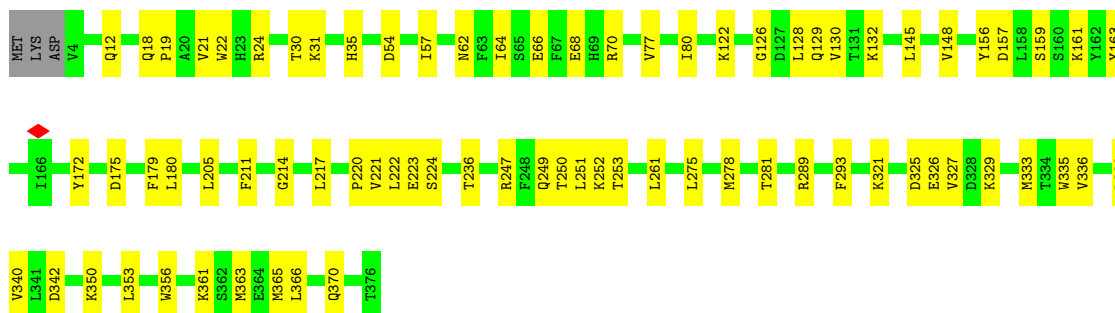
• Molecule 29: 26S proteasome non-ATPase regulatory subunit 7

Chain Z: 69% 18% 12%



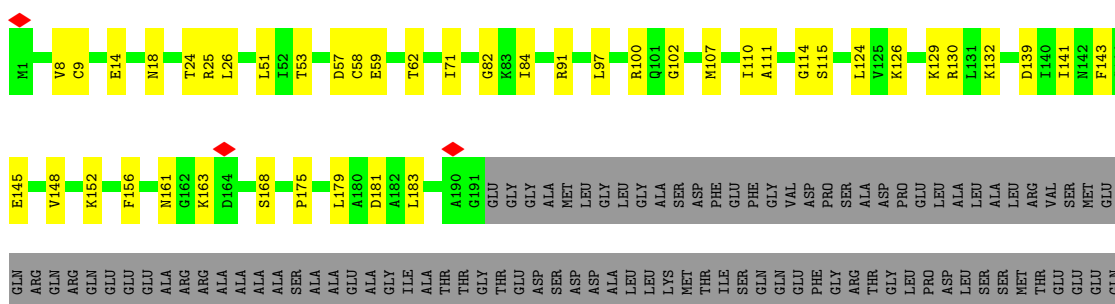
• Molecule 30: 26S proteasome non-ATPase regulatory subunit 13

Chain a: 79% 20%



• Molecule 31: 26S proteasome non-ATPase regulatory subunit 4

Chain b: 39% 12% 49%



ILE	ALA	TYR	ALA	GLN	MET	SER	GLN	GLY	ALA	GLU	PHE	GLY	GLN	ALA	GLU	SER	ALA	ASP	ASP	ASP	THR	SER	GLU	PRO	ALA	LYS	GLU	ASP	LYS	ASP	ASP	ASP	VAL	MET	GLN	ASP	PRO	GLU	PHE	LEU	GLN	SER	VAL	LEU	GLU	ASN	PRO	GLY	VAL	ASP
PRO	ASN	ASN	GLU	MET	ILE	ARG	ASN	ALA	MET	GLY	SER	ALA	SER	GLN	ALA	THR	LYS	ASP	GLY	LYS	LYS	ASP	GLU	LYS	LYS	GLU	GLU	ASP	LYS	LYS	ASP	ASP	VAL	MET	GLN	ASP	PRO	GLU	PHE	LEU	GLN	SER	VAL	LEU	GLU	ASN	PRO	GLY	VAL	ASP

- Molecule 32: 26S proteasome non-ATPase regulatory subunit 14

Chain c: 

MET	ASP	ARG	LEU	LEU	ARG	LEU	GLY	GLY	MET	PRO	GLY	LEU	GLY	GLN	GLY	PRO	THR	ASP	ALA	PRO	K24	E29	L36	A37	M41	M57	L58	G59	V69	I70	D71	V72	M98	E106	M121	V125	M164	M167	P174	R175	Q176	S179	G182
N185	K186	A191	L196	Y200	I203	K209	E213	Q214	K215	M216	M226	L231	Y234	K253	E262	D263	K264	Q269	L270	A271	I272	K273	Q278	R282	Q298	V307	V308	F309	K310														

- Molecule 33: 26S proteasome non-ATPase regulatory subunit 8

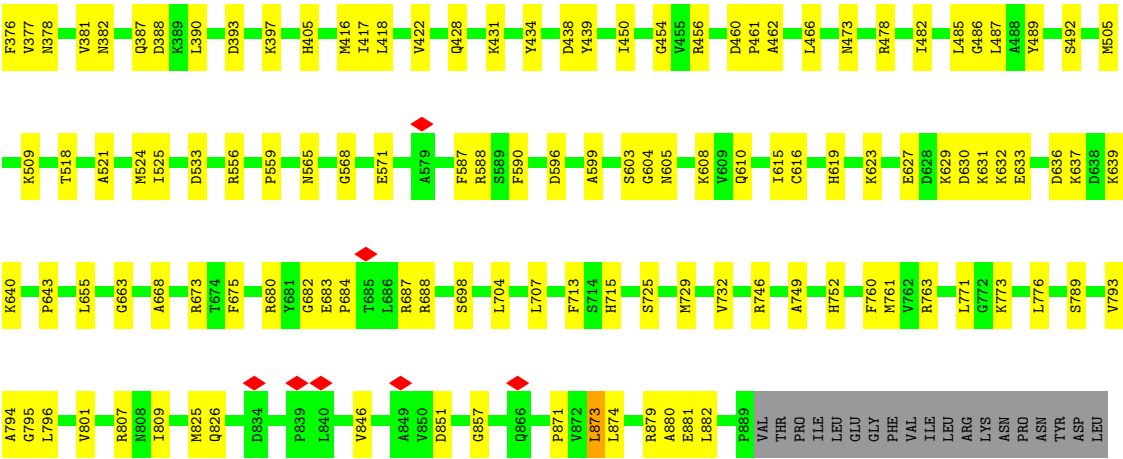
Chain d: 

MET	PHE	ILE	LYS	GLY	ARG	ALA	PRO	ARG	ALA	PRO	GLY	PRO	ARG	GLU	ARG	GLY	GLY	GLN	VAL	VAL	ALA	PRO	PRO	ALA	ARG	ALA	LEU	GLY	GLY	THR	SER	THR	SER	ARG	PRO	HIS	PHE	ARG	ARG	ALA	SER	VAL	CYS	ARG	ARG	ARG	CYS	ARG	LYS	SER	GLY	GLY	LEU	LEU	ALA	ALA																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
SER	ARG	LYS	MET	ALA	ALA	ALA	VAL	VAL	ASN	GLY	ALA	ALA	PHE	GLY	SER	SER	GLY	PRO	ALA	ALA	ALA	LEU	GLN	ALA	ALA	ALA	THR	GLY	M1	Y2	E3	Q4	L5	M15	K18	L23	G24	R25	L26	K27	T39	K45	L48	W61	R65	Q77																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
Y81	K86	E87	Q88	L89	P90	E91	H96	Q97	L98	L103	F105	R111	E114	T117	E118	L119	K125	M130	V131	K134	L143	M144	E145	G146	F166	I182	K188	F200	K205	M206	A210	W215	V216	Q229	Q230	K231	P232	T235																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
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- Molecule 34: 26S proteasome non-ATPase regulatory subunit 2

Chain f: 

M1	E2	R6	D7	K8	A9	P10	V11	Q12	P13	Q14	Q15	S16	P17	A18	A19	A20	P21	G22	G23	T24	D25	E26	K27	P28	S29	G30	K31	E32	R33	R34	D35	A36	G37	D38	K39	D40	K41	E42	Q43	E44	L45	S46	E47	E48	D49	K50	Q51	L52	Q53	D54	E57	M58	L59	V60	E61	R62	L63
G64	E65	K66	R72	P73	A74	L75	E76	E77	L78	R79	R80	Q81	R82	R83	S84	S85	H89	V92	P93	K94	L99	R100	P101	H102	Y103	G104	K105	I109	Y110	M113	A114	P115	G116	E117	M118	R120	A123	D124	I125	L126	S127	V128	M131	T132	M133	S134	G135	E136	R137								
L140	E150	V154	E157	H161	E165	K168	D174	D175	K178	V179	Q180	R181	K189	E190	P193	I191	V192	P193	E203	L207	L208	M209	Q213	Y214	D215	M216	L217	E218	K219	A225	K228	L231	Y232	L233	T234	P243	E244	N245	S246	A247	L248	L249	R250	G251													
A252	F259	S260	R261	L266	R267	L270	C285	K286	V289	K292	F296	M297	H301	G302	V303	F304	L307	S308	E309	D310	V311	E312	E313	D316	I320	K321	S322	N323	V324	Q325	E341	D346	K350	N356	R357	F358	G362	S363	Q364	V365	S374	S375															



● Molecule 35: 26S proteasome complex subunit DSS1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66910	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.024	Depositor
Minimum map value	-0.005	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	438.4, 438.4, 438.4	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: ATP, ZN, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.18	0/3283	0.47	0/4433
2	B	0.18	0/3254	0.48	0/4388
3	C	0.19	0/3146	0.50	0/4226
4	D	0.21	0/3089	0.50	0/4168
5	E	0.17	0/3145	0.46	1/4233 (0.0%)
6	F	0.16	0/3173	0.42	0/4273
7	G	0.19	0/1901	0.43	0/2572
7	g	0.17	0/1913	0.45	2/2589 (0.1%)
8	H	0.17	0/1840	0.38	0/2495
8	h	0.17	0/1844	0.40	0/2497
9	I	0.17	0/1963	0.41	0/2650
9	i	0.17	0/1985	0.42	0/2677
10	J	0.17	0/1887	0.40	0/2553
10	j	0.17	0/1887	0.41	0/2549
11	K	0.17	0/1841	0.34	0/2486
11	k	0.15	0/1809	0.36	0/2444
12	L	0.17	0/1911	0.33	0/2584
12	l	0.16	0/1896	0.33	0/2565
13	M	0.16	0/1925	0.37	0/2592
13	m	0.17	0/1916	0.40	0/2580
14	N	0.16	0/1548	0.31	0/2097
14	n	0.17	0/1536	0.33	0/2080
15	O	0.16	0/1672	0.37	0/2267
15	o	0.15	0/1686	0.37	0/2282
16	P	0.18	0/1616	0.40	0/2180
16	p	0.17	0/1620	0.41	0/2184
17	Q	0.16	0/1621	0.35	0/2194
17	q	0.16	0/1611	0.35	0/2182
18	R	0.15	0/1590	0.34	0/2147
18	r	0.18	0/1580	0.38	0/2135
19	S	0.17	0/1671	0.37	0/2252
19	s	0.17	0/1680	0.39	0/2264

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	T	0.17	0/1716	0.36	0/2323
20	t	0.16	0/1720	0.37	0/2328
22	x	0.15	0/4002	0.37	0/5390
23	y	0.17	0/607	0.47	0/816
24	U	0.19	0/6945	0.53	1/9382 (0.0%)
25	V	0.18	0/3681	0.42	0/4969
26	W	0.20	0/3683	0.55	3/4952 (0.1%)
27	X	0.19	0/3053	0.46	0/4115
28	Y	0.23	0/3261	0.55	0/4393
29	Z	0.20	0/2324	0.52	0/3150
30	a	0.18	0/3053	0.48	0/4133
31	b	0.20	0/1478	0.53	0/2001
32	c	0.21	0/2302	0.53	0/3110
33	d	0.20	0/2162	0.56	0/2919
34	f	0.20	0/6980	0.53	2/9433 (0.0%)
35	e	0.21	0/437	0.48	0/595
All	All	0.18	0/112443	0.45	9/151827 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	g	224	ASN	CA-C-N	-7.81	112.86	120.83
7	g	224	ASN	C-N-CA	-7.81	112.86	120.83
26	W	96	GLN	CB-CA-C	-6.21	109.42	116.63
34	f	99	LEU	CA-C-N	5.67	135.63	121.80
34	f	99	LEU	C-N-CA	5.67	135.63	121.80
24	U	763	VAL	N-CA-C	-5.47	107.04	111.91
26	W	94	ARG	CA-C-N	5.36	131.78	121.54
26	W	94	ARG	C-N-CA	5.36	131.78	121.54
5	E	41	GLU	N-CA-CB	5.30	118.50	110.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3229	0	3261	55	0
2	B	3207	0	3278	46	0
3	C	3105	0	3219	68	0
4	D	3039	0	3076	59	0
5	E	3097	0	3174	44	0
6	F	3133	0	3220	49	0
7	G	1867	0	1867	14	0
7	g	1879	0	1872	19	0
8	H	1801	0	1773	15	0
8	h	1805	0	1798	12	0
9	I	1933	0	1923	16	0
9	i	1955	0	1955	17	0
10	J	1861	0	1846	19	0
10	j	1861	0	1865	20	0
11	K	1813	0	1796	10	0
11	k	1782	0	1766	14	0
12	L	1876	0	1856	14	0
12	l	1861	0	1839	16	0
13	M	1890	0	1880	17	0
13	m	1881	0	1868	9	0
14	N	1521	0	1494	7	0
14	n	1510	0	1483	6	0
15	O	1645	0	1648	10	0
15	o	1659	0	1681	11	0
16	P	1587	0	1598	13	0
16	p	1591	0	1609	15	0
17	Q	1588	0	1584	14	0
17	q	1578	0	1569	10	0
18	R	1559	0	1523	11	0
18	r	1549	0	1506	8	0
19	S	1641	0	1639	12	0
19	s	1650	0	1645	16	0
20	T	1683	0	1662	14	0
20	t	1687	0	1666	8	0
21	v	170	0	44	1	0
22	x	3929	0	3915	59	0
23	y	601	0	629	16	0
24	U	6828	0	6884	98	0
25	V	3612	0	3682	48	0
26	W	3635	0	3762	71	0
27	X	3009	0	3113	36	0
28	Y	3202	0	3204	56	0
29	Z	2281	0	2312	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	a	2995	0	3012	50	0
31	b	1458	0	1505	28	0
32	c	2260	0	2276	31	0
33	d	2116	0	2146	33	0
34	f	6866	0	6866	149	0
35	e	425	0	328	12	0
36	A	27	0	12	1	0
36	B	27	0	12	0	0
37	C	31	0	12	3	0
37	D	31	0	12	0	0
37	E	31	0	12	2	0
37	F	31	0	12	1	0
38	c	1	0	0	0	0
All	All	110889	0	111189	1279	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 (1279) 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)
24:U:890:LYS:HG3	24:U:891:VAL:HG23	1.66	0.77
25:V:309:MET:HE1	25:V:331:LEU:HB3	1.66	0.77
34:f:58:MET:HG2	34:f:62:ARG:HE	1.51	0.73
34:f:127:SER:HA	34:f:131:MET:HB3	1.69	0.73
2:B:74:MET:HE2	34:f:610:GLN:HA	1.71	0.72
3:C:351:MET:HE3	3:C:387:VAL:HG13	1.73	0.70
5:E:352:MET:HE1	6:F:220:PRO:HG3	1.74	0.69
3:C:185:GLY:HA3	3:C:311:ILE:HG12	1.74	0.69
28:Y:10:GLY:HA2	28:Y:210:SER:HA	1.73	0.68
4:D:199:PRO:HG3	4:D:329:ARG:HH21	1.59	0.68
30:a:247:ARG:O	30:a:251:LEU:HB2	1.93	0.67
3:C:45:LEU:HB3	4:D:61:ILE:HG21	1.76	0.67
22:x:98:ALA:HA	22:x:101:MET:HE3	1.76	0.67
16:P:12:MET:HG2	16:P:171:MET:HE2	1.76	0.66
11:k:236:GLU:HA	11:k:239:LYS:HE3	1.78	0.65
26:W:436:MET:HB2	32:c:226:MET:HE1	1.78	0.65
14:n:4:MET:HG3	14:n:127:ILE:HG22	1.79	0.65
34:f:596:ASP:O	34:f:639:LYS:NZ	2.29	0.65
4:D:202:VAL:HG23	4:D:329:ARG:HB3	1.78	0.65
29:Z:43:TRP:HB3	29:Z:48:LEU:HD13	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:370:GLN:HG2	33:d:244:LYS:HG3	1.80	0.64
9:I:155:ASN:ND2	10:J:77:THR:OG1	2.31	0.64
4:D:338:ARG:HE	4:D:364:VAL:HG12	1.61	0.64
15:o:143:ARG:H	15:o:146:MET:HE2	1.62	0.64
22:x:197:GLN:HA	23:y:74:ARG:HD3	1.79	0.64
34:f:682:GLY:HA2	34:f:688:ARG:HH22	1.62	0.64
24:U:265:ILE:HD11	24:U:326:ILE:HG23	1.79	0.64
6:F:39:GLU:HA	6:F:43:GLN:HB2	1.80	0.63
26:W:371:THR:HG22	26:W:372:ARG:HG3	1.80	0.63
28:Y:141:VAL:HG11	28:Y:164:ALA:HB2	1.81	0.63
24:U:333:MET:SD	24:U:333:MET:N	2.71	0.63
2:B:181:GLN:O	2:B:241:ASN:ND2	2.32	0.63
24:U:424:ALA:HA	24:U:427:LEU:HG	1.79	0.63
34:f:590:PHE:HE2	34:f:631:LYS:HB2	1.64	0.63
1:A:213:LEU:HA	1:A:319:MET:HB2	1.82	0.62
30:a:68:GLU:HG2	30:a:70:ARG:H	1.64	0.62
22:x:50:GLY:HA2	34:f:460:ASP:HB2	1.82	0.62
24:U:216:VAL:HG23	24:U:220:LEU:HD13	1.82	0.62
31:b:124:LEU:HD13	31:b:156:PHE:HB2	1.81	0.62
30:a:64:ILE:O	30:a:68:GLU:HB3	2.00	0.62
25:V:440:LYS:NZ	33:d:143:LEU:O	2.32	0.62
34:f:292:LYS:O	34:f:807:ARG:NH2	2.32	0.61
29:Z:72:HIS:HE1	29:Z:111:LEU:HD21	1.64	0.61
8:H:93:LEU:HD13	8:H:113:ARG:HB3	1.81	0.61
24:U:898:CYS:SG	24:U:899:ARG:N	2.74	0.61
26:W:377:ARG:O	26:W:381:LEU:HB2	1.99	0.61
31:b:24:THR:HG22	31:b:26:LEU:H	1.66	0.61
10:j:154:HIS:HB3	11:k:59:MET:HE1	1.83	0.61
24:U:17:PRO:HB3	24:U:21:GLU:HB2	1.81	0.61
24:U:806:CYS:O	24:U:874:ASN:ND2	2.33	0.61
31:b:18:ASN:ND2	31:b:145:GLU:OE2	2.33	0.61
31:b:97:LEU:HB3	31:b:107:MET:HE1	1.83	0.61
28:Y:204:THR:HG21	28:Y:246:ILE:HD11	1.83	0.61
27:X:408:SER:HB3	28:Y:376:LEU:HD13	1.81	0.61
2:B:313:LEU:O	2:B:346:ARG:NH1	2.34	0.60
31:b:148:VAL:HG11	31:b:175:PRO:HG3	1.84	0.60
34:f:571:GLU:OE2	34:f:608:LYS:NZ	2.34	0.60
4:D:378:ILE:HG12	4:D:402:ALA:HB1	1.84	0.60
6:F:87:PRO:O	6:F:155:LYS:NZ	2.34	0.60
26:W:152:ILE:HG13	26:W:165:ILE:HD12	1.84	0.60
4:D:119:ILE:O	4:D:121:ARG:NH1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:121:ARG:HA	4:D:124:LEU:HD23	1.84	0.60
7:g:141:ILE:HG22	7:g:151:VAL:HG22	1.84	0.60
31:b:179:LEU:HD23	31:b:181:ASP:H	1.67	0.60
13:m:34:SER:OG	13:m:65:ARG:NH1	2.32	0.60
34:f:292:LYS:HD2	34:f:879:ARG:HG3	1.84	0.59
20:t:99:ARG:HG2	20:t:106:LEU:HG	1.83	0.59
24:U:666:LYS:NZ	24:U:702:THR:O	2.32	0.59
28:Y:177:ARG:NH2	28:Y:203:ASP:O	2.33	0.59
26:W:138:VAL:HG22	26:W:139:GLU:HG3	1.85	0.59
12:l:132:LEU:HB2	12:l:147:THR:HB	1.85	0.59
30:a:289:ARG:HA	30:a:333:MET:HE1	1.84	0.59
34:f:266:LEU:HB3	34:f:270:LEU:HD23	1.84	0.59
34:f:61:GLU:HB2	34:f:65:GLU:HG2	1.85	0.59
2:B:406:ALA:HB1	2:B:411:ARG:HH12	1.68	0.58
24:U:792:ASN:HB3	24:U:914:LEU:HB3	1.85	0.58
25:V:470:ARG:O	25:V:473:GLN:NE2	2.36	0.58
33:d:229:GLN:HB3	33:d:231:LYS:HG2	1.85	0.58
1:A:98:CYS:HA	1:A:141:GLY:HA2	1.86	0.58
1:A:312:ARG:HB2	1:A:315:ILE:HB	1.84	0.58
22:x:239:LYS:HD3	22:x:244:ASP:HB2	1.85	0.58
24:U:587:ALA:HB2	24:U:621:SER:HB3	1.85	0.58
1:A:339:ARG:HH12	6:F:402:GLU:HG2	1.68	0.58
13:M:34:SER:OG	13:M:65:ARG:NH1	2.35	0.58
24:U:381:THR:HG22	24:U:412:HIS:HA	1.83	0.58
18:r:44:THR:HG21	18:r:100:MET:HE3	1.85	0.58
20:t:98:SER:O	20:t:102:LYS:NZ	2.36	0.58
28:Y:92:GLU:HB3	28:Y:99:GLU:HG2	1.84	0.58
3:C:297:ARG:HH21	4:D:274:ARG:HG3	1.68	0.58
5:E:237:ALA:O	6:F:308:ARG:NH2	2.37	0.58
6:F:410:ARG:NH1	6:F:419:ASP:OD1	2.36	0.58
24:U:656:LEU:HD22	24:U:672:LEU:HD13	1.86	0.58
26:W:401:THR:HG23	26:W:402:ILE:HD12	1.85	0.58
4:D:280:GLY:O	4:D:283:ARG:NH1	2.37	0.57
32:c:278:GLN:O	32:c:282:ARG:N	2.36	0.57
35:e:35:ASP:HB3	35:e:37:HIS:HD2	1.68	0.57
1:A:306:LEU:O	1:A:312:ARG:NH1	2.37	0.57
19:S:181:SER:OG	15:o:198:ARG:NH1	2.37	0.57
10:j:47:LYS:O	10:j:205:ASN:ND2	2.36	0.57
22:x:222:SER:HA	22:x:225:GLU:HG2	1.85	0.57
28:Y:160:ASN:HA	28:Y:163:LYS:HG2	1.86	0.57
29:Z:212:LEU:HA	29:Z:215:VAL:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:W:257:GLN:OE1	26:W:262:LYS:NZ	2.38	0.57
30:a:122:LYS:HD3	30:a:130:VAL:HG23	1.86	0.57
33:d:45:LYS:HZ1	33:d:89:LEU:H	1.52	0.57
13:M:187:ARG:O	13:M:191:LYS:NZ	2.36	0.57
25:V:90:GLU:OE2	25:V:92:ARG:NH1	2.37	0.57
8:H:143:ARG:NH1	8:H:144:PRO:O	2.35	0.57
33:d:91:GLU:OE2	33:d:96:HIS:NE2	2.37	0.57
14:N:4:MET:HE1	14:N:159:ALA:HB3	1.86	0.57
22:x:256:LYS:HB3	22:x:265:VAL:HG13	1.85	0.57
34:f:341:GLU:OE1	34:f:387:GLN:NE2	2.37	0.57
1:A:306:LEU:HD23	1:A:336:ARG:HB3	1.85	0.57
2:B:107:MET:HB3	3:C:96:VAL:HB	1.85	0.57
16:p:65:GLN:OE1	17:q:86:ARG:NH2	2.38	0.57
8:H:119:GLN:HG3	9:I:81:SER:HB2	1.87	0.57
10:j:38:ARG:O	10:j:213:ARG:NH2	2.38	0.57
26:W:443:THR:HG21	29:Z:204:LYS:HD2	1.86	0.57
34:f:80:ARG:HE	34:f:83:ARG:HH12	1.51	0.57
34:f:673:ARG:HD2	34:f:707:LEU:HD21	1.87	0.57
2:B:243:THR:HG23	2:B:245:ALA:H	1.70	0.56
9:i:8:ARG:HH21	10:j:5:ARG:HH22	1.52	0.56
22:x:405:SER:O	22:x:414:ASN:ND2	2.38	0.56
25:V:177:ASN:O	25:V:179:LYS:NZ	2.37	0.56
32:c:174:PRO:O	32:c:176:GLN:NE2	2.38	0.56
9:i:219:GLU:OE1	9:i:220:ASN:ND2	2.38	0.56
1:A:214:LEU:HD23	1:A:343:PHE:HE2	1.70	0.56
25:V:345:ARG:HH21	35:e:43:TRP:HA	1.70	0.56
25:V:473:GLN:OE1	25:V:477:HIS:NE2	2.37	0.56
26:W:220:GLU:HG3	26:W:221:LYS:HG3	1.86	0.56
33:d:39:THR:HA	33:d:86:LYS:HE3	1.86	0.56
34:f:323:ASN:ND2	34:f:454:GLY:O	2.38	0.56
34:f:616:CYS:O	34:f:629:LYS:NZ	2.37	0.56
17:Q:58:GLU:OE1	17:Q:62:LYS:NZ	2.39	0.56
34:f:311:VAL:HG12	34:f:313:GLU:H	1.70	0.56
4:D:176:GLU:OE2	4:D:329:ARG:NH1	2.38	0.56
4:D:274:ARG:HG2	4:D:275:PHE:HD1	1.70	0.56
22:x:43:ARG:HH21	34:f:434:TYR:HB2	1.69	0.56
25:V:175:MET:HE2	25:V:183:GLU:HB2	1.88	0.56
3:C:403:LYS:HA	3:C:406:LYS:HD3	1.88	0.56
9:I:123:GLN:NE2	10:J:125:ARG:O	2.39	0.56
12:L:196:ARG:NH1	12:L:237:GLU:O	2.37	0.56
2:B:107:MET:HE3	2:B:151:LEU:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:37:ARG:NH1	14:n:165:GLU:OE2	2.37	0.56
19:s:27:THR:HB	19:s:40:SER:H	1.71	0.56
26:W:328:LEU:HD21	26:W:351:TRP:HE1	1.70	0.56
28:Y:17:LEU:HD22	28:Y:212:GLU:HA	1.88	0.56
33:d:111:ARG:HB3	33:d:114:GLU:HB2	1.88	0.56
5:E:122:MET:HG2	5:E:196:LEU:HD22	1.87	0.56
7:G:155:ASP:OD1	7:G:159:TYR:N	2.39	0.56
28:Y:220:VAL:HG21	28:Y:249:VAL:HG21	1.87	0.56
34:f:640:LYS:HG2	34:f:643:PRO:HG3	1.88	0.56
1:A:129:VAL:O	22:x:334:LYS:NZ	2.37	0.56
3:C:53:ASN:ND2	24:U:642:GLU:O	2.39	0.56
3:C:375:ARG:NH2	3:C:382:ASP:OD2	2.39	0.56
10:j:158:ALA:HB3	11:k:58:LEU:HD21	1.87	0.56
19:s:125:ASP:OD1	19:s:129:SER:N	2.39	0.56
34:f:320:ILE:HB	34:f:325:GLN:HB2	1.88	0.56
28:Y:197:ALA:HB3	28:Y:226:VAL:HG21	1.88	0.55
1:A:99:THR:HG22	1:A:115:VAL:HA	1.89	0.55
15:O:163:ILE:HG12	15:O:170:GLY:HA2	1.88	0.55
9:i:178:ASP:OD2	9:i:195:LYS:NZ	2.39	0.55
26:W:115:ILE:HB	26:W:120:ILE:HB	1.89	0.55
12:l:204:ASP:OD1	12:l:239:ARG:NH1	2.36	0.55
27:X:248:ILE:HD12	27:X:251:LEU:HD21	1.88	0.55
28:Y:300:ARG:NH1	28:Y:333:GLU:OE2	2.39	0.55
10:J:65:LEU:HD13	10:J:69:VAL:HG12	1.87	0.55
25:V:150:ARG:NH1	25:V:157:THR:O	2.39	0.55
2:B:54:PRO:HB2	2:B:61:LYS:HG3	1.88	0.55
3:C:143:VAL:O	3:C:205:HIS:NE2	2.38	0.55
27:X:134:VAL:HB	27:X:149:LEU:HD23	1.87	0.55
2:B:196:GLU:O	2:B:349:ARG:NH1	2.39	0.55
2:B:227:PRO:O	2:B:232:LYS:NZ	2.40	0.55
13:M:52:LEU:HA	13:M:209:PHE:HA	1.87	0.55
24:U:770:TRP:HA	32:c:179:SER:HB3	1.87	0.55
28:Y:96:GLY:O	28:Y:130:LYS:NZ	2.40	0.55
5:E:62:LYS:NZ	5:E:63:GLN:O	2.40	0.55
15:O:22:GLU:HG2	15:O:27:ALA:HB2	1.89	0.55
24:U:131:GLU:O	24:U:135:ASN:ND2	2.40	0.55
2:B:254:GLU:O	2:B:257:GLN:NE2	2.39	0.55
18:R:192:VAL:HG11	16:p:205:ASP:HB3	1.88	0.55
24:U:12:LEU:HD23	24:U:20:LYS:HD2	1.88	0.55
34:f:749:ALA:O	34:f:752:HIS:ND1	2.36	0.55
1:A:428:ARG:HE	1:A:429:TYR:H	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:83:PHE:O	17:Q:87:ASN:ND2	2.37	0.55
17:q:83:PHE:O	17:q:87:ASN:ND2	2.40	0.55
28:Y:187:TYR:HB3	28:Y:192:ARG:HB3	1.88	0.55
34:f:378:ASN:OD1	34:f:382:ASN:ND2	2.34	0.55
7:g:6:SER:OG	7:g:11:ARG:NH1	2.37	0.55
17:q:44:LEU:HD11	17:q:102:LEU:HD23	1.89	0.55
27:X:80:ILE:HG22	27:X:81:SER:H	1.72	0.55
28:Y:32:ARG:NH1	28:Y:34:ASP:OD1	2.38	0.55
3:C:342:ILE:HG13	3:C:380:GLN:HG2	1.88	0.54
7:G:138:MET:HB3	7:G:154:CYS:HB2	1.87	0.54
24:U:233:LEU:HD22	24:U:268:LEU:HD11	1.89	0.54
24:U:666:LYS:H	24:U:669:ILE:HD12	1.71	0.54
3:C:281:ASP:OD2	3:C:307:ARG:NH2	2.39	0.54
5:E:23:ASP:OD2	5:E:27:LYS:NZ	2.39	0.54
7:g:185:LYS:HD2	7:g:186:LYS:HB2	1.89	0.54
7:g:186:LYS:NZ	7:g:188:ASP:O	2.41	0.54
34:f:683:GLU:OE1	34:f:687:ARG:NH1	2.40	0.54
10:J:2:SER:OG	10:J:3:TYR:N	2.36	0.54
19:s:204:ARG:NH1	19:s:206:GLU:OE2	2.41	0.54
34:f:556:ARG:HH21	34:f:587:PHE:HZ	1.55	0.54
3:C:194:THR:HG21	3:C:317:PHE:HB3	1.89	0.54
1:A:333:ARG:NH1	6:F:229:PRO:O	2.40	0.54
22:x:87:VAL:HG22	22:x:90:GLU:H	1.72	0.54
24:U:504:ASP:OD1	24:U:535:TYR:OH	2.26	0.54
25:V:416:ARG:HH11	25:V:457:TYR:HB3	1.73	0.54
30:a:293:PHE:HB3	30:a:329:LYS:HB3	1.90	0.54
34:f:244:GLU:HG3	34:f:248:LEU:HD22	1.88	0.54
6:F:304:ARG:NH2	6:F:307:GLN:OE1	2.40	0.54
23:y:42:ARG:HE	23:y:72:ARG:HG2	1.71	0.54
24:U:191:LYS:HA	24:U:194:ARG:HG2	1.88	0.54
20:T:174:ARG:NH1	20:T:206:GLU:O	2.40	0.54
33:d:145:GLU:HG3	33:d:146:GLY:H	1.72	0.54
34:f:100:ARG:NH2	34:f:103:TYR:O	2.41	0.54
34:f:301:HIS:HB3	34:f:321:MET:HG2	1.89	0.54
34:f:313:GLU:OE2	34:f:316:ASP:N	2.41	0.54
2:B:80:ARG:O	2:B:84:GLN:NE2	2.41	0.54
4:D:283:ARG:HD3	4:D:287:ARG:HH22	1.72	0.54
25:V:227:VAL:HG12	25:V:231:LEU:HD13	1.89	0.54
5:E:122:MET:HA	5:E:125:GLU:HB2	1.89	0.54
24:U:580:ARG:HB3	24:U:614:VAL:HG12	1.89	0.54
2:B:71:TYR:HA	2:B:74:MET:SD	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:40:GLN:HG3	25:V:495:ARG:HH21	1.70	0.54
4:D:228:ILE:HB	4:D:262:ILE:HG22	1.89	0.54
5:E:205:ASP:OD1	5:E:211:SER:OG	2.26	0.54
18:R:9:ARG:NH2	18:R:146:ASP:OD1	2.41	0.54
10:j:185:ASP:OD1	10:j:189:LYS:NZ	2.40	0.54
11:k:181:LEU:HA	11:k:184:VAL:HG22	1.90	0.54
13:m:8:ASP:O	13:m:22:GLN:NE2	2.41	0.54
28:Y:43:ALA:O	28:Y:46:ARG:NH1	2.40	0.54
34:f:72:ARG:O	34:f:72:ARG:NH1	2.36	0.54
7:G:137:CYS:SG	7:G:138:MET:N	2.80	0.53
19:S:27:THR:HB	19:S:40:SER:H	1.72	0.53
22:x:139:ALA:O	22:x:150:GLN:NE2	2.41	0.53
22:x:422:ALA:HB3	22:x:479:LEU:HB3	1.91	0.53
25:V:121:PHE:O	25:V:128:ARG:NH1	2.41	0.53
26:W:248:ARG:HD3	26:W:290:ILE:HD11	1.90	0.53
10:J:30:SER:OG	10:J:48:LYS:NZ	2.40	0.53
11:K:155:HIS:NE2	11:K:157:ASP:OD1	2.41	0.53
23:y:27:LYS:HB3	23:y:38:PRO:HB3	1.90	0.53
23:y:56:LEU:HB3	23:y:61:ILE:HD11	1.90	0.53
3:C:113:ARG:NH2	3:C:129:ASN:O	2.41	0.53
31:b:14:GLU:N	31:b:82:GLY:O	2.42	0.53
13:M:40:ARG:NE	13:M:146:ALA:O	2.41	0.53
19:s:148:LEU:HD23	19:s:178:VAL:HG12	1.90	0.53
23:y:63:LYS:HD3	23:y:64:GLU:HG2	1.91	0.53
25:V:218:TYR:HD2	25:V:227:VAL:HG22	1.73	0.53
26:W:314:LEU:HD22	26:W:365:ILE:HD12	1.90	0.53
33:d:87:GLU:HA	33:d:89:LEU:HD23	1.91	0.53
34:f:637:LYS:HE2	34:f:655:LEU:HD22	1.91	0.53
3:C:69:GLN:HB2	3:C:118:ASN:HD22	1.73	0.53
5:E:348:THR:OG1	6:F:218:GLN:OE1	2.26	0.53
37:E:501:ATP:O3G	6:F:344:ARG:NH1	2.42	0.53
9:I:119:GLN:HG3	10:J:78:ALA:HB1	1.89	0.53
22:x:301:GLN:HA	22:x:308:ASN:HA	1.90	0.53
4:D:99:ASN:HA	4:D:115:ILE:HG12	1.91	0.53
10:j:120:GLN:HE21	11:k:133:MET:HG3	1.74	0.53
32:c:29:GLU:HB2	32:c:203:ILE:HD11	1.91	0.53
4:D:191:TYR:HA	4:D:196:ILE:HD12	1.91	0.53
4:D:203:LEU:HA	4:D:309:MET:HB2	1.90	0.53
19:S:125:ASP:OD1	19:S:129:SER:N	2.41	0.53
22:x:211:LEU:HA	22:x:215:LEU:HD23	1.89	0.53
27:X:306:LEU:O	27:X:314:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:277:MET:HE2	5:E:295:LEU:HD21	1.90	0.53
25:V:287:ARG:NH2	35:e:17:ASP:OD2	2.42	0.53
28:Y:41:LEU:HD13	28:Y:61:LEU:HD21	1.90	0.53
34:f:680:ARG:NH2	34:f:760:PHE:O	2.42	0.53
3:C:44:ARG:HE	25:V:491:VAL:HG22	1.73	0.53
7:G:165:ALA:HB1	7:G:179:LEU:HD13	1.90	0.53
29:Z:26:ILE:HD11	29:Z:35:VAL:HG22	1.90	0.53
2:B:103:ARG:HB3	2:B:160:ILE:HG21	1.91	0.53
3:C:239:ARG:NH2	3:C:284:GLU:OE1	2.42	0.53
30:a:236:THR:HB	30:a:249:GLN:HE22	1.74	0.53
34:f:45:LEU:HD11	34:f:57:GLU:HA	1.89	0.53
3:C:316:GLU:HG2	3:C:318:PRO:HD3	1.91	0.52
13:m:230:ASP:OD1	13:m:230:ASP:N	2.39	0.52
16:p:193:ASP:OD1	16:p:193:ASP:N	2.42	0.52
28:Y:15:PRO:HG2	28:Y:147:ILE:HG22	1.91	0.52
22:x:463:ILE:HA	22:x:466:LEU:HD12	1.91	0.52
24:U:376:MET:HE1	24:U:738:ASP:HB2	1.91	0.52
4:D:363:TYR:O	4:D:403:TYR:OH	2.27	0.52
25:V:278:GLU:HA	25:V:285:TRP:HZ2	1.74	0.52
29:Z:144:VAL:HA	29:Z:151:THR:HB	1.91	0.52
35:e:54:ASN:OD1	35:e:57:ARG:NH2	2.38	0.52
12:L:125:ARG:NH1	12:L:126:ARG:O	2.43	0.52
22:x:1:MET:SD	22:x:21:ASN:ND2	2.82	0.52
22:x:82:PRO:HG2	34:f:397:LYS:HD3	1.90	0.52
23:y:42:ARG:NH2	23:y:71:LEU:O	2.42	0.52
26:W:28:LEU:HD11	26:W:66:ILE:HG22	1.91	0.52
10:j:90:GLU:HG3	10:j:110:TYR:CZ	2.45	0.52
10:j:140:GLY:O	10:j:213:ARG:NH1	2.42	0.52
18:r:64:ARG:NH1	18:r:67:GLU:OE1	2.43	0.52
24:U:210:LYS:NZ	24:U:211:PRO:O	2.41	0.52
24:U:656:LEU:HD21	24:U:671:LEU:HD23	1.91	0.52
26:W:449:GLU:OE2	26:W:453:HIS:NE2	2.38	0.52
27:X:130:GLU:HG3	27:X:153:LEU:HD21	1.90	0.52
27:X:255:LEU:HD22	27:X:267:VAL:HG13	1.92	0.52
34:f:604:GLY:O	34:f:610:GLN:NE2	2.41	0.52
3:C:232:ARG:NH1	3:C:279:GLN:OE1	2.40	0.52
25:V:454:GLU:HG3	25:V:455:LYS:HG2	1.92	0.52
31:b:51:LEU:HD23	31:b:71:ILE:HG23	1.91	0.52
3:C:254:ILE:HG23	3:C:269:VAL:HG22	1.91	0.52
6:F:298:SER:OG	6:F:304:ARG:NH2	2.43	0.52
16:P:38:ASP:OD1	16:P:38:ASP:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:195:LEU:HD22	10:j:206:ILE:HG12	1.92	0.52
3:C:212:ILE:HG21	3:C:234:LEU:HD11	1.91	0.52
15:O:214:GLU:HG2	16:P:198:ARG:HG2	1.91	0.52
34:f:825:MET:H	34:f:851:ASP:HB2	1.74	0.52
2:B:194:ILE:HG22	2:B:198:LYS:HE2	1.92	0.52
5:E:216:ARG:HA	5:E:263:GLN:HE22	1.74	0.52
9:i:46:ALA:HB1	9:i:197:LEU:HD11	1.91	0.52
22:x:435:HIS:NE2	22:x:451:ASP:OD1	2.43	0.52
25:V:479:ARG:HB2	29:Z:264:SER:HB2	1.92	0.52
3:C:184:LYS:HA	3:C:290:LYS:HG3	1.91	0.51
5:E:168:LYS:HE2	5:E:275:MET:HE1	1.92	0.51
22:x:197:GLN:HG3	23:y:74:ARG:HB2	1.91	0.51
10:j:38:ARG:HB3	10:j:181:ILE:HD12	1.92	0.51
28:Y:48:ASN:HD21	28:Y:74:LYS:HB3	1.75	0.51
33:d:4:GLN:OE1	33:d:25:ARG:NH1	2.43	0.51
34:f:267:ARG:HH22	34:f:303:VAL:HG22	1.75	0.51
12:L:41:LYS:HG3	12:L:42:THR:HG23	1.93	0.51
23:y:6:LYS:NZ	23:y:10:GLY:O	2.42	0.51
31:b:110:ILE:HG22	31:b:139:ASP:HB2	1.91	0.51
34:f:405:HIS:ND1	34:f:794:ALA:O	2.43	0.51
34:f:655:LEU:HD11	34:f:675:PHE:HB2	1.91	0.51
6:F:94:ILE:HD12	6:F:123:VAL:HG12	1.92	0.51
16:p:126:LEU:HD12	16:p:127:ILE:HG23	1.93	0.51
22:x:161:ASP:O	22:x:165:LYS:NZ	2.39	0.51
22:x:321:PRO:O	22:x:418:TYR:OH	2.28	0.51
24:U:353:LEU:HD11	24:U:376:MET:HG3	1.92	0.51
24:U:475:HIS:NE2	24:U:507:VAL:O	2.36	0.51
24:U:894:MET:SD	24:U:894:MET:N	2.83	0.51
28:Y:175:ASP:OD1	28:Y:175:ASP:N	2.43	0.51
5:E:22:ILE:HG23	6:F:55:MET:HE1	1.91	0.51
9:i:68:LEU:HB2	9:i:72:MET:HB2	1.92	0.51
4:D:107:THR:HG22	5:E:77:PRO:HG3	1.93	0.51
19:S:99:ARG:HH21	19:S:102:PHE:HD2	1.58	0.51
20:T:25:ASP:OD1	20:T:41:ARG:NH2	2.43	0.51
20:T:27:LEU:HD11	20:T:34:ALA:HB1	1.93	0.51
16:p:34:MET:HG3	16:p:183:MET:HE2	1.93	0.51
30:a:250:THR:HA	30:a:253:THR:HG22	1.93	0.51
3:C:187:LEU:HD23	3:C:314:LYS:HG2	1.93	0.51
7:G:141:ILE:HG22	7:G:151:VAL:HG22	1.93	0.51
9:i:119:GLN:NE2	10:j:79:ASP:OD1	2.44	0.51
30:a:278:MET:HA	30:a:281:THR:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:f:189:LYS:NZ	34:f:190:GLU:OE2	2.44	0.51
3:C:258:ARG:HD2	3:C:273:MET:HG2	1.91	0.51
27:X:407:MET:HE2	29:Z:266:ILE:HG13	1.93	0.51
29:Z:24:ASN:O	29:Z:28:LYS:NZ	2.44	0.51
34:f:809:ILE:HD11	34:f:857:GLY:HA2	1.91	0.51
1:A:217:PRO:O	1:A:222:LYS:NZ	2.43	0.51
6:F:294:LYS:HA	6:F:339:ASP:HB3	1.93	0.51
8:h:204:THR:OG1	8:h:206:ASP:OD1	2.27	0.51
22:x:249:VAL:HG11	22:x:275:LEU:HD21	1.93	0.51
34:f:826:GLN:HB2	34:f:846:VAL:HG13	1.92	0.51
1:A:51:ASP:OD1	1:A:51:ASP:N	2.44	0.51
2:B:73:LEU:HD13	24:U:833:LEU:HB3	1.93	0.51
4:D:248:ARG:HA	4:D:295:GLN:HE22	1.76	0.51
6:F:46:ARG:NH2	30:a:62:ASN:OD1	2.44	0.51
13:M:108:LEU:HD22	13:M:139:SER:HB3	1.93	0.51
8:h:58:ASP:OD2	8:h:60:ARG:NH1	2.44	0.51
29:Z:113:LYS:NZ	29:Z:117:PRO:O	2.39	0.51
34:f:243:PRO:O	34:f:246:SER:OG	2.28	0.51
2:B:375:ALA:HB2	2:B:412:MET:HE1	1.93	0.50
6:F:44:ARG:O	6:F:48:LEU:HB2	2.09	0.50
8:H:181:ASP:OD1	8:H:181:ASP:N	2.44	0.50
24:U:12:LEU:O	33:d:77:GLN:NE2	2.43	0.50
24:U:889:LEU:HA	24:U:892:LEU:HD23	1.92	0.50
26:W:71:VAL:HG11	26:W:107:GLN:HB3	1.93	0.50
34:f:231:LEU:HA	34:f:234:THR:HG22	1.92	0.50
34:f:286:LYS:HA	34:f:289:VAL:HB	1.93	0.50
12:L:47:VAL:HG12	12:L:195:LEU:HD22	1.92	0.50
17:q:4:LEU:HD22	17:q:45:LEU:HD23	1.93	0.50
30:a:145:LEU:HD12	30:a:148:VAL:HB	1.92	0.50
2:B:168:ASP:OD1	2:B:168:ASP:N	2.44	0.50
16:P:193:ASP:OD1	16:P:193:ASP:N	2.44	0.50
22:x:5:SER:HA	22:x:19:GLU:HA	1.92	0.50
22:x:332:PHE:HA	23:y:8:LEU:HD13	1.93	0.50
26:W:81:ASP:N	26:W:81:ASP:OD1	2.43	0.50
26:W:299:ILE:HG22	26:W:301:LYS:H	1.77	0.50
32:c:270:LEU:HA	32:c:273:LYS:HG2	1.93	0.50
11:K:9:ASP:O	11:K:23:GLN:NE2	2.44	0.50
12:L:173:GLU:OE2	13:M:56:LYS:NZ	2.43	0.50
16:P:35:VAL:HG12	16:P:36:THR:HG23	1.92	0.50
24:U:499:THR:O	24:U:503:GLN:NE2	2.43	0.50
25:V:289:LEU:HB3	25:V:312:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:214:GLY:HA3	30:a:340:VAL:HG11	1.92	0.50
30:a:249:GLN:HG2	30:a:252:LYS:HE3	1.93	0.50
32:c:182:GLY:O	32:c:185:ASN:ND2	2.42	0.50
33:d:114:GLU:HA	33:d:117:THR:HG22	1.94	0.50
13:m:5:THR:HG23	13:m:7:TYR:H	1.75	0.50
24:U:701:ILE:HG21	24:U:810:THR:H	1.77	0.50
3:C:49:ARG:HE	4:D:64:GLU:HG2	1.77	0.50
4:D:410:ASP:OD1	4:D:411:GLU:N	2.41	0.50
29:Z:67:VAL:HG21	31:b:91:ARG:HD2	1.94	0.50
29:Z:68:TRP:HH2	29:Z:111:LEU:HD13	1.76	0.50
30:a:353:LEU:HD12	30:a:356:TRP:HD1	1.77	0.50
34:f:261:ARG:HH21	34:f:296:PHE:HB2	1.76	0.50
34:f:871:PRO:HG3	34:f:882:LEU:HG	1.94	0.50
2:B:249:ARG:HG3	2:B:283:PHE:HD2	1.77	0.50
5:E:237:ALA:HB1	6:F:308:ARG:HE	1.77	0.50
13:M:8:ASP:O	13:M:22:GLN:NE2	2.44	0.50
7:g:190:THR:O	7:g:194:THR:OG1	2.24	0.50
24:U:836:THR:HA	24:U:839:ALA:HB3	1.92	0.50
33:d:206:MET:SD	33:d:206:MET:N	2.83	0.50
7:G:243:ALA:O	7:G:245:ARG:NH1	2.45	0.50
8:H:86:LEU:HD13	8:H:134:LEU:HD11	1.94	0.50
25:V:86:VAL:HG21	25:V:160:LEU:HD13	1.93	0.50
34:f:789:SER:HA	34:f:793:VAL:HG23	1.94	0.50
3:C:186:VAL:HA	3:C:313:ARG:HB2	1.93	0.50
9:I:49:ARG:HH22	9:I:60:PHE:HZ	1.59	0.50
20:T:126:ASP:OD1	20:T:130:VAL:N	2.45	0.50
28:Y:105:MET:HE1	28:Y:140:ILE:HD11	1.93	0.50
28:Y:181:LYS:HB2	28:Y:213:LEU:HD23	1.94	0.50
19:S:43:CYS:HB2	19:S:194:ARG:HH21	1.76	0.49
24:U:264:VAL:HG13	24:U:329:LEU:HD21	1.93	0.49
26:W:247:TYR:HA	26:W:250:ILE:HG12	1.93	0.49
30:a:156:TYR:HB3	30:a:179:PHE:HB2	1.94	0.49
37:C:501:ATP:O3A	4:D:323:ARG:NH1	2.45	0.49
13:M:83:ASP:HB3	13:M:131:PHE:HD1	1.76	0.49
22:x:101:MET:HG3	22:x:103:LEU:H	1.77	0.49
26:W:237:GLU:HG2	26:W:238:GLY:H	1.77	0.49
27:X:409:LYS:HG2	28:Y:376:LEU:HD21	1.93	0.49
34:f:39:LYS:HG3	34:f:120:ARG:HD3	1.93	0.49
34:f:636:ASP:N	34:f:636:ASP:OD1	2.44	0.49
4:D:77:GLU:HG2	4:D:80:LYS:HE3	1.94	0.49
10:J:42:VAL:HG13	10:J:210:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:4:ARG:NH2	9:i:5:TYR:OH	2.45	0.49
24:U:571:CYS:SG	24:U:601:ARG:NH1	2.80	0.49
25:V:175:MET:HE3	25:V:180:ARG:HB2	1.94	0.49
27:X:407:MET:HE1	29:Z:265:LEU:HB3	1.93	0.49
34:f:189:LYS:HG2	34:f:190:GLU:HG2	1.93	0.49
1:A:33:LEU:HD22	3:C:173:GLU:HB3	1.94	0.49
5:E:242:ARG:NH2	5:E:286:ASP:OD2	2.45	0.49
6:F:376:SER:HB3	6:F:414:GLU:HG3	1.93	0.49
17:Q:59:TYR:O	17:Q:63:ASN:ND2	2.45	0.49
19:S:114:ASP:OD1	19:S:118:LYS:N	2.46	0.49
24:U:94:SER:HB3	24:U:97:VAL:HG12	1.95	0.49
26:W:166:LEU:HD23	26:W:169:LEU:HD11	1.94	0.49
31:b:141:ILE:HG21	31:b:183:LEU:HG	1.93	0.49
34:f:633:GLU:HB2	34:f:636:ASP:HB3	1.95	0.49
27:X:360:ASP:OD1	27:X:360:ASP:N	2.44	0.49
31:b:9:CYS:HB3	31:b:111:ALA:HA	1.95	0.49
33:d:125:LYS:HE3	33:d:130:ASN:HB2	1.94	0.49
34:f:473:ASN:OD1	34:f:509:LYS:NZ	2.45	0.49
1:A:347:ASP:OD2	1:A:350:GLY:N	2.45	0.49
19:S:145:LEU:HD22	19:S:178:VAL:HB	1.95	0.49
24:U:7:GLY:N	24:U:37:GLU:O	2.45	0.49
25:V:343:PRO:O	35:e:43:TRP:NE1	2.44	0.49
28:Y:48:ASN:HB3	28:Y:114:ILE:HD12	1.95	0.49
13:M:99:ARG:NH2	13:M:105:ASN:OD1	2.42	0.49
24:U:799:LYS:HB2	24:U:923:GLU:HB3	1.93	0.49
29:Z:102:HIS:CE1	29:Z:104:ASN:HB3	2.47	0.49
16:P:177:ARG:NH2	19:s:150:ASP:OD2	2.46	0.49
9:i:216:LEU:HD12	9:i:225:ILE:HG12	1.93	0.49
24:U:742:HIS:O	24:U:883:ARG:NE	2.41	0.49
25:V:108:LEU:HD23	25:V:174:PHE:HB2	1.95	0.49
28:Y:301:ILE:HG13	28:Y:343:LEU:HD12	1.95	0.49
6:F:124:ILE:HD12	6:F:134:LEU:HD21	1.94	0.49
17:Q:31:ASP:OD1	17:Q:31:ASP:N	2.45	0.49
26:W:82:LEU:O	26:W:86:ASN:ND2	2.44	0.49
32:c:58:LEU:HG	32:c:106:GLU:HG2	1.95	0.49
1:A:336:ARG:NH2	37:F:501:ATP:O1G	2.43	0.49
2:B:223:ILE:HA	2:B:329:MET:HB2	1.94	0.49
10:j:79:ASP:HB3	10:j:127:PHE:HD1	1.78	0.49
14:n:4:MET:HE1	14:n:159:ALA:HB3	1.94	0.49
26:W:94:ARG:HH21	26:W:96:GLN:HA	1.78	0.49
29:Z:236:LEU:HD11	30:a:335:TRP:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:124:LEU:HD21	31:b:152:LYS:HB2	1.94	0.49
34:f:94:LYS:HZ3	34:f:137:ARG:HD2	1.78	0.49
3:C:233:GLU:HA	3:C:236:VAL:HG12	1.95	0.48
5:E:3:ASP:OD1	5:E:3:ASP:N	2.46	0.48
7:g:103:TYR:O	15:o:81:ARG:NH2	2.46	0.48
10:j:146:GLN:NE2	10:j:147:THR:O	2.46	0.48
22:x:199:ASP:OD2	23:y:42:ARG:NH2	2.46	0.48
28:Y:192:ARG:HH21	28:Y:195:LYS:HB3	1.78	0.48
28:Y:231:LEU:HG	28:Y:236:LEU:HD12	1.94	0.48
29:Z:91:ILE:HD12	29:Z:115:TYR:HB3	1.94	0.48
1:A:112:ILE:HG13	1:A:122:VAL:HG22	1.95	0.48
3:C:224:ILE:HG13	3:C:225:GLY:H	1.78	0.48
22:x:115:TYR:CE2	22:x:116:MET:HE2	2.48	0.48
30:a:128:LEU:O	30:a:132:LYS:NZ	2.46	0.48
30:a:159:SER:OG	30:a:175:ASP:OD2	2.23	0.48
3:C:305:LEU:HD12	3:C:311:ILE:HD12	1.94	0.48
6:F:224:LEU:HB2	6:F:348:LEU:HD23	1.95	0.48
11:K:121:LEU:HD23	11:K:160:GLY:HA3	1.94	0.48
26:W:179:LYS:HD3	26:W:183:VAL:HG21	1.95	0.48
26:W:372:ARG:HH11	30:a:327:VAL:HG11	1.78	0.48
34:f:713:PHE:HB2	34:f:752:HIS:CE1	2.48	0.48
34:f:713:PHE:HB2	34:f:752:HIS:HE1	1.78	0.48
34:f:789:SER:HB2	34:f:796:LEU:H	1.77	0.48
10:J:67:ASP:OD1	10:J:67:ASP:N	2.45	0.48
15:o:63:LEU:HD11	15:o:79:ALA:HB2	1.94	0.48
15:o:146:MET:HB3	15:o:150:GLU:HG3	1.95	0.48
19:s:13:LEU:HD11	19:s:149:LEU:HD11	1.96	0.48
22:x:239:LYS:HD2	22:x:245:GLN:HG3	1.95	0.48
33:d:15:ASN:O	33:d:65:ARG:NH2	2.47	0.48
34:f:115:PRO:HD2	34:f:118:ASN:HD21	1.78	0.48
3:C:221:GLN:HG2	3:C:222:LYS:HG2	1.96	0.48
8:H:148:GLN:OE1	8:H:158:TRP:NE1	2.39	0.48
25:V:85:ALA:HB2	25:V:93:PHE:HB2	1.95	0.48
34:f:24:THR:HG21	34:f:34:ARG:HD2	1.96	0.48
34:f:63:LEU:HA	34:f:66:LYS:HE2	1.94	0.48
34:f:175:ASP:HA	34:f:179:VAL:HG21	1.94	0.48
34:f:603:SER:OG	34:f:605:ASN:OD1	2.31	0.48
1:A:212:VAL:HB	1:A:318:LEU:HD23	1.95	0.48
2:B:356:PRO:O	2:B:361:LYS:NZ	2.47	0.48
3:C:399:MET:SD	3:C:399:MET:N	2.84	0.48
7:G:46:ASP:OD1	7:G:46:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:x:8:VAL:HA	22:x:69:LEU:HB2	1.95	0.48
26:W:149:LEU:HB2	26:W:185:PHE:HE1	1.78	0.48
15:O:21:THR:HG22	15:O:26:VAL:HA	1.96	0.48
18:R:182:ASP:OD1	18:R:182:ASP:N	2.46	0.48
22:x:225:GLU:HG3	22:x:226:THR:HG23	1.96	0.48
23:y:1:MET:HG2	23:y:19:PRO:HG3	1.94	0.48
2:B:275:GLU:O	2:B:322:ARG:NH2	2.47	0.48
4:D:133:HIS:HB3	4:D:137:ASN:H	1.78	0.48
14:N:144:ARG:NH2	14:N:151:GLU:OE1	2.46	0.48
27:X:422:THR:O	29:Z:283:ARG:NE	2.47	0.48
29:Z:77:ASN:O	29:Z:81:MET:HG3	2.13	0.48
31:b:126:LYS:HA	31:b:129:LYS:HE3	1.96	0.48
32:c:57:MET:HG3	32:c:72:VAL:HG22	1.96	0.48
34:f:630:ASP:OD1	34:f:630:ASP:N	2.46	0.48
1:A:124:ASP:HB2	6:F:86:LEU:HD22	1.96	0.48
11:K:66:LYS:NZ	11:K:78:MET:O	2.38	0.48
31:b:62:THR:HG21	31:b:71:ILE:HA	1.94	0.48
1:A:28:GLY:HA2	34:f:58:MET:HE2	1.95	0.48
4:D:272:THR:H	4:D:289:LEU:HD11	1.78	0.48
4:D:339:ARG:NH2	27:X:198:ASN:O	2.47	0.48
11:k:70:ILE:HD11	11:k:89:ILE:HD12	1.95	0.48
12:l:47:VAL:HG12	12:l:195:LEU:HD22	1.96	0.48
24:U:229:VAL:HA	24:U:232:ILE:HG22	1.96	0.48
34:f:190:GLU:HB2	34:f:193:PRO:HG2	1.96	0.48
3:C:182:GLN:OE1	3:C:286:THR:OG1	2.29	0.47
4:D:249:ASP:OD1	4:D:252:ARG:NH2	2.43	0.47
8:h:148:GLN:NE2	8:h:150:ASP:OD1	2.47	0.47
24:U:416:GLU:HA	24:U:450:HIS:HE1	1.79	0.47
30:a:363:MET:HE2	32:c:307:VAL:HG11	1.96	0.47
34:f:125:ILE:HD12	34:f:128:VAL:HB	1.94	0.47
34:f:346:ASP:H	34:f:390:LEU:HD22	1.79	0.47
1:A:382:GLY:HA3	36:A:501:ADP:C5	2.50	0.47
2:B:125:THR:OG1	2:B:126:SER:N	2.45	0.47
2:B:153:ASN:HD22	2:B:160:ILE:HD11	1.79	0.47
19:S:144:MET:HE1	19:S:185:ARG:HB2	1.96	0.47
20:T:26:MET:HE2	20:T:188:GLN:HG3	1.97	0.47
30:a:35:HIS:NE2	31:b:14:GLU:O	2.47	0.47
31:b:18:ASN:OD1	31:b:25:ARG:NE	2.42	0.47
3:C:20:LEU:HD22	24:U:149:GLN:HB2	1.97	0.47
4:D:297:ASP:OD2	4:D:326:ARG:NE	2.47	0.47
13:M:161:TRP:HB3	13:M:181:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:o:112:SER:HB3	15:o:125:VAL:HG11	1.94	0.47
26:W:158:ASP:OD2	26:W:160:LYS:NZ	2.38	0.47
28:Y:297:ARG:NH2	35:e:45:ASP:OD1	2.45	0.47
29:Z:67:VAL:HG11	31:b:91:ARG:HG2	1.95	0.47
33:d:200:PHE:HB2	33:d:205:LYS:HZ3	1.78	0.47
1:A:165:GLN:HG3	1:A:167:GLU:H	1.79	0.47
15:O:62:ASN:HB3	15:O:82:MET:HE1	1.95	0.47
11:k:13:ASN:HB3	12:l:126:ARG:HB3	1.96	0.47
27:X:102:ALA:HB3	27:X:105:GLN:HE22	1.79	0.47
28:Y:10:GLY:CA	28:Y:210:SER:HA	2.43	0.47
2:B:67:ARG:HD3	34:f:225:ALA:HA	1.97	0.47
2:B:116:ILE:HG22	2:B:117:ASP:H	1.79	0.47
2:B:135:ILE:HD12	2:B:159:VAL:HB	1.96	0.47
4:D:98:GLN:OE1	4:D:121:ARG:NE	2.45	0.47
8:h:119:GLN:HA	8:h:122:THR:HG22	1.95	0.47
25:V:349:ARG:HH12	35:e:37:HIS:HE1	1.62	0.47
34:f:428:GLN:HA	34:f:431:LYS:HE2	1.96	0.47
1:A:37:GLY:HA2	34:f:128:VAL:HG13	1.97	0.47
1:A:40:THR:HG23	34:f:132:THR:HG23	1.96	0.47
3:C:222:LYS:HB3	3:C:226:GLU:HG3	1.96	0.47
7:G:80:MET:HG3	7:G:87:SER:HB3	1.97	0.47
22:x:263:GLU:OE1	22:x:311:TYR:OH	2.27	0.47
25:V:492:LYS:O	25:V:495:ARG:NH1	2.47	0.47
26:W:220:GLU:OE2	26:W:257:GLN:NE2	2.48	0.47
28:Y:48:ASN:HA	28:Y:70:LEU:HD13	1.97	0.47
30:a:325:ASP:OD1	30:a:326:GLU:N	2.47	0.47
34:f:350:LYS:HA	34:f:356:ASN:HD21	1.80	0.47
1:A:140:VAL:HG12	1:A:152:PRO:HA	1.96	0.47
3:C:209:CYS:SG	3:C:210:THR:N	2.87	0.47
5:E:148:VAL:HG13	5:E:149:ILE:HG13	1.97	0.47
8:H:24:TYR:O	8:H:28:ALA:HB3	2.14	0.47
13:M:50:GLU:OE2	13:M:201:HIS:ND1	2.43	0.47
7:g:155:ASP:OD1	7:g:159:TYR:N	2.42	0.47
16:p:35:VAL:HG12	16:p:36:THR:HG23	1.97	0.47
17:q:180:VAL:HG13	17:q:191:LEU:HB2	1.96	0.47
24:U:360:VAL:HG13	24:U:365:CYS:HB3	1.97	0.47
24:U:369:THR:O	24:U:373:ASN:ND2	2.48	0.47
24:U:609:ASP:O	24:U:615:ARG:NH1	2.44	0.47
24:U:802:TYR:O	24:U:878:LEU:N	2.48	0.47
24:U:903:PHE:HD1	24:U:915:LYS:HG3	1.78	0.47
25:V:337:LEU:HD21	25:V:364:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:281:GLY:H	27:X:284:THR:HG22	1.78	0.47
31:b:143:PHE:HZ	31:b:183:LEU:HD21	1.80	0.47
32:c:269:GLN:HA	32:c:272:ILE:HG12	1.96	0.47
35:e:27:TRP:H	35:e:27:TRP:CD1	2.33	0.47
2:B:326:LYS:HA	2:B:326:LYS:HD3	1.67	0.47
8:H:177:ARG:HH12	27:X:161:ASP:H	1.63	0.47
7:g:191:PHE:HE1	7:g:219:VAL:HG21	1.80	0.47
17:q:53:THR:HG22	17:q:100:VAL:HG12	1.97	0.47
24:U:447:GLY:HA3	24:U:480:GLY:HA2	1.96	0.47
26:W:28:LEU:HD22	26:W:65:ARG:HH21	1.78	0.47
29:Z:223:ASN:HB3	29:Z:227:ILE:HB	1.96	0.47
29:Z:251:LEU:O	32:c:234:TYR:OH	2.31	0.47
30:a:18:GLN:HB3	30:a:22:TRP:HD1	1.78	0.47
34:f:84:SER:O	34:f:120:ARG:NH2	2.48	0.47
22:x:67:MET:SD	22:x:67:MET:N	2.88	0.47
24:U:904:LYS:HB2	24:U:912:ILE:HD12	1.97	0.47
26:W:438:LEU:HB3	29:Z:234:PHE:HE1	1.80	0.47
26:W:440:ASN:OD1	29:Z:204:LYS:NZ	2.47	0.47
30:a:30:THR:OG1	30:a:31:LYS:NZ	2.47	0.47
34:f:217:LEU:HD11	34:f:259:PHE:HB2	1.97	0.47
2:B:376:ASP:N	2:B:376:ASP:OD1	2.48	0.47
22:x:443:LYS:HB2	22:x:446:GLU:HB3	1.97	0.47
24:U:470:ASN:HA	24:U:474:ARG:HG2	1.97	0.47
30:a:217:LEU:HA	30:a:222:LEU:HD11	1.97	0.47
4:D:282:ASP:OD2	5:E:251:ARG:NH1	2.48	0.46
6:F:357:PRO:O	6:F:362:ARG:NH1	2.48	0.46
10:J:4:ASP:OD1	10:J:4:ASP:N	2.48	0.46
12:L:88:MET:HE3	12:L:112:ILE:HG21	1.97	0.46
7:g:202:LEU:HB3	7:g:210:PHE:HE2	1.80	0.46
12:l:196:ARG:NH1	12:l:237:GLU:O	2.48	0.46
12:l:226:ASP:OD1	12:l:226:ASP:N	2.46	0.46
13:m:68:ASN:OD1	13:m:224:HIS:ND1	2.43	0.46
32:c:186:LYS:HZ2	32:c:191:ALA:HB3	1.80	0.46
33:d:48:LEU:HD22	33:d:81:TYR:HE1	1.80	0.46
4:D:259:PRO:HB3	4:D:304:ASN:HB2	1.96	0.46
9:I:161:ALA:HB3	10:J:53:LEU:HD13	1.97	0.46
22:x:205:ILE:HA	22:x:208:MET:HE2	1.96	0.46
24:U:871:PRO:O	24:U:876:GLN:NE2	2.48	0.46
30:a:19:PRO:HA	30:a:22:TRP:HB2	1.97	0.46
33:d:230:GLN:NE2	33:d:232:PRO:HD3	2.31	0.46
34:f:94:LYS:HD2	34:f:100:ARG:HH11	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:f:180:GLN:OE1	34:f:219:LYS:NZ	2.49	0.46
4:D:157:ASP:OD1	4:D:157:ASP:N	2.42	0.46
5:E:171:LEU:HB2	5:E:295:LEU:HD13	1.97	0.46
5:E:328:TYR:HA	5:E:331:ILE:HD12	1.97	0.46
6:F:52:ILE:O	6:F:56:LYS:HB2	2.15	0.46
6:F:380:ASN:HD22	6:F:383:GLU:HG3	1.80	0.46
12:l:23:GLU:HA	12:l:26:MET:HB2	1.96	0.46
12:l:172:LEU:O	12:l:176:MET:HB3	2.15	0.46
2:B:166:ASP:N	2:B:166:ASP:OD1	2.48	0.46
3:C:217:SER:HA	3:C:253:SER:HB3	1.97	0.46
5:E:149:ILE:HD11	5:E:276:ILE:HD11	1.97	0.46
17:Q:35:MET:HB3	17:Q:45:LEU:HG	1.97	0.46
19:S:19:ASP:OD1	19:S:19:ASP:N	2.49	0.46
7:g:49:VAL:HG22	7:g:219:VAL:HG23	1.97	0.46
11:k:41:GLN:NE2	11:k:151:PRO:O	2.47	0.46
24:U:770:TRP:CD1	32:c:179:SER:H	2.34	0.46
25:V:483:CYS:O	25:V:487:HIS:ND1	2.48	0.46
28:Y:109:GLU:O	28:Y:113:ARG:NH1	2.45	0.46
34:f:422:VAL:HG21	34:f:461:PRO:HG3	1.97	0.46
1:A:362:MET:HE3	2:B:216:ILE:HD11	1.98	0.46
4:D:313:ARG:HH21	5:E:242:ARG:HG2	1.80	0.46
7:g:153:LYS:HB3	7:g:163:PHE:HE2	1.79	0.46
24:U:752:THR:HG22	24:U:908:ILE:HD11	1.98	0.46
25:V:354:LYS:HG2	25:V:358:MET:HE1	1.96	0.46
25:V:482:PHE:O	25:V:486:ILE:HG12	2.16	0.46
28:Y:69:LEU:HD23	28:Y:73:MET:HE1	1.98	0.46
1:A:23:ARG:HH12	34:f:1:MET:HE1	1.80	0.46
1:A:158:ASP:OD1	1:A:158:ASP:N	2.49	0.46
2:B:412:MET:O	34:f:50:LYS:NZ	2.48	0.46
3:C:303:SER:HB2	3:C:306:LEU:HB2	1.97	0.46
7:G:112:ASP:N	7:G:112:ASP:OD1	2.45	0.46
16:P:159:ASP:OD1	16:P:159:ASP:N	2.43	0.46
18:R:44:THR:HG22	18:R:100:MET:H	1.81	0.46
19:S:185:ARG:NH1	15:o:26:VAL:O	2.42	0.46
18:r:130:SER:OG	18:r:167:ASP:OD2	2.28	0.46
22:x:222:SER:O	22:x:226:THR:OG1	2.27	0.46
24:U:570:LEU:HD22	24:U:578:LEU:HD11	1.96	0.46
24:U:623:GLY:HA3	24:U:658:ILE:HG13	1.98	0.46
34:f:165:GLU:O	34:f:168:LYS:NZ	2.43	0.46
1:A:101:ILE:HA	1:A:113:ILE:HG12	1.97	0.46
4:D:76:GLN:HA	4:D:79:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:364:ARG:HH21	6:F:368:ILE:HG13	1.81	0.46
20:T:110:MET:HE2	20:T:110:MET:HB2	1.86	0.46
34:f:615:ILE:O	34:f:619:HIS:ND1	2.49	0.46
1:A:116:LYS:HG3	1:A:117:GLN:H	1.79	0.46
12:L:160:SER:O	12:L:169:ARG:NH1	2.48	0.46
15:O:1:THR:N	15:O:168:GLY:O	2.48	0.46
25:V:311:ASN:HB3	28:Y:385:ARG:HH21	1.81	0.46
26:W:385:SER:OG	26:W:386:VAL:N	2.48	0.46
28:Y:191:ILE:HD12	35:e:39:TRP:HA	1.98	0.46
30:a:54:ASP:N	30:a:54:ASP:OD1	2.47	0.46
5:E:251:ARG:HB3	5:E:255:ARG:HH12	1.81	0.46
9:I:118:LYS:HZ1	9:I:150:SER:HG	1.57	0.46
16:p:45:MET:HE3	16:p:71:LEU:HD22	1.98	0.46
24:U:428:PRO:HG2	24:U:439:GLU:HB3	1.97	0.46
29:Z:212:LEU:HD13	30:a:350:LYS:HG2	1.97	0.46
30:a:77:VAL:HA	30:a:80:ILE:HG12	1.98	0.46
34:f:285:CYS:HB2	34:f:881:GLU:HB3	1.96	0.46
34:f:416:MET:HE3	34:f:450:ILE:HD13	1.97	0.46
2:B:60:LEU:HD11	34:f:219:LYS:HD2	1.97	0.46
5:E:331:ILE:HG23	5:E:371:VAL:HG21	1.98	0.46
24:U:801:GLN:HB3	24:U:877:LEU:HD12	1.97	0.46
26:W:78:LYS:HE2	26:W:111:TYR:HE1	1.80	0.46
27:X:225:TRP:HB2	27:X:261:LEU:HD13	1.98	0.46
30:a:220:PRO:HA	30:a:223:GLU:HG2	1.98	0.46
34:f:228:LYS:HD3	34:f:233:LEU:HB3	1.97	0.46
34:f:637:LYS:HD3	34:f:637:LYS:HA	1.77	0.46
6:F:98:ASP:N	6:F:98:ASP:OD1	2.49	0.45
9:I:38:LEU:HD23	9:I:160:LYS:HG2	1.98	0.45
10:J:42:VAL:HG11	10:J:191:VAL:HG21	1.97	0.45
22:x:43:ARG:HH11	22:x:74:SER:HG	1.63	0.45
26:W:431:LYS:HE2	29:Z:237:LEU:HB3	1.98	0.45
27:X:221:GLU:O	27:X:223:LYS:NZ	2.37	0.45
33:d:2:TYR:HB3	33:d:5:LEU:HD22	1.99	0.45
1:A:199:GLU:O	1:A:203:ASN:ND2	2.50	0.45
2:B:296:ASP:OD1	2:B:296:ASP:N	2.50	0.45
3:C:254:ILE:HD12	3:C:254:ILE:H	1.82	0.45
12:L:107:ARG:HH21	20:T:81:HIS:HB2	1.79	0.45
12:L:215:VAL:HB	12:L:221:PHE:HD1	1.81	0.45
20:T:86:ARG:NH1	20:T:133:GLU:OE2	2.49	0.45
11:k:52:LYS:NZ	11:k:216:GLU:OE2	2.49	0.45
25:V:225:ASP:OD1	25:V:228:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:W:390:GLU:O	26:W:394:SER:OG	2.28	0.45
29:Z:72:HIS:CE1	29:Z:111:LEU:HD21	2.49	0.45
31:b:100:ARG:NH1	31:b:102:GLY:O	2.49	0.45
32:c:121:TRP:HB3	32:c:191:ALA:HA	1.97	0.45
1:A:127:ASP:OD1	1:A:127:ASP:N	2.49	0.45
1:A:399:ALA:O	1:A:400:ARG:NH1	2.39	0.45
5:E:11:ASP:OD2	5:E:15:LYS:NZ	2.49	0.45
5:E:246:GLY:O	5:E:251:ARG:NH2	2.50	0.45
8:H:206:ASP:OD1	8:H:206:ASP:N	2.47	0.45
17:Q:30:ASP:OD1	17:Q:30:ASP:N	2.49	0.45
10:j:201:SER:OG	10:j:205:ASN:OD1	2.34	0.45
11:k:167:ALA:HB3	12:l:56:LEU:HD13	1.99	0.45
12:l:139:ASP:N	12:l:139:ASP:OD1	2.46	0.45
22:x:46:VAL:HG22	22:x:71:MET:HG2	1.97	0.45
29:Z:126:VAL:HG23	29:Z:127:LYS:HD3	1.99	0.45
25:V:212:TYR:HA	25:V:253:LEU:HD11	1.99	0.45
27:X:110:CYS:HB3	27:X:133:LEU:HD12	1.97	0.45
28:Y:71:ASN:HA	28:Y:74:LYS:HG2	1.99	0.45
28:Y:213:LEU:HD13	28:Y:213:LEU:HA	1.86	0.45
34:f:157:GLU:O	34:f:161:HIS:ND1	2.49	0.45
2:B:107:MET:HE1	2:B:160:ILE:HD12	1.98	0.45
2:B:224:LEU:HD13	2:B:328:ILE:HG23	1.99	0.45
5:E:145:LEU:HD22	5:E:183:LEU:HD21	1.98	0.45
9:i:53:HIS:HB3	9:i:56:LEU:HD23	1.98	0.45
16:p:125:ASP:OD1	16:p:129:CYS:N	2.40	0.45
27:X:357:SER:OG	27:X:358:LYS:N	2.48	0.45
2:B:153:ASN:OD1	2:B:154:HIS:N	2.47	0.45
4:D:238:LYS:HG2	21:v:18:UNK:HA	1.98	0.45
14:N:4:MET:HE3	14:N:156:THR:HG23	1.98	0.45
24:U:541:HIS:HB2	24:U:544:ILE:HG22	1.99	0.45
26:W:248:ARG:HE	26:W:289:ARG:HH12	1.64	0.45
26:W:273:TYR:HB2	26:W:276:LEU:HB2	1.99	0.45
27:X:401:LEU:HB3	28:Y:369:THR:HG22	1.97	0.45
30:a:180:LEU:HD11	30:a:221:VAL:HG21	1.97	0.45
33:d:182:ILE:HG23	33:d:215:TRP:HE1	1.81	0.45
4:D:274:ARG:NH1	4:D:275:PHE:O	2.50	0.45
6:F:33:VAL:HG23	6:F:34:LEU:HD12	1.98	0.45
24:U:253:TYR:HA	24:U:261:LEU:HD21	1.97	0.45
26:W:67:LEU:HD12	26:W:100:ALA:HB1	1.99	0.45
30:a:211:PHE:HD2	30:a:275:LEU:HD13	1.82	0.45
30:a:220:PRO:O	30:a:224:SER:OG	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:f:364:GLN:NE2	34:f:365:VAL:O	2.50	0.45
34:f:417:ILE:HG22	34:f:418:LEU:HD12	1.98	0.45
1:A:353:HIS:HA	1:A:356:LYS:HE2	1.98	0.45
1:A:394:MET:HA	1:A:397:ILE:HD12	1.99	0.45
6:F:183:GLU:HG3	6:F:238:ARG:HB3	1.97	0.45
15:O:195:LYS:NZ	19:s:184:GLU:OE2	2.42	0.45
12:l:72:ILE:HG22	12:l:134:ILE:HG12	1.99	0.45
25:V:208:ALA:HB1	25:V:249:THR:HG21	1.98	0.45
27:X:201:TYR:HD2	27:X:202:CYS:HB2	1.82	0.45
34:f:450:ILE:HG12	34:f:487:LEU:HD22	1.99	0.45
34:f:456:ARG:HD3	34:f:492:SER:HB3	1.98	0.45
34:f:473:ASN:HA	34:f:478:ARG:HH21	1.80	0.45
34:f:521:ALA:HA	34:f:524:MET:HG3	1.99	0.45
34:f:873:LEU:HD13	34:f:880:ALA:HA	1.99	0.45
1:A:213:LEU:HD22	1:A:340:LYS:HG3	1.99	0.45
3:C:161:ILE:HA	3:C:164:VAL:HG12	1.99	0.45
3:C:223:PHE:O	3:C:225:GLY:N	2.50	0.45
3:C:251:ILE:HB	3:C:293:MET:HE1	1.99	0.45
6:F:292:GLY:HA2	6:F:310:MET:HE1	1.98	0.45
18:R:41:LEU:HD23	18:R:103:GLY:HA3	1.99	0.45
19:s:172:MET:HE1	19:s:195:ILE:HD13	1.99	0.45
22:x:259:GLU:OE2	22:x:310:LEU:N	2.49	0.45
26:W:162:ALA:HB2	26:W:192:LEU:HB3	1.97	0.45
26:W:391:ALA:O	26:W:395:ASN:ND2	2.50	0.45
27:X:335:LEU:O	27:X:339:ILE:HG12	2.17	0.45
28:Y:156:LEU:HD23	28:Y:159:ARG:HH12	1.81	0.45
29:Z:285:ALA:HA	29:Z:288:LYS:HG2	1.98	0.45
9:I:42:GLY:HA3	9:I:186:LEU:HD21	1.98	0.45
14:N:179:ILE:HG12	14:N:184:VAL:HG22	1.99	0.45
9:i:136:TYR:HE1	9:i:150:SER:HB3	1.82	0.45
24:U:772:TRP:CD1	24:U:774:PRO:HD2	2.52	0.45
26:W:118:LEU:H	26:W:119:PRO:HD2	1.81	0.45
29:Z:251:LEU:HG	29:Z:252:LYS:HG2	1.98	0.45
17:Q:25:ILE:HG22	17:Q:26:VAL:HG13	1.99	0.44
15:o:63:LEU:HD23	15:o:63:LEU:HA	1.87	0.44
26:W:190:MET:HE3	26:W:190:MET:HB3	1.91	0.44
34:f:382:ASN:HB3	34:f:388:ASP:HB3	1.99	0.44
1:A:308:GLY:HA2	6:F:238:ARG:HH21	1.82	0.44
2:B:260:LEU:HD12	2:B:307:ARG:HH12	1.82	0.44
3:C:29:GLU:HG2	25:V:201:ARG:CZ	2.47	0.44
3:C:333:SER:HA	3:C:336:MET:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:294:LYS:N	6:F:337:ILE:O	2.50	0.44
8:H:49:GLU:O	8:H:64:LYS:NZ	2.46	0.44
10:J:50:VAL:HB	10:J:54:GLN:HB3	1.98	0.44
17:Q:78:THR:O	17:Q:82:ASN:ND2	2.50	0.44
14:n:127:ILE:HD11	14:n:136:TYR:CD1	2.51	0.44
16:p:134:ASP:OD1	16:p:134:ASP:N	2.51	0.44
3:C:194:THR:N	37:C:501:ATP:O2B	2.45	0.44
4:D:155:THR:OG1	4:D:156:SER:N	2.49	0.44
5:E:368:MET:HB3	5:E:372:ARG:HH12	1.82	0.44
8:H:165:LYS:HE3	8:H:165:LYS:HB2	1.80	0.44
24:U:900:TYR:HA	24:U:917:THR:HG21	1.98	0.44
26:W:80:TRP:HB3	26:W:123:ARG:HE	1.82	0.44
27:X:316:ASP:HB3	27:X:319:ILE:HD11	1.99	0.44
29:Z:190:ARG:HE	29:Z:193:ASN:HD22	1.66	0.44
3:C:89:VAL:HG23	3:C:90:HIS:H	1.83	0.44
4:D:276:ASP:OD1	4:D:282:ASP:HB2	2.17	0.44
5:E:81:VAL:HG12	5:E:105:LEU:HD23	1.99	0.44
12:L:204:ASP:N	12:L:204:ASP:OD1	2.49	0.44
25:V:124:ASN:HA	25:V:128:ARG:HD3	1.99	0.44
32:c:253:LYS:HD2	32:c:253:LYS:HA	1.76	0.44
33:d:105:PHE:HB2	33:d:166:PHE:CZ	2.52	0.44
4:D:265:ASP:HA	4:D:310:ALA:HB3	1.98	0.44
15:O:106:THR:OG1	15:O:109:HIS:NE2	2.36	0.44
11:k:99:HIS:HB2	11:k:107:MET:HE3	1.99	0.44
27:X:358:LYS:HB2	27:X:358:LYS:HE3	1.76	0.44
31:b:8:VAL:HA	31:b:110:ILE:HG13	1.99	0.44
33:d:131:VAL:HA	33:d:134:LYS:HB3	1.98	0.44
34:f:568:GLY:N	34:f:599:ALA:O	2.41	0.44
34:f:680:ARG:HB2	34:f:715:HIS:HA	2.00	0.44
2:B:136:LEU:HD12	2:B:160:ILE:HG12	1.98	0.44
15:o:22:GLU:HG2	15:o:27:ALA:HB2	1.99	0.44
25:V:486:ILE:HG21	29:Z:271:ALA:HB1	1.99	0.44
27:X:394:ASP:N	27:X:394:ASP:OD1	2.45	0.44
28:Y:13:LYS:H	28:Y:13:LYS:HG2	1.56	0.44
30:a:361:LYS:HG2	30:a:365:MET:HE1	2.00	0.44
34:f:623:LYS:HD2	34:f:623:LYS:HA	1.76	0.44
34:f:773:LYS:HA	34:f:776:LEU:HD23	2.00	0.44
26:W:55:ARG:HD3	26:W:96:GLN:HG3	2.00	0.44
28:Y:298:GLU:OE2	28:Y:342:ARG:NH1	2.51	0.44
30:a:12:GLN:HE21	30:a:19:PRO:HB3	1.82	0.44
31:b:130:ARG:HD2	31:b:130:ARG:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:d:23:LEU:O	33:d:27:LYS:HG2	2.18	0.44
34:f:209:MET:HE3	34:f:209:MET:HB3	1.93	0.44
3:C:27:LYS:HG3	3:C:31:LEU:HD23	1.99	0.44
3:C:223:PHE:HD2	3:C:224:ILE:HG23	1.83	0.44
5:E:168:LYS:HE3	5:E:270:LEU:HD12	2.00	0.44
5:E:182:LEU:HD22	37:E:501:ATP:H2'	1.99	0.44
8:H:74:LEU:HD11	8:H:134:LEU:HB3	1.99	0.44
13:M:150:MET:HE3	13:M:150:MET:HB3	1.91	0.44
18:R:3:THR:HG23	18:R:16:ALA:HB2	1.98	0.44
22:x:115:TYR:HB2	22:x:200:ALA:HB2	1.99	0.44
24:U:846:LYS:HG3	24:U:847:GLU:HG2	2.00	0.44
29:Z:45:LYS:HA	29:Z:45:LYS:HD3	1.72	0.44
33:d:15:ASN:HB2	33:d:18:LYS:HB2	1.99	0.44
5:E:145:LEU:HA	5:E:148:VAL:HG12	2.00	0.44
14:N:166:ARG:NH1	20:t:34:ALA:O	2.45	0.44
7:g:125:TYR:HA	7:g:131:MET:HE2	2.00	0.44
13:m:43:ASP:OD1	13:m:43:ASP:N	2.47	0.44
24:U:496:LEU:HA	24:U:499:THR:HG22	2.00	0.44
27:X:369:ILE:HD12	27:X:374:PHE:HD2	1.82	0.44
34:f:505:MET:HG2	34:f:518:THR:HG23	2.00	0.44
2:B:88:LEU:HD13	2:B:88:LEU:HA	1.85	0.43
3:C:60:ARG:NH2	4:D:71:GLU:OE2	2.51	0.43
5:E:349:GLU:OE1	5:E:373:LYS:NZ	2.36	0.43
10:J:3:TYR:OH	11:K:9:ASP:OD2	2.28	0.43
19:s:45:LYS:HD2	19:s:203:ILE:HD12	2.00	0.43
22:x:136:TYR:O	22:x:157:ARG:NH1	2.51	0.43
24:U:471:ASP:OD1	24:U:471:ASP:N	2.45	0.43
26:W:268:LYS:HB2	26:W:336:PRO:HG2	2.00	0.43
34:f:39:LYS:NZ	34:f:85:SER:OG	2.40	0.43
4:D:392:TYR:HB3	5:E:161:ARG:HH21	1.81	0.43
7:G:191:PHE:HE1	7:G:219:VAL:HG21	1.83	0.43
9:I:35:LEU:HD21	9:I:197:LEU:HG	1.99	0.43
16:p:135:ASP:OD1	16:p:136:PHE:N	2.49	0.43
22:x:21:ASN:HB3	22:x:24:GLU:HB2	1.98	0.43
22:x:112:ASN:HB3	23:y:74:ARG:HH12	1.83	0.43
26:W:152:ILE:HG23	26:W:161:GLU:HB3	1.99	0.43
28:Y:148:GLY:O	28:Y:152:MET:N	2.50	0.43
33:d:210:ALA:HA	33:d:216:VAL:HA	2.00	0.43
34:f:725:SER:O	34:f:725:SER:OG	2.34	0.43
34:f:729:MET:HA	34:f:732:VAL:HG12	1.99	0.43
1:A:32:LEU:O	34:f:53:GLN:NE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:LEU:HD22	1:A:316:LYS:HB2	2.00	0.43
8:H:101:TYR:HE1	16:P:90:MET:HE2	1.84	0.43
7:g:141:ILE:HD12	7:g:220:VAL:HG12	1.99	0.43
24:U:86:ASP:OD1	24:U:86:ASP:N	2.50	0.43
24:U:583:MET:HA	24:U:586:VAL:HG12	2.00	0.43
31:b:53:THR:HG22	31:b:59:GLU:H	1.83	0.43
3:C:162:LYS:O	3:C:166:GLU:HB2	2.18	0.43
3:C:168:PRO:HG3	3:C:175:PHE:HE2	1.83	0.43
3:C:175:PHE:HD2	3:C:182:GLN:HG2	1.83	0.43
3:C:231:VAL:HG11	3:C:276:LEU:HB3	2.00	0.43
4:D:154:LEU:HA	4:D:158:GLN:HE21	1.84	0.43
11:K:215:ILE:HD11	11:K:238:ILE:HD11	1.99	0.43
19:s:99:ARG:HD3	19:s:104:TYR:CE2	2.54	0.43
20:t:53:ALA:HB2	20:t:110:MET:HG3	1.99	0.43
24:U:135:ASN:HB3	24:U:159:ARG:HH12	1.84	0.43
26:W:190:MET:SD	26:W:190:MET:N	2.81	0.43
28:Y:224:VAL:HG22	28:Y:228:MET:HE2	2.01	0.43
28:Y:376:LEU:HD23	28:Y:376:LEU:HA	1.87	0.43
29:Z:265:LEU:HD23	29:Z:265:LEU:HA	1.91	0.43
1:A:105:ASP:HB2	1:A:110:LYS:HB2	1.99	0.43
3:C:268:GLU:OE2	3:C:272:THR:OG1	2.37	0.43
7:G:186:LYS:HD3	7:G:186:LYS:HA	1.81	0.43
19:s:145:LEU:HD22	19:s:178:VAL:HB	2.01	0.43
28:Y:220:VAL:HA	28:Y:223:THR:HG22	2.00	0.43
30:a:157:ASP:O	30:a:161:LYS:NZ	2.52	0.43
34:f:466:LEU:HB3	34:f:485:LEU:HB2	2.00	0.43
34:f:533:ASP:OD1	34:f:565:ASN:ND2	2.52	0.43
3:C:391:MET:HG2	3:C:392:GLN:HG2	2.01	0.43
4:D:163:MET:HB2	4:D:166:ASP:HB3	2.01	0.43
5:E:116:ASP:O	5:E:118:LEU:N	2.52	0.43
9:I:71:ASP:OD1	9:I:71:ASP:N	2.51	0.43
17:q:170:ARG:HA	17:q:170:ARG:HD3	1.90	0.43
19:s:213:ASP:OD1	19:s:213:ASP:N	2.52	0.43
27:X:157:LEU:HB3	27:X:166:LEU:HD11	2.00	0.43
27:X:173:GLU:HA	27:X:176:THR:HG22	2.00	0.43
29:Z:82:PHE:HA	29:Z:85:VAL:HG12	2.01	0.43
30:a:18:GLN:HB3	30:a:22:TRP:CD1	2.53	0.43
33:d:103:LEU:HD21	33:d:119:LEU:HD21	2.01	0.43
3:C:62:GLU:OE1	4:D:114:ARG:NH2	2.51	0.43
6:F:251:LEU:HD13	6:F:283:ILE:HG23	2.01	0.43
10:J:211:MET:HB2	10:J:217:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:58:THR:O	17:Q:85:ARG:NH2	2.51	0.43
9:i:180:LYS:H	9:i:184:MET:HE2	1.84	0.43
18:r:182:ASP:OD1	18:r:182:ASP:N	2.48	0.43
24:U:208:LEU:HD23	24:U:210:LYS:H	1.83	0.43
32:c:186:LYS:NZ	32:c:191:ALA:HB3	2.32	0.43
34:f:698:SER:HB3	34:f:704:LEU:HD22	2.01	0.43
35:e:35:ASP:HB3	35:e:37:HIS:CD2	2.52	0.43
11:K:167:ALA:HB3	12:L:56:LEU:HD21	2.01	0.43
18:R:100:MET:HE3	18:R:100:MET:HB2	1.83	0.43
9:i:207:SER:OG	9:i:209:GLU:OE1	2.34	0.43
11:k:119:LEU:HD23	11:k:119:LEU:HA	1.88	0.43
12:l:140:MET:HE3	12:l:140:MET:HB3	1.85	0.43
19:s:38:ARG:NH2	19:s:212:LYS:O	2.51	0.43
22:x:273:LEU:HD12	23:y:47:GLY:HA3	2.01	0.43
24:U:333:MET:HA	24:U:336:GLU:HG3	2.01	0.43
27:X:415:TYR:OH	27:X:419:LYS:NZ	2.49	0.43
34:f:213:GLN:HB2	34:f:249:LEU:HD21	2.01	0.43
34:f:663:GLY:HA3	34:f:668:ALA:HB3	2.00	0.43
34:f:771:LEU:HD23	34:f:773:LYS:H	1.83	0.43
1:A:118:PHE:HA	6:F:129:ARG:HH22	1.83	0.43
3:C:299:ASP:OD1	3:C:299:ASP:N	2.44	0.43
6:F:364:ARG:HE	6:F:368:ILE:HG13	1.84	0.43
9:I:105:ILE:HD13	9:I:110:LEU:HD13	2.01	0.43
22:x:89:VAL:HG13	22:x:91:ASP:H	1.83	0.43
24:U:146:LYS:HD2	24:U:148:LYS:HE2	2.01	0.43
24:U:576:PRO:HB3	24:U:611:ASN:HD22	1.83	0.43
26:W:148:THR:O	26:W:152:ILE:HG12	2.17	0.43
26:W:183:VAL:HA	26:W:186:ILE:HG22	2.00	0.43
26:W:205:ILE:O	26:W:209:ILE:HG12	2.18	0.43
27:X:310:ARG:HA	27:X:314:ARG:NH2	2.34	0.43
28:Y:285:ASP:OD1	28:Y:286:TRP:N	2.51	0.43
29:Z:209:ARG:NH1	30:a:350:LYS:O	2.51	0.43
34:f:131:MET:O	34:f:131:MET:HG3	2.18	0.43
34:f:178:LYS:HA	34:f:181:ARG:HB2	1.99	0.43
34:f:486:GLY:HA2	34:f:525:ILE:HD11	2.01	0.43
18:R:148:GLU:HB3	18:R:151:GLN:HG3	2.01	0.43
10:j:40:ILE:HG22	10:j:212:ARG:HG2	2.00	0.43
11:k:146:VAL:HG11	11:k:222:PRO:HA	2.00	0.43
13:m:46:VAL:HG22	13:m:215:TRP:HB3	1.99	0.43
24:U:744:VAL:HA	24:U:785:PRO:HA	2.01	0.43
32:c:209:LYS:HD2	32:c:214:GLN:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:f:250:ARG:HH11	34:f:252:ALA:HB3	1.83	0.43
2:B:374:LEU:HA	2:B:414:VAL:HG21	2.00	0.42
4:D:126:PRO:HG2	4:D:128:ALA:HB3	1.99	0.42
20:T:50:MET:HE2	20:T:197:VAL:HG13	2.01	0.42
7:g:138:MET:SD	7:g:140:LEU:HG	2.59	0.42
15:o:163:ILE:HG12	15:o:170:GLY:HA2	2.01	0.42
24:U:469:SER:O	24:U:474:ARG:NH1	2.52	0.42
25:V:476:PHE:HE2	28:Y:370:ILE:HD11	1.84	0.42
26:W:74:CYS:HA	26:W:77:ALA:HB3	2.01	0.42
29:Z:9:VAL:HG12	29:Z:48:LEU:HB2	2.00	0.42
29:Z:124:ILE:HA	29:Z:135:THR:HG22	2.00	0.42
31:b:114:GLY:HA2	31:b:143:PHE:HB2	2.01	0.42
34:f:297:MET:SD	34:f:456:ARG:NH2	2.92	0.42
1:A:215:PHE:HE1	1:A:340:LYS:HB3	1.84	0.42
1:A:287:ASP:HB2	12:L:2:PHE:HA	2.00	0.42
22:x:142:ALA:HB3	22:x:148:SER:HA	2.01	0.42
24:U:481:LEU:HD23	24:U:496:LEU:HD11	2.01	0.42
26:W:216:GLU:HA	26:W:219:THR:HB	2.00	0.42
28:Y:203:ASP:N	28:Y:203:ASP:OD1	2.48	0.42
31:b:84:ILE:HD12	31:b:115:SER:HB2	2.01	0.42
34:f:405:HIS:CE1	34:f:795:GLY:HA2	2.54	0.42
3:C:80:MET:HE1	3:C:86:LEU:HB2	2.01	0.42
5:E:235:ILE:HD13	5:E:277:MET:HG3	2.00	0.42
16:P:53:LEU:HB3	16:P:60:VAL:HG22	2.00	0.42
7:g:170:VAL:HG13	7:g:171:LYS:HG2	2.00	0.42
20:t:25:ASP:OD1	20:t:41:ARG:NH2	2.49	0.42
27:X:415:TYR:HE1	32:c:262:GLU:HG3	1.85	0.42
28:Y:379:ARG:O	28:Y:379:ARG:NH1	2.48	0.42
32:c:36:LEU:HD11	32:c:71:ASP:HA	2.01	0.42
4:D:194:ILE:HG13	4:D:196:ILE:HG13	2.01	0.42
5:E:147:GLU:HG3	5:E:151:LEU:HG	2.01	0.42
18:R:98:GLY:HA2	18:R:115:ASP:HA	2.01	0.42
12:l:116:THR:HG22	12:l:128:TYR:HD2	1.83	0.42
16:p:47:ASP:OD1	16:p:47:ASP:N	2.50	0.42
24:U:475:HIS:HE2	24:U:507:VAL:C	2.25	0.42
26:W:153:LYS:HA	26:W:153:LYS:HD3	1.90	0.42
32:c:231:LEU:O	32:c:298:GLN:NE2	2.49	0.42
34:f:462:ALA:HB3	34:f:489:TYR:CZ	2.54	0.42
1:A:163:MET:HE3	1:A:163:MET:HB2	1.91	0.42
5:E:130:VAL:HG22	5:E:131:SER:H	1.84	0.42
20:T:20:VAL:HG23	20:T:120:SER:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:x:361:PRO:HA	22:x:364:GLN:HG3	2.01	0.42
24:U:486:MET:HG2	24:U:518:LEU:HD21	2.01	0.42
24:U:736:ILE:HD13	24:U:736:ILE:HA	1.86	0.42
29:Z:83:LYS:HD3	29:Z:87:ALA:HA	2.01	0.42
30:a:366:LEU:HD13	33:d:244:LYS:HZ3	1.84	0.42
32:c:164:ASN:OD1	32:c:167:MET:N	2.52	0.42
33:d:98:LEU:HD12	33:d:98:LEU:HA	1.85	0.42
33:d:231:LYS:HD2	33:d:231:LYS:HA	1.69	0.42
6:F:43:GLN:HG2	30:a:66:GLU:HG2	2.01	0.42
7:G:167:ALA:HB3	7:G:176:THR:HG23	2.02	0.42
17:Q:44:LEU:HD11	17:Q:102:LEU:HD22	2.01	0.42
26:W:170:GLN:O	26:W:173:THR:OG1	2.29	0.42
33:d:210:ALA:HB1	33:d:216:VAL:HG23	2.02	0.42
1:A:89:SER:HA	1:A:93:LEU:HD23	2.01	0.42
37:C:501:ATP:PG	4:D:323:ARG:HH22	2.42	0.42
6:F:172:VAL:HG12	6:F:274:LEU:HD13	2.01	0.42
6:F:368:ILE:HG23	6:F:371:ARG:HH22	1.85	0.42
20:T:63:LEU:HD21	20:T:106:LEU:HD13	2.01	0.42
7:g:55:LYS:HE3	7:g:55:LYS:HB2	1.89	0.42
8:h:195:LEU:HA	8:h:195:LEU:HD23	1.86	0.42
16:p:68:LYS:HA	16:p:68:LYS:HD2	1.77	0.42
17:q:18:ASP:OD1	17:q:18:ASP:N	2.53	0.42
26:W:96:GLN:HB3	26:W:97:LEU:H	1.62	0.42
4:D:47:LEU:HD23	4:D:47:LEU:HA	1.90	0.42
4:D:164:TYR:HB2	4:D:222:HIS:CG	2.55	0.42
6:F:120:LYS:HB2	6:F:137:ILE:HD11	2.01	0.42
8:h:93:LEU:HD13	8:h:113:ARG:HB3	2.01	0.42
28:Y:314:LEU:HD22	28:Y:319:MET:HE3	2.02	0.42
34:f:377:VAL:O	34:f:381:VAL:HG12	2.20	0.42
34:f:673:ARG:HB3	34:f:707:LEU:HD11	2.01	0.42
1:A:169:LYS:HD3	1:A:169:LYS:HA	1.84	0.42
4:D:60:TYR:CD1	24:U:603:LEU:HG	2.55	0.42
4:D:144:PRO:HA	4:D:145:PRO:HD3	1.93	0.42
5:E:348:THR:HG22	5:E:352:MET:HE2	2.02	0.42
6:F:125:LYS:HA	6:F:131:THR:HA	2.02	0.42
6:F:332:THR:HG21	6:F:338:LEU:HD11	2.01	0.42
9:I:108:GLU:OE2	10:J:60:ARG:NH2	2.37	0.42
10:j:119:THR:HG22	10:j:126:PRO:HB3	2.02	0.42
11:k:189:MET:HE3	11:k:194:ALA:HA	2.01	0.42
14:n:174:ILE:HB	14:n:189:LEU:HB2	2.01	0.42
18:r:6:PHE:HB3	18:r:139:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:U:185:MET:HG3	24:U:194:ARG:HH21	1.84	0.42
24:U:416:GLU:OE1	24:U:450:HIS:ND1	2.53	0.42
27:X:93:LEU:HD22	27:X:129:LEU:HD13	2.02	0.42
28:Y:301:ILE:HD13	28:Y:342:ARG:HD2	2.01	0.42
32:c:215:LYS:HE2	32:c:215:LYS:HB3	1.84	0.42
1:A:195:LEU:HD23	1:A:195:LEU:HA	1.91	0.42
2:B:183:THR:OG1	2:B:184:TYR:N	2.48	0.42
4:D:391:ARG:HG2	4:D:393:ILE:H	1.85	0.42
5:E:234:GLU:HB2	6:F:311:LEU:HD13	2.01	0.42
5:E:234:GLU:HG3	6:F:311:LEU:HB3	2.00	0.42
6:F:372:LYS:HA	6:F:372:LYS:HD3	1.95	0.42
7:G:86:ASP:OD1	13:M:120:HIS:NE2	2.41	0.42
10:J:79:ASP:HB3	10:J:127:PHE:HD1	1.85	0.42
9:i:143:TYR:HB2	9:i:146:GLN:HE21	1.85	0.42
13:m:27:MET:HA	13:m:30:VAL:HG12	2.02	0.42
16:p:143:ALA:HA	16:p:146:MET:HE3	2.02	0.42
28:Y:237:ARG:O	28:Y:241:ILE:HB	2.20	0.42
34:f:627:GLU:OE1	34:f:631:LYS:NZ	2.48	0.42
4:D:80:LYS:O	4:D:83:GLN:HG2	2.20	0.41
8:H:39:LYS:NZ	9:I:57:ASP:OD2	2.49	0.41
8:h:189:HIS:HA	8:h:233:ILE:HD11	2.02	0.41
18:r:105:ASP:OD1	18:r:105:ASP:N	2.52	0.41
22:x:124:ARG:HG2	22:x:130:LYS:HD2	2.02	0.41
22:x:322:ALA:N	22:x:411:GLY:O	2.53	0.41
24:U:688:LEU:HD22	24:U:713:TYR:HE1	1.85	0.41
24:U:703:CYS:HA	24:U:704:PRO:HD3	1.81	0.41
25:V:466:ILE:HG21	33:d:235:THR:HB	2.02	0.41
26:W:366:MET:SD	26:W:378:MET:HE1	2.60	0.41
29:Z:68:TRP:HZ3	29:Z:70:LEU:HB2	1.85	0.41
32:c:59:GLY:HA3	32:c:69:VAL:HA	2.02	0.41
2:B:361:LYS:HG3	2:B:390:LEU:HD11	2.01	0.41
3:C:265:GLY:O	4:D:283:ARG:NH2	2.53	0.41
3:C:365:GLU:OE2	4:D:329:ARG:NH2	2.53	0.41
15:O:63:LEU:HD12	15:O:63:LEU:HA	1.92	0.41
17:Q:35:MET:SD	17:Q:181:ARG:HD3	2.60	0.41
7:g:10:ASP:OD1	7:g:10:ASP:N	2.53	0.41
8:h:135:LEU:HD22	8:h:146:LEU:HD11	2.01	0.41
19:s:10:GLY:HA3	19:s:42:LYS:HE2	2.02	0.41
20:t:96:MET:HE3	20:t:127:MET:HA	2.01	0.41
22:x:124:ARG:NH2	22:x:164:ASP:OD1	2.43	0.41
22:x:152:ILE:HG12	22:x:178:PHE:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:x:170:ILE:HD12	22:x:171:PRO:HD2	2.01	0.41
26:W:455:LEU:HD11	29:Z:102:HIS:HA	2.02	0.41
29:Z:35:VAL:HB	29:Z:97:THR:HG22	2.02	0.41
29:Z:232:ASP:O	29:Z:236:LEU:HB2	2.19	0.41
32:c:37:ALA:O	32:c:41:MET:HB2	2.20	0.41
34:f:124:ASP:OD1	34:f:125:ILE:N	2.53	0.41
35:e:16:ASP:OD1	35:e:16:ASP:N	2.53	0.41
5:E:344:ARG:HG2	6:F:218:GLN:HE22	1.85	0.41
6:F:438:TYR:OH	11:K:19:GLY:O	2.36	0.41
15:O:202:TYR:HE2	19:s:148:LEU:HD11	1.86	0.41
19:S:43:CYS:O	19:S:194:ARG:NH2	2.53	0.41
22:x:124:ARG:HH22	22:x:163:MET:HB3	1.86	0.41
25:V:398:LEU:HA	25:V:401:ASN:HB2	2.03	0.41
32:c:213:GLU:HA	32:c:216:MET:HG3	2.02	0.41
34:f:117:GLU:HB2	34:f:120:ARG:HB2	2.02	0.41
34:f:131:MET:HA	34:f:134:SER:HB2	2.03	0.41
34:f:150:GLU:H	34:f:150:GLU:HG2	1.60	0.41
34:f:346:ASP:HB3	34:f:374:SER:HB3	2.02	0.41
34:f:559:PRO:HG3	34:f:588:ARG:HH11	1.86	0.41
1:A:402:LYS:HA	1:A:402:LYS:HD3	1.88	0.41
7:G:80:MET:HE1	7:G:138:MET:SD	2.61	0.41
12:L:80:ASP:OD2	12:L:126:ARG:NH1	2.51	0.41
7:g:73:THR:HG22	7:g:74:GLU:H	1.86	0.41
10:j:36:ARG:NH1	10:j:142:PRO:O	2.51	0.41
15:o:206:LYS:HD2	15:o:206:LYS:HA	1.87	0.41
16:p:2:SER:OG	16:p:3:ILE:N	2.54	0.41
18:r:135:ALA:O	18:r:139:MET:HG2	2.20	0.41
26:W:131:VAL:HG11	26:W:144:ARG:HB2	2.02	0.41
27:X:46:LYS:HA	27:X:46:LYS:HD3	1.87	0.41
29:Z:59:ASP:HB2	29:Z:69:PHE:HB3	2.03	0.41
34:f:101:PRO:HB3	34:f:140:LEU:HD22	2.01	0.41
34:f:203:GLU:HG3	34:f:244:GLU:HG2	2.01	0.41
35:e:56:LEU:HD12	35:e:56:LEU:HA	1.90	0.41
2:B:135:ILE:HG12	2:B:141:LYS:HE3	2.03	0.41
4:D:401:LYS:HA	4:D:401:LYS:HD2	1.83	0.41
8:H:213:CYS:HB2	8:H:218:PHE:HD1	1.84	0.41
9:I:123:GLN:HE22	10:J:118:TYR:HD2	1.68	0.41
11:K:84:ASP:HB3	11:K:137:PHE:HD2	1.85	0.41
12:L:155:ASP:HB3	13:M:62:SER:HB2	2.01	0.41
14:N:104:ASP:OD1	14:N:104:ASP:N	2.53	0.41
16:P:34:MET:O	18:r:166:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:48:ASP:OD1	19:S:48:ASP:N	2.52	0.41
9:i:49:ARG:NH1	9:i:211:VAL:O	2.52	0.41
9:i:143:TYR:HB2	9:i:146:GLN:NE2	2.35	0.41
22:x:105:CYS:SG	22:x:106:GLY:N	2.94	0.41
24:U:751:ARG:HH22	24:U:912:ILE:HD11	1.86	0.41
30:a:356:TRP:HH2	32:c:309:PHE:HD1	1.67	0.41
34:f:1:MET:HB3	34:f:2:GLU:H	1.70	0.41
5:E:205:ASP:OD1	5:E:205:ASP:N	2.51	0.41
9:I:185:THR:OG1	9:I:186:LEU:N	2.54	0.41
16:P:12:MET:HE3	16:P:12:MET:HB2	1.85	0.41
22:x:204:TRP:CD2	22:x:208:MET:HE1	2.56	0.41
22:x:255:MET:HE2	22:x:311:TYR:HD2	1.86	0.41
24:U:198:LEU:HD21	24:U:222:PHE:HB2	2.02	0.41
25:V:447:ILE:HD12	25:V:447:ILE:HA	1.94	0.41
26:W:140:ILE:HG23	26:W:142:ARG:HD3	2.01	0.41
26:W:294:LYS:HE2	26:W:294:LYS:HB2	1.90	0.41
28:Y:231:LEU:HD12	28:Y:234:PRO:HD2	2.02	0.41
30:a:205:LEU:HD23	30:a:261:LEU:HD11	2.02	0.41
31:b:132:LYS:HE2	31:b:163:LYS:HE2	2.02	0.41
34:f:393:ASP:OD1	34:f:393:ASP:N	2.52	0.41
10:J:199:VAL:HG22	10:J:201:SER:H	1.85	0.41
13:M:197:ILE:HG21	13:M:211:LEU:HD13	2.03	0.41
20:T:53:ALA:HB2	20:T:110:MET:HG3	2.02	0.41
8:h:86:LEU:HD13	8:h:134:LEU:HD11	2.03	0.41
12:l:214:ILE:HD12	12:l:224:TYR:HE2	1.86	0.41
17:q:31:ASP:OD1	17:q:31:ASP:N	2.53	0.41
17:q:142:ILE:HD11	17:q:166:GLU:HG2	2.03	0.41
20:t:124:TYR:HE1	20:t:139:THR:HG22	1.85	0.41
28:Y:184:GLN:HB3	28:Y:197:ALA:HA	2.02	0.41
30:a:366:LEU:HD23	30:a:366:LEU:HA	1.96	0.41
31:b:161:ASN:HD22	31:b:168:SER:H	1.69	0.41
34:f:105:LYS:HG2	34:f:109:ILE:HD12	2.02	0.41
34:f:134:SER:HA	34:f:137:ARG:HD3	2.02	0.41
1:A:204:LEU:HD12	1:A:204:LEU:HA	1.93	0.41
3:C:118:ASN:OD1	3:C:118:ASN:N	2.51	0.41
3:C:248:MET:HB3	3:C:251:ILE:HD11	2.02	0.41
6:F:432:LYS:HE2	6:F:432:LYS:HB2	1.93	0.41
17:Q:22:ALA:HA	17:Q:27:GLN:HA	2.03	0.41
8:h:68:ILE:HG12	8:h:74:LEU:HD22	2.03	0.41
12:l:112:ILE:HD13	12:l:112:ILE:HA	1.89	0.41
24:U:374:SER:HB3	24:U:407:SER:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:U:809:SER:O	24:U:874:ASN:ND2	2.52	0.41
25:V:123:SER:H	25:V:150:ARG:NH2	2.19	0.41
26:W:70:VAL:HG11	26:W:90:LEU:HD11	2.02	0.41
26:W:215:GLN:OE1	26:W:215:GLN:N	2.51	0.41
28:Y:179:ARG:HD2	28:Y:182:VAL:HB	2.03	0.41
28:Y:381:GLN:O	28:Y:385:ARG:HG2	2.20	0.41
30:a:247:ARG:HH21	30:a:251:LEU:HA	1.86	0.41
34:f:133:MET:HA	34:f:136:GLU:HB2	2.03	0.41
34:f:438:ASP:OD1	34:f:439:TYR:N	2.53	0.41
1:A:282:GLY:O	1:A:284:ARG:N	2.52	0.41
3:C:85:VAL:HG21	3:C:123:LEU:HD11	2.03	0.41
3:C:138:MET:HE3	3:C:237:MET:HE2	2.02	0.41
3:C:212:ILE:HB	3:C:246:ILE:HA	2.02	0.41
4:D:278:GLN:HE22	4:D:283:ARG:HB3	1.86	0.41
4:D:337:ASP:OD1	4:D:337:ASP:N	2.50	0.41
6:F:193:LYS:HB3	6:F:193:LYS:HE3	1.86	0.41
6:F:249:LEU:HD23	6:F:283:ILE:HG12	2.02	0.41
16:P:15:LYS:HE3	16:P:121:ILE:HG12	2.02	0.41
8:h:203:MET:HA	8:h:207:ASN:HD21	1.85	0.41
10:j:168:VAL:O	10:j:172:LEU:HG	2.20	0.41
23:y:36:ILE:O	23:y:41:GLN:NE2	2.52	0.41
24:U:135:ASN:HA	24:U:138:PHE:HB2	2.02	0.41
24:U:201:LEU:HD12	24:U:201:LEU:HA	1.94	0.41
26:W:72:LYS:HA	26:W:75:TYR:HB3	2.02	0.41
26:W:84:ASN:O	26:W:88:MET:HG2	2.21	0.41
26:W:118:LEU:HD13	26:W:118:LEU:HA	1.92	0.41
26:W:182:ARG:HD2	26:W:182:ARG:HA	1.86	0.41
28:Y:387:ILE:HD12	28:Y:387:ILE:HA	1.90	0.41
31:b:57:ASP:OD1	31:b:58:CYS:N	2.54	0.41
33:d:61:TRP:O	33:d:65:ARG:HB2	2.20	0.41
34:f:191:ILE:H	34:f:191:ILE:HD12	1.86	0.41
34:f:482:ILE:HD12	34:f:518:THR:HB	2.03	0.41
34:f:629:LYS:HD3	34:f:632:LYS:HD2	2.02	0.41
34:f:683:GLU:HA	34:f:684:PRO:HD3	1.91	0.41
34:f:732:VAL:HB	34:f:746:ARG:HH22	1.85	0.41
6:F:211:LYS:HE3	6:F:211:LYS:HB2	1.94	0.41
20:T:25:ASP:HA	20:T:187:PHE:HA	2.03	0.41
7:g:128:ASN:HB2	7:g:131:MET:HE1	2.03	0.41
10:j:183:THR:HG22	10:j:185:ASP:H	1.86	0.41
13:m:35:THR:HA	13:m:166:GLY:HA3	2.03	0.41
16:p:88:MET:HE2	16:p:88:MET:HB3	1.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:x:212:GLN:NE2	22:x:244:ASP:OD1	2.54	0.41
24:U:412:HIS:CE1	24:U:422:LEU:HD11	2.56	0.41
24:U:643:SER:O	24:U:649:ARG:NH1	2.50	0.41
24:U:819:VAL:HA	24:U:820:PRO:HD3	1.95	0.41
26:W:344:THR:OG1	26:W:345:GLU:N	2.54	0.41
34:f:397:LYS:HD2	34:f:397:LYS:HA	1.85	0.41
1:A:208:PRO:HA	1:A:209:PRO:HD3	1.97	0.40
1:A:241:ILE:HB	1:A:244:GLU:HG3	2.03	0.40
2:B:365:PHE:HB3	2:B:380:LEU:HD21	2.02	0.40
3:C:386:ALA:HA	3:C:390:VAL:HG23	2.03	0.40
4:D:271:ALA:HA	4:D:289:LEU:HD11	2.02	0.40
17:Q:26:VAL:HG21	18:R:136:TYR:HE2	1.86	0.40
18:R:3:THR:HG21	18:R:44:THR:OG1	2.21	0.40
22:x:454:LYS:HA	22:x:454:LYS:HD3	1.91	0.40
23:y:30:ILE:HD13	23:y:30:ILE:HA	1.97	0.40
24:U:506:ALA:HB1	24:U:543:LYS:HD2	2.03	0.40
24:U:794:ASP:OD1	24:U:794:ASP:N	2.54	0.40
25:V:337:LEU:HB3	25:V:398:LEU:HD11	2.03	0.40
27:X:350:ILE:HD12	27:X:350:ILE:HA	1.89	0.40
30:a:163:TYR:HB2	30:a:172:TYR:CD1	2.56	0.40
30:a:321:LYS:HE3	30:a:336:VAL:HG21	2.03	0.40
34:f:376:PHE:HE1	34:f:801:VAL:HG21	1.86	0.40
1:A:333:ARG:HA	1:A:334:PRO:HD3	1.92	0.40
3:C:86:LEU:HD21	3:C:94:LYS:HG2	2.04	0.40
5:E:300:HIS:NE2	5:E:302:ASP:OD1	2.54	0.40
10:J:7:ILE:HG13	10:J:8:THR:HG23	2.03	0.40
9:i:13:SER:OG	9:i:17:ARG:N	2.54	0.40
9:i:238:LYS:HE3	9:i:238:LYS:HB3	1.81	0.40
20:t:9:THR:OG1	20:t:10:SER:N	2.52	0.40
23:y:27:LYS:HD3	23:y:41:GLN:HB2	2.03	0.40
24:U:387:ARG:NH2	24:U:426:TYR:OH	2.54	0.40
25:V:201:ARG:NH1	25:V:241:ARG:O	2.43	0.40
29:Z:74:TYR:OH	32:c:98:MET:O	2.29	0.40
33:d:188:LYS:HZ2	33:d:188:LYS:HG3	1.75	0.40
34:f:127:SER:O	34:f:132:THR:N	2.52	0.40
34:f:215:ASP:O	34:f:219:LYS:HG2	2.20	0.40
34:f:304:PHE:O	34:f:308:SER:OG	2.39	0.40
1:A:427:PRO:HD3	11:K:53:ARG:HH12	1.85	0.40
2:B:178:LYS:HA	2:B:178:LYS:HD2	1.97	0.40
3:C:49:ARG:HD2	24:U:639:LEU:HD21	2.03	0.40
13:M:66:LEU:HD13	13:M:214:SER:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:122:ARG:HG2	14:n:202:LEU:HD21	2.03	0.40
17:Q:43:LEU:HB2	17:Q:183:ILE:HD11	2.04	0.40
12:l:22:ILE:HD13	12:l:22:ILE:HA	1.94	0.40
26:W:273:TYR:HA	26:W:276:LEU:HD23	2.04	0.40
26:W:436:MET:HA	26:W:439:VAL:HG12	2.02	0.40
27:X:303:GLU:OE2	27:X:307:THR:OG1	2.40	0.40
28:Y:70:LEU:HD23	28:Y:73:MET:HE2	2.03	0.40
30:a:21:VAL:HA	30:a:24:ARG:HD3	2.02	0.40
34:f:154:TRP:HA	34:f:157:GLU:HG2	2.02	0.40
34:f:761:MET:HG3	34:f:763:ARG:H	1.85	0.40
13:M:43:ASP:OD1	13:M:43:ASP:N	2.54	0.40
19:s:19:ASP:N	19:s:19:ASP:OD1	2.53	0.40
25:V:123:SER:H	25:V:150:ARG:HH21	1.69	0.40
25:V:182:LYS:HE2	25:V:182:LYS:HB2	1.87	0.40
25:V:255:LEU:HD23	25:V:255:LEU:HA	1.89	0.40
26:W:243:ILE:HA	26:W:246:HIS:HB3	2.04	0.40
30:a:54:ASP:HA	30:a:57:ILE:HG22	2.03	0.40
34:f:10:PRO:HG2	34:f:59:LEU:HD22	2.03	0.40
34:f:707:LEU:HA	34:f:707:LEU:HD12	1.89	0.40
1:A:111:TYR:HE2	1:A:125:LEU:HD23	1.86	0.40
8:h:222:THR:N	8:h:225:GLU:OE1	2.51	0.40
22:x:76:ASP:N	22:x:76:ASP:OD1	2.54	0.40
22:x:108:THR:OG1	22:x:169:SER:O	2.36	0.40
24:U:465:LEU:HD11	24:U:477:GLY:HA3	2.04	0.40
24:U:770:TRP:HD1	32:c:179:SER:H	1.69	0.40
26:W:428:TRP:CZ2	26:W:432:LEU:HD11	2.57	0.40
30:a:126:GLY:HA3	30:a:129:GLN:HE22	1.86	0.40
32:c:57:MET:HB3	32:c:69:VAL:HG21	2.03	0.40
32:c:196:LEU:HD12	32:c:200:TYR:HE1	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	411/433 (95%)	361 (88%)	48 (12%)	2 (0%)	24	57
2	B	409/440 (93%)	367 (90%)	42 (10%)	0	100	100
3	C	394/398 (99%)	351 (89%)	39 (10%)	4 (1%)	12	44
4	D	378/418 (90%)	337 (89%)	40 (11%)	1 (0%)	36	67
5	E	387/403 (96%)	357 (92%)	30 (8%)	0	100	100
6	F	396/439 (90%)	360 (91%)	36 (9%)	0	100	100
7	G	238/246 (97%)	225 (94%)	13 (6%)	0	100	100
7	g	242/246 (98%)	234 (97%)	8 (3%)	0	100	100
8	H	230/234 (98%)	216 (94%)	14 (6%)	0	100	100
8	h	230/234 (98%)	220 (96%)	10 (4%)	0	100	100
9	I	246/261 (94%)	234 (95%)	12 (5%)	0	100	100
9	i	248/261 (95%)	238 (96%)	10 (4%)	0	100	100
10	J	237/248 (96%)	225 (95%)	12 (5%)	0	100	100
10	j	237/248 (96%)	226 (95%)	11 (5%)	0	100	100
11	K	236/241 (98%)	229 (97%)	7 (3%)	0	100	100
11	k	232/241 (96%)	223 (96%)	9 (4%)	0	100	100
12	L	238/269 (88%)	225 (94%)	13 (6%)	0	100	100
12	l	236/269 (88%)	224 (95%)	12 (5%)	0	100	100
13	M	240/255 (94%)	232 (97%)	8 (3%)	0	100	100
13	m	238/255 (93%)	235 (99%)	3 (1%)	0	100	100
14	N	201/239 (84%)	197 (98%)	4 (2%)	0	100	100
14	n	200/239 (84%)	194 (97%)	6 (3%)	0	100	100
15	O	218/277 (79%)	212 (97%)	6 (3%)	0	100	100
15	o	218/277 (79%)	209 (96%)	9 (4%)	0	100	100
16	P	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
16	p	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
17	Q	197/201 (98%)	191 (97%)	6 (3%)	0	100	100
17	q	197/201 (98%)	192 (98%)	5 (2%)	0	100	100
18	R	199/263 (76%)	194 (98%)	5 (2%)	0	100	100
18	r	199/263 (76%)	194 (98%)	5 (2%)	0	100	100
19	S	211/241 (88%)	205 (97%)	6 (3%)	0	100	100
19	s	211/241 (88%)	202 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	214/264 (81%)	206 (96%)	8 (4%)	0	100	100
20	t	214/264 (81%)	206 (96%)	8 (4%)	0	100	100
22	x	492/494 (100%)	469 (95%)	22 (4%)	1 (0%)	43	74
23	y	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
24	U	868/953 (91%)	785 (90%)	83 (10%)	0	100	100
25	V	442/534 (83%)	432 (98%)	10 (2%)	0	100	100
26	W	444/456 (97%)	415 (94%)	28 (6%)	1 (0%)	43	74
27	X	378/422 (90%)	357 (94%)	21 (6%)	0	100	100
28	Y	387/389 (100%)	349 (90%)	35 (9%)	3 (1%)	16	49
29	Z	284/324 (88%)	243 (86%)	41 (14%)	0	100	100
30	a	371/376 (99%)	345 (93%)	26 (7%)	0	100	100
31	b	189/377 (50%)	170 (90%)	19 (10%)	0	100	100
32	c	285/310 (92%)	244 (86%)	41 (14%)	0	100	100
33	d	255/350 (73%)	222 (87%)	33 (13%)	0	100	100
34	f	887/908 (98%)	778 (88%)	107 (12%)	2 (0%)	43	74
35	e	48/70 (69%)	41 (85%)	7 (15%)	0	100	100
All	All	13990/15458 (90%)	13036 (93%)	940 (7%)	14 (0%)	49	79

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	PRO
3	C	224	ILE
4	D	416	PHE
22	x	87	VAL
34	f	100	ARG
28	Y	8	GLU
1	A	66	LYS
3	C	90	HIS
3	C	91	PRO
26	W	140	ILE
28	Y	2	PRO
34	f	110	TYR
3	C	131	VAL
28	Y	211	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	349/372 (94%)	344 (99%)	5 (1%)	59	71
2	B	357/385 (93%)	353 (99%)	4 (1%)	65	74
3	C	340/346 (98%)	338 (99%)	2 (1%)	78	79
4	D	333/366 (91%)	331 (99%)	2 (1%)	78	79
5	E	341/353 (97%)	341 (100%)	0	100	100
6	F	344/379 (91%)	344 (100%)	0	100	100
7	G	202/210 (96%)	201 (100%)	1 (0%)	81	80
7	g	201/210 (96%)	200 (100%)	1 (0%)	81	80
8	H	187/191 (98%)	187 (100%)	0	100	100
8	h	188/191 (98%)	188 (100%)	0	100	100
9	I	202/221 (91%)	202 (100%)	0	100	100
9	i	206/221 (93%)	206 (100%)	0	100	100
10	J	197/211 (93%)	197 (100%)	0	100	100
10	j	196/211 (93%)	196 (100%)	0	100	100
11	K	197/203 (97%)	197 (100%)	0	100	100
11	k	195/203 (96%)	195 (100%)	0	100	100
12	L	202/230 (88%)	202 (100%)	0	100	100
12	l	201/230 (87%)	201 (100%)	0	100	100
13	M	198/212 (93%)	198 (100%)	0	100	100
13	m	198/212 (93%)	197 (100%)	1 (0%)	81	80
14	N	158/181 (87%)	158 (100%)	0	100	100
14	n	156/181 (86%)	156 (100%)	0	100	100
15	O	178/228 (78%)	178 (100%)	0	100	100
15	o	181/228 (79%)	181 (100%)	0	100	100
16	P	172/174 (99%)	172 (100%)	0	100	100
16	p	173/174 (99%)	173 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Q	168/171 (98%)	168 (100%)	0	100	100
17	q	166/171 (97%)	166 (100%)	0	100	100
18	R	156/202 (77%)	156 (100%)	0	100	100
18	r	154/202 (76%)	154 (100%)	0	100	100
19	S	175/199 (88%)	175 (100%)	0	100	100
19	s	177/199 (89%)	177 (100%)	0	100	100
20	T	178/215 (83%)	178 (100%)	0	100	100
20	t	179/215 (83%)	179 (100%)	0	100	100
22	x	439/439 (100%)	438 (100%)	1 (0%)	87	85
23	y	68/68 (100%)	68 (100%)	0	100	100
24	U	748/816 (92%)	748 (100%)	0	100	100
25	V	390/460 (85%)	390 (100%)	0	100	100
26	W	410/416 (99%)	409 (100%)	1 (0%)	87	85
27	X	327/362 (90%)	327 (100%)	0	100	100
28	Y	344/344 (100%)	331 (96%)	13 (4%)	29	55
29	Z	257/295 (87%)	250 (97%)	7 (3%)	39	62
30	a	333/336 (99%)	331 (99%)	2 (1%)	78	79
31	b	167/312 (54%)	167 (100%)	0	100	100
32	c	252/268 (94%)	251 (100%)	1 (0%)	84	81
33	d	231/294 (79%)	231 (100%)	0	100	100
34	f	745/763 (98%)	742 (100%)	3 (0%)	84	81
35	e	44/63 (70%)	42 (96%)	2 (4%)	24	50
All	All	11960/13133 (91%)	11914 (100%)	46 (0%)	81	81

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	LEU
1	A	65	ILE
1	A	66	LYS
1	A	373	LEU
1	A	403	ILE
2	B	88	LEU
2	B	89	GLU

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Mol	Chain	Res	Type
2	B	94	GLU
2	B	125	THR
3	C	109	THR
3	C	210	THR
4	D	82	ILE
4	D	84	SER
7	G	17	SER
7	g	224	ASN
13	m	236	GLU
22	x	78	LEU
26	W	118	LEU
28	Y	3	LEU
28	Y	5	ASN
28	Y	6	LEU
28	Y	11	LEU
28	Y	13	LYS
28	Y	205	VAL
28	Y	208	PHE
28	Y	209	THR
28	Y	210	SER
28	Y	211	TYR
28	Y	212	GLU
28	Y	213	LEU
28	Y	214	MET
29	Z	143	GLU
29	Z	144	VAL
29	Z	145	HIS
29	Z	149	THR
29	Z	151	THR
29	Z	175	LEU
29	Z	176	LEU
30	a	339	ARG
30	a	342	ASP
32	c	125	VAL
34	f	150	GLU
34	f	873	LEU
34	f	874	LEU
35	e	60	LEU
35	e	61	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	A	305	GLN
1	A	379	ASN
1	A	414	ASN
2	B	119	ASN
2	B	120	HIS
2	B	314	ASN
3	C	32	GLN
3	C	50	ASN
3	C	53	ASN
4	D	99	ASN
4	D	158	GLN
4	D	294	ASN
4	D	295	GLN
5	E	45	ASN
5	E	55	GLN
5	E	121	ASN
5	E	155	ASN
5	E	226	GLN
5	E	263	GLN
5	E	345	ASN
6	F	83	ASN
6	F	92	ASN
6	F	102	ASN
6	F	333	ASN
6	F	417	HIS
7	G	33	ASN
7	G	53	GLN
7	G	75	ASN
7	G	128	ASN
7	G	224	ASN
8	H	52	GLN
8	H	109	GLN
9	I	84	ASN
9	I	95	GLN
9	I	109	GLN
9	I	142	HIS
9	I	146	GLN
9	I	240	HIS
10	J	200	GLN
10	J	215	GLN
12	L	4	ASN
12	L	43	HIS

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Mol	Chain	Res	Type
13	M	32	ASN
13	M	143	ASN
14	N	77	HIS
14	N	110	GLN
14	N	158	ASN
14	N	193	GLN
17	Q	82	ASN
17	Q	101	ASN
17	Q	132	HIS
18	R	162	GLN
18	R	175	ASN
18	R	178	HIS
19	S	159	GLN
20	T	3	ASN
8	h	169	ASN
9	i	30	HIS
12	l	53	GLN
13	m	143	ASN
14	n	77	HIS
14	n	110	GLN
17	q	8	GLN
17	q	61	GLN
17	q	99	HIS
17	q	101	ASN
18	r	175	ASN
19	s	108	ASN
20	t	2	GLN
20	t	157	GLN
22	x	308	ASN
24	U	89	ASN
24	U	128	GLN
24	U	135	ASN
24	U	139	GLN
24	U	362	ASN
24	U	373	ASN
24	U	384	GLN
24	U	500	ASN
24	U	527	GLN
24	U	721	HIS
24	U	888	GLN
25	V	78	HIS
25	V	146	GLN

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Mol	Chain	Res	Type
25	V	283	ASN
26	W	156	ASN
26	W	218	ASN
26	W	236	HIS
26	W	395	ASN
26	W	426	ASN
27	X	105	GLN
27	X	329	ASN
28	Y	5	ASN
28	Y	273	GLN
28	Y	367	GLN
29	Z	243	GLN
29	Z	256	GLN
30	a	12	GLN
30	a	231	GLN
30	a	288	HIS
30	a	332	HIS
31	b	158	ASN
32	c	77	GLN
32	c	92	GLN
32	c	149	GLN
32	c	256	ASN
32	c	298	GLN
33	d	141	GLN
33	d	229	GLN
34	f	53	GLN
34	f	148	GLN
34	f	199	ASN
34	f	213	GLN
34	f	472	HIS
34	f	650	GLN
34	f	815	HIS
34	f	855	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	ADP	B	501	-	28,29,29	1.40	4 (14%)	43,45,45	1.88	8 (18%)
37	ATP	E	501	-	32,33,33	0.45	0	48,52,52	0.29	0
37	ATP	F	501	-	32,33,33	0.47	0	48,52,52	0.33	0
37	ATP	D	501	-	32,33,33	0.48	0	48,52,52	0.30	0
36	ADP	A	501	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	10 (23%)
37	ATP	C	501	-	32,33,33	0.52	0	48,52,52	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	ADP	B	501	-	-	5/16/32/32	0/3/3/3
37	ATP	E	501	-	-	4/22/38/38	0/3/3/3
37	ATP	F	501	-	-	3/22/38/38	0/3/3/3
37	ATP	D	501	-	-	10/22/38/38	0/3/3/3
36	ADP	A	501	-	-	2/16/32/32	0/3/3/3
37	ATP	C	501	-	-	6/22/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	B	501	ADP	C5-C4	4.72	1.47	1.39
36	A	501	ADP	C5-C4	4.60	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	B	501	ADP	C5-C6	2.65	1.48	1.41
36	A	501	ADP	C5-C6	2.58	1.48	1.41
36	B	501	ADP	C5-N7	-2.40	1.34	1.39
36	A	501	ADP	C5-N7	-2.38	1.34	1.39
36	A	501	ADP	C8-N7	2.26	1.36	1.31
36	B	501	ADP	C8-N7	2.23	1.36	1.31

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	B	501	ADP	C5-C4-N3	-6.02	118.42	126.72
36	A	501	ADP	C5-C4-N3	-5.86	118.65	126.72
36	B	501	ADP	N3-C4-N9	4.89	135.48	127.17
36	A	501	ADP	N3-C4-N9	4.59	134.98	127.17
36	B	501	ADP	C2-N3-C4	3.74	120.95	111.83
36	A	501	ADP	C2-N3-C4	3.65	120.75	111.83
36	A	501	ADP	C4-C5-N7	-3.54	106.53	110.58
36	B	501	ADP	C4-C5-N7	-3.32	106.78	110.58
36	B	501	ADP	N3-C2-N1	-3.17	123.78	128.58
36	A	501	ADP	N3-C2-N1	-3.14	123.84	128.58
36	B	501	ADP	C3'-C2'-C1'	2.71	106.58	101.46
36	A	501	ADP	C4-N9-C8	2.64	108.51	105.74
36	B	501	ADP	C4-N9-C8	2.60	108.46	105.74
36	A	501	ADP	C5-N7-C8	2.55	107.46	103.45
36	A	501	ADP	C3'-C2'-C1'	2.52	106.22	101.46
36	B	501	ADP	C5-N7-C8	2.48	107.35	103.45
36	A	501	ADP	C2'-C1'-N9	-2.03	108.26	113.30
36	A	501	ADP	C6-C5-N7	2.03	136.00	132.09

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	A	501	ADP	C5'-O5'-PA-O3A
36	B	501	ADP	C5'-O5'-PA-O2A
36	B	501	ADP	C5'-O5'-PA-O3A
36	B	501	ADP	C3'-C4'-C5'-O5'
37	C	501	ATP	C5'-O5'-PA-O2A
37	D	501	ATP	PB-O3B-PG-O3G
37	D	501	ATP	C5'-O5'-PA-O2A
37	F	501	ATP	O4'-C4'-C5'-O5'
36	B	501	ADP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
37	C	501	ATP	C3'-C4'-C5'-O5'
37	C	501	ATP	O4'-C4'-C5'-O5'
37	F	501	ATP	C3'-C4'-C5'-O5'
37	D	501	ATP	O4'-C4'-C5'-O5'
36	A	501	ADP	C5'-O5'-PA-O1A
37	C	501	ATP	C5'-O5'-PA-O1A
37	C	501	ATP	C5'-O5'-PA-O3A
37	D	501	ATP	C5'-O5'-PA-O1A
37	D	501	ATP	C5'-O5'-PA-O3A
37	E	501	ATP	C5'-O5'-PA-O3A
37	C	501	ATP	C4'-C5'-O5'-PA
37	E	501	ATP	PG-O3B-PB-O2B
36	B	501	ADP	C4'-C5'-O5'-PA
37	F	501	ATP	C4'-C5'-O5'-PA
37	D	501	ATP	PB-O3B-PG-O1G
37	D	501	ATP	PG-O3B-PB-O1B
37	E	501	ATP	C4'-C5'-O5'-PA
37	D	501	ATP	C4'-C5'-O5'-PA
37	D	501	ATP	C2'-C1'-N9-C8
37	D	501	ATP	PG-O3B-PB-O2B
37	E	501	ATP	PA-O3A-PB-O2B

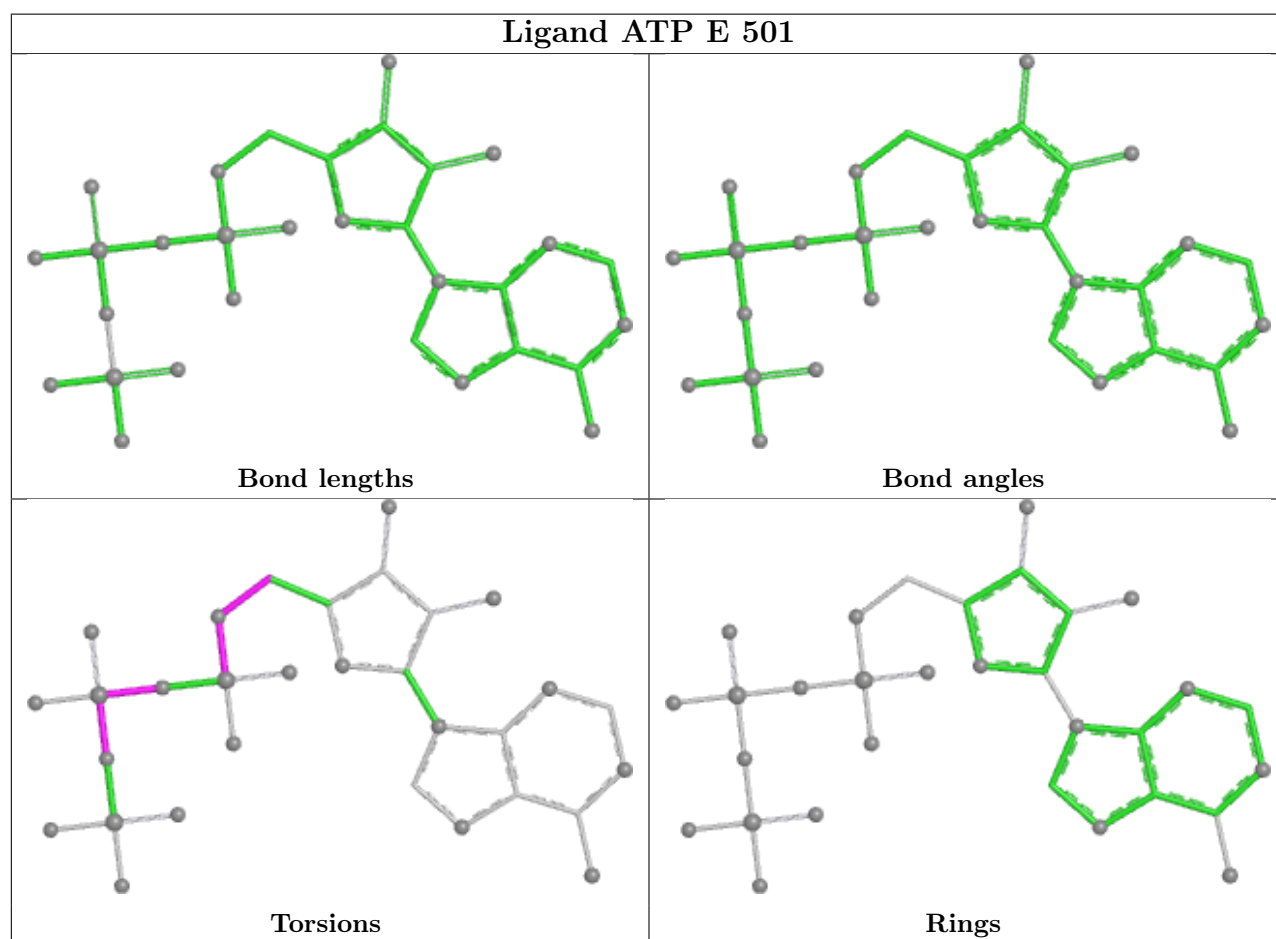
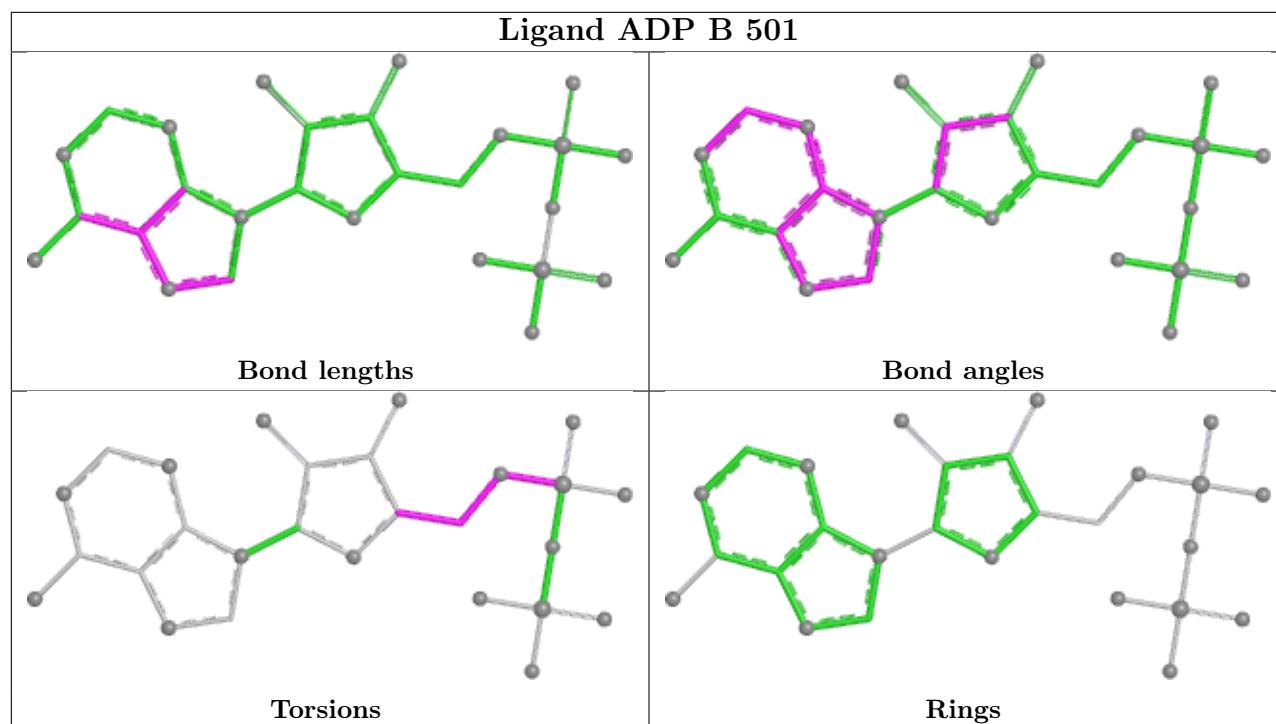
There are no ring outliers.

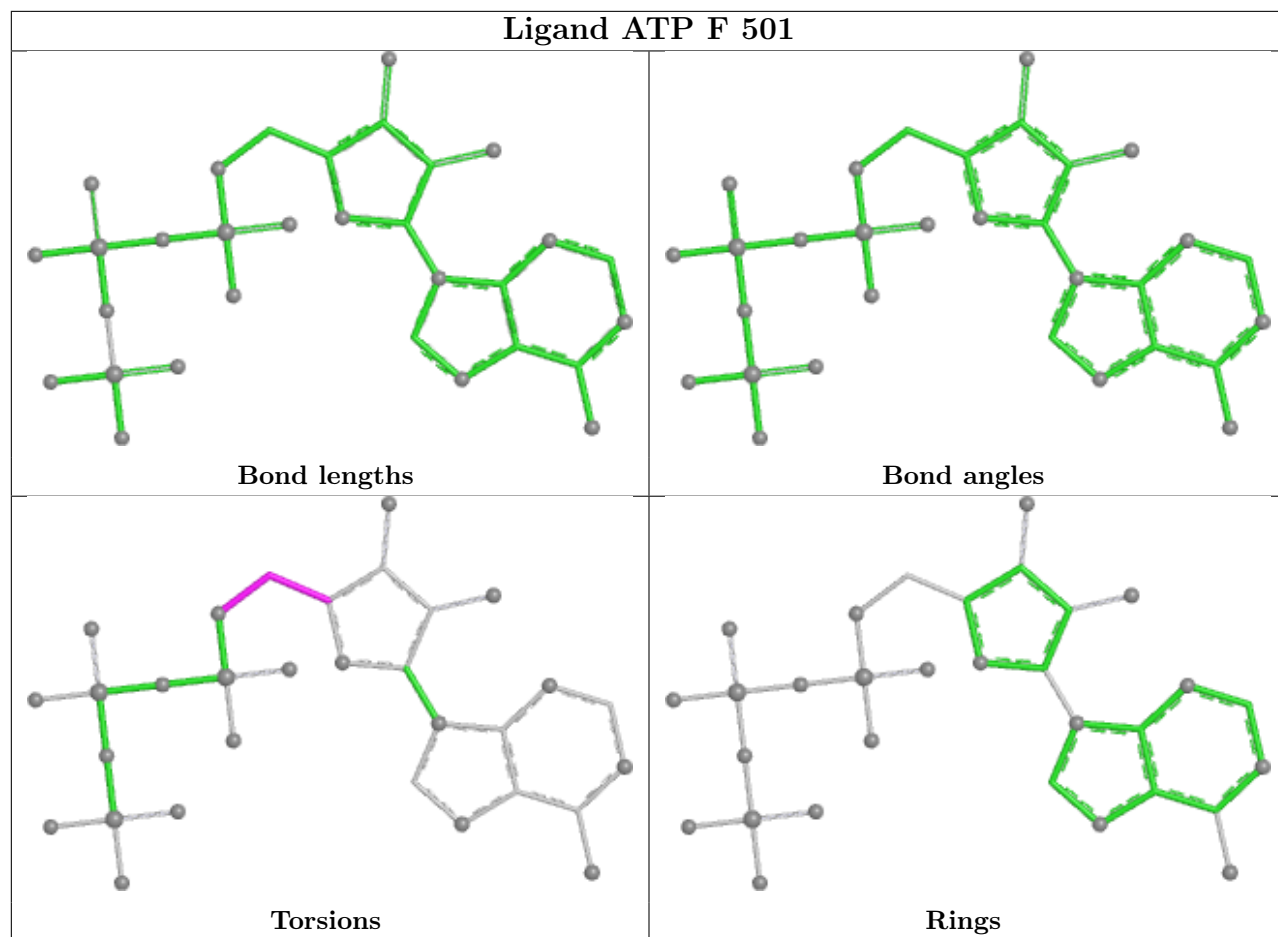
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	E	501	ATP	2	0
37	F	501	ATP	1	0
36	A	501	ADP	1	0
37	C	501	ATP	3	0

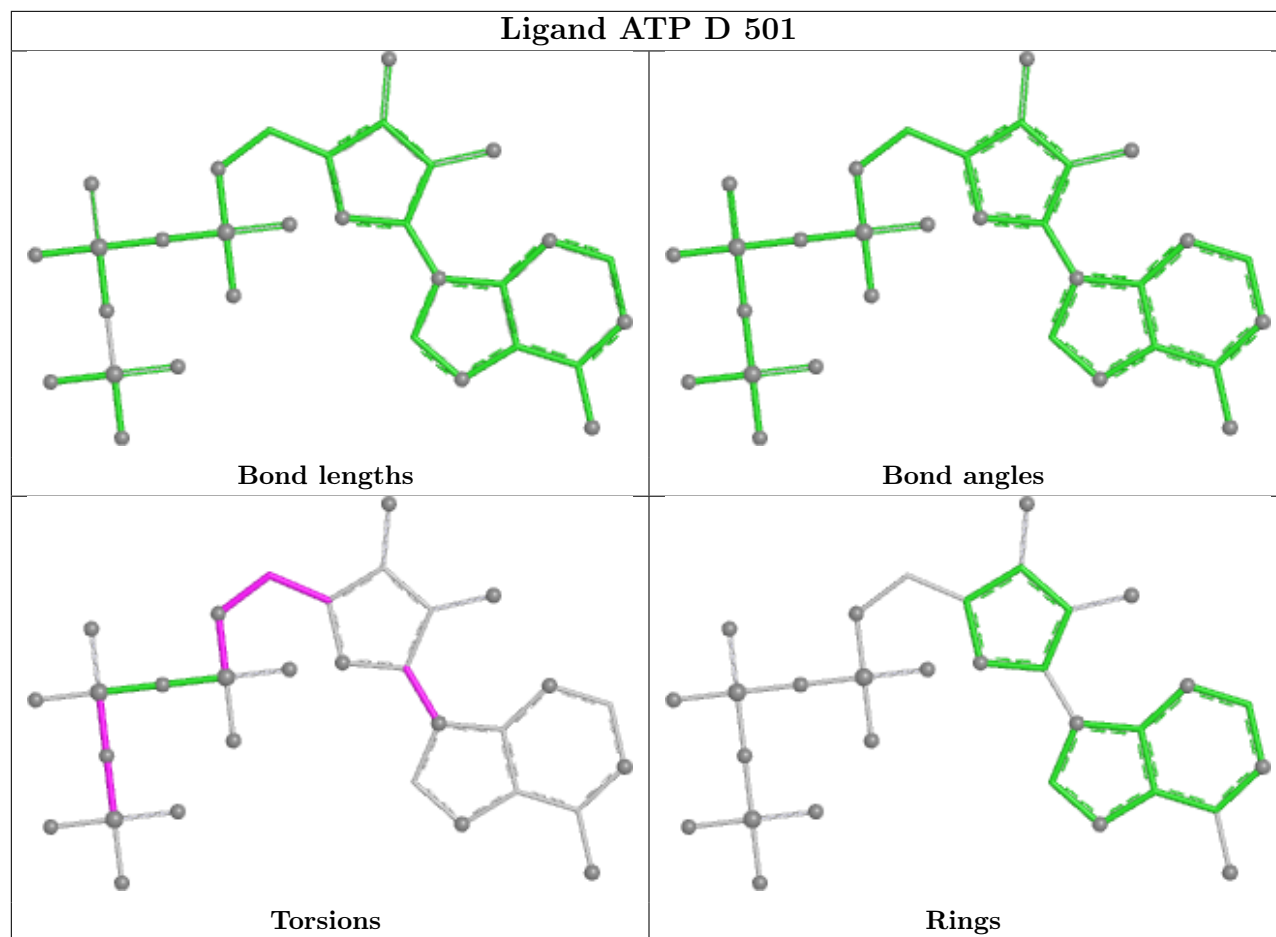
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

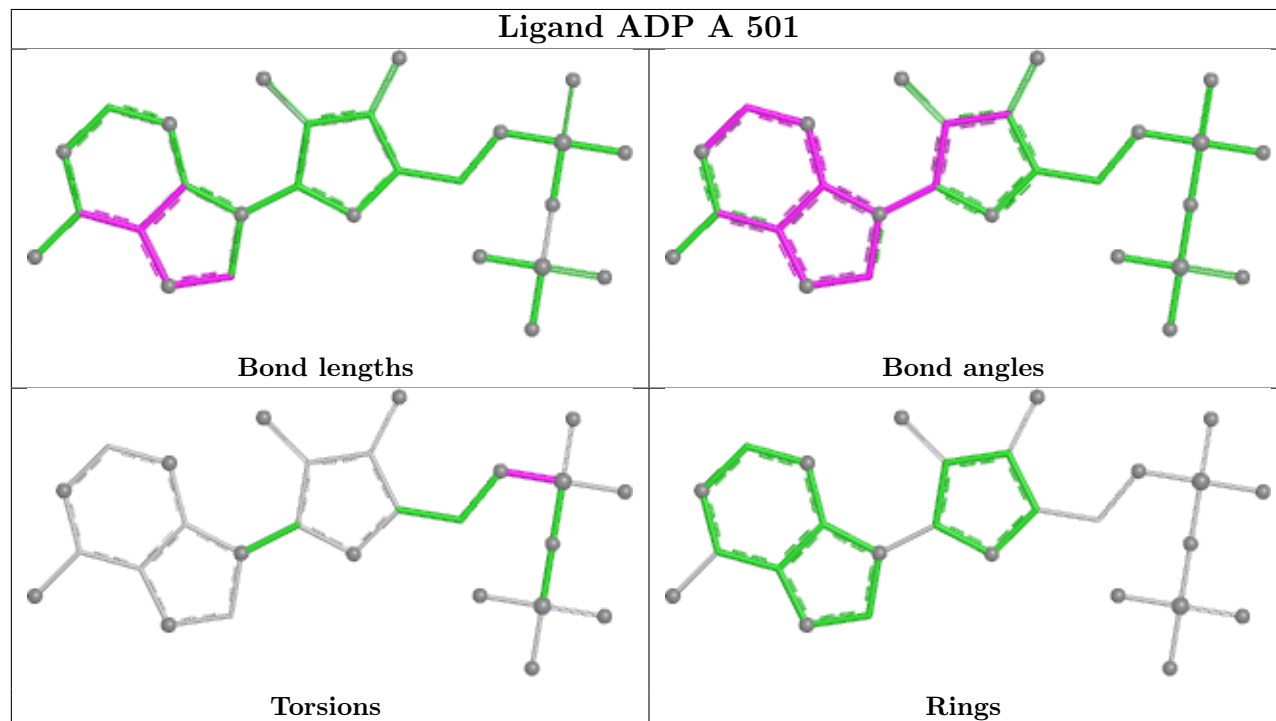


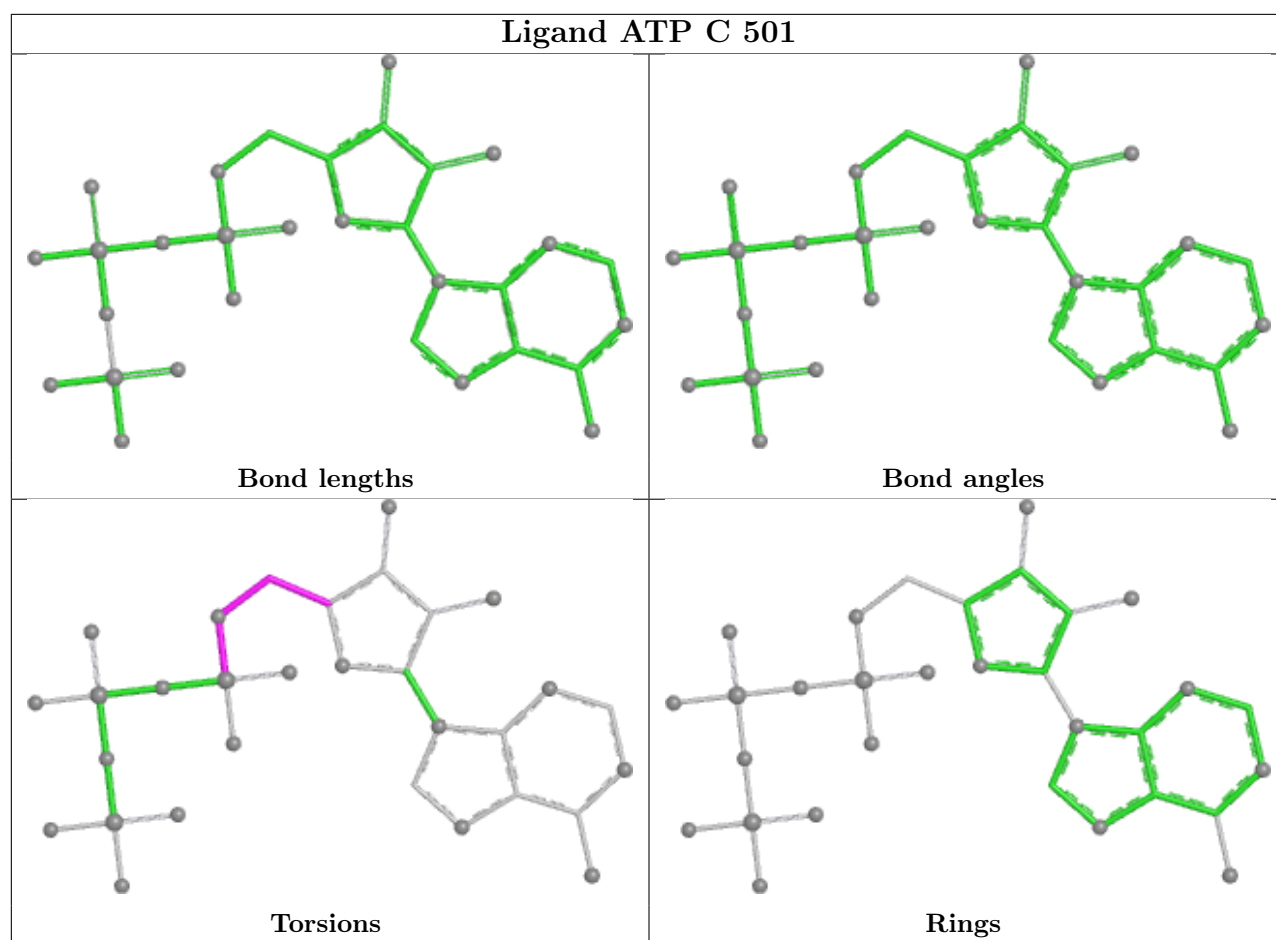


Ligand ATP D 501



Ligand ADP A 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.

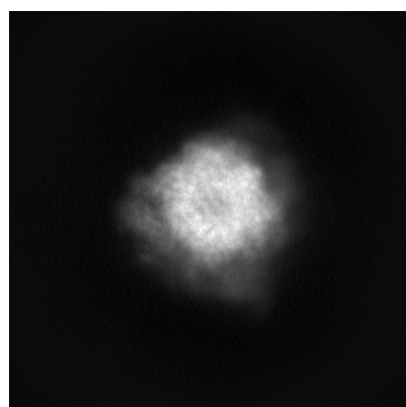
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32275. These allow visual inspection of the internal detail of the map and identification of artifacts.

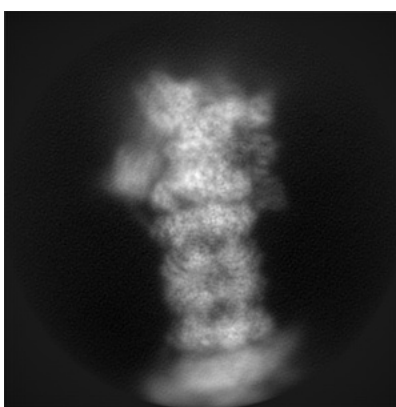
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

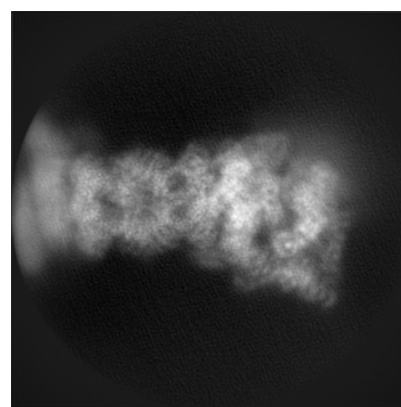
6.1.1 Primary map



X



Y

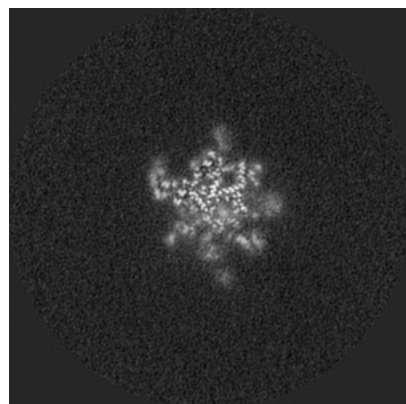


Z

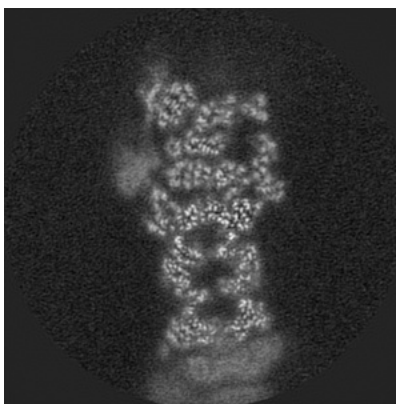
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

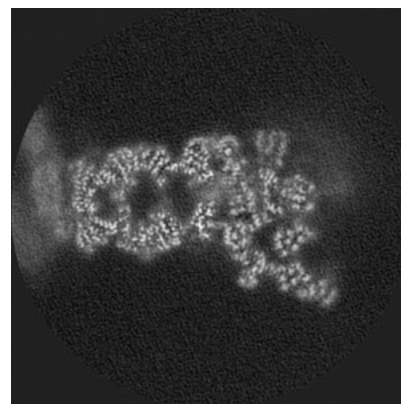
6.2.1 Primary map



X Index: 320



Y Index: 320

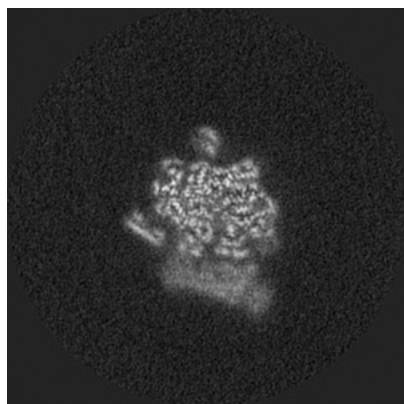


Z Index: 320

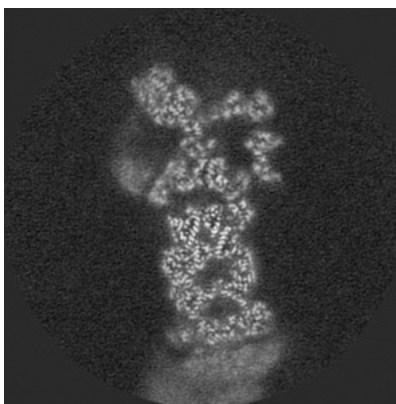
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

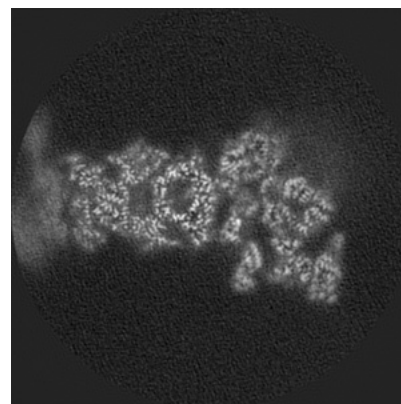
6.3.1 Primary map



X Index: 359



Y Index: 302

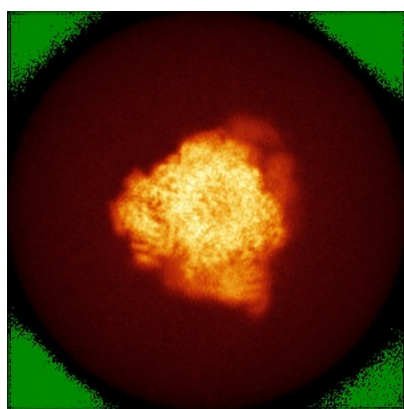


Z Index: 298

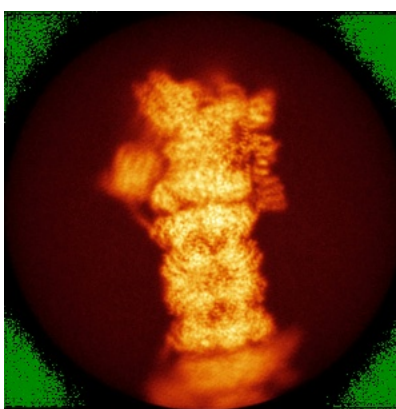
The images above show the largest variance slices of the map in three orthogonal directions.

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

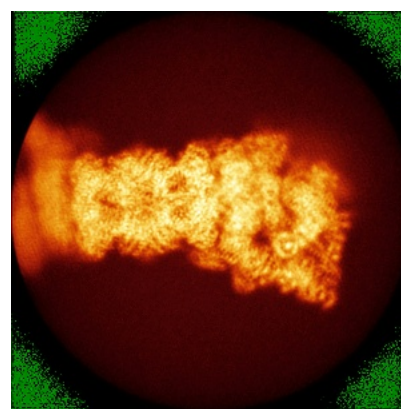
6.4.1 Primary map



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

This section was not generated.

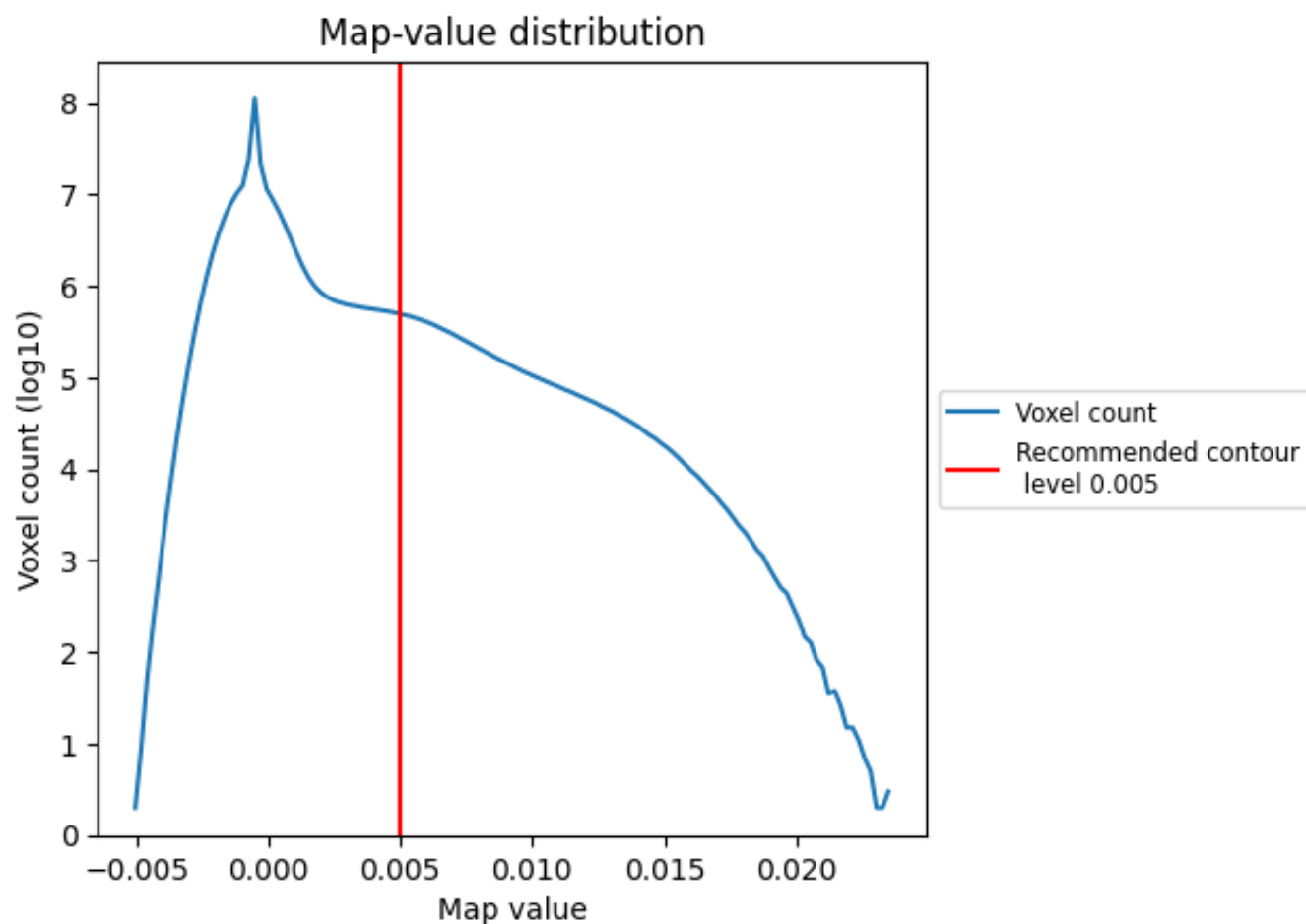
6.6 Mask visualisation

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

7 Map analysis [i](#)

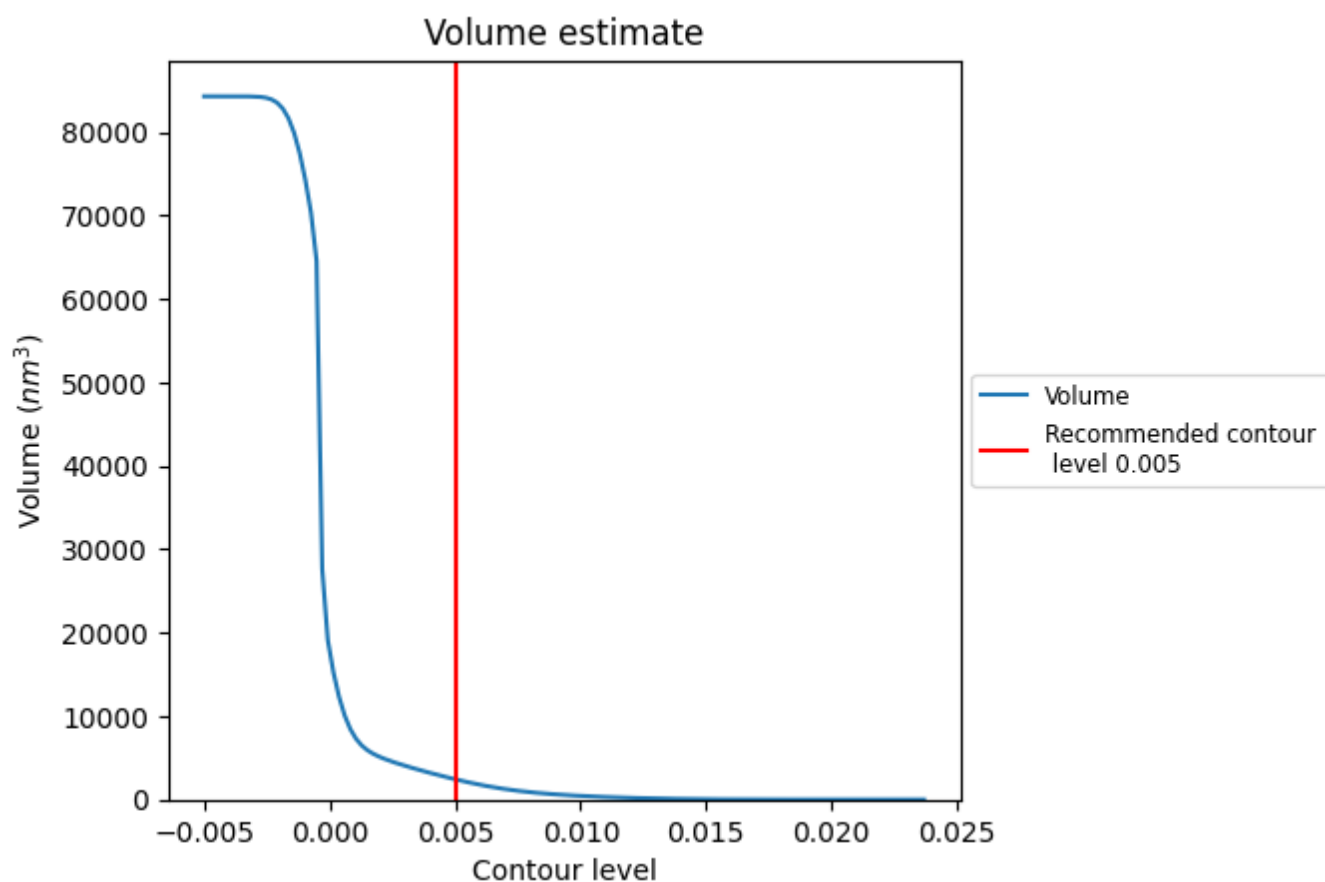
This section contains the results of statistical analysis of the map.

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.

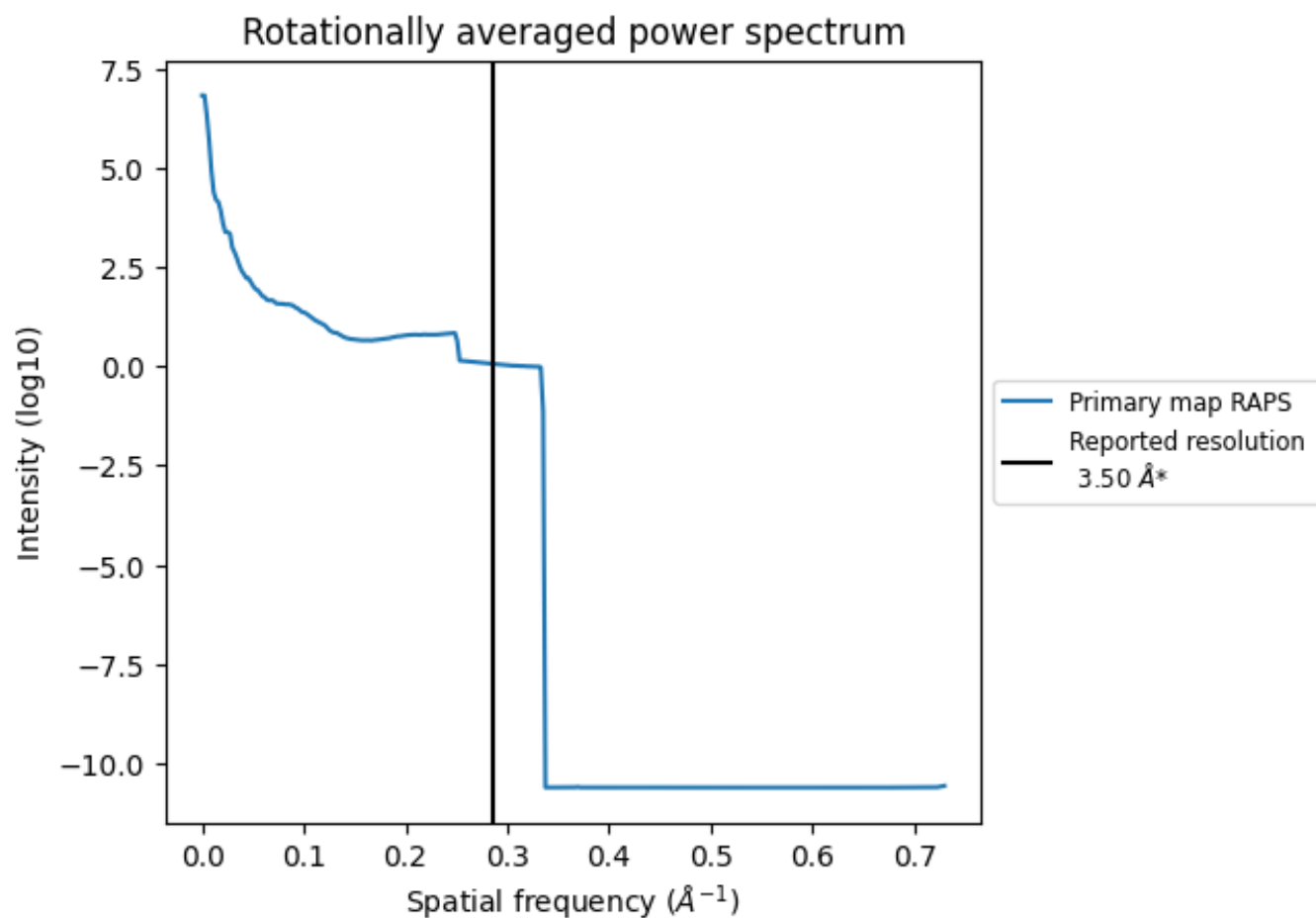
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2426 nm³; this corresponds to an approximate mass of 2191 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 0.286 Å⁻¹

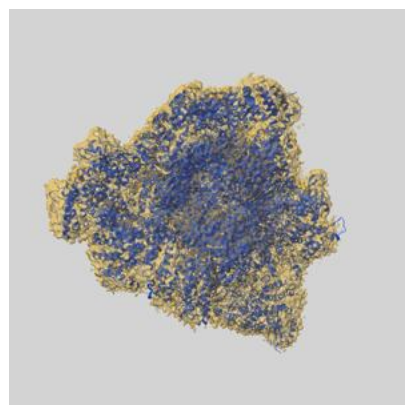
8 Fourier-Shell correlation ⓘ

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

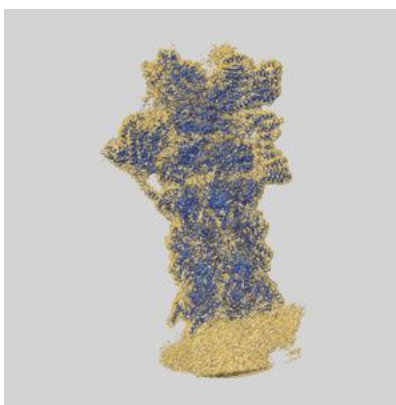
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32275 and PDB model 7W3A. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

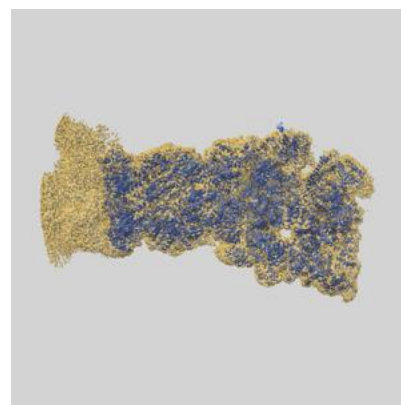
9.1 Map-model overlay [i](#)



X



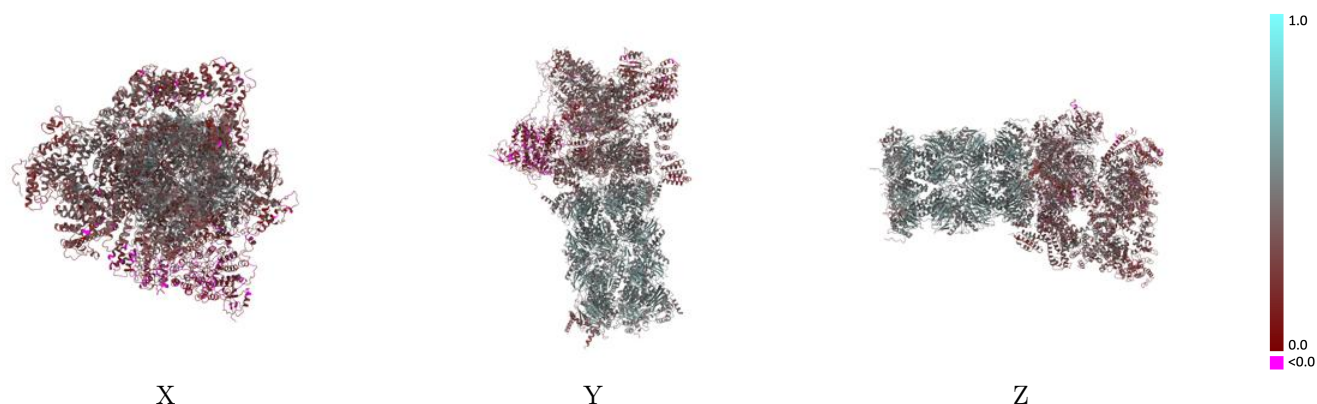
Y



Z

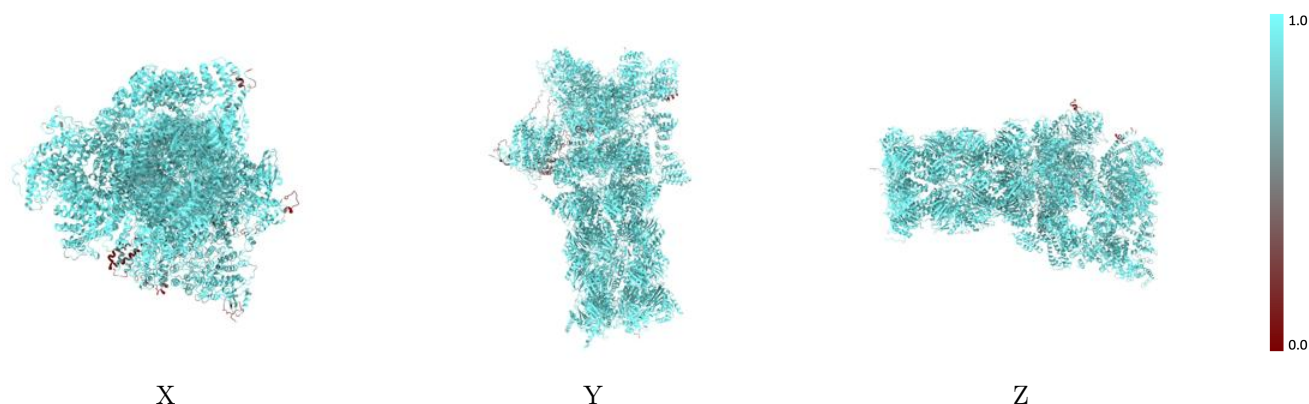
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



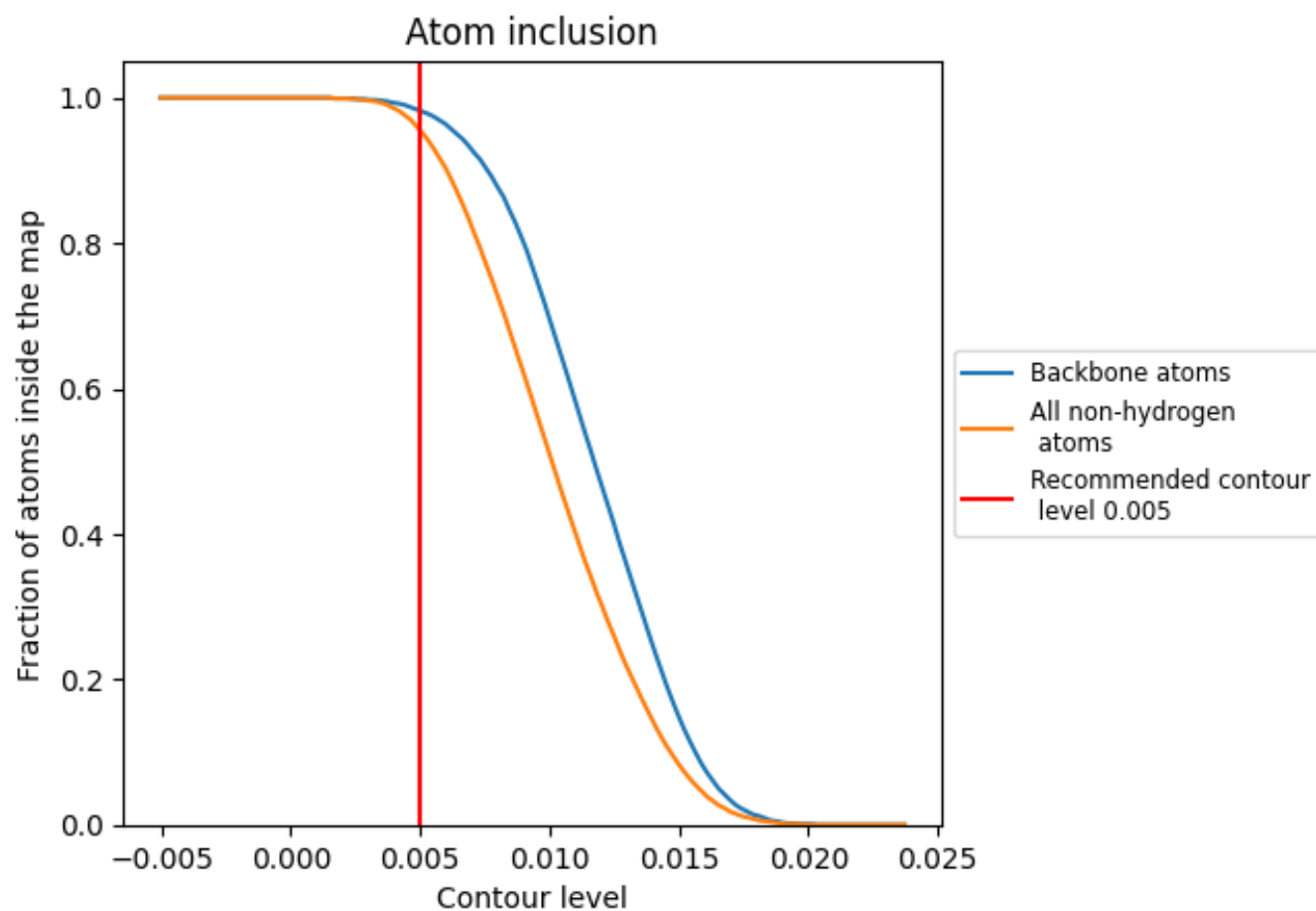
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9550	 0.3900
A	 0.9430	 0.3320
B	 0.9250	 0.3000
C	 0.9630	 0.3300
D	 0.9730	 0.3670
E	 0.9580	 0.3680
F	 0.9420	 0.3660
G	 0.9870	 0.4970
H	 0.9890	 0.4940
I	 0.9840	 0.4810
J	 0.9810	 0.4780
K	 0.9840	 0.4900
L	 0.9920	 0.5040
M	 0.9870	 0.5010
N	 0.9880	 0.5190
O	 0.9930	 0.5120
P	 0.9920	 0.5220
Q	 0.9900	 0.5170
R	 0.9950	 0.5210
S	 0.9930	 0.5090
T	 0.9860	 0.5260
U	 0.9230	 0.3270
V	 0.9500	 0.3300
W	 0.9310	 0.2950
X	 0.9610	 0.3500
Y	 0.9540	 0.3300
Z	 0.9730	 0.3350
a	 0.9460	 0.2830
b	 0.9470	 0.2680
c	 0.9660	 0.3420
d	 0.9250	 0.2580
e	 0.9450	 0.3200
f	 0.8630	 0.1480
g	 0.9780	 0.4950
h	 0.9830	 0.4980



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Chain	Atom inclusion	Q-score
i	 0.9740	 0.4700
j	 0.9690	 0.4350
k	 0.9770	 0.4740
l	 0.9890	 0.5060
m	 0.9780	 0.4930
n	 0.9950	 0.5270
o	 0.9900	 0.5170
p	 0.9940	 0.5220
q	 0.9950	 0.5190
r	 0.9960	 0.5250
s	 0.9900	 0.5130
t	 0.9880	 0.5220
v	 0.9880	 0.3420
x	 0.8520	 0.2700
y	 0.9410	 0.3260