



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:02 PM UTC

PDB ID : 9NKG / pdb_00009nkg
EMDB ID : EMD-49508
Title : Structure of substrate engaged MIDN-bound human 26S proteasome, EB-MIDN (Composite map)
Authors : Peddada, N.; Beutler, B.
Deposited on : 2025-02-28
Resolution : 2.80 Å(reported)
Based on initial model : 6mse

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

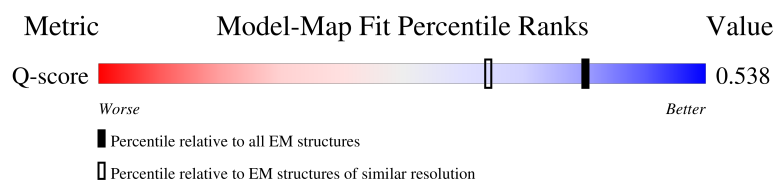
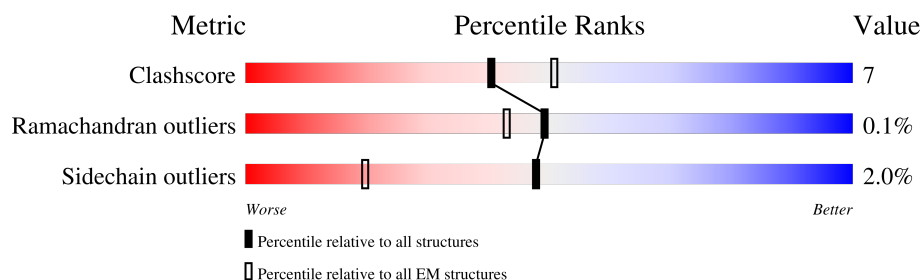
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	11806 (2.30 - 3.30)

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	G	246	
1	g	246	
2	H	234	
2	h	234	

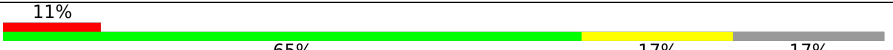
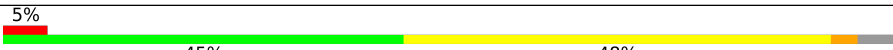
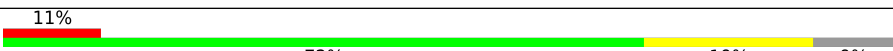
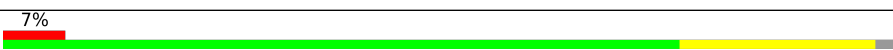
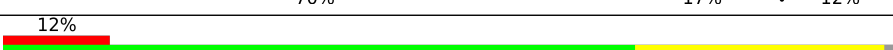
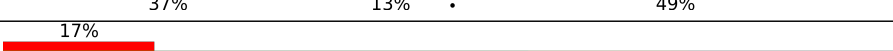
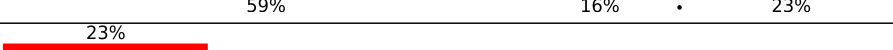
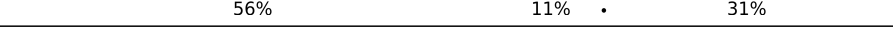
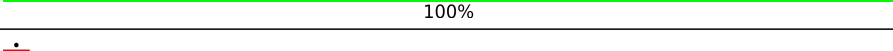
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Mol	Chain	Length	Quality of chain
3	I	261	
3	i	261	
4	J	248	
4	j	248	
5	K	241	
5	k	241	
6	L	263	
6	l	263	
7	M	255	
7	m	255	
8	N	239	
8	n	239	
9	O	277	
9	o	277	
10	P	205	
10	p	205	
11	Q	201	
11	q	201	
12	R	263	
12	r	263	
13	S	241	
13	s	241	
14	T	264	
14	t	264	
15	A	433	

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Mol	Chain	Length	Quality of chain
16	B	440	
17	C	406	
18	D	418	
19	E	403	
20	F	439	
21	V	534	
22	W	456	
23	X	422	
24	Y	389	
25	Z	324	
26	a	376	
27	b	377	
28	d	350	
29	e	70	
30	v	12	
31	U	953	
32	c	310	
33	f	908	
34	z	468	

2 Entry composition [i](#)

There are 39 unique types of molecules in this entry. The entry contains 201518 atoms, of which 98452 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 Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	G	240	Total	C	H	N	O	S	0	0
			3394	1106	1656	304	316	12		
1	g	240	Total	C	H	N	O	S	0	0
			3445	1124	1687	306	316	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	H	229	Total	C	H	N	O	S	0	0
			3252	1080	1590	288	288	6		
2	h	229	Total	C	H	N	O	S	0	0
			3252	1080	1590	288	288	6		

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	I	247	Total	C	H	N	O	S	0	0
			3543	1150	1741	322	320	10		
3	i	247	Total	C	H	N	O	S	0	0
			3503	1143	1717	320	313	10		

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	J	232	Total	C	H	N	O	S	0	0
			3151	1038	1518	306	284	5		
4	j	232	Total	C	H	N	O	S	0	0
			3151	1038	1518	306	284	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	K	233	Total	C	H	N	O	S	0	0
			3264	1062	1597	287	307	11		
5	k	233	Total	C	H	N	O	S	0	0
			3249	1056	1589	287	306	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	9	TYR	ASP	conflict	UNP P28066
k	9	TYR	ASP	conflict	UNP P28066

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	L	233	Total	C	H	N	O	S	0	0
			3359	1090	1649	318	293	9		
6	l	233	Total	C	H	N	O	S	0	0
			3352	1089	1645	315	293	10		

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	M	239	Total	C	H	N	O	S	0	0
			3440	1131	1680	308	311	10		
7	m	239	Total	C	H	N	O	S	0	0
			3444	1131	1683	308	312	10		

- Molecule 8 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	N	202	Total	C	H	N	O	S	0	0
			2891	928	1422	257	272	12		
8	n	202	Total	C	H	N	O	S	0	0
			2881	926	1416	256	271	12		

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	O	220	Total	C	H	N	O	S	0	0
			3139	1005	1559	272	294	9		
9	o	220	Total	C	H	N	O	S	0	0
			3131	1003	1555	272	292	9		

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	P	204	Total	C	H	N	O	S	0	0
			3096	992	1550	262	273	19		
10	p	204	Total	C	H	N	O	S	0	0
			3081	989	1543	263	268	18		

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	Q	196	Total	C	H	N	O	S	0	0
			2986	974	1477	259	268	8		
11	q	196	Total	C	H	N	O	S	0	0
			2981	973	1475	259	266	8		

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	R	200	Total	C	H	N	O	S	0	0
			2953	957	1449	271	267	9		
12	r	200	Total	C	H	N	O	S	0	0
			2938	954	1438	270	267	9		

- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	S	212	Total	C	H	N	O	S	0	0
			3163	1016	1579	279	279	10		
13	s	212	Total	C	H	N	O	S	0	0
			3168	1017	1581	279	281	10		

- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	T	212	Total	C	H	N	O	S	0	0
			3102	1003	1526	280	282	11		
14	t	212	Total	C	H	N	O	S	0	0
			3079	998	1511	279	280	11		

- Molecule 15 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	A	390	Total	C	H	N	O	S	0	0
			6166	1928	3106	537	578	17		

- Molecule 16 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	B	393	Total	C	H	N	O	S	0	0
			6129	1936	3053	524	601	15		

- Molecule 17 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	C	389	Total	C	H	N	O	S	0	0
			6264	1932	3193	550	571	18		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
18	D	380	Total	C	H	N	O	S	0	0
			6114	1923	3075	524	579	13		

- Molecule 19 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	E	389	Total	C	H	N	O	S	0	0
			6248	1947	3150	552	582	17		

- Molecule 20 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	F	415	Total	C	H	N	O	S	0	0
			6569	2038	3318	561	634	18		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	V	442	Total	C	H	N	O	S	0	0
			7239	2290	3647	639	650	13		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	440	Total	C	N	O	S	0	0
			3588	2272	612	681	23		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace	
23	X	384	Total	C	H	N	O	S	0	0
			6174	1935	3134	513	580	12		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace	
24	Y	380	Total	C	H	N	O	S	0	0
			6260	1995	3133	535	580	17		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Z	286	Total	C	H	N	O	S	0	0
			4593	1457	2312	392	427	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
26	a	373	Total	C	H	N	O	S	0	0
			6007	1911	3012	510	559	15		

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	b	191	Total	C	H	N	O	S	0	0
			2963	910	1505	261	279	8		

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	d	270	Total	C	H	N	O	S	0	0
			4366	1407	2189	357	404	9		

- Molecule 29 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	48	Total	C	H	N	O	0	0
			687	236	298	62	91		

- Molecule 30 is a protein called unknown density (substrate density).

Mol	Chain	Residues	Atoms				AltConf	Trace
30	v	12	Total	C	N	O	0	0
			60	36	12	12		

- Molecule 31 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	U	814	Total	C	H	N	O	S	0	0
			12714	4028	6370	1080	1192	44		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
32	c	283	Total	C	H	N	O	S	0	0
			4473	1412	2241	385	418	17		

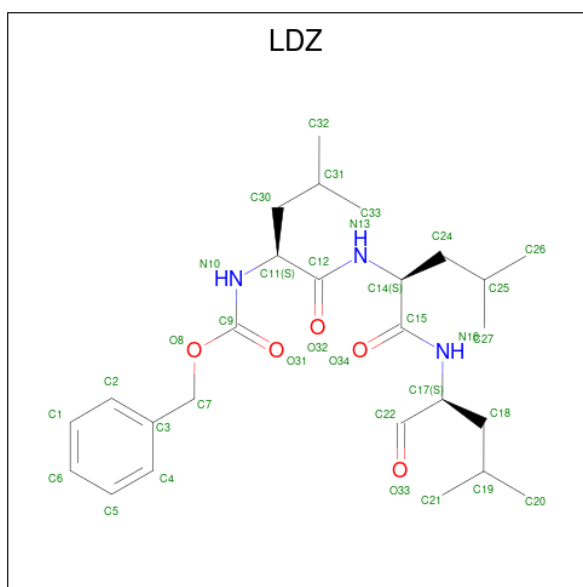
- Molecule 33 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	f	836	Total	C	H	N	O	S	0	0
			12946	4084	6486	1097	1234	45		

- Molecule 34 is a protein called Midnolin.

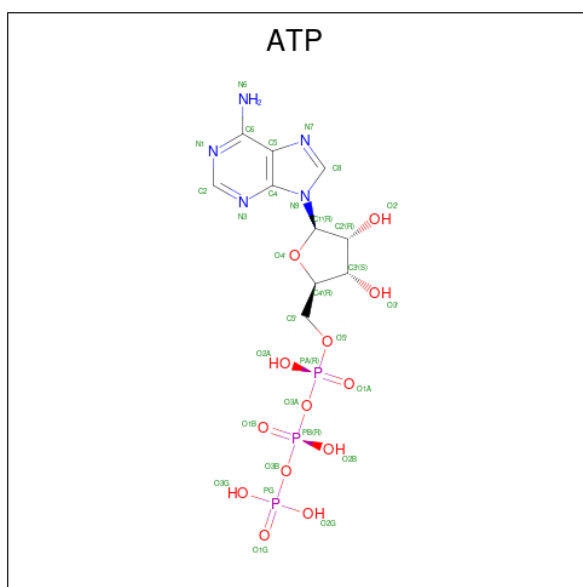
Mol	Chain	Residues	Atoms						AltConf	Trace
34	z	117	Total	C	H	N	O	S	0	0
			1904	566	983	185	167	3		

- Molecule 35 is N-[(benzyloxy)carbonyl]-L-leucyl-N-[(2S)-4-methyl-1-oxopentan-2-yl]-L-leucinamide (CCD ID: LDZ) (formula: C₂₆H₄₁N₃O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
35	N	1	Total	C	H	N	O	0
			75	26	41	3	5	
35	O	1	Total	C	H	N	O	0
			75	26	41	3	5	
35	R	1	Total	C	H	N	O	0
			75	26	41	3	5	
35	n	1	Total	C	H	N	O	0
			75	26	41	3	5	
35	o	1	Total	C	H	N	O	0
			75	26	41	3	5	
35	r	1	Total	C	H	N	O	0
			75	26	41	3	5	

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

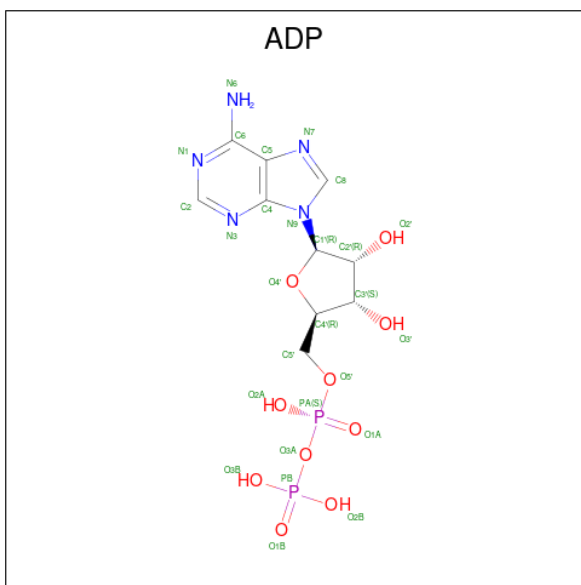


Mol	Chain	Residues	Atoms						AltConf
36	A	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
36	B	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
36	D	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
36	F	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
37	A	1	Total	Mg	0
			1	1	
37	B	1	Total	Mg	0
			1	1	
37	D	1	Total	Mg	0
			1	1	
37	F	1	Total	Mg	0
			1	1	

- Molecule 38 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
38	E	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

- Molecule 39 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

3 Residue-property plots [i](#)

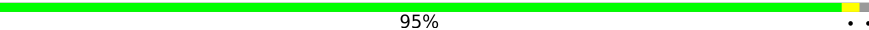
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Proteasome subunit alpha type-6

Chain G: 



- Molecule 1: Proteasome subunit alpha type-6

Chain g: 



- Molecule 2: Proteasome subunit alpha type-2

Chain H: 



- Molecule 2: Proteasome subunit alpha type-2

Chain h: 



- Molecule 3: Proteasome subunit alpha type-4

Chain I: 



- Molecule 3: Proteasome subunit alpha type-4

Chain i:  91% 5%



- Molecule 4: Proteasome subunit alpha type-7

Chain J:  89% 6%



- Molecule 4: Proteasome subunit alpha type-7

Chain j:  87% 6% 6%



- Molecule 5: Proteasome subunit alpha type-5

Chain K:  91% 5%



- Molecule 5: Proteasome subunit alpha type-5

Chain k:  93%



- Molecule 6: Proteasome subunit alpha type-1

Chain L:  83% 5% 11%



HIS

- Molecule 6: Proteasome subunit alpha type-1

Chain l:  83% 5% 11%



- Molecule 7: Proteasome subunit alpha type-3

Chain M:  88% 6% 6%



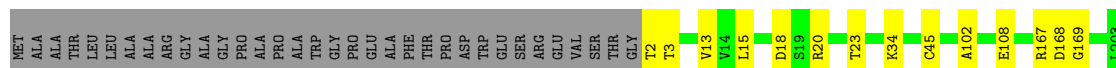
- Molecule 7: Proteasome subunit alpha type-3

Chain m:  89% 6%



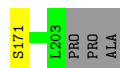
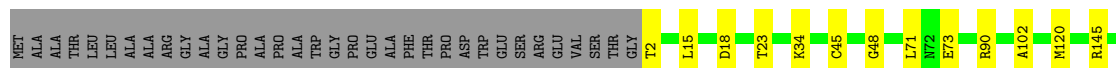
- Molecule 8: Proteasome subunit beta type-6

Chain N:  79% 6% 15%



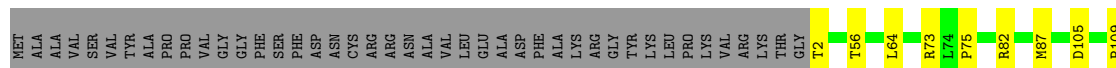
- Molecule 8: Proteasome subunit beta type-6

Chain n:  79% 6% 15%



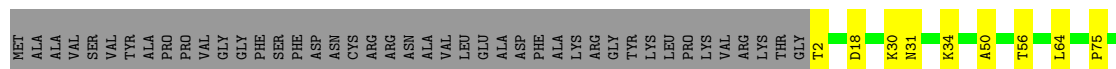
- Molecule 9: Proteasome subunit beta type-7

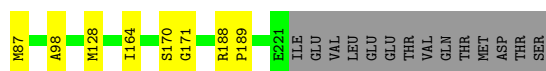
Chain O:  74% 6% 21%



- Molecule 9: Proteasome subunit beta type-7

Chain o:  73% 6% 21%





- Molecule 10: Proteasome subunit beta type-3

Chain P: 94% 5%



- Molecule 10: Proteasome subunit beta type-3

Chain p: 93% 6%



- Molecule 11: Proteasome subunit beta type-2

Chain Q: 90% 8%



- Molecule 11: Proteasome subunit beta type-2

Chain q: 96%



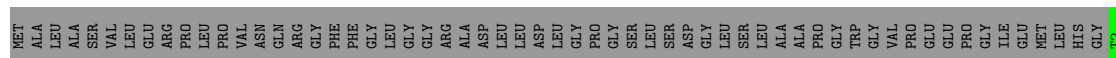
- Molecule 12: Proteasome subunit beta type-5

Chain R: 70% 6% 24%



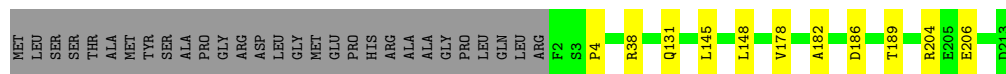
- Molecule 12: Proteasome subunit beta type-5

Chain r: 67% 9% 24%



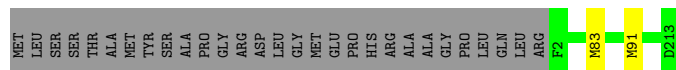
- Molecule 13: Proteasome subunit beta type-1

Chain S:  83% 5% 12%



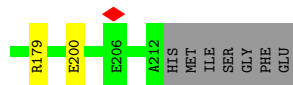
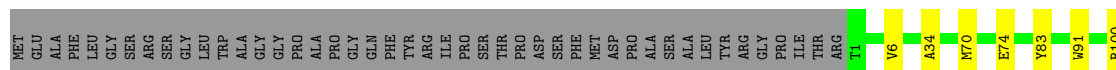
- Molecule 13: Proteasome subunit beta type-1

Chain s:  87% 12%



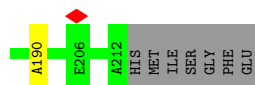
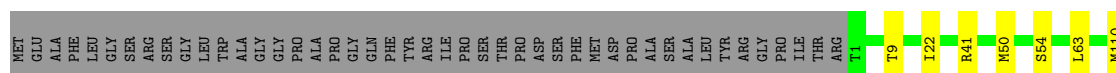
- Molecule 14: Proteasome subunit beta type-4

Chain T:  77% 20%



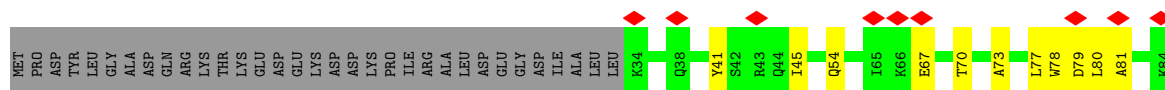
- Molecule 14: Proteasome subunit beta type-4

Chain t:  77% 20%



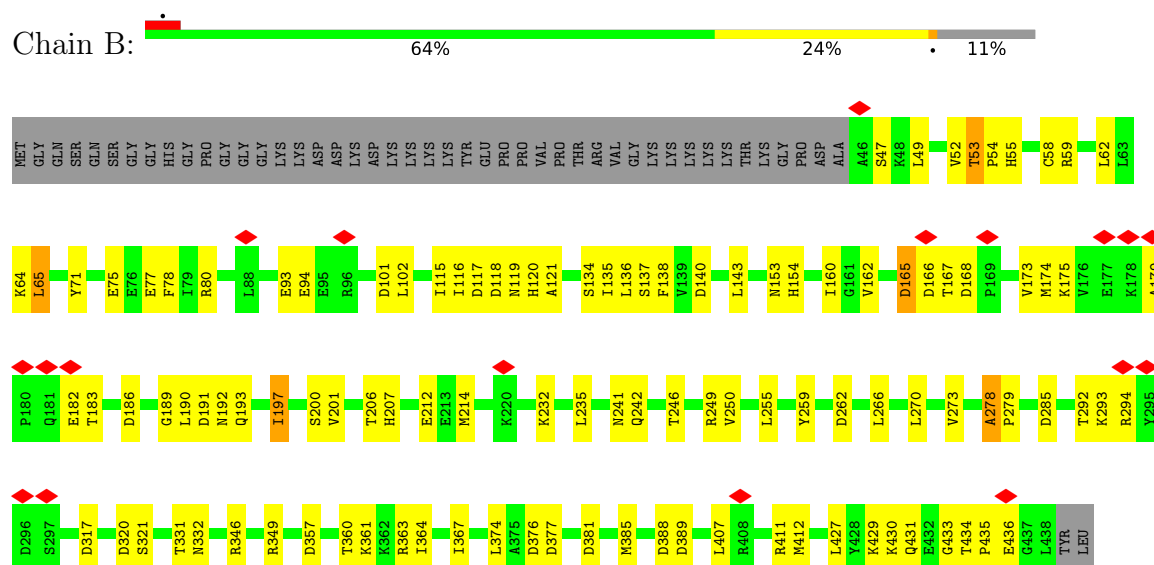
- Molecule 15: 26S proteasome regulatory subunit 7

Chain A:  76% 14% 10%



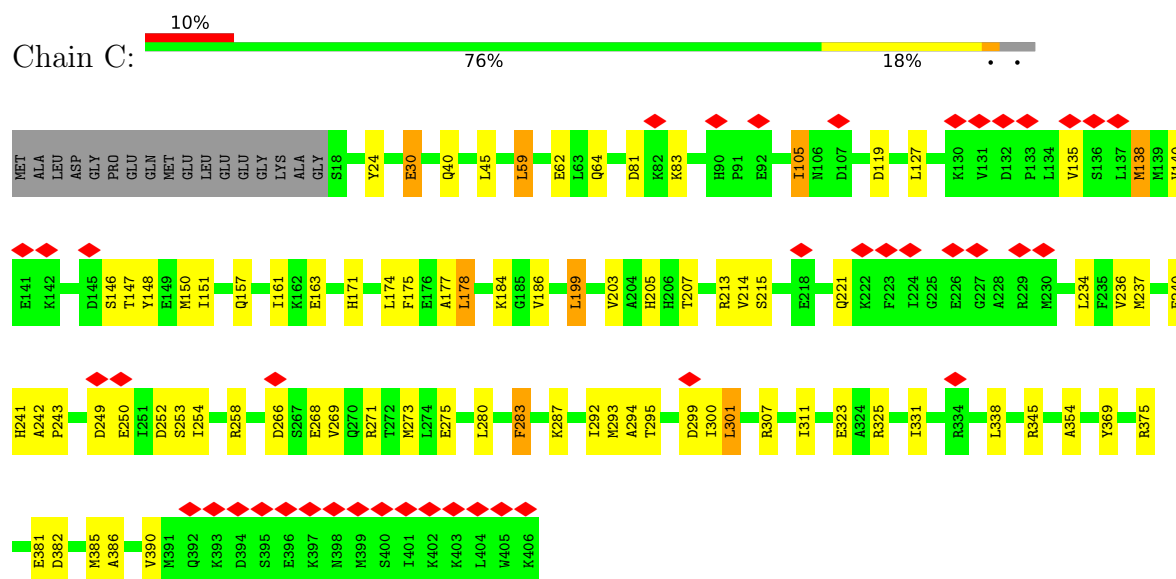
- Molecule 16: 26S proteasome regulatory subunit 4

Chain B:



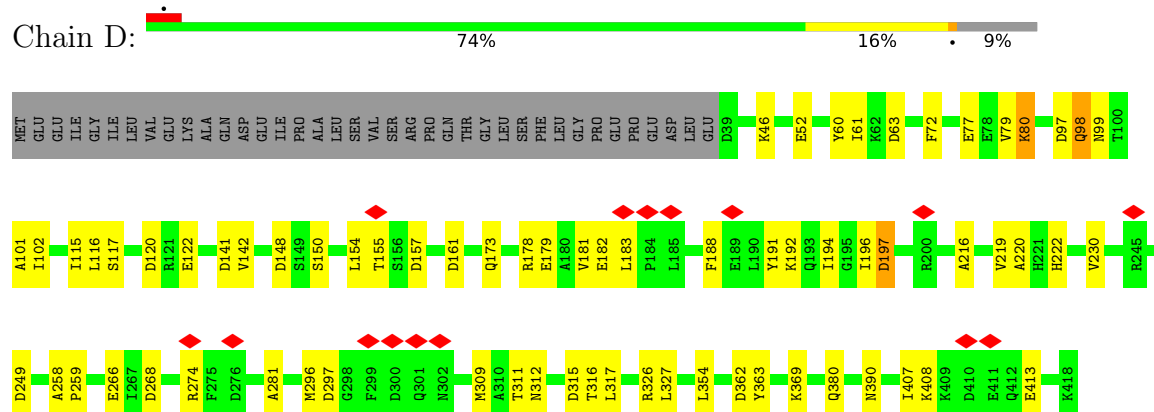
- Molecule 17: 26S protease regulatory subunit 8

Chain C:

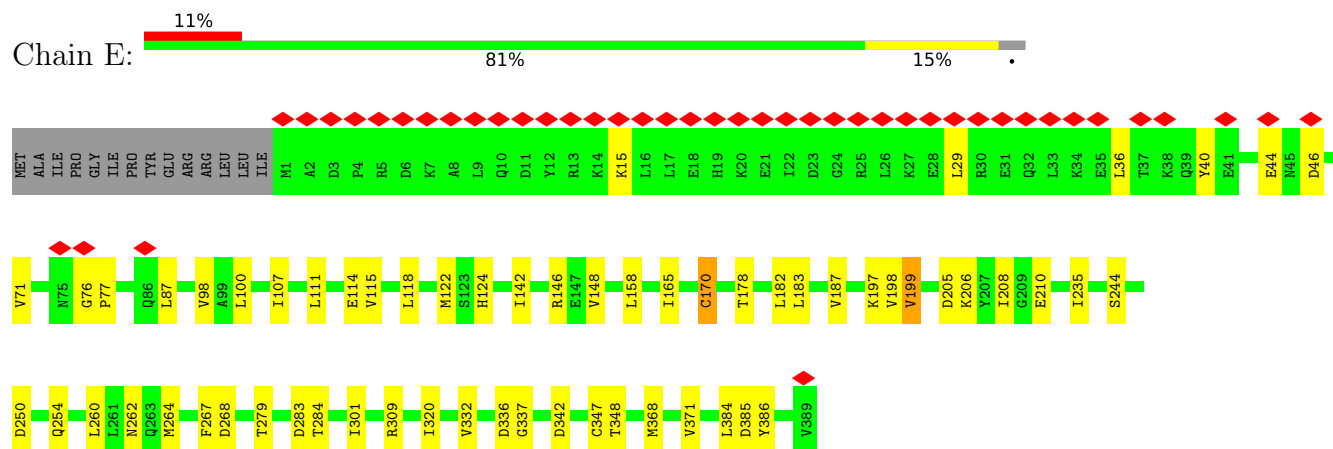


- Molecule 18: 26S proteasome regulatory subunit 6B

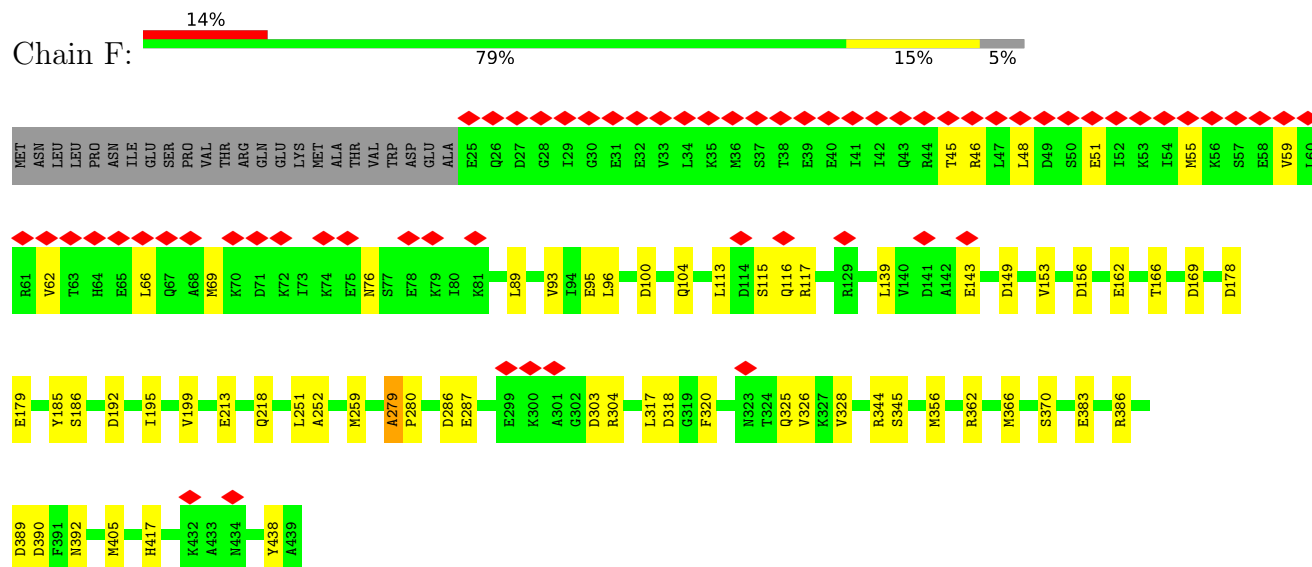
Chain D:



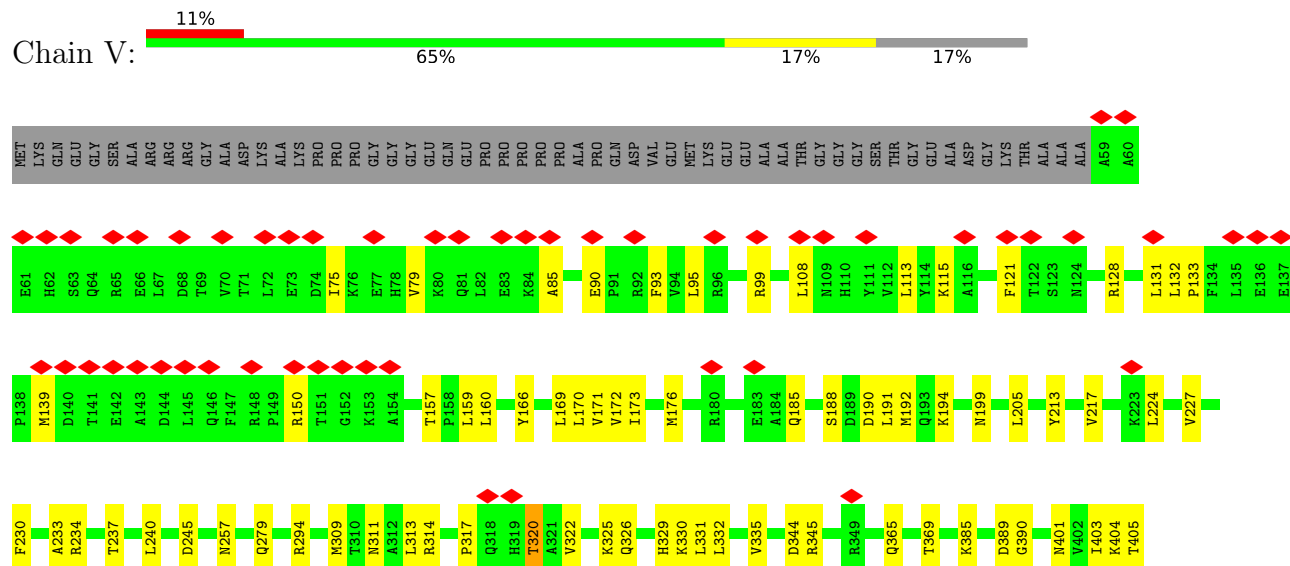
Chain E:

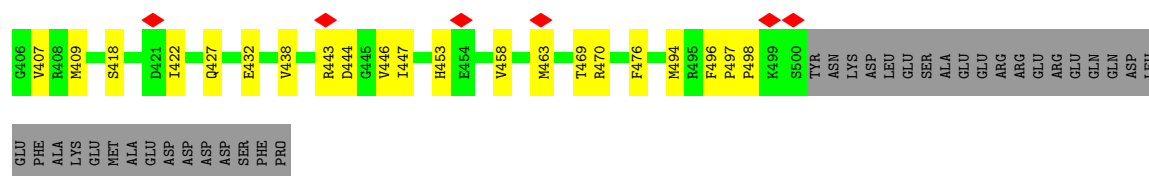


Chain F:

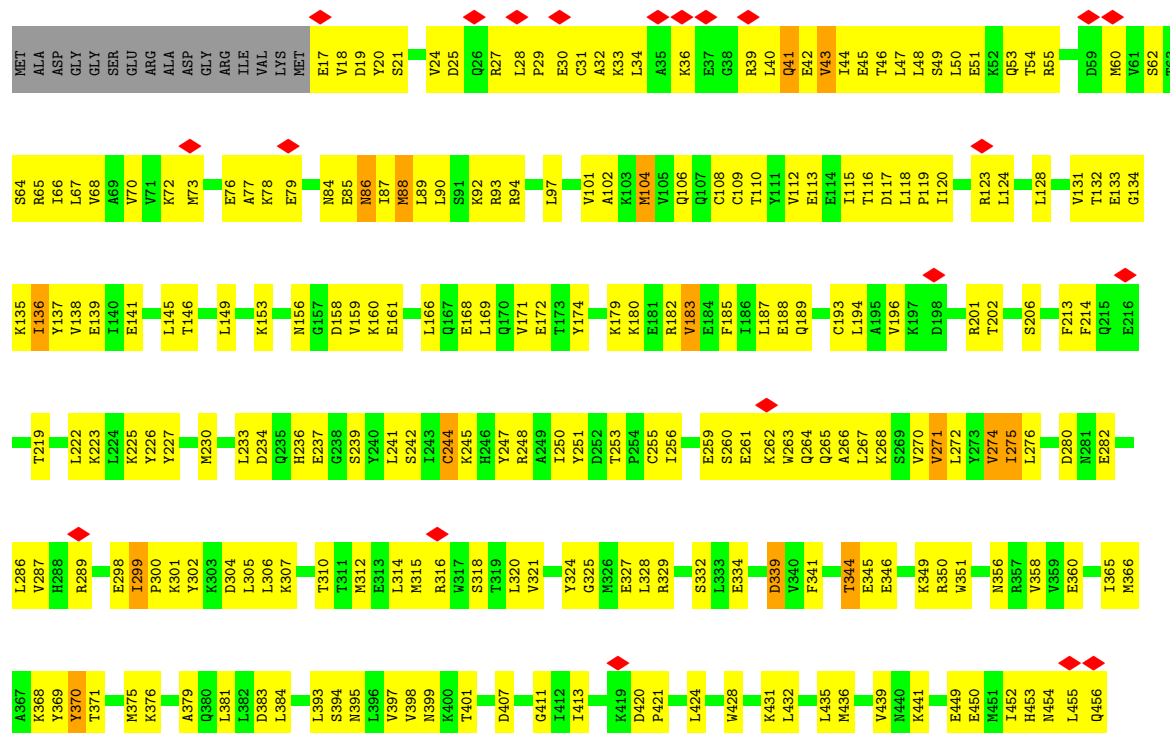


Chain V:

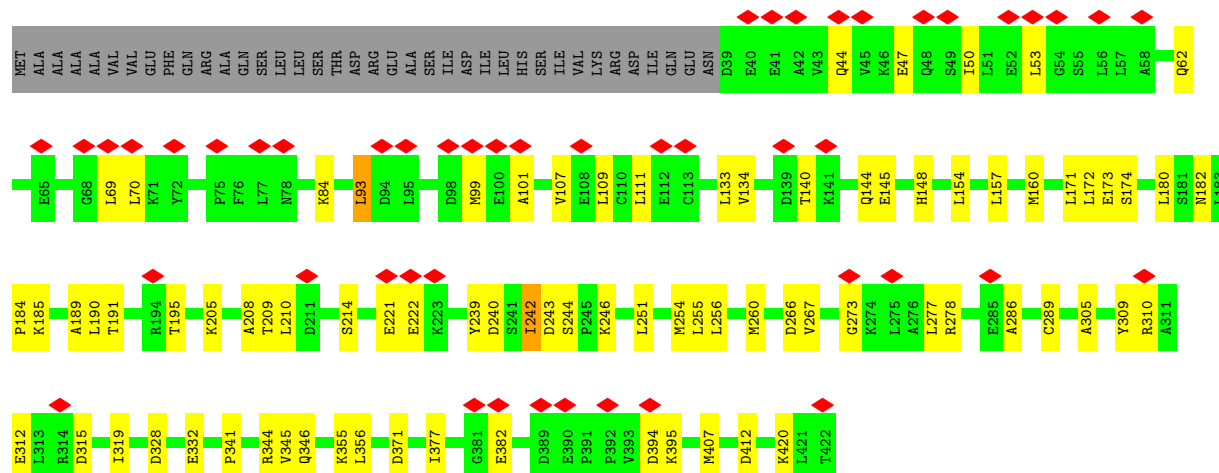




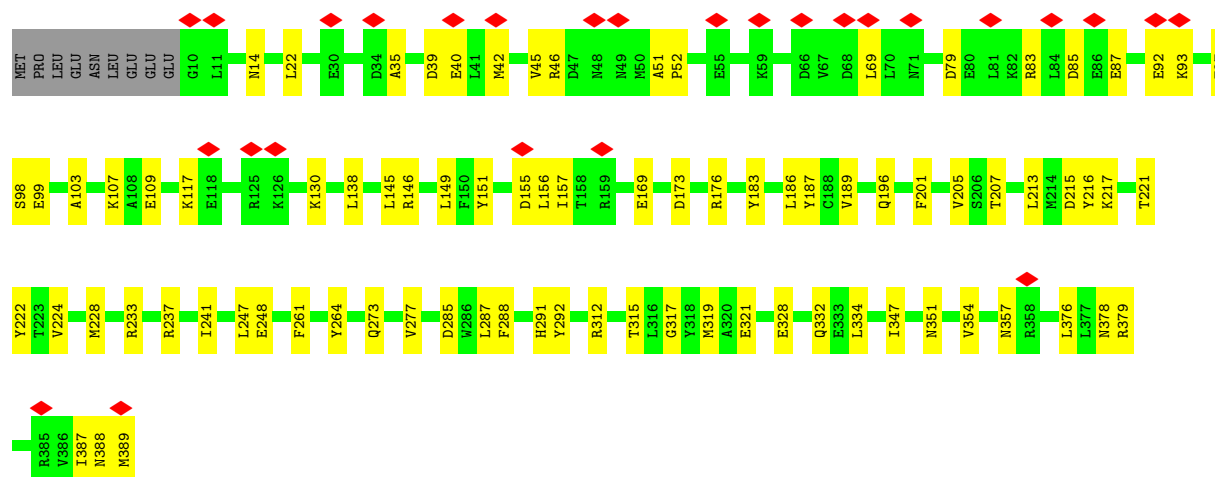
• Molecule 22: 26S proteasome non-ATPase regulatory subunit 12



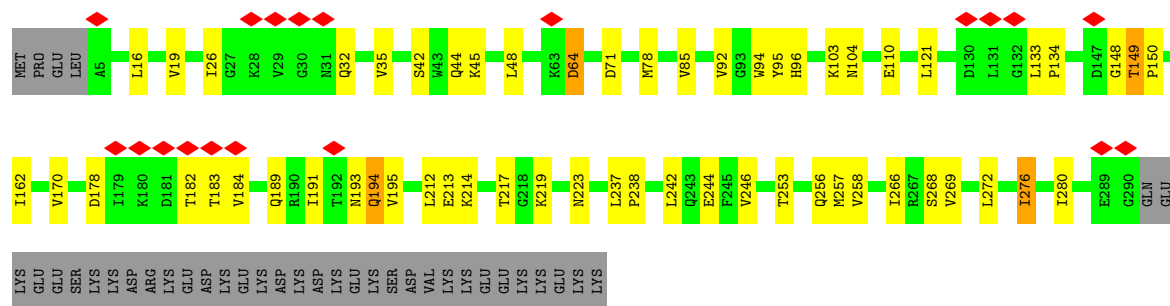
• Molecule 23: 26S proteasome non-ATPase regulatory subunit 11



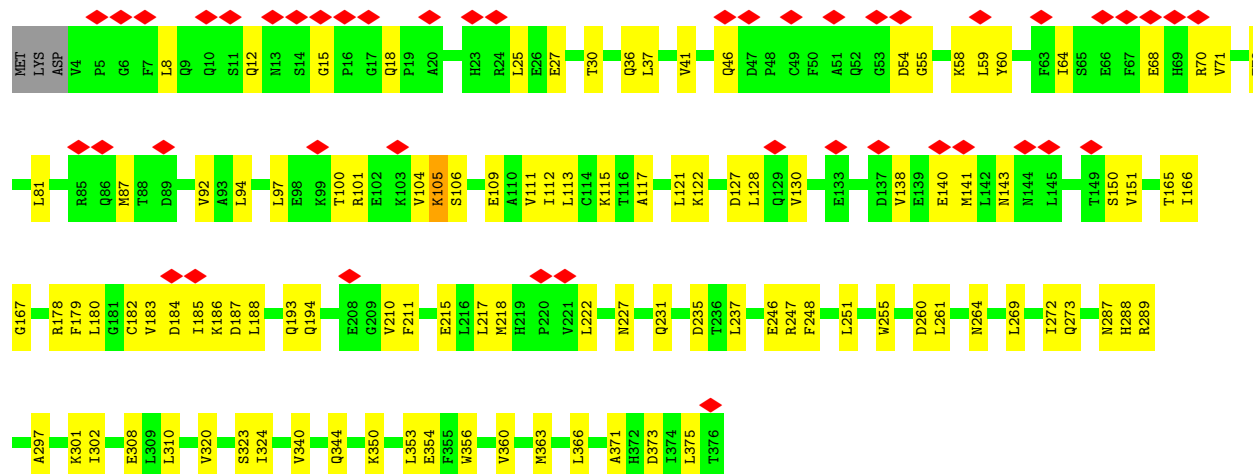
Chain Y: 7% 76% 22%



Chain Z: 6% 70% 17% 12%

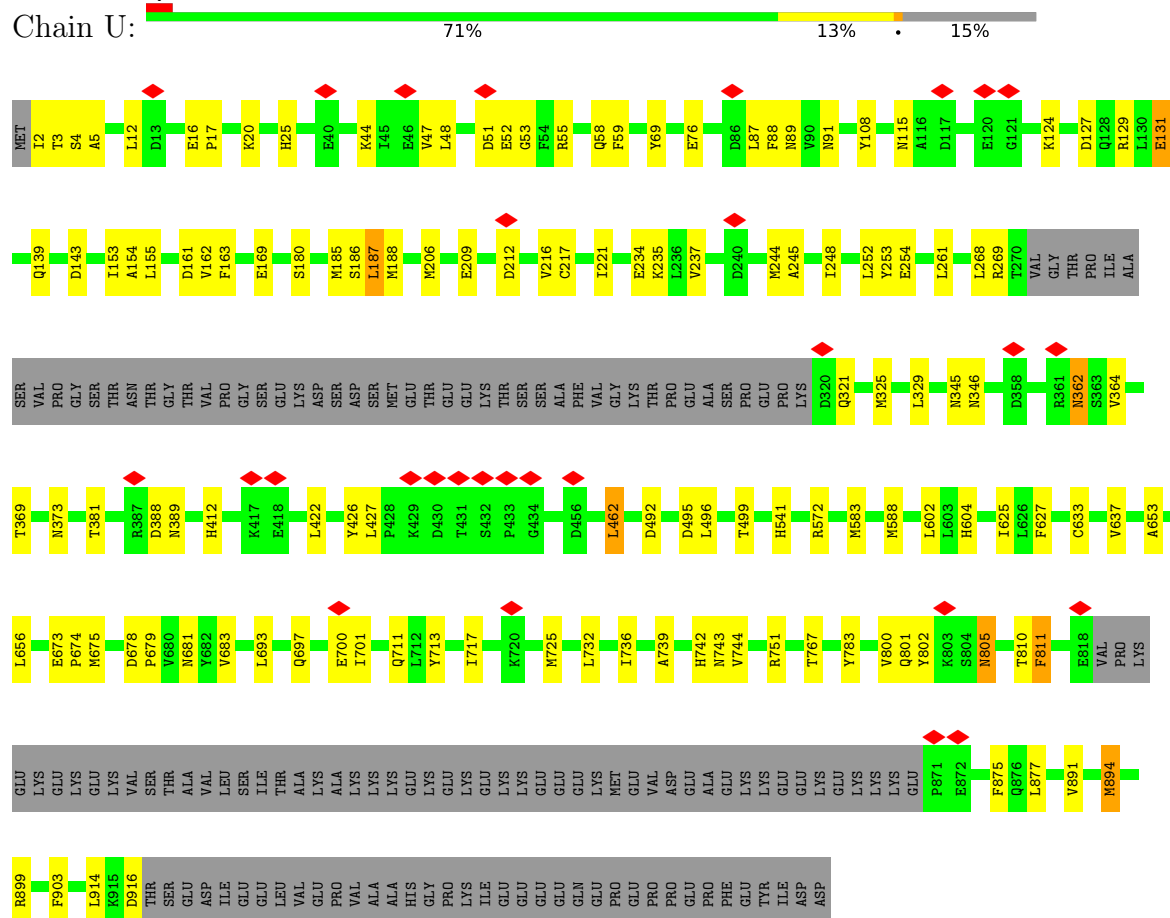


Chain a:

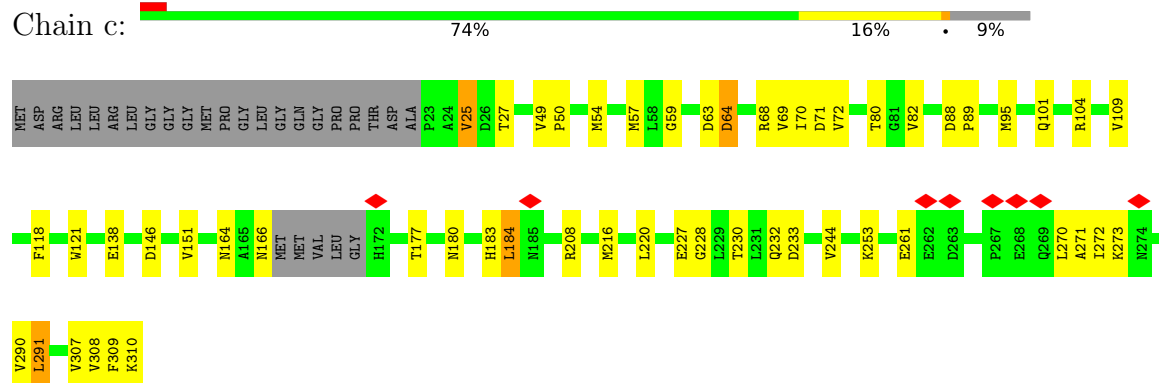


There are no outlier residues recorded for this chain.

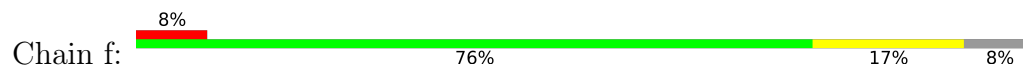
• Molecule 31: 26S proteasome non-ATPase regulatory subunit 1



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



• Molecule 33: 26S proteasome non-ATPase regulatory subunit 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	232000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.841	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.165	Depositor
Map size (Å)	687.36, 687.36, 687.36	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.074, 1.074, 1.074	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LDZ, ADP, ATP, ZN, MG

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	G	0.12	0/1767	0.27	0/2398
1	g	0.10	0/1790	0.22	0/2429
2	H	0.12	0/1701	0.29	0/2318
2	h	0.11	0/1701	0.25	0/2318
3	I	0.12	0/1831	0.29	0/2487
3	i	0.10	0/1815	0.23	0/2466
4	J	0.10	0/1657	0.25	0/2261
4	j	0.10	0/1657	0.25	0/2261
5	K	0.12	0/1694	0.28	0/2301
5	k	0.10	0/1686	0.22	0/2290
6	L	0.11	0/1744	0.26	0/2371
6	l	0.10	0/1741	0.27	0/2367
7	M	0.11	0/1795	0.26	0/2434
7	m	0.10	0/1796	0.22	0/2435
8	N	0.11	0/1495	0.23	0/2026
8	n	0.10	0/1491	0.21	0/2021
9	O	0.10	0/1607	0.24	0/2185
9	o	0.11	0/1603	0.23	0/2180
10	P	0.12	0/1575	0.26	0/2128
10	p	0.12	0/1567	0.25	0/2118
11	Q	0.10	0/1541	0.22	0/2092
11	q	0.11	0/1538	0.26	0/2088
12	R	0.10	0/1535	0.22	0/2080
12	r	0.11	0/1531	0.25	0/2076
13	S	0.10	0/1614	0.24	0/2178
13	s	0.10	0/1617	0.24	0/2182
14	T	0.12	0/1606	0.26	0/2179
14	t	0.11	0/1598	0.25	0/2170
15	A	0.15	0/3110	0.34	0/4196
16	B	0.15	0/3120	0.35	0/4210
17	C	0.15	0/3112	0.34	0/4182
18	D	0.15	0/3089	0.33	0/4168

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	E	0.14	0/3146	0.26	0/4233
20	F	0.13	0/3292	0.27	0/4435
21	V	0.14	0/3662	0.37	2/4946 (0.0%)
22	W	0.13	0/3636	0.25	0/4891
23	X	0.14	0/3084	0.34	0/4157
24	Y	0.14	0/3185	0.30	0/4290
25	Z	0.15	0/2324	0.31	0/3150
26	a	0.14	0/3053	0.33	0/4133
27	b	0.14	0/1478	0.33	0/2001
28	d	0.15	0/2223	0.34	0/3007
29	e	0.12	0/398	0.31	0/542
31	U	0.15	0/6458	0.30	0/8740
32	c	0.15	0/2274	0.31	0/3072
33	f	0.14	0/6569	0.32	0/8893
34	z	0.11	0/928	0.25	0/1241
All	All	0.13	0/104434	0.29	2/141326 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	V	494	MET	CA-C-N	10.40	137.66	122.99
21	V	494	MET	C-N-CA	10.40	137.66	122.99

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	G	1738	1656	1656	17	0
1	g	1758	1687	1687	4	0
2	H	1662	1590	1590	18	0
2	h	1662	1590	1590	12	0
3	I	1802	1741	1741	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	i	1786	1717	1717	5	0
4	J	1633	1518	1518	7	0
4	j	1633	1518	1518	10	0
5	K	1667	1597	1596	11	0
5	k	1660	1589	1589	6	0
6	L	1710	1649	1649	13	0
6	l	1707	1645	1645	9	0
7	M	1760	1680	1680	10	0
7	m	1761	1683	1683	7	0
8	N	1469	1422	1422	10	0
8	n	1465	1416	1416	10	0
9	O	1580	1559	1559	12	0
9	o	1576	1555	1555	12	0
10	P	1546	1550	1552	7	0
10	p	1538	1543	1545	9	0
11	Q	1509	1477	1477	9	0
11	q	1506	1475	1475	3	0
12	R	1504	1449	1449	12	0
12	r	1500	1438	1438	15	0
13	S	1584	1579	1579	7	0
13	s	1587	1581	1581	1	0
14	T	1576	1526	1528	6	0
14	t	1568	1511	1513	4	0
15	A	3060	3106	3106	61	0
16	B	3076	3053	3128	103	0
17	C	3071	3193	3193	69	0
18	D	3039	3075	3075	49	0
19	E	3098	3150	3174	45	0
20	F	3251	3318	3318	46	0
21	V	3592	3647	3647	66	0
22	W	3588	0	3704	254	0
23	X	3040	3134	3134	70	0
24	Y	3127	3133	3133	56	0
25	Z	2281	2312	2312	50	0
26	a	2995	3012	3012	84	0
27	b	1458	1505	1505	37	0
28	d	2177	2189	2189	55	0
29	e	389	298	298	10	0
30	v	60	0	15	0	0
31	U	6344	6370	6374	95	0
32	c	2232	2241	2242	42	0
33	f	6460	6486	6487	112	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	z	921	983	983	13	0
35	N	34	41	41	2	0
35	O	34	41	41	2	0
35	R	34	41	41	4	0
35	n	34	41	41	5	0
35	o	34	41	41	2	0
35	r	34	41	41	1	0
36	A	31	12	12	1	0
36	B	31	12	12	1	0
36	D	31	12	12	0	0
36	F	31	12	12	0	0
37	A	1	0	0	0	0
37	B	1	0	0	0	0
37	D	1	0	0	0	0
37	F	1	0	0	0	0
38	E	27	12	12	2	0
39	c	1	0	0	0	0
All	All	103066	98452	102283	1442	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 7.

All (1442) 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)
22:W:47:LEU:HD22	22:W:70:VAL:HG22	1.41	0.98
22:W:67:LEU:HD12	22:W:104:MET:HE3	1.50	0.92
16:B:434:THR:HB	16:B:435:PRO:HD3	1.52	0.91
22:W:115:ILE:HD12	22:W:116:THR:H	1.35	0.91
22:W:264:GLN:HG2	22:W:299:ILE:HD11	1.53	0.90
28:d:282:ILE:HG21	28:d:315:TYR:HA	1.53	0.90
22:W:33:LYS:HA	22:W:36:LYS:HE2	1.54	0.90
22:W:346:GLU:OE2	22:W:346:GLU:N	2.07	0.87
8:N:2:THR:OG1	35:N:301:LDZ:O33	1.94	0.85
33:f:423:ASP:OD1	34:z:403:ARG:NH1	2.09	0.85
22:W:301:LYS:HD3	22:W:327:GLU:HG2	1.57	0.84
1:G:19:GLU:N	1:G:19:GLU:OE1	2.12	0.83
20:F:279:ALA:HB1	20:F:280:PRO:HD2	1.60	0.83
1:g:158:GLY:O	2:h:83:ARG:NH2	2.12	0.82
21:V:139:MET:HE3	21:V:139:MET:HA	1.60	0.82
4:J:140:GLY:O	4:J:213:ARG:NH1	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:452:ILE:HG22	22:W:453:HIS:CD2	2.14	0.82
24:Y:155:ASP:OD1	24:Y:156:LEU:N	2.12	0.81
22:W:234:ASP:HB3	22:W:239:SER:HB2	1.61	0.81
15:A:207:GLU:N	15:A:207:GLU:OE2	2.13	0.81
1:G:120:ASP:OD1	2:H:83:ARG:NH1	2.14	0.81
31:U:221:ILE:HD11	31:U:252:LEU:HD23	1.63	0.81
1:g:17:SER:OG	1:g:19:GLU:OE2	1.98	0.80
33:f:245:ASN:OD1	33:f:246:SER:N	2.15	0.80
33:f:315:GLU:OE1	33:f:315:GLU:N	2.14	0.80
22:W:201:ARG:HG2	22:W:201:ARG:HH11	1.47	0.79
28:d:125:GLU:OE2	28:d:125:GLU:N	2.16	0.79
9:o:2:THR:N	9:o:170:SER:HG	1.80	0.79
22:W:370:TYR:OH	26:a:308:GLU:OE2	2.01	0.79
15:A:349:GLU:OE1	15:A:349:GLU:N	2.15	0.79
26:a:55:GLY:O	26:a:58:LYS:NZ	2.14	0.79
22:W:64:SER:O	22:W:68:VAL:HG12	1.83	0.78
31:U:76:GLU:OE2	31:U:76:GLU:N	2.16	0.78
17:C:268:GLU:N	17:C:268:GLU:OE1	2.17	0.78
22:W:41:GLN:O	22:W:44:ILE:HG13	1.83	0.77
22:W:78:LYS:N	22:W:78:LYS:HE2	1.99	0.77
31:U:744:VAL:HG21	31:U:783:TYR:HB3	1.67	0.77
33:f:791:VAL:HG12	33:f:823:ALA:HB1	1.67	0.77
15:A:375:ARG:NE	15:A:375:ARG:O	2.18	0.77
12:R:2:THR:N	12:R:131:SER:HG	1.83	0.76
17:C:240:GLU:OE1	17:C:241:HIS:ND1	2.19	0.76
22:W:29:PRO:O	22:W:33:LYS:HG2	1.85	0.76
33:f:222:ASP:OD1	33:f:223:GLU:N	2.19	0.76
10:p:143:GLU:N	10:p:143:GLU:OE2	2.16	0.76
32:c:71:ASP:OD1	32:c:72:VAL:N	2.19	0.76
22:W:67:LEU:HD13	22:W:90:LEU:HD13	1.66	0.76
2:H:34:SER:OG	2:H:76:SER:OG	2.03	0.75
22:W:46:THR:O	22:W:50:LEU:HG	1.87	0.75
25:Z:193:ASN:OD1	25:Z:194:GLN:NE2	2.19	0.75
33:f:316:ASP:OD1	33:f:317:LEU:N	2.18	0.75
22:W:47:LEU:HD13	22:W:70:VAL:HG21	1.68	0.75
19:E:342:ASP:OD1	20:F:345:SER:OG	2.03	0.75
17:C:203:VAL:O	17:C:207:THR:HG22	1.86	0.75
22:W:450:GLU:O	22:W:454:ASN:HB2	1.87	0.74
1:g:120:ASP:OD1	2:h:83:ARG:NH1	2.19	0.74
22:W:67:LEU:CD1	22:W:90:LEU:HD13	2.17	0.74
22:W:141:GLU:OE1	22:W:141:GLU:N	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:174:TYR:O	22:W:182:ARG:NH1	2.20	0.74
21:V:330:LYS:NZ	21:V:389:ASP:OD2	2.19	0.74
22:W:239:SER:HB3	22:W:242:SER:OG	1.88	0.74
21:V:463:MET:SD	21:V:463:MET:N	2.61	0.73
31:U:58:GLN:HB2	31:U:87:LEU:HD12	1.70	0.73
33:f:665:GLU:N	33:f:665:GLU:OE1	2.21	0.73
34:z:32:SER:N	34:z:92:ASP:OD1	2.21	0.73
1:g:174:GLU:N	1:g:174:GLU:OE2	2.22	0.73
23:X:256:LEU:HD22	23:X:319:ILE:HD13	1.71	0.73
22:W:369:TYR:O	22:W:370:TYR:HB2	1.87	0.72
18:D:148:ASP:OD1	18:D:150:SER:N	2.22	0.72
22:W:40:LEU:O	22:W:44:ILE:HG23	1.89	0.72
22:W:244:CYS:O	22:W:248:ARG:HG3	1.89	0.72
4:J:40:ILE:HD11	4:J:210:VAL:HG13	1.70	0.72
22:W:33:LYS:HD3	22:W:36:LYS:CE	2.19	0.72
26:a:104:VAL:O	26:a:106:SER:N	2.22	0.72
22:W:168:GLU:HA	22:W:168:GLU:OE1	1.90	0.71
32:c:244:VAL:HG11	32:c:291:LEU:HD13	1.72	0.71
33:f:157:GLU:N	33:f:157:GLU:OE1	2.21	0.71
2:H:34:SER:HG	2:H:76:SER:HG	1.38	0.71
15:A:182:GLU:N	15:A:182:GLU:OE2	2.20	0.71
23:X:62:GLN:N	23:X:62:GLN:OE1	2.24	0.71
26:a:46:GLN:N	26:a:46:GLN:OE1	2.23	0.71
33:f:237:VAL:HG21	33:f:249:LEU:HG	1.71	0.71
22:W:32:ALA:O	22:W:36:LYS:HG2	1.91	0.71
22:W:345:GLU:HG3	22:W:346:GLU:OE2	1.91	0.71
26:a:141:MET:SD	26:a:141:MET:N	2.63	0.71
22:W:25:ASP:OD1	22:W:65:ARG:NH2	2.24	0.70
26:a:60:TYR:CZ	26:a:64:ILE:HD11	2.25	0.70
22:W:43:VAL:O	22:W:47:LEU:HG	1.90	0.70
22:W:51:GLU:HB2	22:W:66:ILE:HG21	1.72	0.70
31:U:161:ASP:OD1	31:U:162:VAL:N	2.24	0.70
9:o:2:THR:OG1	35:o:301:LDZ:O33	2.06	0.70
22:W:60:MET:HA	22:W:97:LEU:HD12	1.72	0.70
22:W:452:ILE:HG22	22:W:453:HIS:HD2	1.55	0.70
31:U:588:MET:HA	31:U:588:MET:HE2	1.74	0.70
17:C:381:GLU:N	17:C:381:GLU:OE1	2.23	0.70
16:B:278:ALA:HB1	16:B:279:PRO:CD	2.22	0.70
24:Y:334:LEU:HB3	24:Y:347:ILE:HD11	1.74	0.70
8:n:2:THR:OG1	35:n:301:LDZ:O33	2.06	0.70
33:f:177:GLU:OE1	33:f:177:GLU:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:152:ASN:OD1	7:M:85:ARG:NH2	2.25	0.69
22:W:346:GLU:HB3	22:W:350:ARG:NH2	2.07	0.69
26:a:36:GLN:NE2	27:b:146:GLU:OE1	2.26	0.69
26:a:344:GLN:N	26:a:344:GLN:OE1	2.25	0.69
16:B:429:LYS:C	16:B:430:LYS:HD2	2.17	0.69
32:c:261:GLU:OE1	32:c:261:GLU:N	2.26	0.69
22:W:50:LEU:O	22:W:54:THR:HG23	1.93	0.69
26:a:122:LYS:HD3	26:a:130:VAL:HG21	1.75	0.68
31:U:139:GLN:NE2	31:U:143:ASP:OD1	2.26	0.68
31:U:237:VAL:HG21	31:U:321:GLN:OE1	1.93	0.68
2:H:64:VAL:O	2:H:219:ARG:NH1	2.25	0.68
18:D:380:GLN:NE2	19:E:165:ILE:O	2.26	0.68
22:W:29:PRO:O	22:W:33:LYS:NZ	2.26	0.68
18:D:274:ARG:NH1	19:E:244:SER:O	2.26	0.68
22:W:260:SER:HA	22:W:263:TRP:CD1	2.29	0.68
27:b:61:LEU:O	27:b:74:LYS:NZ	2.26	0.68
15:A:41:TYR:OH	33:f:210:GLU:OE2	2.08	0.68
16:B:430:LYS:HA	16:B:430:LYS:HE3	1.75	0.68
18:D:101:ALA:HB2	18:D:115:ILE:HD11	1.76	0.68
23:X:221:GLU:N	23:X:221:GLU:OE1	2.27	0.68
23:X:382:GLU:N	23:X:382:GLU:OE1	2.27	0.68
23:X:312:GLU:OE1	23:X:312:GLU:N	2.27	0.68
27:b:101:GLN:NE2	32:c:101:GLN:OE1	2.27	0.67
18:D:362:ASP:OD1	18:D:363:TYR:N	2.28	0.67
21:V:345:ARG:NH2	29:e:46:ASP:OD2	2.28	0.67
33:f:173:LEU:HD11	33:f:177:GLU:HB2	1.76	0.67
33:f:885:GLU:N	33:f:885:GLU:OE1	2.27	0.67
33:f:729:MET:HG2	33:f:741:LEU:HD11	1.75	0.67
13:S:148:LEU:HD23	13:S:178:VAL:HG12	1.77	0.67
21:V:320:THR:HG22	29:e:18:GLU:OE1	1.95	0.67
33:f:313:GLU:N	33:f:313:GLU:OE2	2.27	0.67
15:A:73:ALA:O	15:A:78:TRP:NE1	2.27	0.67
23:X:99:MET:SD	23:X:101:ALA:N	2.68	0.67
26:a:227:ASN:O	26:a:231:GLN:NE2	2.27	0.67
22:W:47:LEU:HD13	22:W:70:VAL:CG2	2.24	0.67
12:R:36:ILE:HD11	12:R:46:MET:SD	2.35	0.66
22:W:117:ASP:OD1	22:W:119:PRO:HD2	1.95	0.66
22:W:84:ASN:O	22:W:87:ILE:HG22	1.94	0.66
22:W:452:ILE:O	22:W:456:GLN:NE2	2.28	0.66
28:d:282:ILE:HG23	28:d:283:LEU:H	1.61	0.66
22:W:19:ASP:OD1	22:W:21:SER:N	2.20	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:217:LYS:O	24:Y:221:THR:HG23	1.96	0.66
26:a:140:GLU:O	26:a:143:ASN:ND2	2.29	0.66
31:U:206:MET:HE3	31:U:216:VAL:HG21	1.77	0.66
31:U:206:MET:CE	31:U:216:VAL:HG21	2.25	0.66
33:f:146:GLY:O	33:f:148:GLN:NE2	2.29	0.65
31:U:155:LEU:HD22	31:U:188:MET:HE1	1.78	0.65
19:E:71:VAL:HG11	19:E:100:LEU:HD21	1.78	0.65
21:V:108:LEU:HD22	21:V:113:LEU:HD12	1.77	0.65
16:B:278:ALA:HB1	16:B:279:PRO:HD2	1.77	0.65
28:d:258:PHE:CE2	28:d:262:ILE:HD11	2.31	0.65
36:A:501:ATP:O2G	16:B:346:ARG:NH2	2.30	0.65
18:D:179:GLU:HG3	18:D:183:LEU:HD22	1.78	0.65
31:U:20:LYS:HD3	31:U:48:LEU:HD21	1.79	0.65
16:B:412:MET:HE2	17:C:177:ALA:HB3	1.79	0.64
27:b:97:LEU:HD13	27:b:107:MET:HE3	1.79	0.64
16:B:49:LEU:HD21	33:f:669:GLU:HB2	1.79	0.64
18:D:98:GLN:O	18:D:99:ASN:ND2	2.30	0.64
28:d:128:PHE:O	28:d:174:TYR:OH	2.07	0.64
20:F:286:ASP:OD1	20:F:287:GLU:N	2.29	0.64
28:d:236:LEU:HD21	28:d:267:ILE:HG13	1.80	0.64
22:W:307:LYS:HA	22:W:310:THR:HG22	1.79	0.64
15:A:101:ILE:HG23	15:A:137:GLY:H	1.62	0.64
33:f:761:MET:HA	33:f:761:MET:HE3	1.78	0.64
4:J:40:ILE:HD11	4:J:210:VAL:CG1	2.28	0.64
18:D:154:LEU:HD13	18:D:154:LEU:O	1.97	0.64
22:W:187:LEU:HD21	22:W:226:TYR:HB2	1.79	0.64
17:C:184:LYS:NZ	17:C:280:LEU:O	2.31	0.64
27:b:10:VAL:HG13	27:b:29:GLN:OE1	1.99	0.63
20:F:366:MET:O	20:F:370:SER:OG	2.14	0.63
22:W:332:SER:HB2	22:W:334:GLU:OE2	1.98	0.63
1:G:103:TYR:O	9:O:82:ARG:NH1	2.32	0.63
31:U:206:MET:HE2	31:U:206:MET:HA	1.79	0.63
18:D:309:MET:HE3	18:D:327:LEU:HD11	1.79	0.63
19:E:98:VAL:HG11	19:E:107:ILE:HG12	1.80	0.63
20:F:389:ASP:OD1	20:F:390:ASP:N	2.30	0.63
17:C:242:ALA:HB3	17:C:243:PRO:HD3	1.80	0.63
21:V:108:LEU:HD22	21:V:113:LEU:CD1	2.28	0.63
22:W:146:THR:HB	22:W:169:LEU:HD11	1.79	0.63
23:X:243:ASP:OD1	23:X:278:ARG:NH1	2.30	0.63
22:W:33:LYS:HA	22:W:36:LYS:CE	2.26	0.63
26:a:363:MET:CE	32:c:307:VAL:HG11	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:70:THR:OG1	17:C:81:ASP:OD2	2.17	0.63
22:W:115:ILE:HD12	22:W:116:THR:N	2.13	0.63
28:d:282:ILE:HG23	28:d:283:LEU:N	2.14	0.63
21:V:407:VAL:HG12	21:V:447:ILE:CD1	2.29	0.63
22:W:90:LEU:HB2	22:W:104:MET:HE1	1.79	0.63
27:b:118:GLU:OE1	27:b:118:GLU:N	2.32	0.62
23:X:222:GLU:OE1	23:X:222:GLU:N	2.32	0.62
31:U:345:ASN:O	31:U:743:ASN:ND2	2.32	0.62
22:W:183:VAL:HG21	22:W:213:PHE:CD2	2.34	0.62
19:E:385:ASP:OD1	19:E:386:TYR:N	2.33	0.62
16:B:360:THR:O	16:B:364:ILE:HD12	2.00	0.62
17:C:266:ASP:O	17:C:271:ARG:NH1	2.33	0.62
19:E:309:ARG:NH1	19:E:332:VAL:O	2.32	0.62
3:I:187:LYS:H	3:I:187:LYS:HE2	1.65	0.62
9:O:2:THR:N	9:O:170:SER:HG	1.98	0.62
22:W:289:ARG:HB2	22:W:289:ARG:CZ	2.30	0.62
31:U:701:ILE:HD13	31:U:810:THR:HA	1.81	0.62
18:D:181:VAL:HG23	18:D:182:GLU:OE1	1.99	0.62
27:b:33:VAL:HG21	27:b:75:LEU:HD11	1.80	0.62
33:f:388:ASP:OD1	33:f:389:LYS:N	2.32	0.62
2:H:8:SER:OG	2:H:122:GLN:O	2.18	0.61
9:O:192:VAL:O	9:O:192:VAL:HG13	2.00	0.61
17:C:295:THR:HG21	17:C:301:LEU:HD12	1.81	0.61
22:W:44:ILE:HA	22:W:47:LEU:CG	2.30	0.61
22:W:206:SER:CB	22:W:230:MET:HE3	2.29	0.61
22:W:260:SER:HA	22:W:263:TRP:NE1	2.15	0.61
26:a:112:ILE:HD12	26:a:112:ILE:H	1.65	0.61
31:U:801:GLN:HB3	31:U:877:LEU:HD12	1.82	0.61
22:W:117:ASP:OD2	22:W:120:ILE:HD13	2.00	0.61
22:W:193:CYS:HA	22:W:196:VAL:HG12	1.82	0.61
16:B:407:LEU:HD21	17:C:175:PHE:CZ	2.36	0.61
22:W:84:ASN:OD1	22:W:123:ARG:NH2	2.32	0.61
4:j:140:GLY:O	4:j:213:ARG:NH1	2.33	0.61
10:p:202:ARG:NH2	10:p:204:ASP:OD2	2.33	0.61
23:X:70:LEU:HD23	23:X:109:LEU:HD21	1.83	0.61
23:X:208:ALA:HB1	23:X:239:TYR:CD2	2.35	0.61
23:X:256:LEU:HD11	23:X:260:MET:HE1	1.80	0.61
28:d:297:LYS:O	28:d:300:THR:OG1	2.18	0.61
22:W:179:LYS:HD2	22:W:182:ARG:HH21	1.65	0.61
26:a:68:GLU:OE2	26:a:71:VAL:N	2.34	0.61
33:f:145:VAL:O	33:f:145:VAL:HG13	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:136:LEU:HD12	16:B:160:ILE:HG22	1.82	0.61
17:C:148:TYR:HA	17:C:151:ILE:HG22	1.82	0.61
26:a:12:GLN:O	26:a:18:GLN:NE2	2.34	0.61
10:p:35:THR:HG22	10:p:37:ASP:H	1.66	0.61
10:p:192:ASP:OD1	10:p:192:ASP:N	2.34	0.61
31:U:212:ASP:O	31:U:216:VAL:HG23	2.01	0.61
22:W:48:LEU:HD21	22:W:93:ARG:CZ	2.31	0.60
5:k:18:GLU:OE1	5:k:18:GLU:N	2.34	0.60
15:A:81:ALA:HB1	16:B:138:PHE:CD2	2.35	0.60
18:D:258:ALA:HB3	18:D:259:PRO:HD3	1.83	0.60
31:U:209:GLU:N	31:U:209:GLU:OE1	2.33	0.60
16:B:206:THR:HG22	16:B:207:HIS:ND1	2.16	0.60
21:V:233:ALA:O	21:V:237:THR:HG23	2.00	0.60
26:a:127:ASP:OD1	26:a:128:LEU:N	2.34	0.60
26:a:140:GLU:N	26:a:140:GLU:OE1	2.34	0.60
22:W:33:LYS:HD3	22:W:36:LYS:NZ	2.16	0.60
22:W:366:MET:O	22:W:370:TYR:HB2	2.02	0.60
22:W:455:LEU:HD22	25:Z:103:LYS:CD	2.30	0.60
2:h:28:VAL:HG13	2:h:76:SER:O	2.01	0.60
18:D:192:LYS:HD2	18:D:192:LYS:C	2.26	0.60
22:W:339:ASP:OD1	22:W:339:ASP:N	2.34	0.60
5:K:18:GLU:OE1	5:K:18:GLU:N	2.35	0.60
16:B:166:ASP:OD1	16:B:167:THR:N	2.34	0.60
31:U:541:HIS:ND1	32:c:63:ASP:OD2	2.33	0.60
33:f:479:LEU:CD2	33:f:517:VAL:HG21	2.31	0.60
22:W:185:PHE:O	22:W:189:GLN:HG3	2.02	0.60
35:n:301:LDZ:H3	35:n:301:LDZ:H38	1.84	0.60
24:Y:215:ASP:OD1	24:Y:216:TYR:N	2.35	0.60
11:q:13:VAL:HG11	11:q:105:ALA:HB1	1.83	0.59
16:B:58:CYS:SG	33:f:232:TYR:OH	2.46	0.59
20:F:104:GLN:OE1	20:F:104:GLN:N	2.35	0.59
22:W:47:LEU:CD2	22:W:70:VAL:HG22	2.24	0.59
33:f:574:GLU:N	33:f:574:GLU:OE1	2.34	0.59
14:T:74:GLU:OE2	14:T:83:TYR:N	2.35	0.59
22:W:33:LYS:HD3	22:W:36:LYS:HE2	1.83	0.59
22:W:435:LEU:HD21	26:a:356:TRP:HH2	1.66	0.59
23:X:371:ASP:OD2	24:Y:233:ARG:NH1	2.35	0.59
24:Y:201:PHE:O	24:Y:205:VAL:HG23	2.03	0.59
2:h:73:LEU:HD23	2:h:86:VAL:HG22	1.83	0.59
17:C:252:ASP:OD1	17:C:253:SER:N	2.35	0.59
22:W:371:THR:HG23	26:a:323:SER:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:157:LEU:O	23:X:160:MET:C	2.46	0.59
4:J:195:LEU:O	4:J:199:VAL:HG12	2.02	0.59
27:b:181:ASP:OD1	27:b:182:ALA:N	2.36	0.59
6:L:65:HIS:NE2	6:L:223:ILE:HD12	2.17	0.59
22:W:55:ARG:HD2	22:W:94:ARG:O	2.02	0.59
22:W:90:LEU:HD23	22:W:93:ARG:HD2	1.85	0.59
22:W:314:LEU:CD1	22:W:381:LEU:HD22	2.33	0.59
21:V:224:LEU:HD22	21:V:257:ASN:OD1	2.02	0.59
22:W:250:ILE:O	22:W:253:THR:HG23	2.03	0.59
23:X:145:GLU:O	23:X:148:HIS:ND1	2.29	0.59
2:h:8:SER:OG	2:h:122:GLN:O	2.20	0.58
22:W:206:SER:HB2	22:W:230:MET:HE3	1.84	0.58
16:B:377:ASP:OD1	16:B:377:ASP:N	2.36	0.58
18:D:407:ILE:O	18:D:407:ILE:CG2	2.51	0.58
22:W:67:LEU:HD11	22:W:90:LEU:HB3	1.84	0.58
31:U:802:TYR:O	31:U:877:LEU:HD13	2.01	0.58
31:U:52:GLU:N	31:U:52:GLU:OE1	2.36	0.58
33:f:422:VAL:HG21	33:f:457:ASN:OD1	2.04	0.58
15:A:86:THR:HG21	16:B:102:LEU:HD13	1.85	0.58
19:E:205:ASP:OD1	19:E:206:LYS:N	2.37	0.58
25:Z:96:HIS:HD2	25:Z:121:LEU:HD11	1.69	0.58
28:d:269:ASP:OD1	28:d:306:ARG:NH2	2.36	0.58
29:e:51:ASP:O	29:e:54:ASN:N	2.36	0.58
15:A:280:ILE:C	15:A:280:ILE:HD12	2.28	0.58
22:W:40:LEU:O	22:W:43:VAL:HG12	2.02	0.58
31:U:17:PRO:O	31:U:55:ARG:NH2	2.36	0.58
10:P:64:GLN:OE1	11:Q:86:ARG:NH2	2.37	0.58
31:U:637:VAL:HG21	31:U:656:LEU:HG	1.85	0.58
26:a:81:LEU:HD21	26:a:117:ALA:HB2	1.86	0.58
33:f:741:LEU:HD12	33:f:744:MET:HE2	1.86	0.58
15:A:101:ILE:HG21	15:A:135:GLU:O	2.03	0.58
17:C:24:TYR:CE1	31:U:153:ILE:HD11	2.39	0.58
22:W:271:VAL:O	22:W:274:VAL:HG12	2.04	0.58
22:W:432:LEU:HD22	32:c:309:PHE:CD2	2.38	0.58
19:E:148:VAL:HG11	19:E:170:CYS:SG	2.44	0.57
22:W:33:LYS:HD3	22:W:36:LYS:HZ3	1.69	0.57
27:b:22:LEU:CD2	27:b:179:LEU:HD22	2.34	0.57
31:U:495:ASP:O	31:U:499:THR:HG23	2.04	0.57
33:f:312:GLU:N	33:f:312:GLU:OE1	2.36	0.57
15:A:67:GLU:N	15:A:67:GLU:OE1	2.37	0.57
17:C:184:LYS:NZ	17:C:283:PHE:O	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:f:646:MET:SD	33:f:646:MET:N	2.77	0.57
33:f:333:LEU:HD22	33:f:829:MET:HE2	1.86	0.57
3:I:35:LEU:HD11	3:I:175:LEU:HD11	1.86	0.57
5:k:117:SER:OG	6:l:82:ARG:NH2	2.36	0.57
18:D:173:GLN:N	18:D:173:GLN:OE1	2.38	0.57
20:F:143:GLU:OE1	20:F:143:GLU:N	2.35	0.57
22:W:45:GLU:OE1	22:W:45:GLU:HA	2.04	0.57
22:W:383:ASP:O	22:W:384:LEU:HD23	2.04	0.57
26:a:363:MET:SD	26:a:366:LEU:HD23	2.44	0.57
33:f:430:ASP:OD1	33:f:431:LYS:N	2.37	0.57
16:B:273:VAL:HG23	16:B:273:VAL:O	2.05	0.57
17:C:294:ALA:O	17:C:295:THR:HG23	2.05	0.57
21:V:365:GLN:O	21:V:369:THR:HG22	2.04	0.57
22:W:455:LEU:HD22	25:Z:103:LYS:HD3	1.86	0.57
31:U:254:GLU:OE1	31:U:751:ARG:NE	2.37	0.57
31:U:346:ASN:OD1	31:U:346:ASN:O	2.22	0.57
18:D:188:PHE:HD2	18:D:188:PHE:O	1.88	0.57
23:X:256:LEU:HD22	23:X:319:ILE:CD1	2.33	0.57
31:U:381:THR:HG22	31:U:381:THR:O	2.04	0.57
22:W:424:LEU:HD11	25:Z:244:GLU:OE1	2.05	0.56
26:a:186:LYS:HE2	26:a:186:LYS:HA	1.87	0.56
27:b:4:GLU:N	27:b:47:ASN:OD1	2.34	0.56
5:K:19:GLY:O	20:F:438:TYR:OH	2.19	0.56
16:B:293:LYS:O	16:B:293:LYS:NZ	2.33	0.56
27:b:151:GLU:OE2	27:b:152:LYS:NZ	2.38	0.56
28:d:87:VAL:HG21	28:d:125:GLU:HG3	1.87	0.56
2:H:227:ASP:O	23:X:84:LYS:NZ	2.29	0.56
15:A:217:PRO:O	15:A:220:THR:OG1	2.23	0.56
16:B:115:ILE:HG22	16:B:117:ASP:H	1.70	0.56
22:W:214:PHE:HA	22:W:219:THR:OG1	2.05	0.56
31:U:633:CYS:O	31:U:637:VAL:HG22	2.05	0.56
33:f:842:VAL:N	33:f:870:THR:OG1	2.39	0.56
9:O:165:PHE:O	13:S:38:ARG:NH2	2.38	0.56
12:r:81:SER:OG	12:r:121:ARG:NE	2.36	0.56
21:V:121:PHE:O	21:V:128:ARG:NH2	2.39	0.56
22:W:223:LYS:CE	22:W:253:THR:HG22	2.35	0.56
16:B:47:SER:O	16:B:47:SER:OG	2.24	0.56
25:Z:182:THR:HG22	25:Z:184:VAL:HG23	1.87	0.56
3:I:30:HIS:O	3:I:50:ARG:NH1	2.39	0.56
22:W:138:VAL:HG23	22:W:141:GLU:HB2	1.86	0.56
23:X:190:LEU:HD11	23:X:214:SER:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:f:102:HIS:O	33:f:102:HIS:ND1	2.39	0.56
33:f:333:LEU:HD22	33:f:829:MET:CE	2.35	0.56
21:V:294:ARG:NH1	21:V:390:GLY:O	2.38	0.56
24:Y:186:LEU:HD22	24:Y:287:LEU:CD1	2.36	0.56
24:Y:222:TYR:OH	24:Y:285:ASP:OD1	2.24	0.56
26:a:371:ALA:O	26:a:375:LEU:HD23	2.06	0.56
27:b:25:ARG:NH1	27:b:146:GLU:OE2	2.38	0.56
20:F:185:TYR:CD1	20:F:195:ILE:HD11	2.40	0.56
22:W:247:TYR:HB3	22:W:270:VAL:HG23	1.87	0.56
26:a:183:VAL:HG13	26:a:183:VAL:O	2.06	0.56
26:a:260:ASP:OD1	26:a:261:LEU:N	2.39	0.56
9:o:18:ASP:OD1	9:o:34:LYS:NZ	2.35	0.56
15:A:80:LEU:HD21	33:f:712:LYS:O	2.06	0.56
15:A:81:ALA:HB2	16:B:137:SER:HB2	1.88	0.56
20:F:178:ASP:OD1	20:F:179:GLU:N	2.39	0.56
24:Y:14:ASN:ND2	24:Y:109:GLU:OE2	2.39	0.56
27:b:123:ASP:OD1	27:b:124:LEU:N	2.39	0.56
17:C:323:GLU:OE1	17:C:323:GLU:N	2.38	0.56
18:D:258:ALA:HB3	18:D:259:PRO:CD	2.36	0.56
25:Z:19:VAL:HG22	25:Z:95:TYR:CE1	2.41	0.56
25:Z:212:LEU:HD12	26:a:353:LEU:HD12	1.87	0.56
16:B:175:LYS:HE2	16:B:246:THR:HG23	1.89	0.55
22:W:315:MET:SD	22:W:358:VAL:HG22	2.46	0.55
26:a:360:VAL:HG22	32:c:308:VAL:HG13	1.87	0.55
26:a:60:TYR:CE2	26:a:64:ILE:HD11	2.41	0.55
31:U:58:GLN:CB	31:U:87:LEU:HD12	2.35	0.55
34:z:87:GLU:OE1	34:z:87:GLU:N	2.36	0.55
9:O:105:ASP:N	9:O:105:ASP:OD1	2.40	0.55
25:Z:94:TRP:CE2	25:Z:121:LEU:HD13	2.41	0.55
31:U:725:MET:HE3	31:U:725:MET:HA	1.87	0.55
2:H:188:HIS:CE1	2:H:192:LEU:HD11	2.41	0.55
24:Y:241:ILE:HD11	24:Y:261:PHE:CE2	2.41	0.55
28:d:114:GLU:HA	28:d:114:GLU:OE2	2.07	0.55
22:W:393:LEU:HD22	22:W:413:ILE:HD13	1.88	0.55
31:U:362:ASN:OD1	31:U:362:ASN:N	2.39	0.55
12:r:36:ILE:HD11	12:r:46:MET:SD	2.47	0.55
17:C:275:GLU:HA	17:C:275:GLU:OE1	2.06	0.55
22:W:108:CYS:SG	22:W:124:LEU:HD11	2.47	0.55
22:W:180:LYS:NZ	22:W:222:LEU:HD11	2.20	0.55
24:Y:14:ASN:O	24:Y:146:ARG:NH1	2.34	0.55
33:f:573:ILE:HG21	33:f:599:ALA:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:17:GLU:OE2	22:W:18:VAL:HG22	2.07	0.55
22:W:289:ARG:HB2	22:W:289:ARG:NH1	2.22	0.55
23:X:70:LEU:HD21	23:X:93:LEU:HD22	1.89	0.55
24:Y:87:GLU:OE1	24:Y:103:ALA:HB2	2.07	0.55
33:f:727:PHE:HB2	33:f:761:MET:HE2	1.88	0.55
18:D:407:ILE:O	18:D:407:ILE:HG22	2.07	0.55
22:W:41:GLN:OE1	22:W:41:GLN:N	2.40	0.55
22:W:44:ILE:HA	22:W:47:LEU:HG	1.87	0.55
23:X:182:ASN:HB3	23:X:185:LYS:HD3	1.89	0.55
24:Y:354:VAL:HG12	24:Y:354:VAL:O	2.07	0.55
27:b:76:HIS:O	27:b:77:THR:OG1	2.20	0.55
17:C:266:ASP:OD2	17:C:266:ASP:C	2.50	0.54
21:V:385:LYS:HE2	21:V:385:LYS:HA	1.88	0.54
22:W:112:VAL:HG22	22:W:124:LEU:HG	1.88	0.54
22:W:428:TRP:O	22:W:432:LEU:HG	2.07	0.54
27:b:22:LEU:O	27:b:24:THR:N	2.40	0.54
15:A:101:ILE:HG22	15:A:138:MET:O	2.05	0.54
22:W:133:GLU:OE1	22:W:133:GLU:C	2.50	0.54
26:a:235:ASP:CG	26:a:251:LEU:HD11	2.31	0.54
31:U:185:MET:HE3	31:U:185:MET:HA	1.88	0.54
12:R:2:THR:N	12:R:131:SER:OG	2.38	0.54
16:B:360:THR:HG22	16:B:364:ILE:HD11	1.88	0.54
18:D:157:ASP:OD1	18:D:157:ASP:N	2.39	0.54
18:D:188:PHE:O	18:D:188:PHE:CD2	2.60	0.54
18:D:281:ALA:HB1	19:E:208:ILE:HD12	1.90	0.54
32:c:272:ILE:N	32:c:272:ILE:HD12	2.22	0.54
3:I:51:ASN:OD1	3:I:51:ASN:O	2.25	0.54
10:P:192:ASP:N	10:P:192:ASP:OD1	2.39	0.54
11:Q:13:VAL:HG11	11:Q:105:ALA:HB1	1.88	0.54
26:a:188:LEU:O	26:a:193:GLN:NE2	2.40	0.54
27:b:100:ARG:NH1	27:b:107:MET:SD	2.81	0.54
3:I:68:LEU:O	3:I:69:ASN:ND2	2.40	0.54
24:Y:183:TYR:CE1	24:Y:213:LEU:HD11	2.42	0.54
26:a:15:GLY:N	26:a:18:GLN:OE1	2.41	0.54
33:f:479:LEU:HD22	33:f:517:VAL:HG21	1.88	0.54
7:m:87:LEU:HD12	7:m:133:CYS:SG	2.48	0.54
10:p:112:ASP:OD1	10:p:115:THR:HG22	2.07	0.54
17:C:375:ARG:NH1	17:C:382:ASP:OD2	2.35	0.54
25:Z:133:LEU:HD22	25:Z:134:PRO:HD2	1.89	0.54
29:e:48:VAL:O	29:e:48:VAL:HG13	2.08	0.54
31:U:805:ASN:OD1	31:U:805:ASN:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:4:PRO:O	14:T:100:ARG:NH1	2.39	0.54
17:C:161:ILE:HG21	17:C:199:LEU:HD21	1.90	0.54
17:C:45:LEU:HB3	18:D:61:ILE:HG21	1.90	0.54
38:E:401:ADP:O3B	20:F:344:ARG:NH1	2.41	0.54
20:F:195:ILE:O	20:F:199:VAL:HG13	2.08	0.54
20:F:251:LEU:HD23	20:F:252:ALA:N	2.23	0.54
22:W:241:LEU:HD11	22:W:286:LEU:HD12	1.90	0.54
22:W:280:ASP:C	22:W:280:ASP:OD1	2.50	0.54
22:W:369:TYR:O	22:W:370:TYR:CB	2.54	0.54
16:B:140:ASP:HB3	16:B:143:LEU:HD12	1.89	0.54
18:D:266:GLU:HA	18:D:266:GLU:OE1	2.08	0.54
18:D:413:GLU:OE1	18:D:413:GLU:N	2.41	0.54
19:E:44:GLU:OE2	20:F:76:ASN:ND2	2.40	0.54
20:F:100:ASP:N	20:F:100:ASP:OD1	2.38	0.54
28:d:242:ASN:O	28:d:246:LEU:HG	2.07	0.54
9:o:64:LEU:HD22	9:o:75:PRO:HB3	1.89	0.53
15:A:86:THR:HG23	16:B:136:LEU:HD22	1.89	0.53
22:W:18:VAL:HG23	22:W:20:TYR:HE1	1.73	0.53
31:U:268:LEU:HD21	31:U:325:MET:CE	2.38	0.53
33:f:659:LEU:HD13	33:f:797:LEU:HD21	1.90	0.53
8:n:71:LEU:O	8:n:73:GLU:N	2.42	0.53
22:W:149:LEU:O	22:W:153:LYS:HG2	2.09	0.53
9:O:64:LEU:HD22	9:O:75:PRO:HB3	1.90	0.53
16:B:434:THR:HB	16:B:435:PRO:CD	2.32	0.53
26:a:104:VAL:HG23	26:a:105:LYS:H	1.73	0.53
31:U:899:ARG:NH1	31:U:916:ASP:OD2	2.41	0.53
31:U:186:SER:O	31:U:188:MET:N	2.41	0.53
33:f:352:HIS:ND1	33:f:353:LEU:HD23	2.24	0.53
9:o:98:ALA:HB1	9:o:128:MET:HE3	1.89	0.53
20:F:383:GLU:OE2	20:F:417:HIS:NE2	2.36	0.53
22:W:251:TYR:HB2	22:W:266:ALA:HB1	1.91	0.53
22:W:393:LEU:O	22:W:397:VAL:HG23	2.08	0.53
23:X:242:ILE:HD12	23:X:242:ILE:O	2.07	0.53
26:a:68:GLU:OE2	26:a:70:ARG:N	2.39	0.53
20:F:213:GLU:HA	20:F:213:GLU:OE2	2.08	0.53
21:V:311:ASN:OD1	21:V:314:ARG:NH2	2.42	0.53
22:W:137:TYR:CD1	22:W:138:VAL:HG12	2.44	0.53
16:B:385:MET:HE2	16:B:385:MET:HA	1.90	0.53
17:C:299:ASP:OD1	17:C:300:ILE:N	2.42	0.53
28:d:219:ASP:OD1	28:d:220:ILE:N	2.42	0.53
12:R:3:THR:N	12:R:18:ASP:OD1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:C:242:ALA:HB3	17:C:243:PRO:CD	2.39	0.53
21:V:317:PRO:O	21:V:325:LYS:NZ	2.35	0.53
22:W:137:TYR:CE1	22:W:138:VAL:HG12	2.43	0.53
22:W:196:VAL:O	22:W:196:VAL:HG22	2.09	0.53
22:W:314:LEU:HD13	22:W:381:LEU:HD22	1.90	0.53
23:X:107:VAL:O	23:X:111:LEU:HD23	2.09	0.53
1:G:174:GLU:N	1:G:174:GLU:OE2	2.41	0.53
15:A:81:ALA:HB1	16:B:138:PHE:HD2	1.72	0.53
17:C:140:VAL:HG12	17:C:140:VAL:O	2.09	0.53
20:F:51:GLU:O	20:F:55:MET:HG3	2.09	0.53
22:W:256:ILE:HD13	22:W:262:LYS:HD2	1.91	0.53
2:h:67:ILE:HG21	2:h:109:LEU:HD21	1.91	0.53
22:W:274:VAL:HG22	22:W:287:VAL:HG23	1.90	0.53
23:X:185:LYS:CD	23:X:185:LYS:H	2.22	0.53
11:Q:38:MET:HE1	11:Q:61:GLN:HB2	1.89	0.52
11:q:111:GLU:HA	11:q:111:GLU:OE2	2.09	0.52
17:C:280:LEU:HD21	17:C:311:ILE:HD13	1.90	0.52
22:W:237:GLU:N	22:W:237:GLU:OE1	2.41	0.52
23:X:255:LEU:HD22	23:X:267:VAL:HG13	1.91	0.52
9:o:56:THR:HG23	9:o:87:MET:CE	2.39	0.52
15:A:110:LYS:NZ	20:F:162:GLU:OE2	2.42	0.52
19:E:210:GLU:N	19:E:210:GLU:OE1	2.43	0.52
21:V:279:GLN:CG	21:V:279:GLN:O	2.57	0.52
22:W:272:LEU:HD22	22:W:341:PHE:CE2	2.44	0.52
6:L:74:ILE:HG22	6:L:132:LEU:CD2	2.40	0.52
21:V:438:VAL:HG11	21:V:458:VAL:HG11	1.91	0.52
16:B:101:ASP:C	16:B:101:ASP:OD1	2.52	0.52
18:D:154:LEU:HD12	18:D:157:ASP:OD1	2.10	0.52
18:D:197:ASP:OD1	18:D:197:ASP:N	2.43	0.52
22:W:77:ALA:C	22:W:78:LYS:HE2	2.35	0.52
24:Y:79:ASP:OD2	24:Y:79:ASP:C	2.52	0.52
26:a:138:VAL:HG23	26:a:138:VAL:O	2.10	0.52
28:d:251:ILE:HG23	28:d:256:TYR:HB2	1.92	0.52
33:f:387:GLN:N	33:f:387:GLN:OE1	2.42	0.52
15:A:238:ILE:HG21	15:A:260:LEU:CD1	2.39	0.52
15:A:307:ASP:OD2	15:A:333:ARG:NH2	2.42	0.52
16:B:427:LEU:O	16:B:430:LYS:HG2	2.09	0.52
19:E:98:VAL:HG12	19:E:100:LEU:HD12	1.92	0.52
22:W:109:CYS:SG	22:W:145:LEU:HD21	2.50	0.52
22:W:394:SER:HB2	23:X:341:PRO:HG3	1.91	0.52
17:C:325:ARG:NH1	17:C:354:ALA:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:435:LEU:HD21	26:a:356:TRP:CH2	2.44	0.52
24:Y:273:GLN:HE21	24:Y:273:GLN:HA	1.75	0.52
28:d:96:GLU:OE2	28:d:96:GLU:HA	2.10	0.52
28:d:121:LEU:HD21	31:U:16:GLU:OE1	2.10	0.52
16:B:53:THR:O	16:B:55:HIS:N	2.42	0.52
20:F:279:ALA:HB1	20:F:280:PRO:CD	2.38	0.52
24:Y:186:LEU:HD22	24:Y:287:LEU:HD11	1.92	0.52
24:Y:241:ILE:O	24:Y:247:LEU:HD11	2.10	0.52
28:d:177:ASP:OD1	28:d:178:TYR:N	2.42	0.52
33:f:470:VAL:HG13	33:f:482:ILE:HD11	1.92	0.52
4:j:42:VAL:CG1	4:j:208:LEU:HD21	2.40	0.52
31:U:388:ASP:OD1	31:U:389:ASN:N	2.43	0.52
6:l:88:MET:CE	6:l:132:LEU:HD13	2.40	0.52
17:C:213:ARG:NH1	17:C:249:ASP:OD2	2.39	0.52
22:W:214:PHE:HA	22:W:219:THR:CB	2.40	0.52
16:B:292:THR:HG22	16:B:293:LYS:N	2.25	0.51
17:C:237:MET:C	17:C:237:MET:SD	2.93	0.51
26:a:363:MET:HE2	32:c:307:VAL:HG11	1.91	0.51
3:I:209:GLU:HA	3:I:209:GLU:OE1	2.09	0.51
5:K:99:HIS:HB2	5:K:107:MET:HE2	1.91	0.51
8:N:15:LEU:HD23	8:N:45:CYS:SG	2.50	0.51
7:m:53:VAL:O	7:m:53:VAL:HG23	2.10	0.51
21:V:404:LYS:HD2	21:V:446:VAL:HG21	1.92	0.51
22:W:97:LEU:O	22:W:101:VAL:HG23	2.11	0.51
22:W:435:LEU:HD11	25:Z:237:LEU:HG	1.92	0.51
18:D:311:THR:HG21	18:D:317:LEU:HD11	1.91	0.51
22:W:113:GLU:O	22:W:113:GLU:OE1	2.28	0.51
33:f:583:VAL:HG12	33:f:584:SER:H	1.74	0.51
34:z:397:LEU:O	34:z:401:GLN:OE1	2.28	0.51
15:A:81:ALA:HB2	16:B:137:SER:CB	2.41	0.51
22:W:72:LYS:HG2	22:W:73:MET:CE	2.40	0.51
26:a:287:ASN:OD1	26:a:288:HIS:N	2.43	0.51
31:U:697:GLN:NE2	31:U:742:HIS:O	2.41	0.51
22:W:49:SER:O	22:W:53:GLN:HG3	2.11	0.51
23:X:157:LEU:O	23:X:160:MET:O	2.28	0.51
21:V:497:PRO:N	21:V:498:PRO:CD	2.73	0.51
22:W:201:ARG:HG2	22:W:201:ARG:NH1	2.23	0.51
23:X:240:ASP:OD1	23:X:240:ASP:C	2.53	0.51
27:b:22:LEU:HD21	27:b:179:LEU:HD22	1.93	0.51
7:M:141:SER:O	7:M:145:GLY:N	2.38	0.51
15:A:199:GLU:N	15:A:199:GLU:OE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:85:ASP:OD1	24:Y:107:LYS:NZ	2.41	0.51
24:Y:357:ASN:CG	24:Y:357:ASN:O	2.52	0.51
31:U:321:GLN:NE2	31:U:325:MET:SD	2.84	0.51
31:U:462:LEU:HD23	31:U:496:LEU:HD22	1.92	0.51
22:W:47:LEU:HD12	22:W:48:LEU:N	2.25	0.51
23:X:50:ILE:HD12	23:X:69:LEU:HD21	1.93	0.51
23:X:185:LYS:H	23:X:185:LYS:HD2	1.75	0.51
24:Y:169:GLU:OE2	24:Y:169:GLU:O	2.28	0.51
26:a:104:VAL:HG23	26:a:105:LYS:N	2.26	0.51
29:e:48:VAL:O	29:e:48:VAL:CG1	2.59	0.51
8:N:20:ARG:O	8:N:34:LYS:NZ	2.44	0.51
16:B:317:ASP:OD2	16:B:317:ASP:C	2.54	0.51
17:C:40:GLN:NE2	21:V:90:GLU:OE2	2.44	0.51
21:V:401:ASN:C	21:V:401:ASN:OD1	2.53	0.51
22:W:17:GLU:HG2	22:W:18:VAL:HG13	1.93	0.51
22:W:160:LYS:HG3	22:W:196:VAL:HG23	1.91	0.51
32:c:54:MET:SD	34:z:102:VAL:HG12	2.51	0.51
33:f:129:LEU:O	33:f:129:LEU:HD23	2.10	0.51
33:f:836:GLU:OE1	33:f:838:ARG:NH2	2.44	0.51
11:Q:168:GLN:NE2	11:Q:175:LEU:O	2.43	0.51
22:W:214:PHE:HB3	22:W:223:LYS:HB2	1.93	0.51
24:Y:224:VAL:O	24:Y:228:MET:HG3	2.11	0.51
27:b:48:ASN:OD1	27:b:48:ASN:N	2.43	0.51
33:f:264:GLU:OE1	33:f:264:GLU:N	2.42	0.51
12:R:46:MET:CE	35:R:301:LDZ:H17	2.41	0.50
12:r:18:ASP:OD1	12:r:34:LYS:NZ	2.44	0.50
27:b:33:VAL:CG2	27:b:75:LEU:HD11	2.41	0.50
3:i:174:MET:SD	3:i:195:LYS:NZ	2.84	0.50
15:A:45:ILE:HD13	16:B:62:LEU:HD23	1.93	0.50
28:d:104:ARG:NH2	28:d:108:ASN:OD1	2.43	0.50
31:U:678:ASP:OD2	31:U:683:VAL:HG11	2.11	0.50
16:B:255:LEU:HD23	16:B:266:LEU:HD23	1.92	0.50
17:C:30:GLU:N	17:C:30:GLU:OE1	2.45	0.50
22:W:368:LYS:HE2	22:W:369:TYR:CE1	2.45	0.50
16:B:80:ARG:HG2	16:B:80:ARG:HH11	1.76	0.50
22:W:304:ASP:HB3	22:W:324:TYR:OH	2.11	0.50
22:W:321:VAL:O	22:W:325:GLY:HA3	2.11	0.50
32:c:27:THR:HG21	32:c:177:THR:HG22	1.93	0.50
33:f:180:GLN:OE1	33:f:180:GLN:N	2.39	0.50
6:L:74:ILE:HG21	6:L:81:ALA:HB1	1.93	0.50
26:a:165:THR:HG22	26:a:166:ILE:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:f:452:ASN:HD22	33:f:462:ALA:HB2	1.76	0.50
16:B:93:GLU:OE1	16:B:93:GLU:HA	2.11	0.50
23:X:242:ILE:HD11	23:X:244:SER:HB2	1.92	0.50
25:Z:191:ILE:HG22	26:a:375:LEU:HD13	1.92	0.50
31:U:91:ASN:OD1	31:U:91:ASN:O	2.29	0.50
16:B:197:ILE:O	16:B:201:VAL:HG22	2.11	0.50
22:W:183:VAL:HG21	22:W:213:PHE:CE2	2.46	0.50
23:X:328:ASP:OD2	23:X:328:ASP:C	2.55	0.50
24:Y:186:LEU:HD12	24:Y:213:LEU:HD13	1.94	0.50
24:Y:237:ARG:HA	24:Y:241:ILE:HG22	1.93	0.50
33:f:133:MET:SD	33:f:135:GLY:N	2.84	0.50
33:f:458:GLU:C	33:f:458:GLU:OE2	2.55	0.50
34:z:42:ARG:NH1	34:z:44:ASP:OD2	2.44	0.50
1:G:158:GLY:O	2:H:83:ARG:NH2	2.45	0.50
5:K:133:MET:HE2	5:K:133:MET:HA	1.93	0.50
12:R:50:ALA:HA	35:R:301:LDZ:H22	1.94	0.50
6:l:84:LEU:HD13	6:l:132:LEU:HD11	1.94	0.50
8:n:18:ASP:OD1	8:n:34:LYS:NZ	2.41	0.50
22:W:112:VAL:HA	22:W:115:ILE:HG22	1.94	0.50
26:a:25:LEU:HD21	26:a:60:TYR:CZ	2.47	0.50
26:a:215:GLU:OE1	26:a:215:GLU:N	2.44	0.50
29:e:18:GLU:OE1	29:e:18:GLU:HA	2.11	0.50
32:c:227:GLU:OE2	32:c:227:GLU:C	2.55	0.50
3:i:35:LEU:N	3:i:46:ALA:O	2.43	0.50
16:B:389:ASP:C	16:B:389:ASP:OD1	2.55	0.50
16:B:430:LYS:HD2	16:B:430:LYS:N	2.27	0.50
21:V:227:VAL:HG22	21:V:227:VAL:O	2.12	0.50
6:L:166:GLN:OE1	20:F:386:ARG:NH1	2.45	0.49
19:E:98:VAL:CG1	19:E:107:ILE:HG23	2.41	0.49
21:V:313:LEU:HD21	21:V:329:HIS:NE2	2.26	0.49
21:V:405:THR:O	21:V:409:MET:HG2	2.12	0.49
22:W:87:ILE:HD11	22:W:128:LEU:CD2	2.42	0.49
23:X:246:LYS:HD2	23:X:246:LYS:N	2.27	0.49
26:a:363:MET:HE3	32:c:307:VAL:HG11	1.93	0.49
33:f:341:GLU:N	33:f:341:GLU:OE1	2.45	0.49
8:N:15:LEU:HD21	8:N:102:ALA:HB3	1.94	0.49
16:B:249:ARG:NH1	16:B:285:ASP:OD1	2.44	0.49
18:D:369:LYS:N	18:D:369:LYS:HE2	2.26	0.49
22:W:318:SER:O	22:W:321:VAL:HG12	2.11	0.49
25:Z:217:THR:HG21	25:Z:219:LYS:HD2	1.94	0.49
33:f:558:LEU:HB2	33:f:559:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:C:240:GLU:OE1	17:C:241:HIS:N	2.44	0.49
22:W:108:CYS:SG	22:W:128:LEU:HD11	2.52	0.49
27:b:10:VAL:HG13	27:b:29:GLN:CD	2.37	0.49
31:U:681:ASN:OD1	31:U:681:ASN:N	2.45	0.49
6:L:150:SER:O	6:L:152:ASN:N	2.42	0.49
9:o:30:LYS:NZ	10:p:150:GLU:OE2	2.46	0.49
12:r:108:ARG:NH1	12:r:108:ARG:HB2	2.27	0.49
15:A:165:GLN:HB3	15:A:167:GLU:OE2	2.12	0.49
22:W:301:LYS:CD	22:W:327:GLU:HG2	2.37	0.49
24:Y:46:ARG:HG2	24:Y:69:LEU:HD21	1.95	0.49
26:a:37:LEU:O	26:a:41:VAL:HG23	2.12	0.49
6:L:16:GLN:N	6:L:16:GLN:OE1	2.46	0.49
23:X:84:LYS:HE2	23:X:84:LYS:HA	1.95	0.49
31:U:127:ASP:OD2	31:U:129:ARG:NH2	2.45	0.49
4:j:42:VAL:HG13	4:j:208:LEU:HD21	1.95	0.49
8:n:23:THR:HB	35:n:301:LDZ:H39	1.94	0.49
26:a:350:LYS:NZ	26:a:354:GLU:OE1	2.46	0.49
33:f:316:ASP:OD1	33:f:316:ASP:C	2.55	0.49
1:G:112:ASP:OD2	9:O:73:ARG:NH2	2.46	0.49
11:Q:96:THR:O	11:Q:96:THR:OG1	2.26	0.49
13:s:83:MET:HE1	13:s:91:MET:SD	2.53	0.49
16:B:250:VAL:HG21	16:B:270:LEU:HD22	1.94	0.49
21:V:309:MET:SD	21:V:331:LEU:HD23	2.53	0.49
21:V:344:ASP:N	21:V:344:ASP:OD1	2.43	0.49
22:W:24:VAL:HG11	22:W:62:SER:HB3	1.94	0.49
22:W:223:LYS:HE2	22:W:253:THR:HG22	1.94	0.49
22:W:259:GLU:OE1	22:W:261:GLU:N	2.45	0.49
22:W:420:ASP:CG	22:W:421:PRO:HD2	2.38	0.49
25:Z:94:TRP:O	25:Z:121:LEU:HD12	2.12	0.49
16:B:174:MET:SD	16:B:250:VAL:HG22	2.53	0.49
21:V:108:LEU:HD11	21:V:170:LEU:HD22	1.95	0.49
22:W:32:ALA:HB3	22:W:33:LYS:NZ	2.28	0.49
23:X:93:LEU:HD11	23:X:109:LEU:CD1	2.43	0.49
8:N:23:THR:O	8:N:23:THR:OG1	2.28	0.49
15:A:255:ARG:NH1	15:A:259:GLU:OE2	2.45	0.49
16:B:153:ASN:OD1	16:B:154:HIS:N	2.46	0.49
18:D:97:ASP:O	18:D:98:GLN:CB	2.61	0.49
22:W:94:ARG:HB3	22:W:94:ARG:CZ	2.42	0.49
33:f:496:ASP:OD1	33:f:497:VAL:HG23	2.13	0.49
15:A:277:ILE:HD11	15:A:280:ILE:HD11	1.95	0.49
22:W:455:LEU:HD22	25:Z:103:LYS:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:f:654:VAL:HG22	33:f:678:LEU:HD21	1.94	0.49
18:D:315:ASP:OD1	18:D:316:THR:N	2.45	0.48
22:W:77:ALA:CB	22:W:79:GLU:HG3	2.42	0.48
22:W:89:LEU:C	22:W:89:LEU:HD23	2.38	0.48
22:W:171:VAL:HG11	22:W:182:ARG:HA	1.95	0.48
22:W:201:ARG:HH11	22:W:201:ARG:CG	2.21	0.48
28:d:142:ILE:HD13	28:d:182:LEU:HD12	1.95	0.48
31:U:244:MET:CE	31:U:903:PHE:CZ	2.96	0.48
32:c:138:GLU:C	32:c:138:GLU:OE2	2.55	0.48
33:f:869:THR:HG22	33:f:871:PRO:HD2	1.95	0.48
16:B:53:THR:O	16:B:54:PRO:C	2.56	0.48
22:W:115:ILE:CD1	22:W:116:THR:H	2.17	0.48
22:W:194:LEU:HG	22:W:202:THR:HG21	1.95	0.48
26:a:81:LEU:HD11	26:a:113:LEU:HG	1.95	0.48
2:h:110:VAL:HG22	2:h:135:ILE:HD13	1.95	0.48
22:W:27:ARG:HG3	22:W:31:CYS:SG	2.53	0.48
22:W:40:LEU:HB3	22:W:41:GLN:OE1	2.14	0.48
23:X:407:MET:CE	25:Z:269:VAL:HG11	2.44	0.48
26:a:218:MET:HE3	26:a:340:VAL:HG11	1.95	0.48
10:p:163:PHE:O	10:p:167:SER:OG	2.22	0.48
16:B:190:LEU:O	16:B:192:ASN:N	2.46	0.48
17:C:151:ILE:HG23	17:C:151:ILE:O	2.12	0.48
19:E:98:VAL:HG12	19:E:100:LEU:CD1	2.44	0.48
20:F:185:TYR:CG	20:F:195:ILE:HD11	2.49	0.48
24:Y:145:LEU:HD23	24:Y:157:ILE:HD13	1.96	0.48
33:f:463:LEU:HD13	33:f:497:VAL:HG22	1.95	0.48
7:M:30:VAL:HG22	7:M:133:CYS:HA	1.94	0.48
7:M:169:ARG:HB3	7:M:169:ARG:NH1	2.29	0.48
6:l:81:ALA:HB2	6:l:130:VAL:HG21	1.94	0.48
9:o:164:ILE:HG23	9:o:171:GLY:HA2	1.96	0.48
15:A:199:GLU:OE1	15:A:200:ARG:N	2.46	0.48
16:B:376:ASP:N	16:B:376:ASP:OD1	2.47	0.48
17:C:386:ALA:O	17:C:390:VAL:HG23	2.14	0.48
20:F:113:LEU:HD21	32:c:80:THR:CG2	2.44	0.48
22:W:289:ARG:HG3	22:W:289:ARG:HH11	1.78	0.48
31:U:412:HIS:CD2	31:U:422:LEU:HD21	2.48	0.48
33:f:662:MET:O	33:f:662:MET:HG2	2.13	0.48
31:U:653:ALA:HB2	31:U:675:MET:CE	2.44	0.48
6:l:88:MET:HE1	6:l:132:LEU:HD13	1.95	0.48
14:t:63:LEU:HD13	14:t:110:MET:CE	2.43	0.48
16:B:77:GLU:C	16:B:77:GLU:OE2	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:278:ALA:CB	16:B:279:PRO:CD	2.91	0.48
19:E:235:ILE:HG22	19:E:279:THR:HB	1.94	0.48
22:W:280:ASP:OD1	22:W:282:GLU:N	2.47	0.48
23:X:53:LEU:HD23	23:X:69:LEU:HD22	1.96	0.48
24:Y:157:ILE:HG21	24:Y:187:TYR:CD1	2.49	0.48
24:Y:376:LEU:HD23	24:Y:376:LEU:O	2.14	0.48
25:Z:44:GLN:O	25:Z:45:LYS:HG2	2.14	0.48
26:a:54:ASP:OD1	26:a:55:GLY:N	2.47	0.48
28:d:161:ILE:HD11	28:d:258:PHE:CZ	2.49	0.48
10:P:202:ARG:NH2	10:P:204:ASP:OD2	2.44	0.48
13:S:204:ARG:NH1	13:S:206:GLU:OE2	2.47	0.48
22:W:66:ILE:O	22:W:70:VAL:HG23	2.13	0.48
22:W:394:SER:O	22:W:398:VAL:HG23	2.13	0.48
26:a:78:GLU:HA	26:a:81:LEU:HD12	1.95	0.48
22:W:112:VAL:CG2	22:W:124:LEU:HG	2.44	0.48
25:Z:272:LEU:O	25:Z:276:ILE:HG13	2.14	0.48
31:U:206:MET:HE2	31:U:206:MET:CA	2.44	0.48
31:U:492:ASP:OD1	31:U:492:ASP:N	2.47	0.48
2:H:67:ILE:HG21	2:H:109:LEU:HD21	1.95	0.48
3:I:91:ARG:HD3	10:P:75:LEU:HD13	1.96	0.48
9:O:109:PRO:O	9:O:110:HIS:ND1	2.46	0.48
19:E:182:LEU:N	38:E:401:ADP:O1A	2.46	0.48
20:F:113:LEU:HD23	20:F:117:ARG:HH21	1.78	0.48
23:X:251:LEU:HA	23:X:254:MET:HE3	1.95	0.48
26:a:27:GLU:HA	26:a:27:GLU:OE2	2.14	0.48
28:d:282:ILE:O	28:d:283:LEU:HB2	2.13	0.48
32:c:64:ASP:OD1	32:c:64:ASP:N	2.47	0.48
33:f:189:LYS:HD2	33:f:189:LYS:O	2.13	0.48
34:z:73:LEU:C	34:z:74:LEU:HD12	2.39	0.48
2:H:74:VAL:HG22	2:H:75:TYR:H	1.78	0.47
20:F:318:ASP:C	20:F:318:ASP:OD1	2.57	0.47
21:V:176:MET:HE2	21:V:217:VAL:HB	1.96	0.47
22:W:19:ASP:OD1	22:W:20:TYR:N	2.47	0.47
25:Z:148:GLY:O	25:Z:150:PRO:HD2	2.13	0.47
28:d:125:GLU:OE1	28:d:126:LEU:HD13	2.13	0.47
31:U:739:ALA:O	31:U:744:VAL:HG12	2.14	0.47
31:U:800:VAL:HG12	31:U:801:GLN:N	2.29	0.47
6:l:176:MET:HE2	7:m:57:LEU:HD23	1.95	0.47
15:A:80:LEU:HB3	15:A:85:GLN:CB	2.44	0.47
22:W:276:LEU:CD1	22:W:350:ARG:HG2	2.43	0.47
23:X:171:LEU:HD13	23:X:210:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:d:121:LEU:HD11	31:U:16:GLU:OE1	2.14	0.47
31:U:810:THR:HG1	31:U:811:PHE:HD1	1.62	0.47
7:M:117:MET:HE2	7:M:117:MET:HA	1.96	0.47
4:j:115:LYS:O	4:j:119:THR:HG23	2.14	0.47
6:l:62:LYS:NZ	6:l:74:ILE:O	2.47	0.47
11:q:96:THR:O	11:q:96:THR:OG1	2.29	0.47
16:B:241:ASN:OD1	16:B:242:GLN:N	2.47	0.47
20:F:178:ASP:OD1	20:F:178:ASP:C	2.55	0.47
24:Y:387:ILE:HD11	25:Z:276:ILE:HG12	1.96	0.47
31:U:693:LEU:HD12	31:U:736:ILE:HG21	1.95	0.47
33:f:107:LYS:HD2	33:f:107:LYS:C	2.40	0.47
33:f:249:LEU:HD21	33:f:271:MET:HE2	1.96	0.47
4:j:121:SER:OG	4:j:124:ARG:NH1	2.48	0.47
22:W:370:TYR:HA	26:a:324:ILE:O	2.15	0.47
25:Z:170:VAL:HG13	32:c:151:VAL:O	2.14	0.47
28:d:125:GLU:CD	28:d:126:LEU:HD13	2.39	0.47
32:c:25:VAL:HG12	32:c:25:VAL:O	2.12	0.47
1:G:112:ASP:OD1	1:G:112:ASP:N	2.46	0.47
13:S:186:ASP:HB3	13:S:189:THR:HG22	1.97	0.47
19:E:250:ASP:O	19:E:254:GLN:HG3	2.14	0.47
21:V:192:MET:HE3	21:V:192:MET:HA	1.95	0.47
21:V:294:ARG:NH2	21:V:390:GLY:O	2.48	0.47
22:W:298:GLU:OE2	22:W:298:GLU:HA	2.14	0.47
22:W:316:ARG:NH2	22:W:383:ASP:OD2	2.48	0.47
6:L:65:HIS:CD2	6:L:223:ILE:HD12	2.50	0.47
22:W:27:ARG:NH2	22:W:46:THR:OG1	2.48	0.47
22:W:156:ASN:OD1	22:W:156:ASN:C	2.57	0.47
26:a:186:LYS:O	26:a:188:LEU:HD22	2.15	0.47
28:d:125:GLU:OE2	28:d:126:LEU:N	2.45	0.47
31:U:234:GLU:OE1	31:U:235:LYS:N	2.47	0.47
2:H:226:LYS:O	2:H:226:LYS:HD3	2.14	0.47
8:N:3:THR:N	8:N:18:ASP:OD2	2.40	0.47
9:o:31:ASN:OD1	9:o:188:ARG:NH2	2.48	0.47
15:A:375:ARG:NE	15:A:375:ARG:C	2.71	0.47
16:B:292:THR:HG22	16:B:293:LYS:H	1.80	0.47
16:B:381:ASP:OD1	16:B:381:ASP:N	2.48	0.47
16:B:412:MET:HE2	17:C:177:ALA:CB	2.44	0.47
17:C:64:GLN:HA	17:C:64:GLN:OE1	2.15	0.47
21:V:188:SER:O	21:V:192:MET:HG2	2.14	0.47
24:Y:97:GLU:O	24:Y:99:GLU:N	2.47	0.47
28:d:232:LEU:HD22	28:d:244:VAL:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:c:146:ASP:C	32:c:146:ASP:OD2	2.57	0.47
21:V:227:VAL:HG23	21:V:230:PHE:HD2	1.79	0.47
22:W:275:ILE:HD11	22:W:306:LEU:HD12	1.97	0.47
32:c:164:ASN:OD1	32:c:166:ASN:N	2.48	0.47
33:f:393:ASP:OD1	33:f:393:ASP:N	2.48	0.47
21:V:85:ALA:HB2	21:V:93:PHE:HB2	1.96	0.47
27:b:171:VAL:HG13	27:b:171:VAL:O	2.14	0.47
2:h:28:VAL:HG11	2:h:132:SER:CB	2.45	0.47
7:m:141:SER:O	7:m:145:GLY:N	2.40	0.47
14:t:9:THR:O	14:t:41:ARG:NH1	2.46	0.47
15:A:54:GLN:OE1	15:A:54:GLN:HA	2.15	0.47
15:A:375:ARG:C	15:A:375:ARG:HE	2.23	0.47
16:B:119:ASN:O	16:B:119:ASN:OD1	2.33	0.47
16:B:179:ALA:HB3	16:B:241:ASN:HB3	1.98	0.47
16:B:189:GLY:HA3	16:B:360:THR:HG23	1.97	0.47
19:E:98:VAL:HG13	19:E:107:ILE:HG23	1.97	0.47
27:b:148:VAL:HG22	27:b:148:VAL:O	2.15	0.47
28:d:122:VAL:O	28:d:125:GLU:OE2	2.33	0.47
16:B:52:VAL:HG12	16:B:52:VAL:O	2.15	0.46
18:D:154:LEU:O	18:D:155:THR:HG22	2.13	0.46
22:W:43:VAL:HA	22:W:46:THR:HG22	1.97	0.46
22:W:455:LEU:HD13	25:Z:103:LYS:HD2	1.97	0.46
25:Z:149:THR:HB	25:Z:150:PRO:HD3	1.97	0.46
28:d:258:PHE:O	28:d:262:ILE:HD12	2.14	0.46
21:V:169:LEU:HA	21:V:172:VAL:HG12	1.97	0.46
6:L:88:MET:HE3	6:L:112:ILE:HD11	1.97	0.46
8:n:2:THR:N	8:n:171:SER:HG	2.13	0.46
22:W:134:GLY:O	22:W:135:LYS:HG3	2.15	0.46
23:X:47:GLU:HA	23:X:50:ILE:HG22	1.97	0.46
25:Z:149:THR:CB	25:Z:150:PRO:CD	2.93	0.46
26:a:94:LEU:HD22	26:a:121:LEU:HD23	1.97	0.46
26:a:165:THR:O	26:a:167:GLY:N	2.43	0.46
26:a:183:VAL:HG22	26:a:185:ILE:O	2.15	0.46
31:U:58:GLN:OE1	31:U:58:GLN:N	2.48	0.46
33:f:92:VAL:HG11	33:f:97:LYS:HE2	1.97	0.46
6:L:72:ILE:HG21	6:L:88:MET:HE1	1.98	0.46
15:A:306:LEU:HD21	15:A:317:VAL:HG21	1.96	0.46
22:W:259:GLU:HB3	22:W:262:LYS:HG3	1.97	0.46
22:W:289:ARG:HH11	22:W:289:ARG:CG	2.28	0.46
25:Z:78:MET:HE1	32:c:95:MET:SD	2.56	0.46
28:d:144:ALA:O	28:d:148:LEU:HD23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:i:118:LYS:NZ	3:i:150:SER:OG	2.49	0.46
17:C:250:GLU:OE2	17:C:250:GLU:HA	2.15	0.46
21:V:132:LEU:N	21:V:133:PRO:HD2	2.30	0.46
22:W:88:MET:O	22:W:92:LYS:HG3	2.16	0.46
32:c:88:ASP:OD1	32:c:88:ASP:O	2.33	0.46
32:c:270:LEU:HD12	32:c:271:ALA:N	2.30	0.46
33:f:496:ASP:OD1	33:f:497:VAL:N	2.48	0.46
1:G:72:ILE:HG21	1:G:114:LEU:HD21	1.97	0.46
16:B:71:TYR:O	16:B:75:GLU:HG3	2.16	0.46
18:D:120:ASP:OD1	18:D:122:GLU:HG2	2.16	0.46
22:W:344:THR:OG1	22:W:345:GLU:N	2.49	0.46
23:X:134:VAL:HG12	23:X:172:LEU:HD23	1.98	0.46
23:X:140:THR:HG22	23:X:140:THR:O	2.16	0.46
9:o:188:ARG:HB3	9:o:189:PRO:CD	2.46	0.46
15:A:87:LEU:HD12	16:B:102:LEU:HD21	1.98	0.46
22:W:301:LYS:HE2	22:W:327:GLU:CB	2.45	0.46
26:a:255:TRP:CD1	26:a:255:TRP:C	2.94	0.46
27:b:176:GLY:O	27:b:178:SER:N	2.45	0.46
8:N:34:LYS:HG2	35:N:301:LDZ:H20	1.97	0.46
7:m:170:GLN:HA	7:m:170:GLN:NE2	2.30	0.46
17:C:287:LYS:O	17:C:287:LYS:HG3	2.16	0.46
19:E:283:ASP:N	19:E:283:ASP:OD1	2.48	0.46
20:F:93:VAL:HG11	20:F:96:LEU:HD21	1.97	0.46
26:a:166:ILE:HG22	26:a:167:GLY:N	2.29	0.46
28:d:94:MET:HE1	28:d:118:ARG:HD3	1.98	0.46
28:d:133:GLY:O	28:d:134:THR:C	2.59	0.46
33:f:185:LEU:HD13	33:f:185:LEU:C	2.41	0.46
15:A:79:ASP:HB3	33:f:712:LYS:HB2	1.98	0.46
15:A:86:THR:CG2	16:B:136:LEU:HD13	2.46	0.46
17:C:307:ARG:CZ	17:C:307:ARG:HB2	2.46	0.46
17:C:345:ARG:HG3	17:C:345:ARG:HH11	1.79	0.46
23:X:109:LEU:HD13	23:X:109:LEU:C	2.41	0.46
26:a:101:ARG:HG3	26:a:101:ARG:HH11	1.81	0.46
31:U:25:HIS:HA	31:U:59:PHE:HE2	1.80	0.46
31:U:381:THR:O	31:U:381:THR:CG2	2.63	0.46
4:j:50:VAL:O	4:j:51:ALA:HB3	2.15	0.46
8:n:48:GLY:O	35:n:301:LDZ:N16	2.44	0.46
12:r:108:ARG:CG	12:r:108:ARG:O	2.64	0.46
12:r:108:ARG:O	12:r:108:ARG:HG3	2.16	0.46
20:F:317:LEU:CD2	20:F:328:VAL:HG21	2.46	0.46
22:W:441:LYS:HD3	22:W:441:LYS:HA	1.66	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:45:LYS:HG3	25:Z:45:LYS:O	2.16	0.46
25:Z:213:GLU:O	25:Z:217:THR:HG22	2.16	0.46
33:f:408:LEU:HD12	33:f:443:GLY:CA	2.46	0.46
33:f:517:VAL:HG23	33:f:557:TRP:CZ3	2.51	0.46
9:O:188:ARG:HB3	9:O:189:PRO:CD	2.46	0.45
4:j:208:LEU:HD23	4:j:209:ALA:N	2.31	0.45
22:W:51:GLU:OE1	22:W:93:ARG:NE	2.49	0.45
22:W:72:LYS:HG2	22:W:73:MET:HE2	1.98	0.45
22:W:172:GLU:OE1	22:W:172:GLU:N	2.35	0.45
31:U:51:ASP:OD1	31:U:53:GLY:N	2.48	0.45
31:U:217:CYS:SG	31:U:248:ILE:HD12	2.56	0.45
33:f:707:LEU:HD22	33:f:741:LEU:HD13	1.97	0.45
7:M:39:ILE:HD12	7:M:193:VAL:HG22	1.98	0.45
16:B:49:LEU:HD11	33:f:669:GLU:HB2	1.98	0.45
20:F:303:ASP:OD1	20:F:304:ARG:N	2.50	0.45
21:V:95:LEU:CD1	21:V:205:LEU:HD23	2.46	0.45
28:d:159:LYS:HA	28:d:258:PHE:CE1	2.51	0.45
33:f:113:MET:SD	33:f:113:MET:N	2.89	0.45
3:I:90:LEU:HG	3:I:114:LEU:HD13	1.99	0.45
8:n:15:LEU:HD23	8:n:45:CYS:SG	2.55	0.45
16:B:411:ARG:HB2	16:B:411:ARG:CZ	2.46	0.45
17:C:62:GLU:OE1	18:D:116:LEU:HD12	2.17	0.45
17:C:119:ASP:OD1	17:C:119:ASP:N	2.50	0.45
19:E:76:GLY:N	19:E:77:PRO:CD	2.79	0.45
21:V:496:PHE:C	21:V:498:PRO:HD2	2.41	0.45
24:Y:117:LYS:HE3	24:Y:151:TYR:CD2	2.51	0.45
26:a:112:ILE:HD12	26:a:112:ILE:N	2.30	0.45
28:d:125:GLU:OE2	28:d:125:GLU:CA	2.63	0.45
28:d:149:GLU:OE1	28:d:187:TYR:HB2	2.16	0.45
31:U:91:ASN:OD1	31:U:91:ASN:C	2.59	0.45
33:f:517:VAL:HG23	33:f:557:TRP:HZ3	1.81	0.45
5:K:171:GLY:N	5:K:174:SER:OG	2.50	0.45
14:t:50:MET:HE1	14:t:190:ALA:O	2.17	0.45
17:C:345:ARG:HG3	17:C:345:ARG:NH1	2.31	0.45
18:D:297:ASP:OD1	18:D:297:ASP:C	2.59	0.45
21:V:322:VAL:O	21:V:326:GLN:HG3	2.15	0.45
23:X:144:GLN:OE1	23:X:180:LEU:HD11	2.17	0.45
27:b:7:MET:HE3	27:b:96:ALA:HB1	1.98	0.45
27:b:22:LEU:HD23	27:b:179:LEU:HD22	1.97	0.45
34:z:81:SER:OG	34:z:82:SER:N	2.48	0.45
2:H:71:ILE:HG21	2:H:109:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:34:SER:OG	7:M:65:ARG:NH1	2.50	0.45
13:S:145:LEU:HD21	13:S:182:ALA:HB2	1.98	0.45
17:C:234:LEU:O	17:C:237:MET:HE3	2.16	0.45
17:C:369:TYR:HD2	17:C:385:MET:HE3	1.80	0.45
17:C:369:TYR:CD2	17:C:385:MET:HE3	2.51	0.45
18:D:141:ASP:OD1	18:D:142:VAL:N	2.49	0.45
3:i:119:GLN:NE2	4:j:79:ASP:OD1	2.50	0.45
3:i:197:LEU:HA	3:i:200:THR:HG22	1.98	0.45
16:B:186:ASP:HA	16:B:367:ILE:HD12	1.98	0.45
17:C:254:ILE:HD13	17:C:269:VAL:HG23	1.98	0.45
24:Y:42:MET:HA	24:Y:45:VAL:HG12	1.99	0.45
24:Y:149:LEU:N	24:Y:157:ILE:HD11	2.32	0.45
26:a:68:GLU:HG3	26:a:71:VAL:HG23	1.97	0.45
26:a:180:LEU:HD22	26:a:222:LEU:HD21	1.98	0.45
3:I:187:LYS:HE2	3:I:187:LYS:N	2.29	0.45
2:h:28:VAL:HG11	2:h:132:SER:HB2	1.99	0.45
10:p:182:MET:HE2	10:p:203:MET:HE3	1.97	0.45
12:r:20:ARG:NE	12:r:30:GLN:OE1	2.46	0.45
14:t:22:ILE:HB	14:t:50:MET:HE3	1.99	0.45
18:D:63:ASP:OD2	31:U:604:HIS:ND1	2.44	0.45
19:E:115:VAL:HG23	19:E:115:VAL:O	2.17	0.45
28:d:159:LYS:HD3	28:d:159:LYS:N	2.32	0.45
2:H:227:ASP:CB	23:X:84:LYS:HE3	2.47	0.45
8:N:167:ARG:NH1	14:T:34:ALA:O	2.45	0.45
16:B:49:LEU:HD21	33:f:669:GLU:CB	2.47	0.45
19:E:40:TYR:CG	20:F:69:MET:HE3	2.52	0.45
24:Y:138:LEU:HD13	24:Y:176:ARG:HG2	1.99	0.45
25:Z:213:GLU:OE1	25:Z:214:LYS:N	2.49	0.45
27:b:55:ALA:O	27:b:56:ASN:C	2.59	0.45
33:f:589:SER:O	33:f:593:THR:HG23	2.17	0.45
34:z:58:LYS:NZ	34:z:62:GLN:OE1	2.50	0.45
12:r:139:VAL:HG21	12:r:163:GLN:HG3	1.98	0.45
15:A:80:LEU:HB3	15:A:85:GLN:HB3	1.99	0.45
15:A:86:THR:HG23	16:B:136:LEU:HD13	1.99	0.45
16:B:93:GLU:O	16:B:94:GLU:HB3	2.17	0.45
16:B:116:ILE:O	16:B:116:ILE:HG22	2.17	0.45
17:C:150:MET:HE3	17:C:331:ILE:HD11	1.99	0.45
21:V:476:PHE:CZ	25:Z:258:VAL:HG22	2.52	0.45
22:W:93:ARG:NH1	22:W:93:ARG:HG2	2.31	0.45
22:W:356:ASN:O	22:W:360:GLU:HG3	2.16	0.45
23:X:286:ALA:HB2	23:X:309:TYR:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:U:713:TYR:O	31:U:717:ILE:HD12	2.17	0.45
33:f:422:VAL:HG23	33:f:423:ASP:N	2.32	0.45
34:z:54:GLU:OE2	34:z:82:SER:OG	2.16	0.45
3:I:71:ASP:HA	3:I:223:THR:HG21	1.97	0.45
21:V:469:THR:HG22	21:V:470:ARG:N	2.32	0.45
28:d:134:THR:O	28:d:135:LYS:C	2.59	0.45
28:d:248:LYS:O	28:d:251:ILE:HD11	2.17	0.45
32:c:89:PRO:HG2	34:z:74:LEU:HD11	1.98	0.45
33:f:411:ALA:HB3	33:f:443:GLY:HA3	1.98	0.45
33:f:583:VAL:HG12	33:f:584:SER:N	2.32	0.45
33:f:706:ILE:O	33:f:710:LEU:HD23	2.16	0.45
4:j:119:THR:HG22	4:j:126:PRO:HB3	1.98	0.44
16:B:93:GLU:CD	16:B:94:GLU:H	2.25	0.44
16:B:332:ASN:OD1	16:B:332:ASN:C	2.59	0.44
21:V:309:MET:HE1	21:V:331:LEU:C	2.42	0.44
22:W:21:SER:O	22:W:24:VAL:HG22	2.17	0.44
24:Y:334:LEU:CB	24:Y:347:ILE:HD11	2.44	0.44
25:Z:16:LEU:HD22	32:c:216:MET:SD	2.57	0.44
12:R:46:MET:HE2	35:R:301:LDZ:H17	1.98	0.44
12:r:177:LEU:HD23	12:r:188:VAL:HG21	1.99	0.44
15:A:99:THR:CG2	15:A:115:VAL:HG22	2.47	0.44
15:A:299:MET:O	15:A:303:ILE:HG13	2.18	0.44
15:A:366:ARG:HG3	15:A:366:ARG:HH11	1.83	0.44
16:B:121:ALA:HB2	16:B:135:ILE:HD11	1.99	0.44
19:E:178:THR:HB	19:E:301:ILE:HG22	1.99	0.44
22:W:44:ILE:HA	22:W:47:LEU:HD11	1.98	0.44
22:W:136:ILE:O	22:W:139:GLU:HG2	2.16	0.44
22:W:298:GLU:OE2	22:W:298:GLU:CA	2.65	0.44
22:W:305:LEU:CD1	22:W:320:LEU:HD11	2.47	0.44
22:W:312:MET:SD	22:W:365:ILE:HD11	2.57	0.44
27:b:93:ALA:O	27:b:97:LEU:HG	2.17	0.44
31:U:426:TYR:C	31:U:427:LEU:HD23	2.42	0.44
1:G:176:THR:HG23	2:H:55:LEU:HD12	1.99	0.44
7:M:87:LEU:HD12	7:M:133:CYS:SG	2.58	0.44
22:W:124:LEU:O	22:W:124:LEU:HD12	2.17	0.44
22:W:223:LYS:HG3	22:W:227:TYR:CE2	2.52	0.44
23:X:256:LEU:HD13	23:X:319:ILE:HD13	2.00	0.44
24:Y:35:ALA:O	24:Y:39:ASP:OD1	2.35	0.44
25:Z:110:GLU:OE2	25:Z:110:GLU:HA	2.17	0.44
26:a:287:ASN:OD1	26:a:287:ASN:C	2.60	0.44
28:d:128:PHE:CE1	28:d:148:LEU:HD21	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:U:700:GLU:OE1	31:U:700:GLU:O	2.36	0.44
33:f:185:LEU:HD13	33:f:185:LEU:O	2.16	0.44
3:I:51:ASN:OD1	3:I:51:ASN:C	2.61	0.44
22:W:305:LEU:HD22	22:W:328:LEU:HD11	1.98	0.44
25:Z:242:LEU:O	25:Z:246:VAL:HG23	2.18	0.44
28:d:258:PHE:C	28:d:258:PHE:CD2	2.95	0.44
31:U:261:LEU:HD23	31:U:329:LEU:O	2.17	0.44
15:A:101:ILE:HG23	15:A:137:GLY:N	2.32	0.44
22:W:18:VAL:HG23	22:W:18:VAL:O	2.18	0.44
22:W:77:ALA:HB3	22:W:79:GLU:HG3	1.99	0.44
23:X:394:ASP:O	23:X:395:LYS:HB2	2.17	0.44
31:U:269:ARG:HG3	31:U:269:ARG:HH11	1.83	0.44
32:c:227:GLU:O	32:c:230:THR:HG22	2.17	0.44
33:f:122:ALA:O	33:f:126:ILE:HG12	2.18	0.44
17:C:254:ILE:HG22	17:C:273:MET:HG2	1.99	0.44
23:X:309:TYR:N	23:X:309:TYR:CD1	2.85	0.44
23:X:355:LYS:O	23:X:356:LEU:HD12	2.18	0.44
31:U:88:PHE:CD1	31:U:88:PHE:C	2.96	0.44
31:U:678:ASP:OD1	31:U:679:PRO:HD2	2.17	0.44
33:f:841:PRO:HA	33:f:870:THR:HB	2.00	0.44
21:V:224:LEU:O	21:V:227:VAL:HG12	2.18	0.44
26:a:68:GLU:CG	26:a:71:VAL:HG23	2.48	0.44
26:a:179:PHE:O	26:a:183:VAL:HG12	2.18	0.44
26:a:217:LEU:HD21	26:a:237:LEU:HB3	1.99	0.44
31:U:583:MET:HE3	31:U:602:LEU:HD23	2.00	0.44
31:U:653:ALA:HB2	31:U:675:MET:HE1	1.99	0.44
31:U:701:ILE:HD13	31:U:810:THR:CA	2.48	0.44
9:O:56:THR:HG23	9:O:87:MET:HE1	2.00	0.44
16:B:173:VAL:O	17:C:258:ARG:NH1	2.50	0.44
19:E:46:ASP:CG	20:F:139:LEU:HD22	2.42	0.44
22:W:42:GLU:HG3	22:W:43:VAL:N	2.32	0.44
22:W:193:CYS:HA	22:W:196:VAL:CG1	2.45	0.44
27:b:35:ILE:HG21	27:b:181:ASP:CB	2.48	0.44
31:U:253:TYR:HA	31:U:261:LEU:HD21	2.00	0.44
32:c:70:ILE:HG21	32:c:104:ARG:NH1	2.33	0.44
5:K:109:VAL:HG21	5:K:152:GLN:HB2	1.98	0.44
35:R:301:LDZ:H21	35:R:301:LDZ:C22	2.48	0.44
16:B:53:THR:HB	16:B:54:PRO:HD2	1.99	0.44
19:E:197:LYS:HE3	20:F:320:PHE:HB2	2.00	0.44
21:V:131:LEU:CD1	21:V:171:VAL:HG11	2.48	0.44
22:W:48:LEU:O	22:W:48:LEU:HD23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:a:273:GLN:HB3	26:a:310:LEU:HD11	2.00	0.44
33:f:173:LEU:HD12	33:f:174:ASP:N	2.33	0.44
33:f:461:PRO:HB3	34:z:395:LEU:HD21	1.99	0.44
8:N:168:ASP:OD1	8:N:169:GLY:N	2.50	0.43
21:V:345:ARG:HD3	29:e:41:ASP:HB3	2.00	0.43
22:W:180:LYS:HZ1	22:W:222:LEU:HD11	1.83	0.43
25:Z:64:ASP:N	25:Z:64:ASP:OD1	2.51	0.43
28:d:161:ILE:HD13	28:d:161:ILE:N	2.32	0.43
31:U:321:GLN:CD	31:U:321:GLN:C	2.86	0.43
1:G:109:ILE:O	1:G:109:ILE:HG23	2.17	0.43
35:O:301:LDZ:O34	35:O:301:LDZ:H32	2.18	0.43
12:R:6:ALA:HA	12:R:14:ILE:O	2.18	0.43
12:r:15:VAL:HG21	12:r:43:LEU:HD11	2.00	0.43
18:D:407:ILE:O	18:D:408:LYS:C	2.61	0.43
19:E:76:GLY:N	19:E:77:PRO:HD2	2.33	0.43
20:F:362:ARG:O	20:F:366:MET:HG3	2.18	0.43
21:V:469:THR:HG22	21:V:470:ARG:H	1.82	0.43
22:W:85:GLU:OE2	22:W:85:GLU:HA	2.18	0.43
22:W:272:LEU:CD2	22:W:341:PHE:HE2	2.31	0.43
26:a:111:VAL:HG12	26:a:115:LYS:HE3	2.00	0.43
33:f:388:ASP:OD1	33:f:388:ASP:C	2.61	0.43
6:L:74:ILE:HG22	6:L:132:LEU:HD23	2.00	0.43
6:L:84:LEU:HD23	6:L:132:LEU:HD11	2.00	0.43
17:C:157:GLN:OE1	17:C:157:GLN:N	2.43	0.43
22:W:20:TYR:O	22:W:24:VAL:HG13	2.17	0.43
23:X:99:MET:SD	23:X:99:MET:C	3.01	0.43
23:X:315:ASP:OD1	23:X:315:ASP:N	2.51	0.43
32:c:57:MET:HE3	32:c:69:VAL:HG21	1.99	0.43
33:f:429:ILE:O	33:f:429:ILE:HG22	2.18	0.43
1:G:155:ASP:HB2	1:G:156:PRO:HD2	2.01	0.43
15:A:303:ILE:HG23	15:A:336:ARG:NE	2.33	0.43
16:B:78:PHE:CZ	33:f:678:LEU:HD12	2.53	0.43
18:D:178:ARG:O	18:D:182:GLU:HB2	2.19	0.43
22:W:407:ASP:OD2	23:X:344:ARG:NH1	2.51	0.43
26:a:186:LYS:O	26:a:187:ASP:C	2.60	0.43
28:d:138:LYS:O	28:d:142:ILE:HG12	2.19	0.43
29:e:45:ASP:OD1	29:e:45:ASP:N	2.51	0.43
31:U:221:ILE:HD11	31:U:252:LEU:CD2	2.43	0.43
2:h:21:ILE:HD11	2:h:121:THR:OG1	2.18	0.43
35:n:301:LDZ:C22	35:n:301:LDZ:H21	2.48	0.43
28:d:156:ILE:HD12	28:d:194:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:e:17:ASP:O	29:e:18:GLU:C	2.61	0.43
31:U:154:ALA:HB2	31:U:162:VAL:HG13	2.01	0.43
2:H:79:GLY:N	2:H:80:PRO:HD2	2.34	0.43
16:B:206:THR:HG22	16:B:207:HIS:CE1	2.52	0.43
20:F:326:VAL:O	20:F:326:VAL:HG13	2.19	0.43
22:W:89:LEU:HD23	22:W:90:LEU:HD23	1.99	0.43
22:W:432:LEU:O	22:W:436:MET:HG3	2.18	0.43
22:W:453:HIS:HA	22:W:456:GLN:HE21	1.82	0.43
5:K:29:GLU:OE1	5:K:29:GLU:HA	2.17	0.43
5:K:104:ASN:OD1	12:R:58:ARG:NH2	2.47	0.43
18:D:268:ASP:OD2	18:D:311:THR:OG1	2.31	0.43
20:F:192:ASP:HA	20:F:195:ILE:HG22	1.99	0.43
22:W:50:LEU:HB2	22:W:66:ILE:CD1	2.48	0.43
22:W:272:LEU:CD1	22:W:302:TYR:HE2	2.32	0.43
23:X:377:ILE:HG21	24:Y:312:ARG:HB2	2.01	0.43
24:Y:92:GLU:C	24:Y:92:GLU:OE2	2.62	0.43
24:Y:273:GLN:HA	24:Y:273:GLN:NE2	2.33	0.43
33:f:733:GLY:HA3	33:f:741:LEU:CD2	2.48	0.43
9:O:140:GLU:OE1	14:T:179:ARG:NH2	2.48	0.43
15:A:252:GLU:OE2	20:F:259:MET:HE2	2.18	0.43
16:B:59:ARG:HE	33:f:209:MET:HE3	1.84	0.43
17:C:163:GLU:OE1	17:C:163:GLU:O	2.36	0.43
17:C:338:LEU:O	24:Y:207:THR:HG23	2.18	0.43
18:D:312:ASN:OD1	18:D:312:ASN:O	2.37	0.43
21:V:95:LEU:O	24:Y:389:MET:HE2	2.18	0.43
21:V:115:LYS:N	21:V:115:LYS:HD2	2.34	0.43
21:V:131:LEU:HD12	21:V:171:VAL:HG21	2.01	0.43
22:W:272:LEU:HD11	22:W:302:TYR:HE2	1.84	0.43
24:Y:83:ARG:CZ	24:Y:83:ARG:HB3	2.49	0.43
26:a:109:GLU:O	26:a:151:VAL:HG11	2.18	0.43
26:a:210:VAL:HG13	26:a:210:VAL:O	2.18	0.43
27:b:97:LEU:O	27:b:100:ARG:HD3	2.17	0.43
28:d:94:MET:HE1	28:d:118:ARG:CD	2.49	0.43
28:d:123:LEU:HD21	28:d:143:LEU:HD23	2.00	0.43
31:U:3:THR:O	31:U:5:ALA:N	2.52	0.43
5:K:236:GLU:C	5:K:236:GLU:OE2	2.62	0.43
17:C:214:VAL:HG21	17:C:234:LEU:HD22	2.00	0.43
22:W:30:GLU:O	22:W:34:LEU:HG	2.19	0.43
25:Z:193:ASN:O	25:Z:195:VAL:N	2.52	0.43
32:c:59:GLY:HA3	32:c:68:ARG:O	2.19	0.43
33:f:399:LEU:HD23	33:f:410:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:f:802:SER:OG	33:f:817:VAL:HG21	2.18	0.43
3:I:58:GLU:OE2	3:I:59:VAL:N	2.52	0.43
5:k:121:LEU:HD22	6:l:79:ALA:HB3	2.00	0.43
15:A:93:LEU:HD21	16:B:120:HIS:NE2	2.34	0.43
15:A:236:CYS:HB3	15:A:270:CYS:HA	2.00	0.43
20:F:95:GLU:O	20:F:96:LEU:HD22	2.19	0.43
21:V:422:ILE:HD11	21:V:458:VAL:HG21	2.00	0.43
21:V:453:HIS:CD2	21:V:453:HIS:O	2.72	0.43
23:X:420:LYS:HB2	25:Z:280:ILE:HD11	2.01	0.43
31:U:108:TYR:OH	31:U:131:GLU:OE2	2.27	0.43
31:U:673:GLU:HB3	31:U:674:PRO:HD3	2.00	0.43
5:K:225:ASN:OD1	5:K:225:ASN:N	2.52	0.42
16:B:192:ASN:OD1	16:B:193:GLN:N	2.51	0.42
19:E:197:LYS:HD2	19:E:198:VAL:N	2.33	0.42
22:W:112:VAL:HA	22:W:115:ILE:CG2	2.49	0.42
23:X:173:GLU:OE1	23:X:174:SER:N	2.52	0.42
28:d:159:LYS:N	28:d:159:LYS:CD	2.81	0.42
7:m:39:ILE:HD12	7:m:193:VAL:HG22	2.01	0.42
22:W:86:ASN:HD22	22:W:86:ASN:HA	1.70	0.42
22:W:158:ASP:HB3	22:W:161:GLU:HB2	2.01	0.42
23:X:171:LEU:HD13	23:X:210:LEU:CD1	2.48	0.42
23:X:273:GLY:O	23:X:277:LEU:HD22	2.19	0.42
23:X:345:VAL:HG22	23:X:346:GLN:N	2.35	0.42
24:Y:328:GLU:O	24:Y:332:GLN:HG3	2.18	0.42
28:d:228:HIS:HB3	28:d:229:PRO:HD3	2.01	0.42
33:f:92:VAL:O	33:f:93:PRO:C	2.61	0.42
10:P:143:GLU:OE1	10:P:143:GLU:N	2.49	0.42
11:Q:20:VAL:HG13	11:Q:27:GLN:HG2	2.00	0.42
8:n:15:LEU:HD21	8:n:102:ALA:HB3	2.01	0.42
16:B:118:ASP:N	16:B:118:ASP:OD1	2.52	0.42
18:D:326:ARG:O	18:D:327:LEU:C	2.62	0.42
25:Z:45:LYS:O	25:Z:45:LYS:CG	2.68	0.42
31:U:602:LEU:HD12	31:U:625:ILE:HD12	2.01	0.42
32:c:82:VAL:HG22	32:c:82:VAL:O	2.19	0.42
6:L:72:ILE:CG2	6:L:88:MET:HE1	2.49	0.42
12:R:193:VAL:HG11	10:p:204:ASP:HB3	2.00	0.42
15:A:86:THR:CG2	16:B:102:LEU:HD13	2.48	0.42
18:D:216:ALA:O	18:D:219:VAL:HG22	2.18	0.42
19:E:36:LEU:CD2	20:F:69:MET:HE2	2.50	0.42
22:W:44:ILE:HA	22:W:47:LEU:CD1	2.49	0.42
22:W:87:ILE:HD11	22:W:128:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:205:LYS:HD2	23:X:205:LYS:C	2.44	0.42
23:X:412:ASP:OD1	24:Y:379:ARG:NH2	2.51	0.42
25:Z:71:ASP:OD1	27:b:63:THR:HG21	2.19	0.42
27:b:33:VAL:HG13	27:b:112:PHE:CE2	2.54	0.42
32:c:183:HIS:O	32:c:184:LEU:HD12	2.19	0.42
33:f:478:ARG:O	33:f:482:ILE:HG12	2.20	0.42
2:h:71:ILE:HG21	2:h:109:LEU:HD23	2.00	0.42
5:k:78:MET:HG3	5:k:82:ILE:HD12	2.01	0.42
15:A:278:ASP:OD2	16:B:294:ARG:NH2	2.53	0.42
16:B:168:ASP:O	16:B:168:ASP:CG	2.63	0.42
16:B:259:TYR:HB2	16:B:262:ASP:OD2	2.19	0.42
22:W:44:ILE:HA	22:W:47:LEU:HD21	2.02	0.42
22:W:128:LEU:HB3	22:W:145:LEU:CD1	2.50	0.42
25:Z:48:LEU:HD21	25:Z:92:VAL:HG11	2.02	0.42
26:a:25:LEU:HD21	26:a:60:TYR:OH	2.20	0.42
31:U:894:MET:HE1	31:U:914:LEU:HD22	2.01	0.42
33:f:226:TYR:OH	33:f:261:ARG:NH1	2.49	0.42
33:f:799:VAL:HG21	33:f:821:LEU:CD2	2.49	0.42
5:K:107:MET:HG2	5:K:111:SER:HB2	2.01	0.42
5:k:180:SER:CB	5:k:201:ILE:HD12	2.50	0.42
17:C:163:GLU:OE1	17:C:163:GLU:C	2.63	0.42
17:C:214:VAL:HG12	17:C:215:SER:N	2.35	0.42
18:D:312:ASN:OD1	18:D:312:ASN:C	2.62	0.42
20:F:115:SER:OG	20:F:116:GLN:N	2.53	0.42
21:V:150:ARG:NH2	21:V:157:THR:O	2.50	0.42
22:W:379:ALA:HB1	22:W:384:LEU:O	2.20	0.42
22:W:453:HIS:HA	22:W:456:GLN:NE2	2.33	0.42
24:Y:189:VAL:HG13	24:Y:288:PHE:CE1	2.55	0.42
25:Z:35:VAL:O	25:Z:96:HIS:HA	2.19	0.42
26:a:246:GLU:HA	26:a:246:GLU:OE2	2.20	0.42
28:d:289:ARG:O	28:d:289:ARG:NE	2.52	0.42
31:U:88:PHE:C	31:U:88:PHE:HD1	2.26	0.42
17:C:62:GLU:OE2	18:D:117:SER:OG	2.37	0.42
19:E:118:LEU:O	19:E:122:MET:HG3	2.20	0.42
21:V:173:ILE:HD11	21:V:213:TYR:CE2	2.54	0.42
22:W:431:LYS:HE3	25:Z:238:PRO:HB3	2.01	0.42
24:Y:248:GLU:OE2	24:Y:248:GLU:C	2.62	0.42
28:d:190:GLN:HG3	28:d:225:TYR:CD2	2.54	0.42
31:U:572:ARG:HH11	31:U:572:ARG:HB3	1.85	0.42
32:c:272:ILE:O	32:c:272:ILE:HG22	2.19	0.42
33:f:470:VAL:HG13	33:f:482:ILE:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:202:ASP:OD2	7:M:202:ASP:C	2.60	0.42
16:B:136:LEU:HD12	16:B:160:ILE:CG2	2.50	0.42
20:F:113:LEU:HD21	32:c:80:THR:HG22	2.00	0.42
21:V:443:ARG:NH2	21:V:444:ASP:OD2	2.52	0.42
22:W:395:ASN:OD1	22:W:399:ASN:ND2	2.53	0.42
23:X:173:GLU:OE1	23:X:189:ALA:HB1	2.19	0.42
24:Y:155:ASP:OD1	24:Y:155:ASP:C	2.62	0.42
26:a:235:ASP:OD1	26:a:247:ARG:NH2	2.53	0.42
27:b:128:ALA:HB2	27:b:156:PHE:CD1	2.54	0.42
33:f:477:MET:HE2	33:f:477:MET:HB3	1.96	0.42
12:r:3:THR:O	12:r:3:THR:HG23	2.20	0.42
16:B:388:ASP:O	16:B:389:ASP:OD1	2.38	0.42
16:B:430:LYS:O	16:B:431:GLN:HB2	2.20	0.42
17:C:293:MET:HE3	17:C:311:ILE:HD13	2.00	0.42
20:F:89:LEU:O	20:F:153:VAL:HG22	2.20	0.42
21:V:190:ASP:O	21:V:194:LYS:HG3	2.20	0.42
22:W:264:GLN:O	22:W:268:LYS:HG3	2.20	0.42
23:X:310:ARG:HB3	23:X:310:ARG:NH1	2.34	0.42
25:Z:149:THR:CB	25:Z:150:PRO:HD3	2.50	0.42
25:Z:162:ILE:HD13	32:c:220:LEU:HD23	2.01	0.42
26:a:25:LEU:HD23	26:a:25:LEU:C	2.44	0.42
33:f:128:VAL:HG21	33:f:154:TRP:CZ3	2.54	0.42
3:I:207:SER:O	3:I:208:ALA:HB3	2.20	0.42
4:J:134:VAL:HG12	4:J:144:LEU:HD13	2.02	0.42
15:A:238:ILE:HG21	15:A:260:LEU:HD13	2.01	0.42
16:B:53:THR:CB	16:B:54:PRO:HD2	2.50	0.42
19:E:260:LEU:O	19:E:264:MET:HG3	2.20	0.42
20:F:45:THR:HG23	20:F:46:ARG:N	2.35	0.42
22:W:349:LYS:HB3	22:W:349:LYS:HE3	1.84	0.42
22:W:435:LEU:O	22:W:439:VAL:HG23	2.20	0.42
25:Z:193:ASN:HB2	32:c:228:GLY:CA	2.50	0.42
32:c:49:VAL:CG1	32:c:50:PRO:HD3	2.50	0.42
32:c:232:GLN:O	32:c:233:ASP:C	2.63	0.42
33:f:432:TYR:CD2	33:f:432:TYR:N	2.88	0.42
33:f:512:MET:HA	33:f:512:MET:HE3	2.01	0.42
10:P:87:MET:HE1	10:P:131:VAL:HG22	2.02	0.41
16:B:182:GLU:OE1	16:B:183:THR:HG23	2.20	0.41
21:V:245:ASP:OD1	21:V:245:ASP:N	2.53	0.41
22:W:118:LEU:HD23	22:W:119:PRO:N	2.35	0.41
23:X:289:CYS:SG	23:X:305:ALA:HB1	2.59	0.41
4:J:89:VAL:HG12	11:Q:66:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:13:VAL:HG21	8:N:102:ALA:HB1	2.02	0.41
12:r:39:ASN:HB2	12:r:40:PRO:HD2	2.02	0.41
16:B:165:ASP:OD1	16:B:165:ASP:N	2.51	0.41
17:C:146:SER:O	17:C:146:SER:OG	2.38	0.41
18:D:281:ALA:HB1	19:E:208:ILE:CD1	2.50	0.41
21:V:75:ILE:O	21:V:79:VAL:HG13	2.19	0.41
21:V:99:ARG:HB2	24:Y:389:MET:CE	2.50	0.41
22:W:28:LEU:HB2	22:W:29:PRO:HD3	2.02	0.41
23:X:208:ALA:HB1	23:X:239:TYR:CE2	2.54	0.41
24:Y:241:ILE:HD13	24:Y:264:TYR:CG	2.55	0.41
26:a:218:MET:O	26:a:218:MET:HG3	2.19	0.41
31:U:44:LYS:O	31:U:47:VAL:HG12	2.20	0.41
31:U:115:ASN:OD1	31:U:124:LYS:N	2.53	0.41
33:f:372:LEU:HD13	33:f:406:GLY:HA2	2.02	0.41
1:G:17:SER:OG	1:G:18:PRO:HD2	2.20	0.41
9:o:50:ALA:HA	35:o:301:LDZ:H19	2.02	0.41
17:C:186:VAL:HG12	17:C:292:ILE:HG12	2.03	0.41
21:V:166:TYR:C	21:V:166:TYR:CD2	2.99	0.41
22:W:40:LEU:HD22	22:W:41:GLN:HE22	1.84	0.41
22:W:314:LEU:HD23	22:W:314:LEU:HA	1.90	0.41
24:Y:22:LEU:HD21	24:Y:40:GLU:OE1	2.19	0.41
26:a:248:PHE:O	26:a:255:TRP:CZ3	2.74	0.41
26:a:264:ASN:N	26:a:264:ASN:HD22	2.19	0.41
31:U:602:LEU:CD1	31:U:625:ILE:HD12	2.51	0.41
31:U:627:PHE:CD1	31:U:627:PHE:C	2.98	0.41
35:O:301:LDZ:H3	10:P:125:LEU:HD21	2.01	0.41
12:r:13:VAL:HG13	12:r:180:VAL:HB	2.02	0.41
16:B:64:LYS:O	16:B:65:LEU:CB	2.68	0.41
20:F:405:MET:HE3	20:F:405:MET:HB3	1.99	0.41
22:W:166:LEU:HD12	22:W:166:LEU:HA	1.88	0.41
22:W:256:ILE:HD12	22:W:262:LYS:HB3	2.02	0.41
22:W:272:LEU:CD2	22:W:341:PHE:CE2	3.04	0.41
24:Y:92:GLU:OE2	24:Y:93:LYS:N	2.53	0.41
28:d:142:ILE:CD1	28:d:182:LEU:HD12	2.50	0.41
34:z:392:VAL:O	34:z:396:GLN:HG3	2.21	0.41
2:H:226:LYS:HD3	2:H:226:LYS:C	2.45	0.41
7:M:50:GLU:OE2	7:M:201:HIS:ND1	2.51	0.41
13:S:131:GLN:OE1	35:r:301:LDZ:H4	2.21	0.41
15:A:99:THR:HG22	15:A:115:VAL:HG22	2.01	0.41
15:A:303:ILE:HG23	15:A:336:ARG:CZ	2.51	0.41
21:V:199:ASN:OD1	21:V:199:ASN:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:233:LEU:O	22:W:236:HIS:HB3	2.19	0.41
22:W:307:LYS:O	22:W:310:THR:HG22	2.20	0.41
26:a:87:MET:SD	26:a:92:VAL:HG23	2.61	0.41
26:a:297:ALA:HB1	26:a:302:ILE:O	2.20	0.41
27:b:11:ASP:O	27:b:16:MET:HE3	2.21	0.41
16:B:332:ASN:OD1	16:B:332:ASN:O	2.39	0.41
16:B:433:GLY:O	16:B:436:GLU:HG3	2.20	0.41
18:D:77:GLU:HA	18:D:80:LYS:HE3	2.01	0.41
22:W:341:PHE:CD1	22:W:351:TRP:HE3	2.39	0.41
33:f:502:LEU:N	33:f:503:PRO:HD2	2.36	0.41
33:f:707:LEU:CD2	33:f:741:LEU:HD13	2.51	0.41
9:O:188:ARG:HB3	9:O:189:PRO:HD3	2.02	0.41
14:T:70:MET:HE1	14:T:91:TRP:CE2	2.56	0.41
16:B:361:LYS:HA	16:B:364:ILE:HD12	2.02	0.41
22:W:138:VAL:O	22:W:138:VAL:HG13	2.20	0.41
23:X:266:ASP:OD2	23:X:266:ASP:N	2.54	0.41
26:a:288:HIS:O	26:a:289:ARG:C	2.63	0.41
31:U:169:GLU:OE1	31:U:169:GLU:O	2.39	0.41
2:H:226:LYS:HA	2:H:226:LYS:HE2	2.02	0.41
12:R:21:ALA:HB2	12:R:32:VAL:HG21	2.02	0.41
4:j:59:VAL:O	4:j:59:VAL:HG22	2.20	0.41
19:E:348:THR:HG23	20:F:218:GLN:O	2.20	0.41
22:W:76:GLU:OE1	22:W:76:GLU:N	2.53	0.41
22:W:180:LYS:HE3	22:W:180:LYS:HB3	1.79	0.41
23:X:184:PRO:HG2	23:X:185:LYS:HD2	2.03	0.41
23:X:407:MET:SD	25:Z:266:ILE:HD13	2.59	0.41
24:Y:173:ASP:OD1	24:Y:173:ASP:N	2.45	0.41
25:Z:182:THR:O	25:Z:183:THR:C	2.63	0.41
25:Z:189:GLN:O	25:Z:193:ASN:ND2	2.53	0.41
26:a:269:LEU:O	26:a:272:ILE:HG22	2.20	0.41
27:b:147:GLU:O	27:b:149:ASN:ND2	2.53	0.41
28:d:142:ILE:HD13	28:d:142:ILE:N	2.36	0.41
28:d:177:ASP:HB2	31:U:2:ILE:HG23	2.03	0.41
32:c:208:ARG:HH11	32:c:208:ARG:HG3	1.86	0.41
33:f:54:ASP:O	33:f:58:MET:HG3	2.21	0.41
33:f:498:LEU:HD13	33:f:531:ASN:ND2	2.36	0.41
33:f:870:THR:O	33:f:872:VAL:N	2.54	0.41
1:G:153:LYS:O	1:G:160:TYR:HA	2.21	0.41
1:G:160:TYR:O	1:G:160:TYR:CD2	2.73	0.41
1:G:205:VAL:HG23	1:G:206:LEU:N	2.36	0.41
11:Q:118:MET:HE2	11:Q:124:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:l:63:ILE:HD12	6:l:211:SER:HB3	2.03	0.41
15:A:394:MET:HE3	16:B:349:ARG:NH2	2.35	0.41
16:B:53:THR:C	16:B:55:HIS:N	2.79	0.41
16:B:64:LYS:O	16:B:65:LEU:HG	2.21	0.41
19:E:15:LYS:HG3	20:F:48:LEU:HD13	2.03	0.41
19:E:111:LEU:HD12	19:E:111:LEU:N	2.35	0.41
21:V:230:PHE:CE1	21:V:234:ARG:HG3	2.56	0.41
21:V:279:GLN:O	21:V:279:GLN:HG3	2.21	0.41
21:V:403:ILE:O	21:V:407:VAL:HG23	2.21	0.41
22:W:19:ASP:CG	22:W:21:SER:HG	2.28	0.41
22:W:102:ALA:O	22:W:106:GLN:HG3	2.21	0.41
22:W:376:LYS:HE3	22:W:376:LYS:HB3	1.90	0.41
23:X:50:ILE:CD1	23:X:69:LEU:HD21	2.51	0.41
24:Y:241:ILE:HD11	24:Y:261:PHE:CD2	2.56	0.41
31:U:163:PHE:HE1	31:U:180:SER:HG	1.68	0.41
33:f:67:ASP:OD2	33:f:70:LEU:HD12	2.21	0.41
8:n:90:ARG:HH11	8:n:90:ARG:HG2	1.85	0.41
12:r:36:ILE:HD13	12:r:57:GLU:CB	2.51	0.41
15:A:213:LEU:C	15:A:214:LEU:HD12	2.45	0.41
15:A:322:ASN:OD1	15:A:322:ASN:C	2.63	0.41
17:C:161:ILE:HG21	17:C:199:LEU:CD2	2.51	0.41
19:E:368:MET:HA	19:E:371:VAL:HG12	2.03	0.41
21:V:332:LEU:HA	21:V:335:VAL:HG12	2.03	0.41
22:W:108:CYS:O	22:W:112:VAL:HG23	2.21	0.41
22:W:128:LEU:HD23	22:W:128:LEU:HA	1.96	0.41
22:W:132:THR:CG2	22:W:138:VAL:HG21	2.51	0.41
22:W:267:LEU:HD12	22:W:267:LEU:HA	1.92	0.41
23:X:44:GLN:O	23:X:47:GLU:HG3	2.21	0.41
25:Z:217:THR:CG2	25:Z:219:LYS:HD2	2.51	0.41
26:a:122:LYS:CD	26:a:130:VAL:HG21	2.48	0.41
33:f:189:LYS:O	33:f:193:PRO:CD	2.69	0.41
3:I:177:GLN:CD	3:I:177:GLN:C	2.89	0.40
12:R:38:ILE:HG23	12:R:61:ALA:HA	2.02	0.40
12:r:6:ALA:HA	12:r:14:ILE:O	2.21	0.40
15:A:377:CYS:O	15:A:377:CYS:SG	2.79	0.40
16:B:232:LYS:NZ	36:B:501:ATP:O2G	2.36	0.40
16:B:357:ASP:OD1	16:B:357:ASP:N	2.49	0.40
16:B:412:MET:HE3	17:C:178:LEU:HD13	2.02	0.40
17:C:83:LYS:HA	17:C:105:ILE:HD11	2.03	0.40
17:C:147:THR:HG22	17:C:205:HIS:CE1	2.55	0.40
19:E:29:LEU:HD22	20:F:62:VAL:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:E:142:ILE:CG1	19:E:183:LEU:HD11	2.51	0.40
19:E:284:THR:O	19:E:284:THR:OG1	2.35	0.40
19:E:336:ASP:OD1	19:E:337:GLY:N	2.55	0.40
24:Y:315:THR:HG22	24:Y:317:GLY:H	1.87	0.40
25:Z:246:VAL:HA	28:d:330:ILE:HD11	2.03	0.40
28:d:301:ASP:N	28:d:301:ASP:OD1	2.54	0.40
33:f:462:ALA:HB3	33:f:489:TYR:CE2	2.57	0.40
11:Q:56:PHE:CE2	11:Q:102:LEU:HD11	2.57	0.40
14:T:6:VAL:HG11	8:n:120:MET:CE	2.51	0.40
2:h:118:GLN:O	2:h:121:THR:HG22	2.21	0.40
9:o:188:ARG:HB3	9:o:189:PRO:HD3	2.03	0.40
15:A:91:GLN:HB2	15:A:92:PRO:HD3	2.02	0.40
17:C:59:LEU:HD12	18:D:72:PHE:CE1	2.55	0.40
17:C:127:LEU:HD13	18:D:102:ILE:HD11	2.03	0.40
17:C:135:VAL:HA	17:C:138:MET:HE1	2.04	0.40
18:D:220:ALA:HB2	19:E:267:PHE:HZ	1.86	0.40
19:E:198:VAL:HG22	19:E:199:VAL:N	2.37	0.40
19:E:384:LEU:HD23	19:E:384:LEU:N	2.36	0.40
21:V:191:LEU:O	21:V:191:LEU:HD12	2.22	0.40
21:V:345:ARG:NH1	29:e:42:ASN:O	2.54	0.40
22:W:34:LEU:O	22:W:39:ARG:HG2	2.21	0.40
22:W:117:ASP:OD2	22:W:120:ILE:HB	2.20	0.40
22:W:149:LEU:O	22:W:149:LEU:HD12	2.21	0.40
22:W:305:LEU:HD13	22:W:320:LEU:HD11	2.02	0.40
23:X:205:LYS:O	23:X:209:THR:HG22	2.21	0.40
23:X:246:LYS:N	23:X:246:LYS:CD	2.85	0.40
26:a:184:ASP:OD1	26:a:185:ILE:N	2.52	0.40
27:b:22:LEU:CB	27:b:23:PRO:CD	2.99	0.40
32:c:118:PHE:O	32:c:121:TRP:NE1	2.40	0.40
33:f:520:LEU:O	33:f:524:MET:HG3	2.22	0.40
1:G:165:ALA:HB3	2:H:55:LEU:HD22	2.03	0.40
16:B:429:LYS:O	16:B:430:LYS:HD2	2.20	0.40
19:E:320:ILE:HD11	19:E:347:CYS:HB3	2.02	0.40
22:W:298:GLU:O	22:W:300:PRO:HD3	2.21	0.40
22:W:369:TYR:O	22:W:370:TYR:CD2	2.75	0.40
22:W:449:GLU:OE1	25:Z:223:ASN:ND2	2.54	0.40
4:J:71:MET:HE3	4:J:131:ALA:HB1	2.04	0.40
7:m:181:MET:HE3	7:m:181:MET:HB3	2.00	0.40
15:A:77:LEU:C	15:A:79:ASP:N	2.79	0.40
15:A:378:PRO:O	15:A:379:ASN:C	2.64	0.40
18:D:194:ILE:HG13	18:D:196:ILE:HG12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:72:LYS:HG2	22:W:73:MET:HE1	2.04	0.40
22:W:90:LEU:CD2	22:W:93:ARG:HD2	2.50	0.40
22:W:188:GLU:OE1	22:W:225:LYS:HE2	2.22	0.40
25:Z:253:THR:O	25:Z:257:MET:HG2	2.20	0.40
26:a:97:LEU:O	26:a:100:THR:HG22	2.22	0.40
27:b:29:GLN:O	27:b:33:VAL:HG22	2.22	0.40
27:b:157:VAL:O	27:b:161:ASN:OD1	2.40	0.40
28:d:262:ILE:HD12	28:d:262:ILE:H	1.85	0.40
31:U:89:ASN:OD1	31:U:89:ASN:C	2.63	0.40
31:U:245:ALA:HB1	31:U:325:MET:SD	2.61	0.40
31:U:364:VAL:HG22	32:c:177:THR:OG1	2.21	0.40
32:c:180:ASN:O	32:c:184:LEU:HD13	2.20	0.40
33:f:110:TYR:O	33:f:111:GLU:C	2.64	0.40
33:f:394:ASP:N	33:f:394:ASP:OD1	2.53	0.40
33:f:832:THR:HG23	33:f:870:THR:HG23	2.04	0.40
33:f:905:ASN:OD1	33:f:905:ASN:N	2.53	0.40
1:G:123:GLN:O	1:G:126:THR:HG22	2.21	0.40
5:k:85:ALA:HB2	5:k:139:VAL:HG21	2.03	0.40
15:A:287:ASP:OD1	15:A:287:ASP:N	2.55	0.40
15:A:372:LEU:HD13	15:A:372:LEU:C	2.46	0.40
16:B:241:ASN:OD1	16:B:241:ASN:C	2.64	0.40
16:B:412:MET:CE	17:C:177:ALA:HB3	2.48	0.40
17:C:171:HIS:HB3	17:C:174:LEU:HD13	2.02	0.40
19:E:368:MET:O	19:E:371:VAL:HG12	2.22	0.40
22:W:201:ARG:NH1	22:W:201:ARG:CG	2.80	0.40
22:W:241:LEU:O	22:W:245:LYS:HG3	2.20	0.40
22:W:256:ILE:CD1	22:W:262:LYS:HB3	2.51	0.40
22:W:407:ASP:O	22:W:411:GLY:N	2.54	0.40
24:Y:51:ALA:HB3	24:Y:52:PRO:HD3	2.04	0.40
24:Y:378:ASN:OD1	24:Y:378:ASN:C	2.64	0.40
28:d:232:LEU:CD2	28:d:244:VAL:HG23	2.51	0.40
33:f:189:LYS:O	33:f:193:PRO:HD2	2.21	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	G	238/246 (97%)	226 (95%)	12 (5%)	0	100	100
1	g	238/246 (97%)	232 (98%)	6 (2%)	0	100	100
2	H	227/234 (97%)	224 (99%)	3 (1%)	0	100	100
2	h	227/234 (97%)	223 (98%)	4 (2%)	0	100	100
3	I	245/261 (94%)	237 (97%)	8 (3%)	0	100	100
3	i	245/261 (94%)	240 (98%)	5 (2%)	0	100	100
4	J	230/248 (93%)	225 (98%)	5 (2%)	0	100	100
4	j	230/248 (93%)	222 (96%)	8 (4%)	0	100	100
5	K	231/241 (96%)	228 (99%)	3 (1%)	0	100	100
5	k	231/241 (96%)	228 (99%)	3 (1%)	0	100	100
6	L	231/263 (88%)	221 (96%)	10 (4%)	0	100	100
6	l	231/263 (88%)	229 (99%)	2 (1%)	0	100	100
7	M	237/255 (93%)	233 (98%)	4 (2%)	0	100	100
7	m	237/255 (93%)	234 (99%)	3 (1%)	0	100	100
8	N	200/239 (84%)	198 (99%)	2 (1%)	0	100	100
8	n	200/239 (84%)	195 (98%)	5 (2%)	0	100	100
9	O	218/277 (79%)	213 (98%)	5 (2%)	0	100	100
9	o	218/277 (79%)	213 (98%)	5 (2%)	0	100	100
10	P	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
10	p	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
11	Q	194/201 (96%)	187 (96%)	7 (4%)	0	100	100
11	q	194/201 (96%)	188 (97%)	6 (3%)	0	100	100
12	R	198/263 (75%)	198 (100%)	0	0	100	100
12	r	198/263 (75%)	196 (99%)	2 (1%)	0	100	100
13	S	210/241 (87%)	207 (99%)	3 (1%)	0	100	100
13	s	210/241 (87%)	209 (100%)	1 (0%)	0	100	100
14	T	210/264 (80%)	198 (94%)	12 (6%)	0	100	100
14	t	210/264 (80%)	201 (96%)	9 (4%)	0	100	100
15	A	388/433 (90%)	366 (94%)	22 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	B	391/440 (89%)	361 (92%)	27 (7%)	3 (1%)	16	44
17	C	387/406 (95%)	357 (92%)	30 (8%)	0	100	100
18	D	378/418 (90%)	350 (93%)	27 (7%)	1 (0%)	36	66
19	E	387/403 (96%)	368 (95%)	19 (5%)	0	100	100
20	F	413/439 (94%)	398 (96%)	14 (3%)	1 (0%)	43	72
21	V	440/534 (82%)	420 (96%)	20 (4%)	0	100	100
22	W	438/456 (96%)	420 (96%)	17 (4%)	1 (0%)	43	72
23	X	382/422 (90%)	366 (96%)	16 (4%)	0	100	100
24	Y	378/389 (97%)	364 (96%)	13 (3%)	1 (0%)	36	66
25	Z	284/324 (88%)	268 (94%)	14 (5%)	2 (1%)	18	47
26	a	371/376 (99%)	330 (89%)	40 (11%)	1 (0%)	36	66
27	b	189/377 (50%)	160 (85%)	28 (15%)	1 (0%)	24	55
28	d	268/350 (77%)	238 (89%)	28 (10%)	2 (1%)	18	47
29	e	46/70 (66%)	36 (78%)	10 (22%)	0	100	100
31	U	808/953 (85%)	762 (94%)	44 (5%)	2 (0%)	43	72
32	c	279/310 (90%)	262 (94%)	16 (6%)	1 (0%)	30	60
33	f	832/908 (92%)	786 (94%)	46 (6%)	0	100	100
34	z	113/468 (24%)	111 (98%)	2 (2%)	0	100	100
All	All	13314/15352 (87%)	12722 (96%)	576 (4%)	16 (0%)	49	77

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	W	370	TYR
25	Z	149	THR
26	a	105	LYS
16	B	65	LEU
16	B	278	ALA
20	F	279	ALA
27	b	22	LEU
16	B	191	ASP
25	Z	194	GLN
28	d	283	LEU
28	d	282	ILE
32	c	25	VAL
18	D	98	GLN

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Mol	Chain	Res	Type
24	Y	98	SER
31	U	4	SER
31	U	187	LEU

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	G	164/210 (78%)	163 (99%)	1 (1%)	78	92
1	g	168/210 (80%)	167 (99%)	1 (1%)	78	92
2	H	150/191 (78%)	148 (99%)	2 (1%)	61	86
2	h	150/191 (78%)	149 (99%)	1 (1%)	76	91
3	I	166/221 (75%)	165 (99%)	1 (1%)	78	92
3	i	160/221 (72%)	159 (99%)	1 (1%)	78	92
4	J	136/211 (64%)	136 (100%)	0	100	100
4	j	136/211 (64%)	134 (98%)	2 (2%)	57	84
5	K	159/203 (78%)	158 (99%)	1 (1%)	78	92
5	k	158/203 (78%)	158 (100%)	0	100	100
6	L	161/224 (72%)	160 (99%)	1 (1%)	78	92
6	l	161/224 (72%)	158 (98%)	3 (2%)	50	81
7	M	162/212 (76%)	162 (100%)	0	100	100
7	m	163/212 (77%)	162 (99%)	1 (1%)	78	92
8	N	141/181 (78%)	140 (99%)	1 (1%)	76	91
8	n	140/181 (77%)	139 (99%)	1 (1%)	76	91
9	O	158/228 (69%)	158 (100%)	0	100	100
9	o	157/228 (69%)	157 (100%)	0	100	100
10	P	159/174 (91%)	157 (99%)	2 (1%)	61	86
10	p	156/174 (90%)	156 (100%)	0	100	100
11	Q	149/171 (87%)	148 (99%)	1 (1%)	76	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	q	148/171 (86%)	148 (100%)	0	100	100
12	R	139/202 (69%)	139 (100%)	0	100	100
12	r	138/202 (68%)	138 (100%)	0	100	100
13	S	158/199 (79%)	158 (100%)	0	100	100
13	s	159/199 (80%)	159 (100%)	0	100	100
14	T	151/215 (70%)	150 (99%)	1 (1%)	76	91
14	t	149/215 (69%)	148 (99%)	1 (1%)	76	91
15	A	333/372 (90%)	329 (99%)	4 (1%)	63	87
16	B	344/385 (89%)	330 (96%)	14 (4%)	27	62
17	C	340/352 (97%)	330 (97%)	10 (3%)	37	73
18	D	333/366 (91%)	319 (96%)	14 (4%)	26	61
19	E	341/353 (97%)	331 (97%)	10 (3%)	37	73
20	F	357/379 (94%)	347 (97%)	10 (3%)	38	73
21	V	388/460 (84%)	380 (98%)	8 (2%)	47	79
22	W	405/416 (97%)	383 (95%)	22 (5%)	20	51
23	X	330/362 (91%)	323 (98%)	7 (2%)	47	79
24	Y	335/344 (97%)	326 (97%)	9 (3%)	39	74
25	Z	257/295 (87%)	247 (96%)	10 (4%)	28	64
26	a	333/336 (99%)	322 (97%)	11 (3%)	33	69
27	b	167/312 (54%)	159 (95%)	8 (5%)	23	56
28	d	233/294 (79%)	224 (96%)	9 (4%)	28	64
29	e	39/63 (62%)	38 (97%)	1 (3%)	40	75
31	U	692/816 (85%)	676 (98%)	16 (2%)	44	78
32	c	249/268 (93%)	241 (97%)	8 (3%)	34	70
33	f	704/763 (92%)	692 (98%)	12 (2%)	53	83
34	z	100/377 (26%)	96 (96%)	4 (4%)	28	63
All	All	10576/12997 (81%)	10367 (98%)	209 (2%)	48	80

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	191	PHE
2	H	47	THR

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Mol	Chain	Res	Type
2	H	101	GLN
3	I	164	ILE
5	K	225	ASN
6	L	198	THR
8	N	108	GLU
10	P	121	CYS
10	P	151	SER
11	Q	141	SER
14	T	200	GLU
1	g	189	TRP
2	h	48	GLU
3	i	43	VAL
4	j	11	SER
4	j	69	VAL
6	l	9	ASP
6	l	35	THR
6	l	211	SER
7	m	37	ILE
8	n	145	ARG
14	t	54	SER
15	A	87	LEU
15	A	93	LEU
15	A	166	VAL
15	A	384	GLU
16	B	53	THR
16	B	134	SER
16	B	162	VAL
16	B	165	ASP
16	B	197	ILE
16	B	200	SER
16	B	212	GLU
16	B	214	MET
16	B	235	LEU
16	B	320	ASP
16	B	321	SER
16	B	331	THR
16	B	363	ARG
16	B	374	LEU
17	C	30	GLU
17	C	59	LEU
17	C	105	ILE
17	C	138	MET

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Mol	Chain	Res	Type
17	C	178	LEU
17	C	199	LEU
17	C	221	GLN
17	C	236	VAL
17	C	283	PHE
17	C	301	LEU
18	D	46	LYS
18	D	52	GLU
18	D	60	TYR
18	D	79	VAL
18	D	80	LYS
18	D	161	ASP
18	D	191	TYR
18	D	197	ASP
18	D	222	HIS
18	D	230	VAL
18	D	249	ASP
18	D	296	MET
18	D	354	LEU
18	D	390	ASN
19	E	87	LEU
19	E	114	GLU
19	E	124	HIS
19	E	146	ARG
19	E	158	LEU
19	E	170	CYS
19	E	187	VAL
19	E	199	VAL
19	E	262	ASN
19	E	268	ASP
20	F	59	VAL
20	F	66	LEU
20	F	149	ASP
20	F	156	ASP
20	F	166	THR
20	F	169	ASP
20	F	186	SER
20	F	325	GLN
20	F	356	MET
20	F	392	ASN
21	V	159	LEU
21	V	160	LEU

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Mol	Chain	Res	Type
21	V	185	GLN
21	V	240	LEU
21	V	320	THR
21	V	418	SER
21	V	427	GLN
21	V	432	GLU
22	W	41	GLN
22	W	43	VAL
22	W	86	ASN
22	W	88	MET
22	W	104	MET
22	W	110	THR
22	W	131	VAL
22	W	136	ILE
22	W	159	VAL
22	W	183	VAL
22	W	244	CYS
22	W	255	CYS
22	W	265	GLN
22	W	271	VAL
22	W	274	VAL
22	W	275	ILE
22	W	299	ILE
22	W	329	ARG
22	W	339	ASP
22	W	344	THR
22	W	375	MET
22	W	401	THR
23	X	93	LEU
23	X	133	LEU
23	X	154	LEU
23	X	191	THR
23	X	195	THR
23	X	242	ILE
23	X	332	GLU
24	Y	130	LYS
24	Y	196	GLN
24	Y	277	VAL
24	Y	291	HIS
24	Y	292	TYR
24	Y	319	MET
24	Y	321	GLU

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Mol	Chain	Res	Type
24	Y	351	ASN
24	Y	388	ASN
25	Z	26	ILE
25	Z	32	GLN
25	Z	42	SER
25	Z	64	ASP
25	Z	85	VAL
25	Z	104	ASN
25	Z	178	ASP
25	Z	256	GLN
25	Z	268	SER
25	Z	276	ILE
26	a	8	LEU
26	a	30	THR
26	a	59	LEU
26	a	150	SER
26	a	178	ARG
26	a	182	CYS
26	a	194	GLN
26	a	211	PHE
26	a	301	LYS
26	a	320	VAL
26	a	373	ASP
27	b	6	THR
27	b	14	GLU
27	b	22	LEU
27	b	36	VAL
27	b	84	ILE
27	b	147	GLU
27	b	160	LEU
27	b	179	LEU
28	d	111	LYS
28	d	143	LEU
28	d	182	LEU
28	d	185	SER
28	d	210	THR
28	d	284	PHE
28	d	300	THR
28	d	315	TYR
28	d	329	THR
29	e	18	GLU
31	U	12	LEU

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Mol	Chain	Res	Type
31	U	69	TYR
31	U	131	GLU
31	U	187	LEU
31	U	362	ASN
31	U	369	THR
31	U	373	ASN
31	U	462	LEU
31	U	711	GLN
31	U	732	LEU
31	U	767	THR
31	U	805	ASN
31	U	811	PHE
31	U	875	PHE
31	U	891	VAL
31	U	894	MET
32	c	64	ASP
32	c	109	VAL
32	c	184	LEU
32	c	253	LYS
32	c	273	LYS
32	c	290	VAL
32	c	291	LEU
32	c	310	LYS
33	f	89	MET
33	f	124	ASP
33	f	240	VAL
33	f	277	LEU
33	f	327	ASN
33	f	428	GLN
33	f	434	TYR
33	f	608	LYS
33	f	681	TYR
33	f	759	LEU
33	f	814	SER
33	f	901	ARG
34	z	33	LEU
34	z	41	THR
34	z	393	GLU
34	z	403	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	68	HIS
1	G	193	GLN
2	H	20	GLN
2	H	101	GLN
2	H	213	ASN
3	I	102	GLN
5	K	97	GLN
6	L	146	GLN
7	M	110	HIS
7	M	120	HIS
8	N	63	GLN
11	Q	65	GLN
11	Q	82	ASN
12	R	71	ASN
13	S	79	ASN
13	S	151	ASN
14	T	65	GLN
14	T	147	GLN
2	h	108	GLN
3	i	230	GLN
4	j	92	GLN
6	l	146	GLN
7	m	120	HIS
7	m	201	HIS
8	n	8	GLN
9	o	36	HIS
10	p	172	ASN
11	q	63	ASN
12	r	176	ASN
13	s	79	ASN
13	s	131	GLN
13	s	151	ASN
13	s	152	GLN
13	s	157	ASN
15	A	414	ASN
16	B	298	ASN
16	B	315	GLN
17	C	40	GLN
17	C	41	ASN
17	C	50	ASN
17	C	124	HIS
17	C	171	HIS
17	C	205	HIS

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Mol	Chain	Res	Type
17	C	343	ASN
18	D	67	ASN
18	D	312	ASN
18	D	376	ASN
20	F	83	ASN
22	W	26	GLN
22	W	107	GLN
22	W	167	GLN
22	W	235	GLN
22	W	288	HIS
22	W	399	ASN
22	W	440	ASN
23	X	127	GLN
23	X	213	GLN
23	X	322	HIS
23	X	346	GLN
23	X	406	ASN
24	Y	14	ASN
24	Y	154	ASN
24	Y	280	GLN
24	Y	378	ASN
25	Z	7	GLN
25	Z	12	HIS
25	Z	189	GLN
25	Z	223	ASN
25	Z	278	ASN
26	a	86	GLN
26	a	194	GLN
26	a	332	HIS
27	b	76	HIS
28	d	195	ASN
28	d	209	HIS
31	U	267	ASN
31	U	338	HIS
31	U	467	ASN
31	U	645	ASN
31	U	647	HIS
31	U	718	ASN
32	c	197	ASN
32	c	274	ASN
32	c	278	GLN
32	c	283	HIS

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Mol	Chain	Res	Type
33	f	224	ASN
33	f	475	ASN
33	f	610	GLN
33	f	752	HIS
34	z	382	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
35	LDZ	R	301	-	33,34,34	0.46	0	42,44,44	0.71	1 (2%)
35	LDZ	o	301	-	33,34,34	0.45	0	42,44,44	0.66	1 (2%)
36	ATP	F	501	37	32,33,33	0.42	0	48,52,52	0.73	0
35	LDZ	n	301	-	33,34,34	0.49	1 (3%)	42,44,44	0.67	0
38	ADP	E	401	-	28,29,29	1.34	4 (14%)	43,45,45	1.91	9 (20%)
35	LDZ	N	301	-	33,34,34	0.50	1 (3%)	42,44,44	0.65	0
35	LDZ	O	301	-	33,34,34	0.49	1 (3%)	42,44,44	0.76	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	ATP	D	502	37	32,33,33	0.45	0	48,52,52	0.75	0
35	LDZ	r	301	-	33,34,34	0.51	0	42,44,44	0.88	1 (2%)
36	ATP	B	501	37	32,33,33	0.48	0	48,52,52	0.75	1 (2%)
36	ATP	A	501	37	32,33,33	0.37	0	48,52,52	0.73	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LDZ	R	301	-	-	7/38/39/39	0/1/1/1
35	LDZ	o	301	-	-	8/38/39/39	0/1/1/1
36	ATP	F	501	37	-	4/22/38/38	0/3/3/3
35	LDZ	n	301	-	-	4/38/39/39	0/1/1/1
38	ADP	E	401	-	-	5/16/32/32	0/3/3/3
35	LDZ	N	301	-	-	8/38/39/39	0/1/1/1
35	LDZ	O	301	-	-	14/38/39/39	0/1/1/1
36	ATP	D	502	37	-	6/22/38/38	0/3/3/3
35	LDZ	r	301	-	-	11/38/39/39	0/1/1/1
36	ATP	B	501	37	-	5/22/38/38	0/3/3/3
36	ATP	A	501	37	-	3/22/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	E	401	ADP	C5-C4	4.38	1.46	1.39
38	E	401	ADP	C5-N7	-2.61	1.34	1.39
38	E	401	ADP	C5-C6	2.32	1.47	1.41
38	E	401	ADP	C8-N7	2.11	1.35	1.31
35	O	301	LDZ	C17-N16	-2.07	1.43	1.46
35	N	301	LDZ	C17-N16	-2.06	1.43	1.46
35	n	301	LDZ	C17-N16	-2.00	1.43	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	E	401	ADP	C5-C4-N3	-6.01	118.44	126.72
38	E	401	ADP	N3-C4-N9	5.01	135.69	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	E	401	ADP	C2-N3-C4	3.84	121.22	111.83
35	r	301	LDZ	C14-N13-C12	3.73	129.67	121.65
38	E	401	ADP	N3-C2-N1	-3.65	123.06	128.58
38	E	401	ADP	C4-C5-N7	-2.99	107.16	110.58
35	O	301	LDZ	C14-N13-C12	2.83	127.73	121.65
38	E	401	ADP	C4-N9-C8	2.76	108.63	105.74
38	E	401	ADP	C5-N7-C8	2.44	107.29	103.45
35	O	301	LDZ	C18-C17-N16	2.35	114.23	110.69
38	E	401	ADP	C3'-C2'-C1'	2.34	105.89	101.46
35	o	301	LDZ	C18-C17-N16	2.21	114.03	110.69
36	B	501	ATP	O3'-C3'-C4'	-2.09	105.09	111.08
35	R	301	LDZ	C15-C14-N13	-2.06	105.55	111.11
38	E	401	ADP	N9-C8-N7	-2.03	111.05	113.94
36	A	501	ATP	O3'-C3'-C2'	-2.02	105.33	111.82
36	A	501	ATP	O3'-C3'-C4'	-2.01	105.31	111.08

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	N	301	LDZ	O8-C9-N10-C11
35	O	301	LDZ	C15-C14-N13-C12
35	R	301	LDZ	C22-C17-C18-C19
35	n	301	LDZ	O31-C9-O8-C7
35	n	301	LDZ	N10-C9-O8-C7
36	D	502	ATP	C5'-O5'-PA-O3A
36	F	501	ATP	C5'-O5'-PA-O2A
36	F	501	ATP	C5'-O5'-PA-O3A
38	E	401	ADP	C5'-O5'-PA-O1A
38	E	401	ADP	C5'-O5'-PA-O2A
38	E	401	ADP	C5'-O5'-PA-O3A
35	N	301	LDZ	O31-C9-N10-C11
35	r	301	LDZ	O31-C9-O8-C7
35	r	301	LDZ	N10-C9-O8-C7
35	O	301	LDZ	C15-C14-C24-C25
35	o	301	LDZ	N10-C9-O8-C7
35	o	301	LDZ	O31-C9-O8-C7
36	A	501	ATP	C3'-C4'-C5'-O5'
36	D	502	ATP	C3'-C4'-C5'-O5'
36	F	501	ATP	O4'-C4'-C5'-O5'
36	B	501	ATP	C3'-C4'-C5'-O5'
35	O	301	LDZ	N10-C9-O8-C7

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Mol	Chain	Res	Type	Atoms
35	r	301	LDZ	C11-C12-N13-C14
35	O	301	LDZ	C11-C30-C31-C33
35	r	301	LDZ	C14-C24-C25-C27
35	r	301	LDZ	O32-C12-N13-C14
35	O	301	LDZ	C11-C30-C31-C32
35	O	301	LDZ	C17-C18-C19-C21
35	r	301	LDZ	C14-C24-C25-C26
35	O	301	LDZ	C17-C18-C19-C20
35	N	301	LDZ	C14-C24-C25-C26
35	O	301	LDZ	O31-C9-O8-C7
35	N	301	LDZ	C14-C24-C25-C27
35	o	301	LDZ	C11-C30-C31-C32
35	o	301	LDZ	C11-C30-C31-C33
36	A	501	ATP	O4'-C4'-C5'-O5'
36	B	501	ATP	O4'-C4'-C5'-O5'
36	D	502	ATP	O4'-C4'-C5'-O5'
35	R	301	LDZ	C11-C30-C31-C33
36	F	501	ATP	C3'-C4'-C5'-O5'
36	B	501	ATP	C4'-C5'-O5'-PA
35	o	301	LDZ	C12-C11-C30-C31
35	O	301	LDZ	C14-C24-C25-C27
35	O	301	LDZ	C14-C24-C25-C26
35	r	301	LDZ	C18-C17-N16-C15
35	R	301	LDZ	N13-C14-C15-N16
35	R	301	LDZ	N13-C14-C15-O34
36	A	501	ATP	C4'-C5'-O5'-PA
35	O	301	LDZ	N13-C14-C24-C25
35	N	301	LDZ	C12-C11-C30-C31
35	o	301	LDZ	N10-C11-C30-C31
35	r	301	LDZ	C30-C11-N10-C9
36	D	502	ATP	C5'-O5'-PA-O1A
36	D	502	ATP	C2'-C1'-N9-C4
35	N	301	LDZ	N10-C11-C30-C31
35	o	301	LDZ	N13-C14-C24-C25
35	n	301	LDZ	C17-C18-C19-C20
36	D	502	ATP	C2'-C1'-N9-C8
35	O	301	LDZ	C22-C17-N16-C15
35	r	301	LDZ	C22-C17-N16-C15
35	r	301	LDZ	N10-C11-C12-O32
35	o	301	LDZ	C22-C17-C18-C19
35	N	301	LDZ	C17-C18-C19-C21
35	r	301	LDZ	N10-C11-C12-N13

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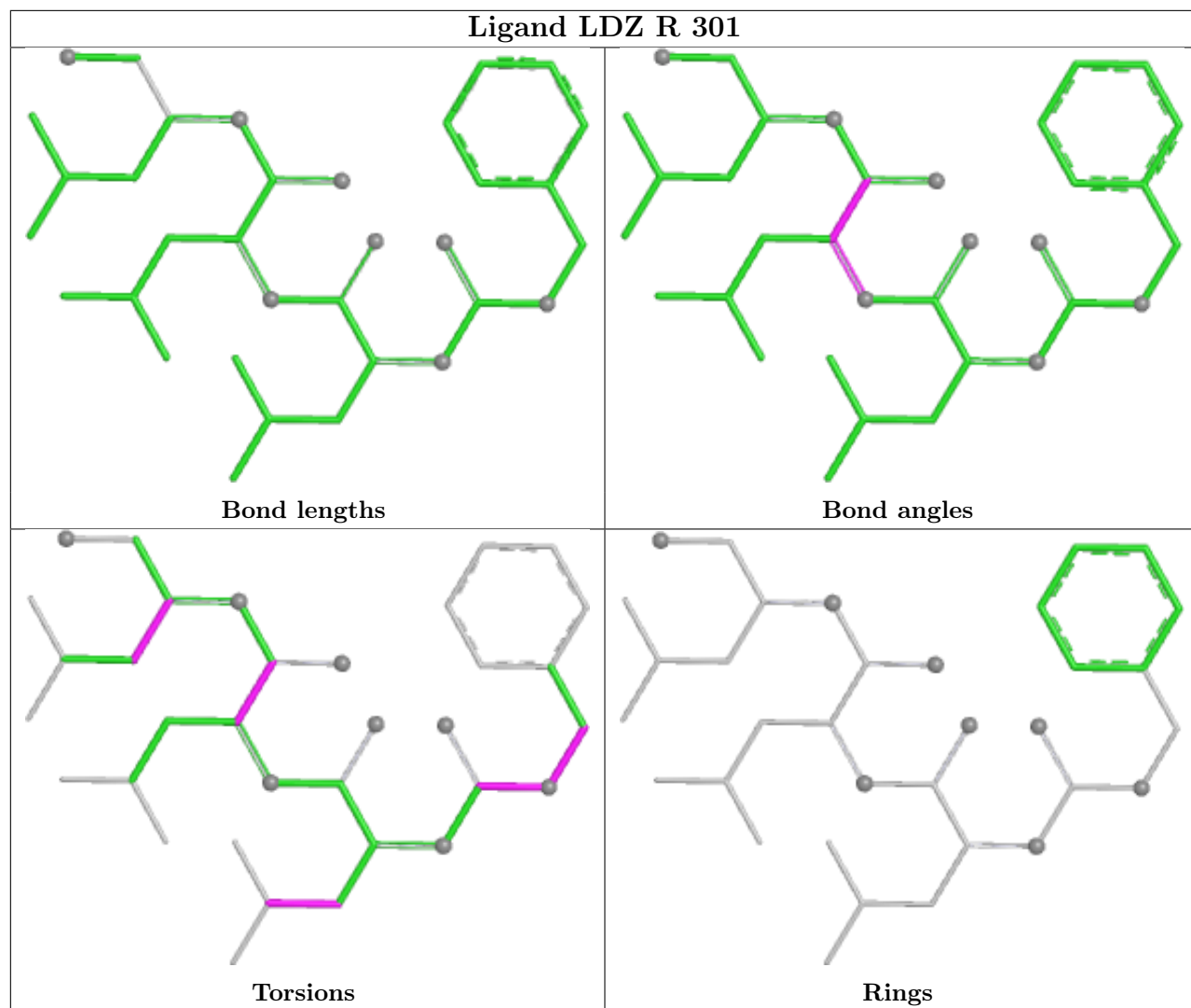
Mol	Chain	Res	Type	Atoms
35	n	301	LDZ	N10-C11-C30-C31
38	E	401	ADP	C2'-C1'-N9-C8
35	O	301	LDZ	C18-C17-N16-C15
36	B	501	ATP	PG-O3B-PB-O1B
36	B	501	ATP	PG-O3B-PB-O2B
35	R	301	LDZ	N16-C17-C18-C19
35	R	301	LDZ	C3-C7-O8-C9
35	N	301	LDZ	C17-C18-C19-C20
35	R	301	LDZ	N10-C9-O8-C7
38	E	401	ADP	C3'-C4'-C5'-O5'
35	O	301	LDZ	C30-C11-C12-O32

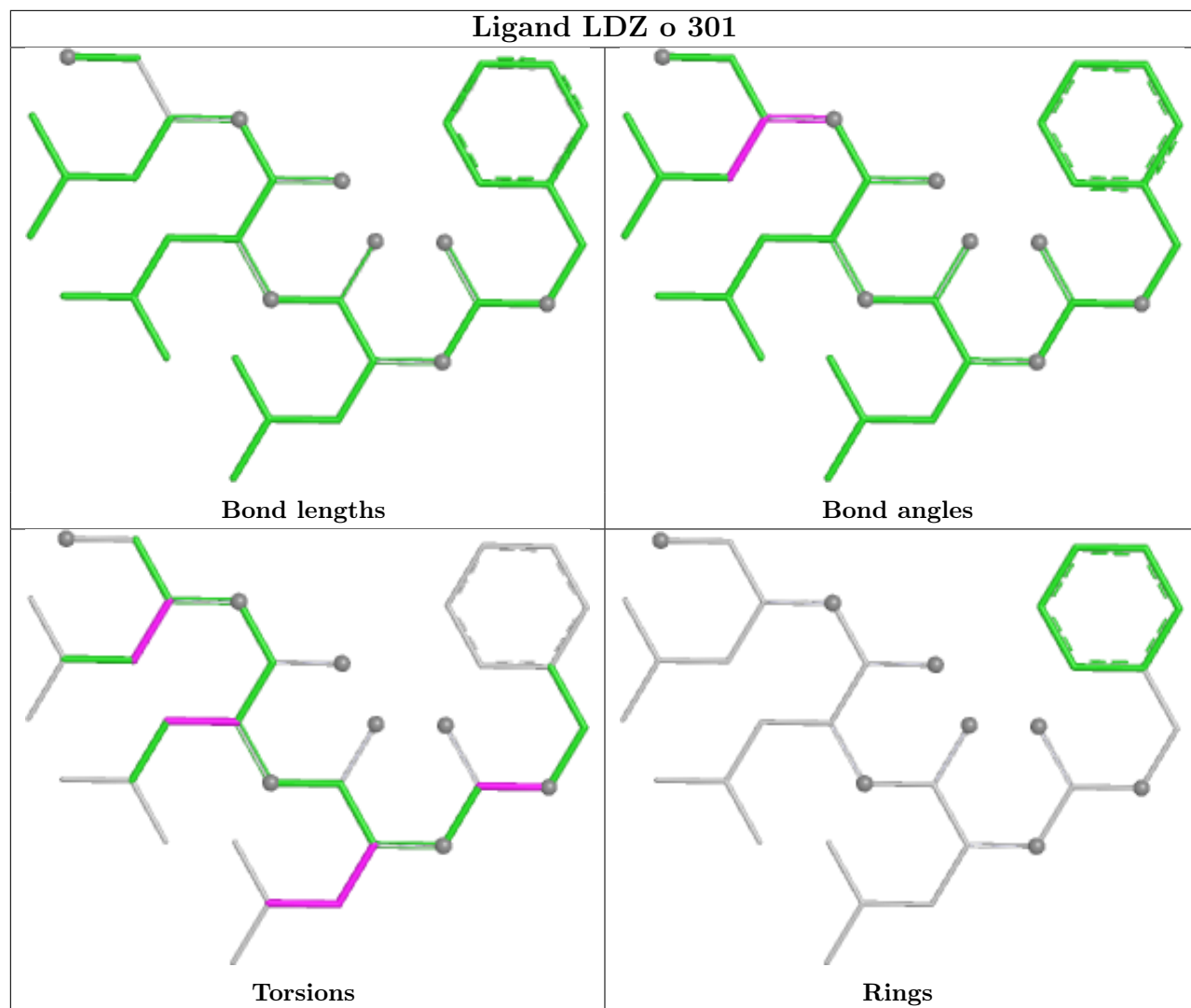
There are no ring outliers.

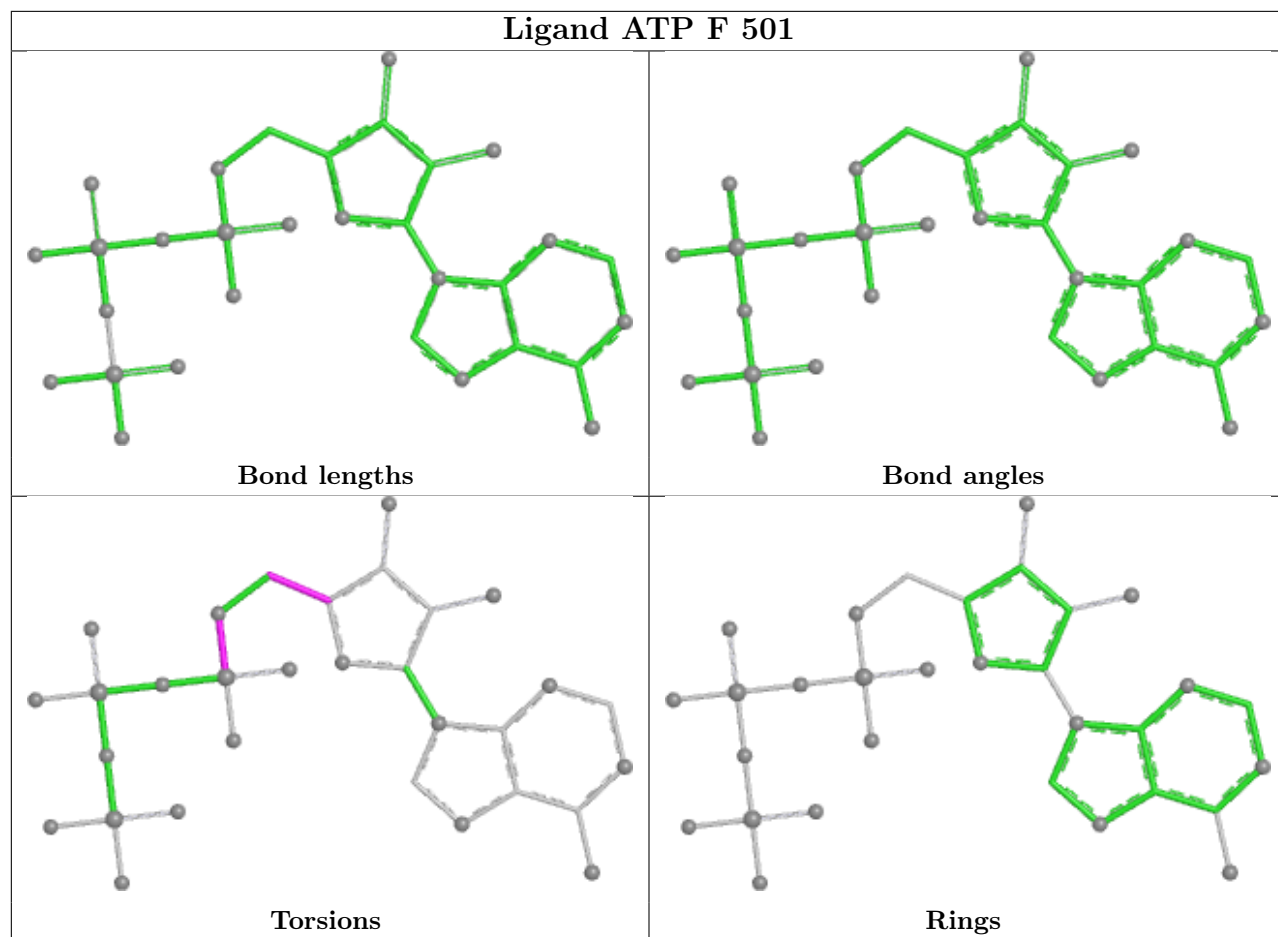
9 monomers are involved in 20 short contacts:

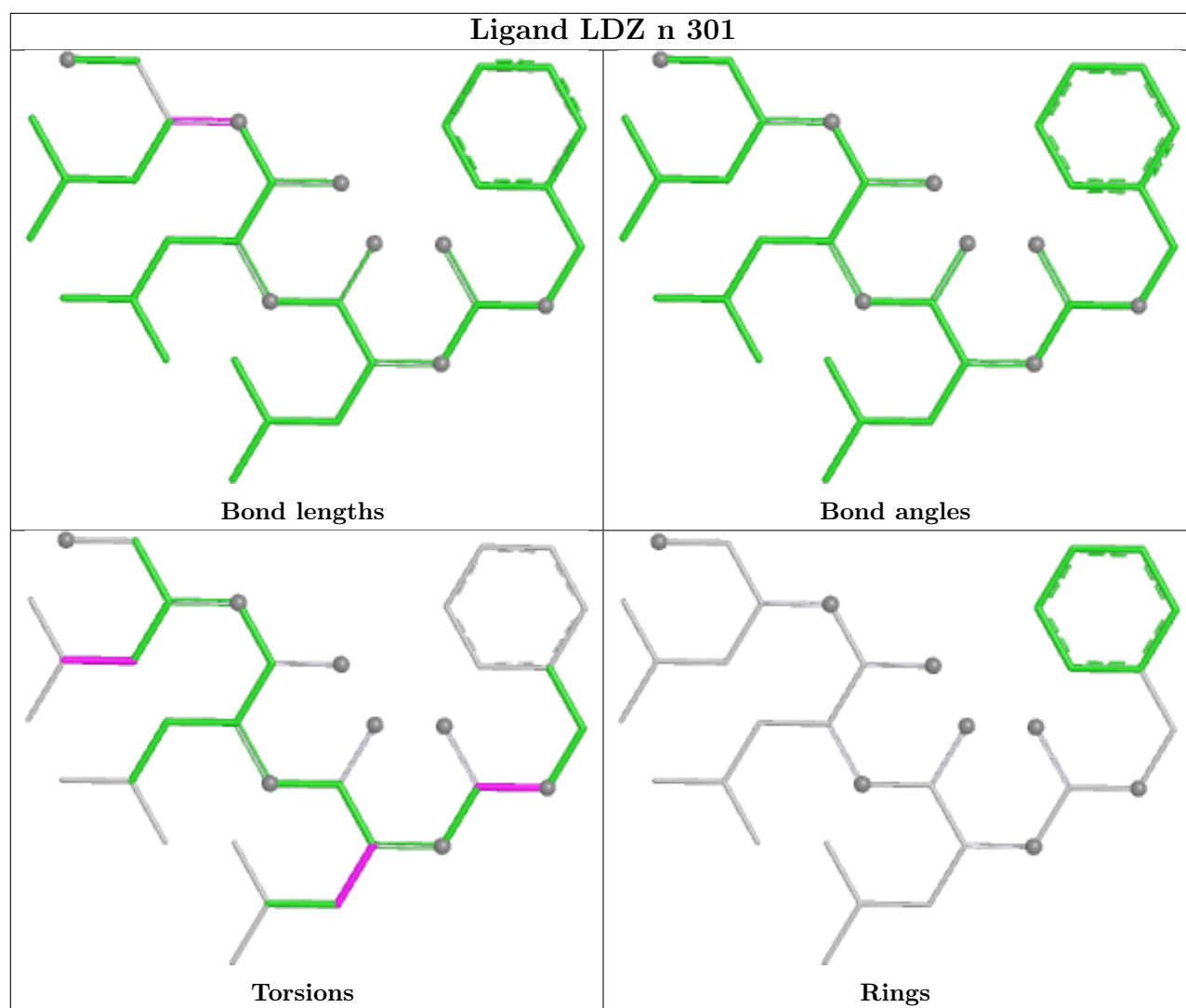
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	R	301	LDZ	4	0
35	o	301	LDZ	2	0
35	n	301	LDZ	5	0
38	E	401	ADP	2	0
35	N	301	LDZ	2	0
35	O	301	LDZ	2	0
35	r	301	LDZ	1	0
36	B	501	ATP	1	0
36	A	501	ATP	1	0

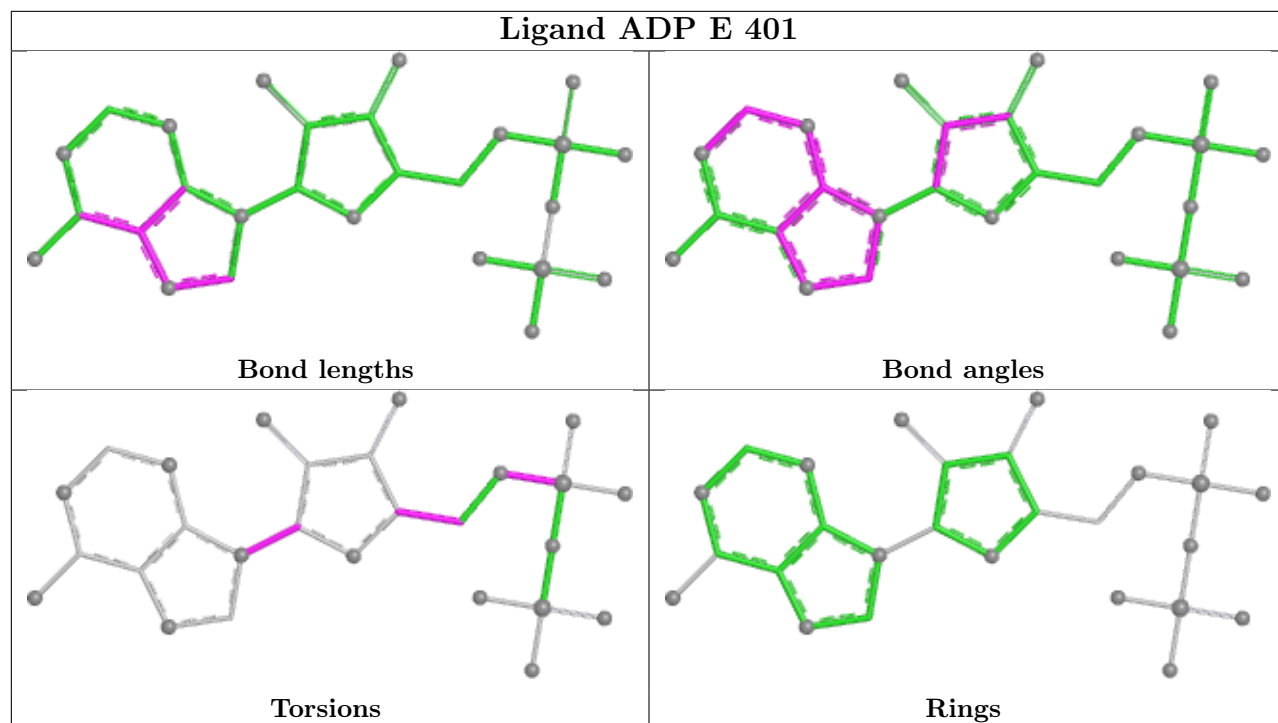
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

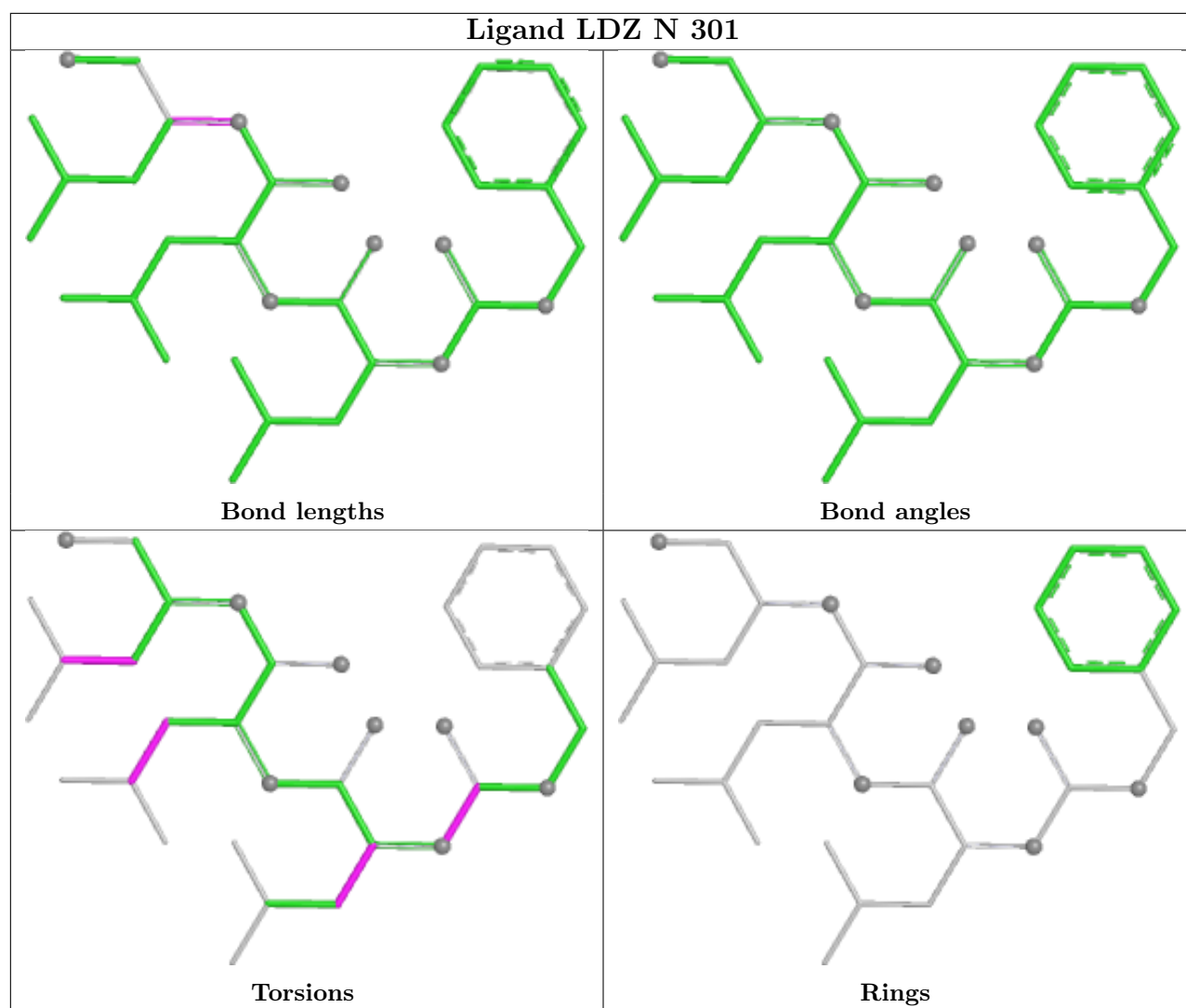


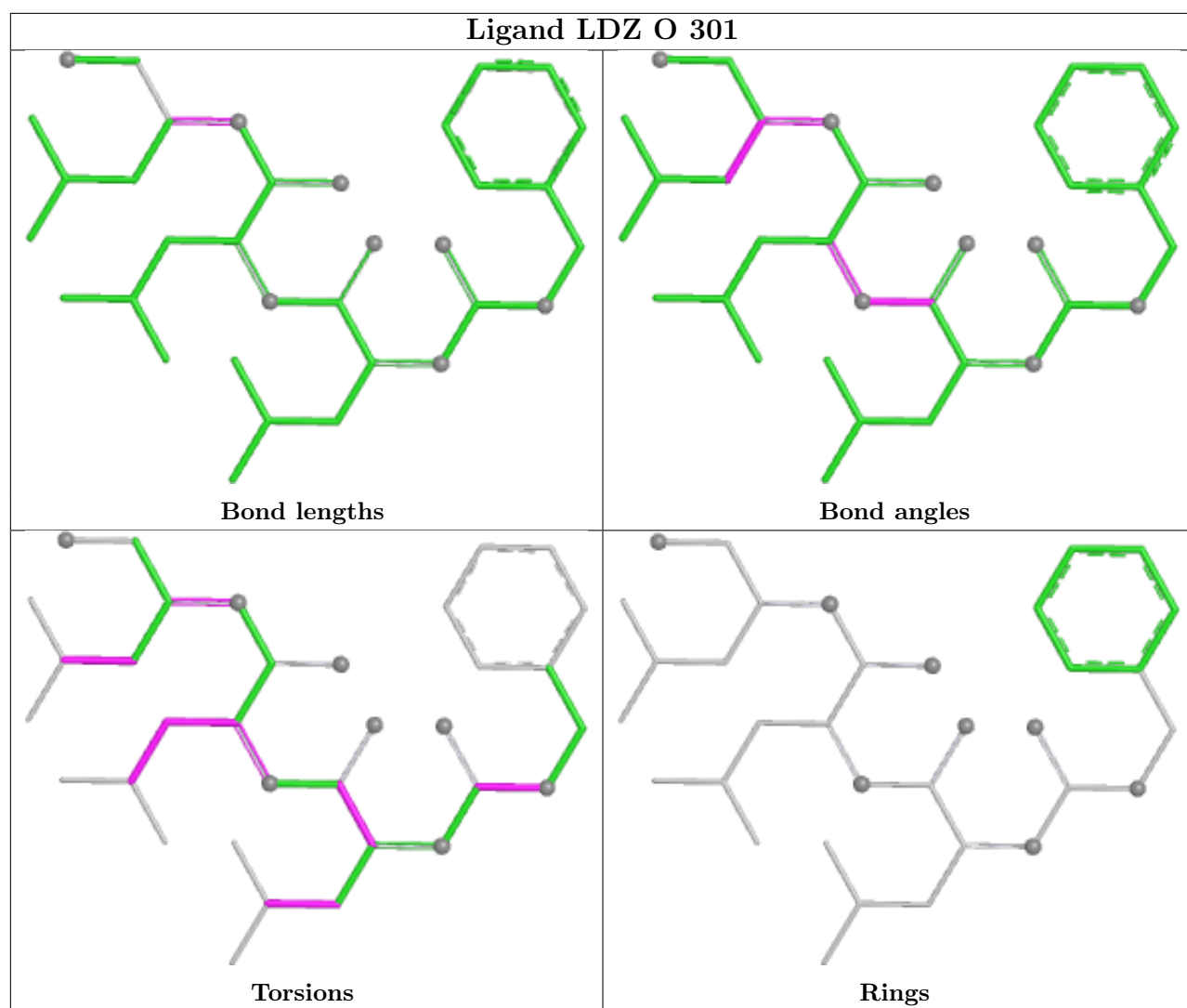


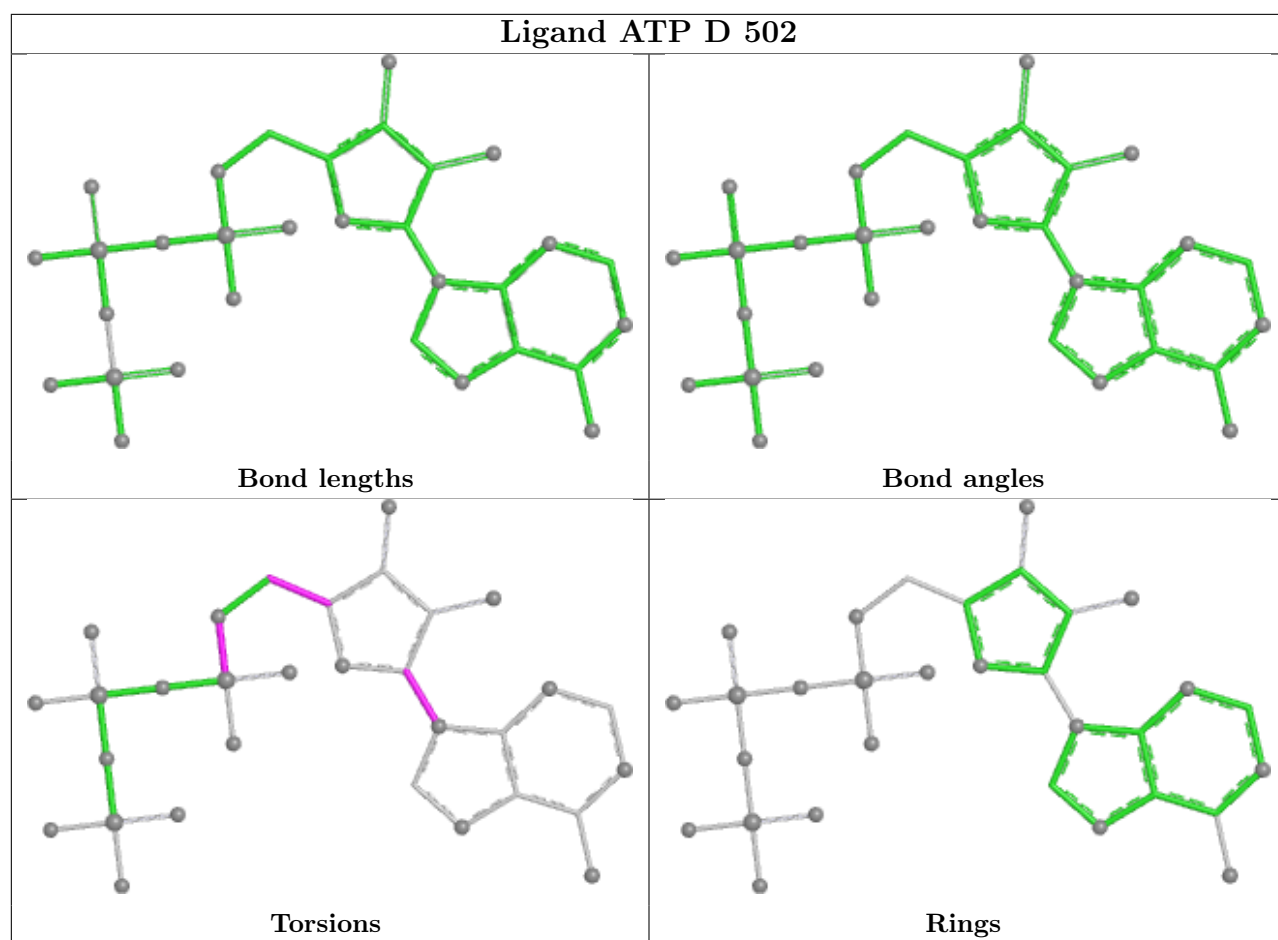


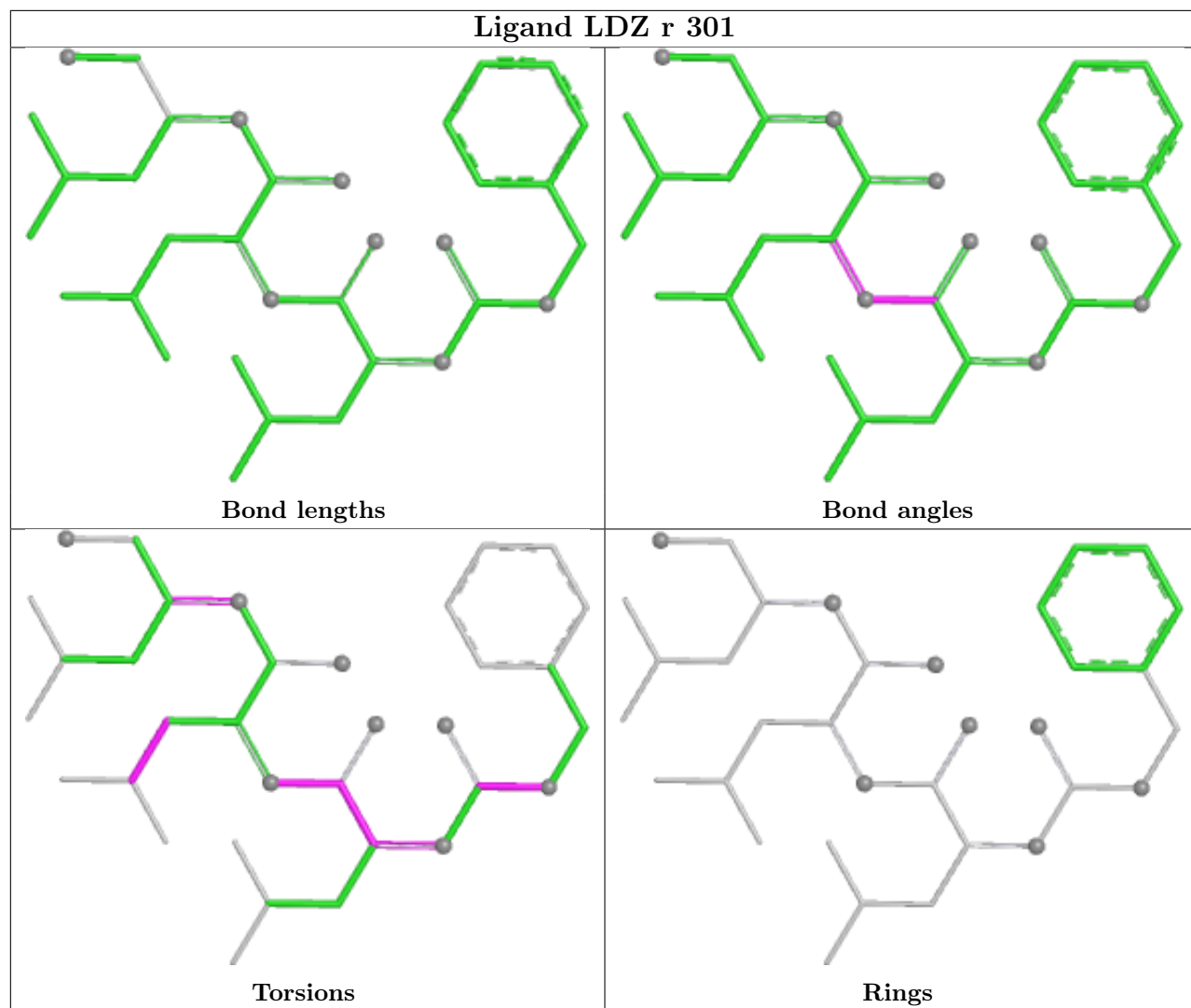


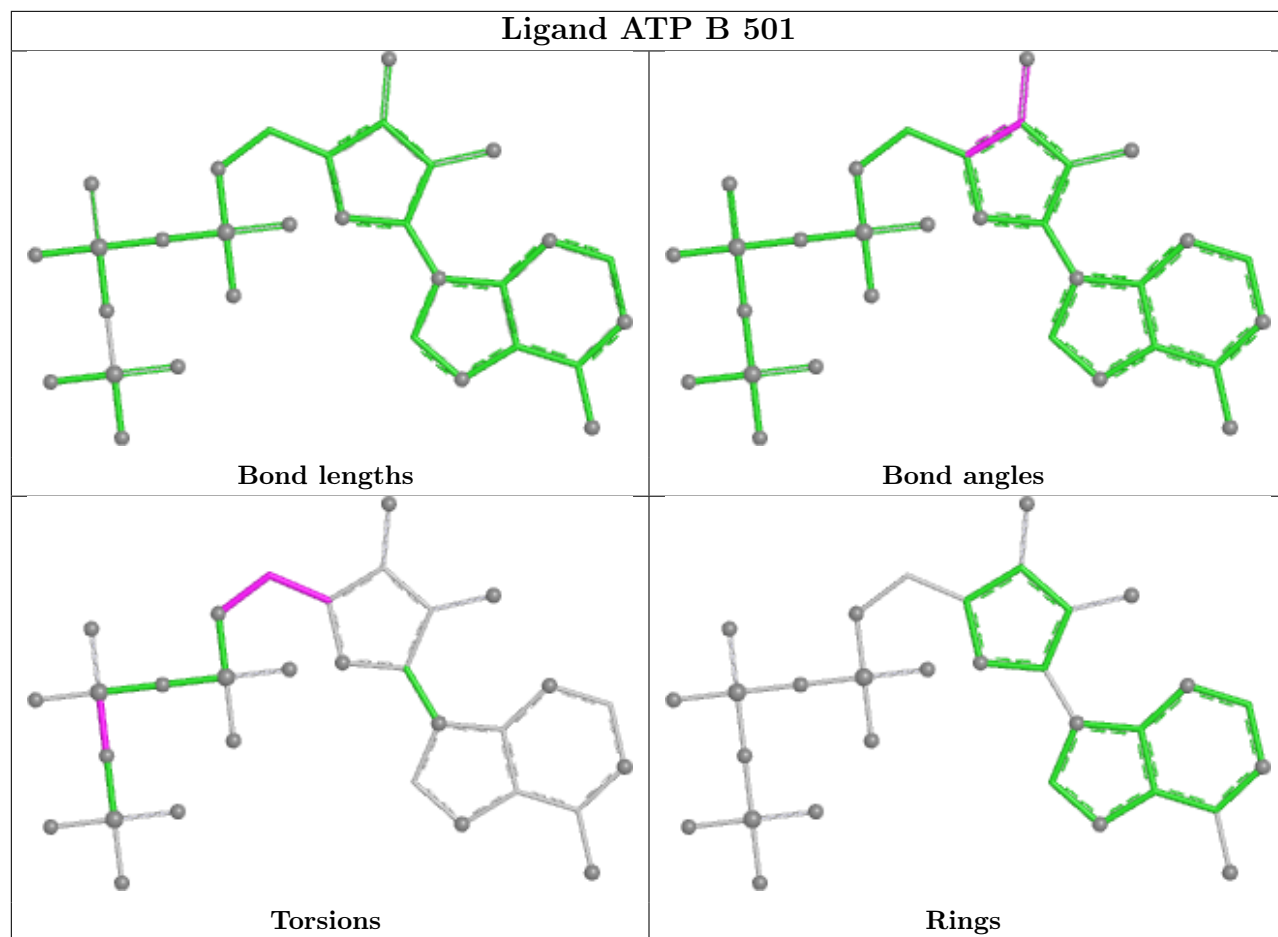


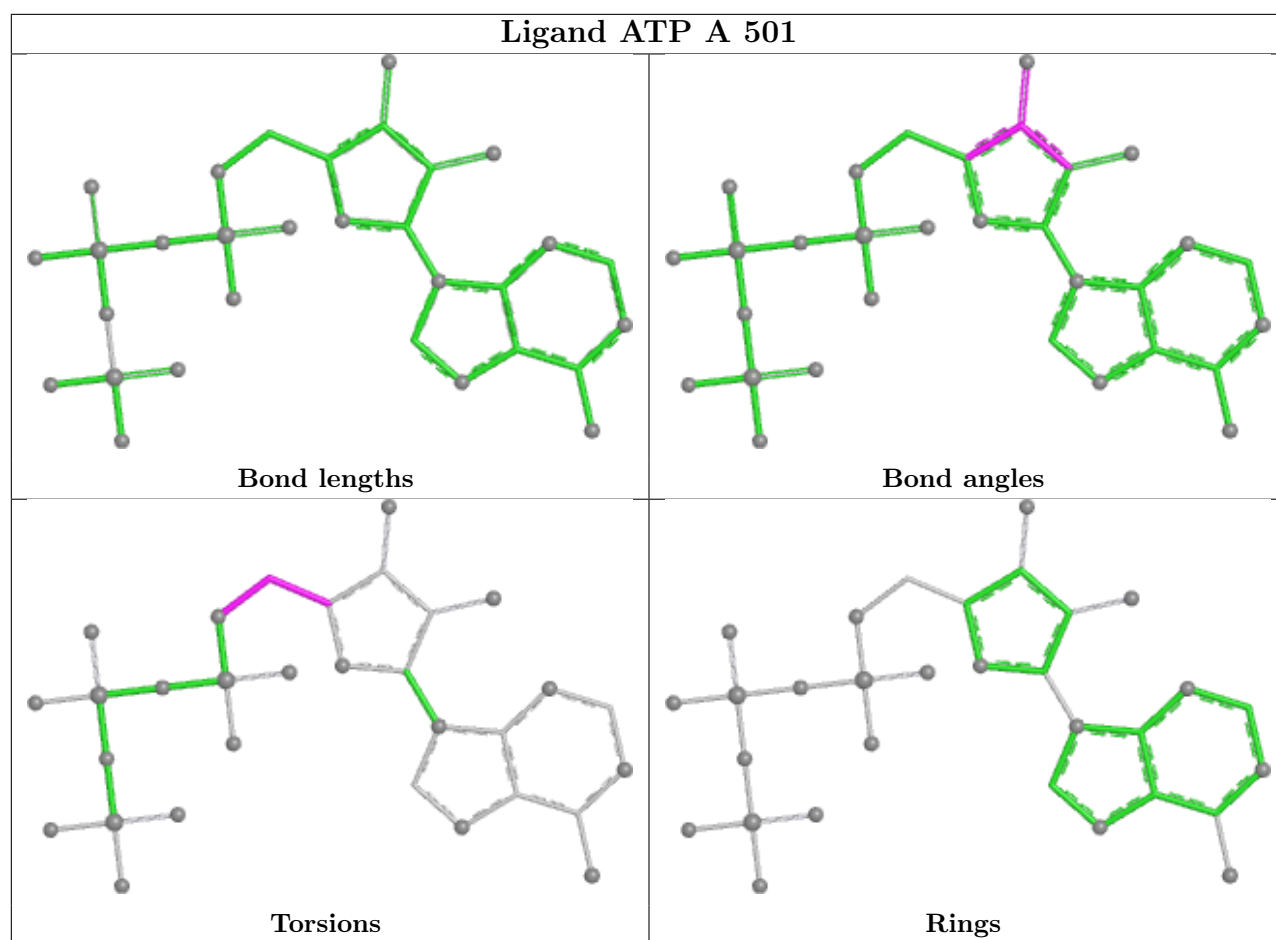












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

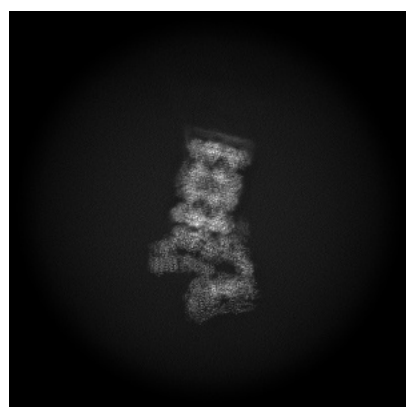
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49508. These allow visual inspection of the internal detail of the map and identification of artifacts.

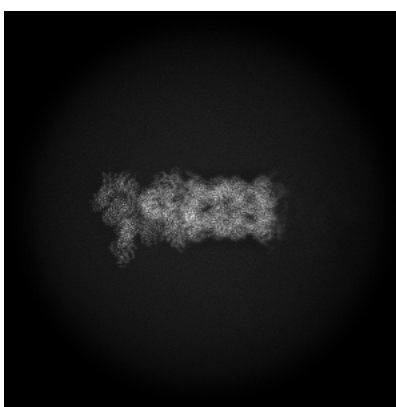
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

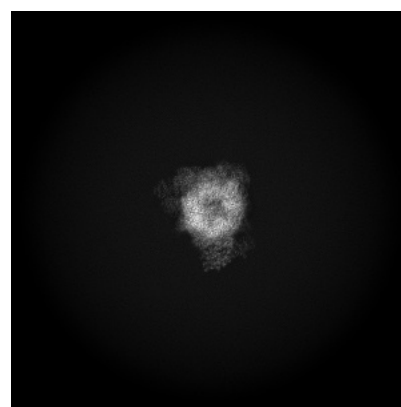
6.1.1 Primary map



X



Y

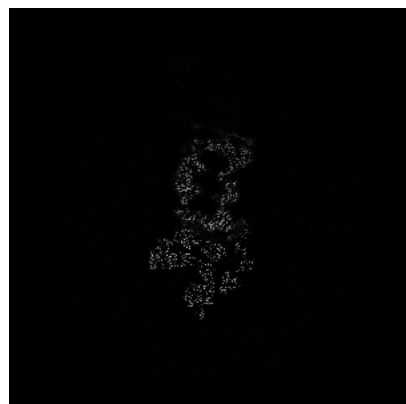


Z

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

6.2 Central slices [i](#)

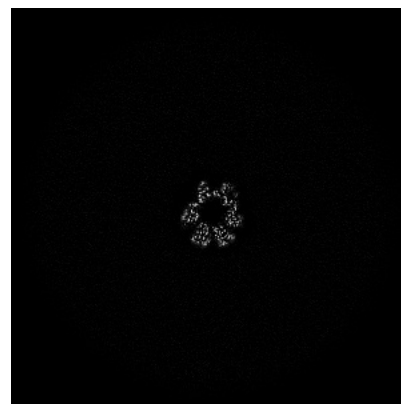
6.2.1 Primary map



X Index: 320



Y Index: 320

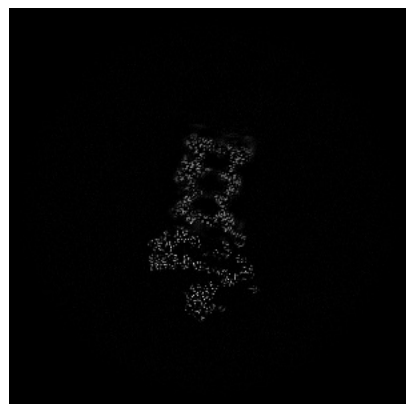


Z Index: 320

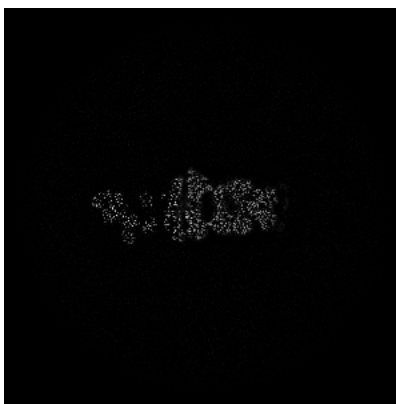
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

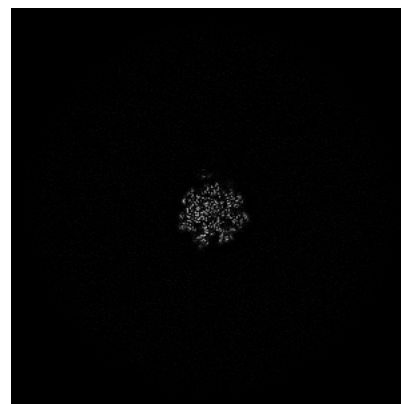
6.3.1 Primary map



X Index: 330



Y Index: 300



Z Index: 303

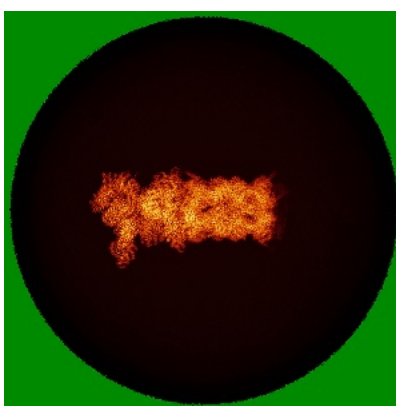
The images above show the largest variance slices of the map in three orthogonal directions.

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

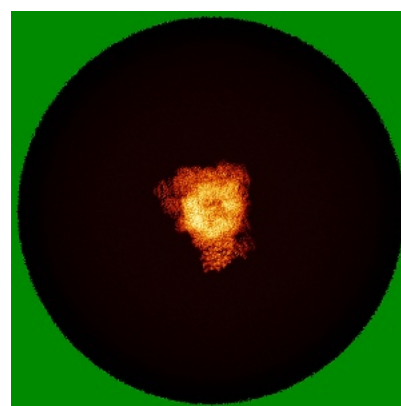
6.4.1 Primary map



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.

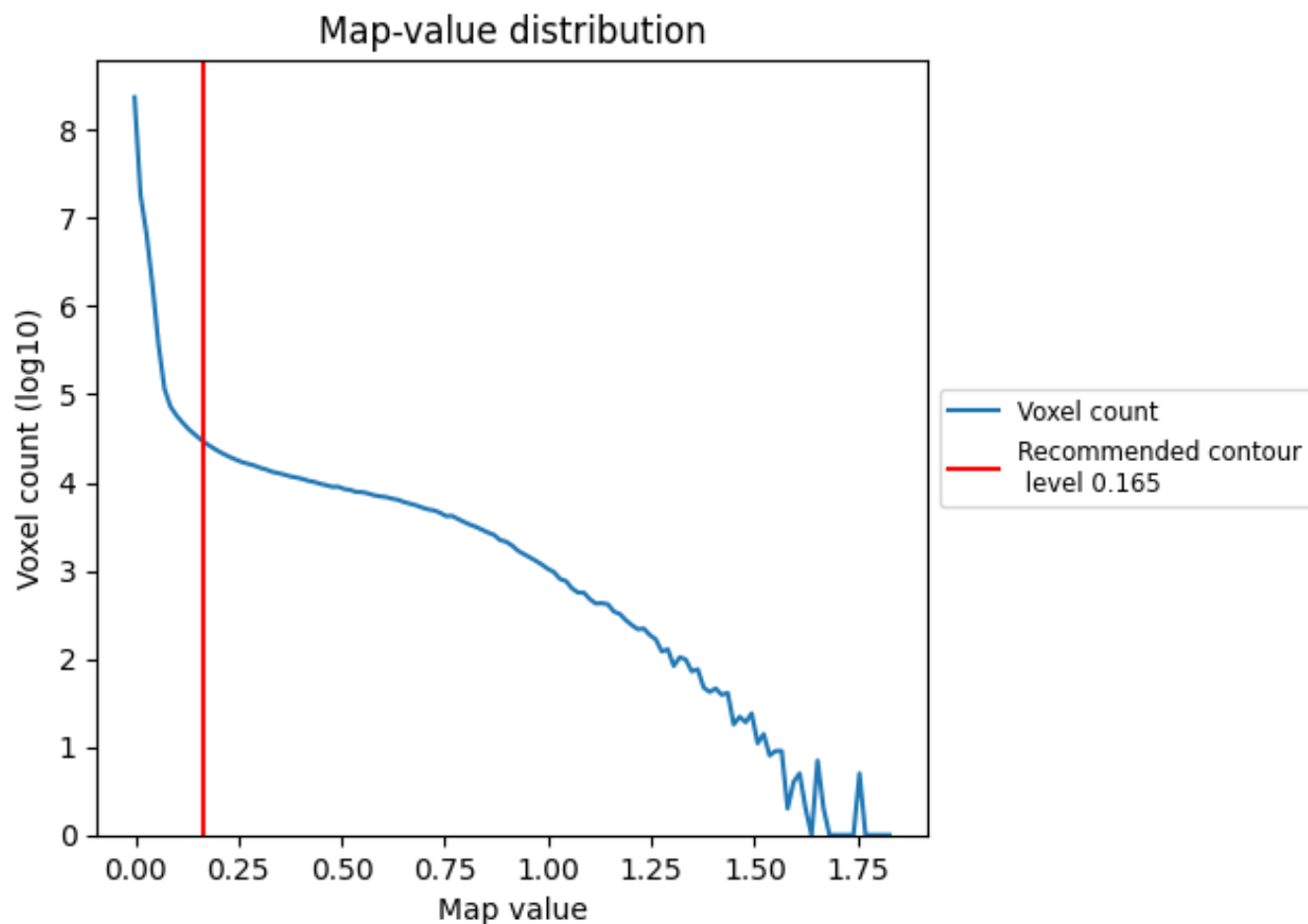
6.6 Mask visualisation

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

7 Map analysis [i](#)

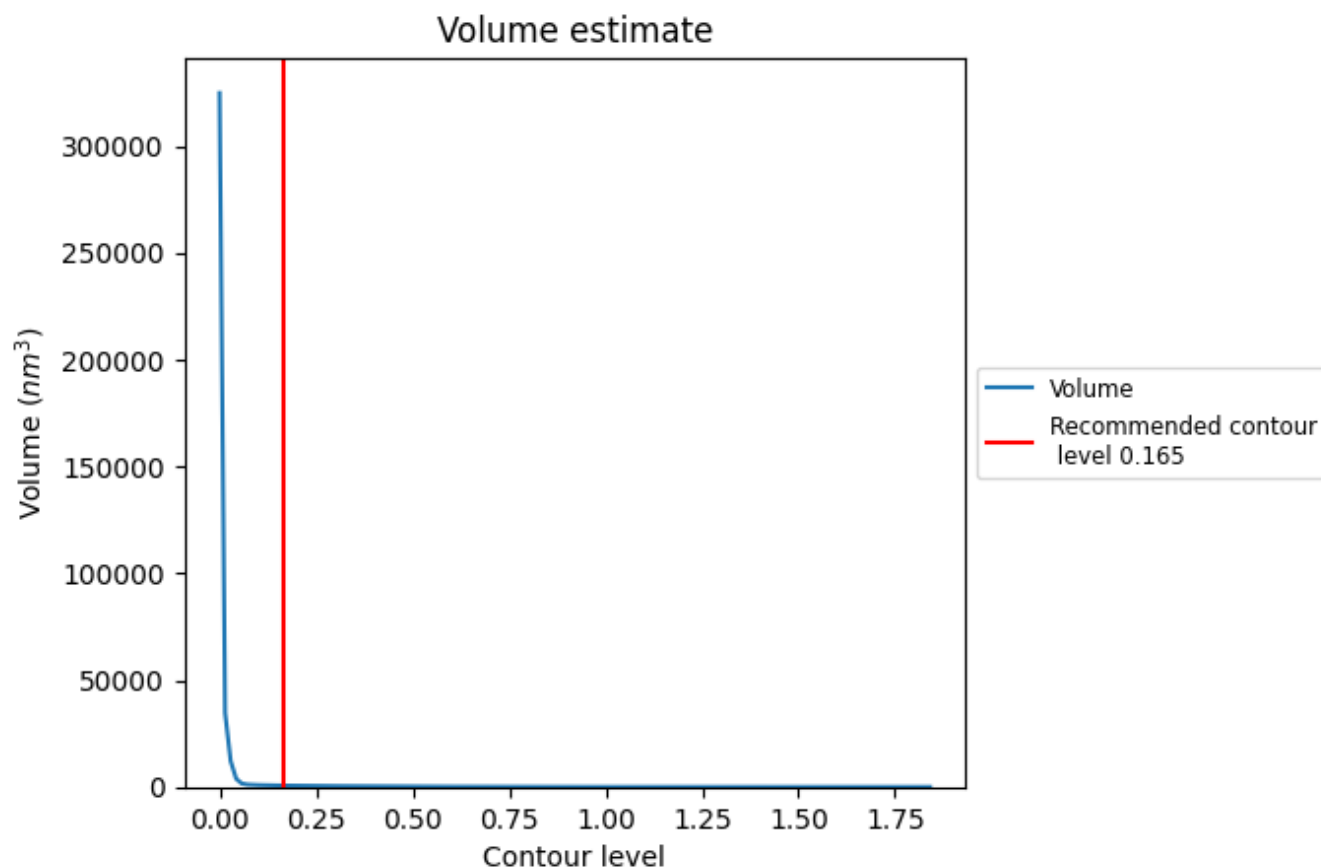
This section contains the results of statistical analysis of the map.

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.

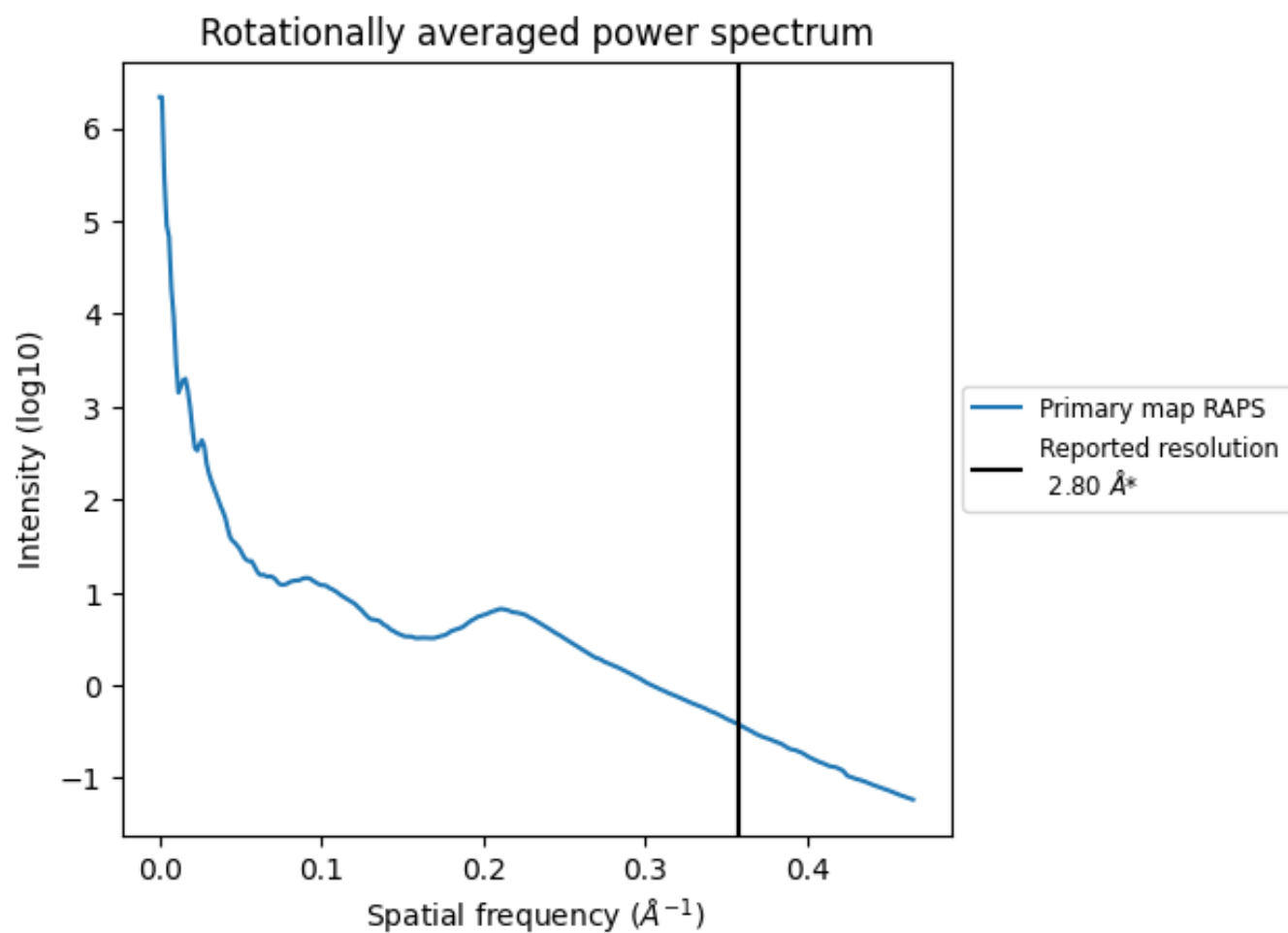
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 644 nm^3 ; this corresponds to an approximate mass of 582 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 0.357 Å⁻¹

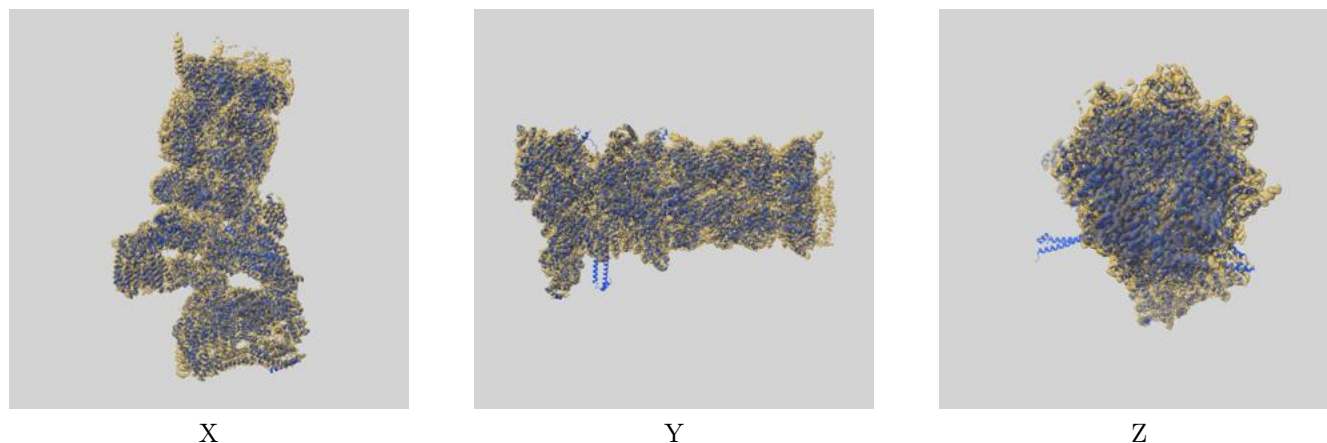
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

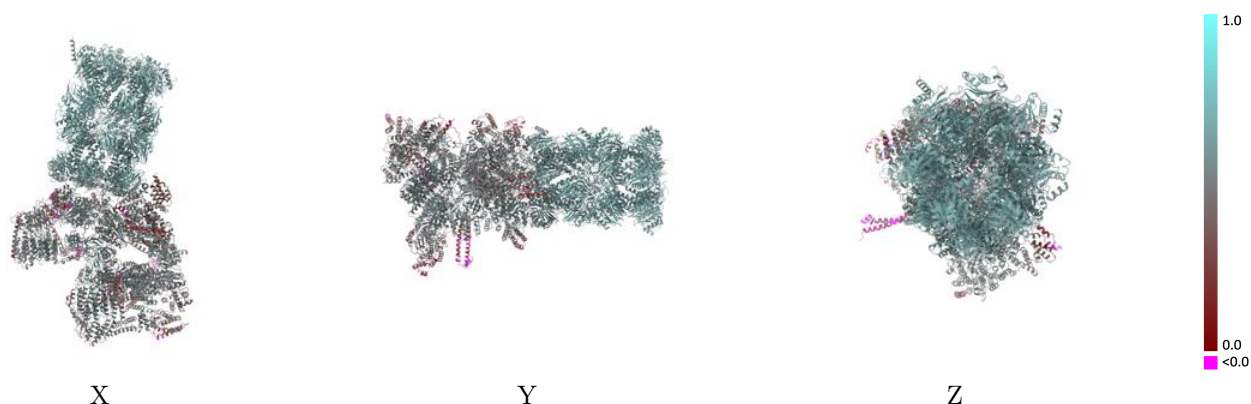
This section contains information regarding the fit between EMDB map EMD-49508 and PDB model 9NKG. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



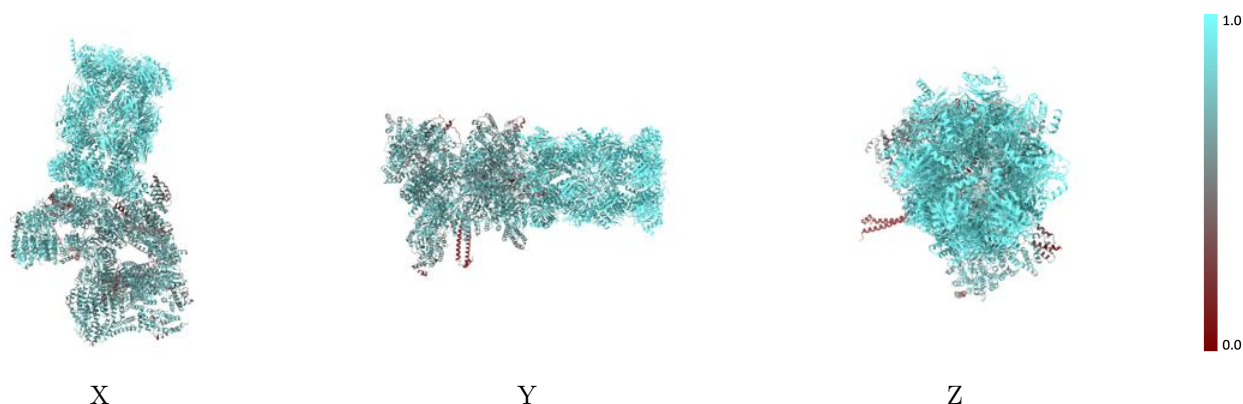
The images above show the 3D surface view of the map at the recommended contour level 0.165 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



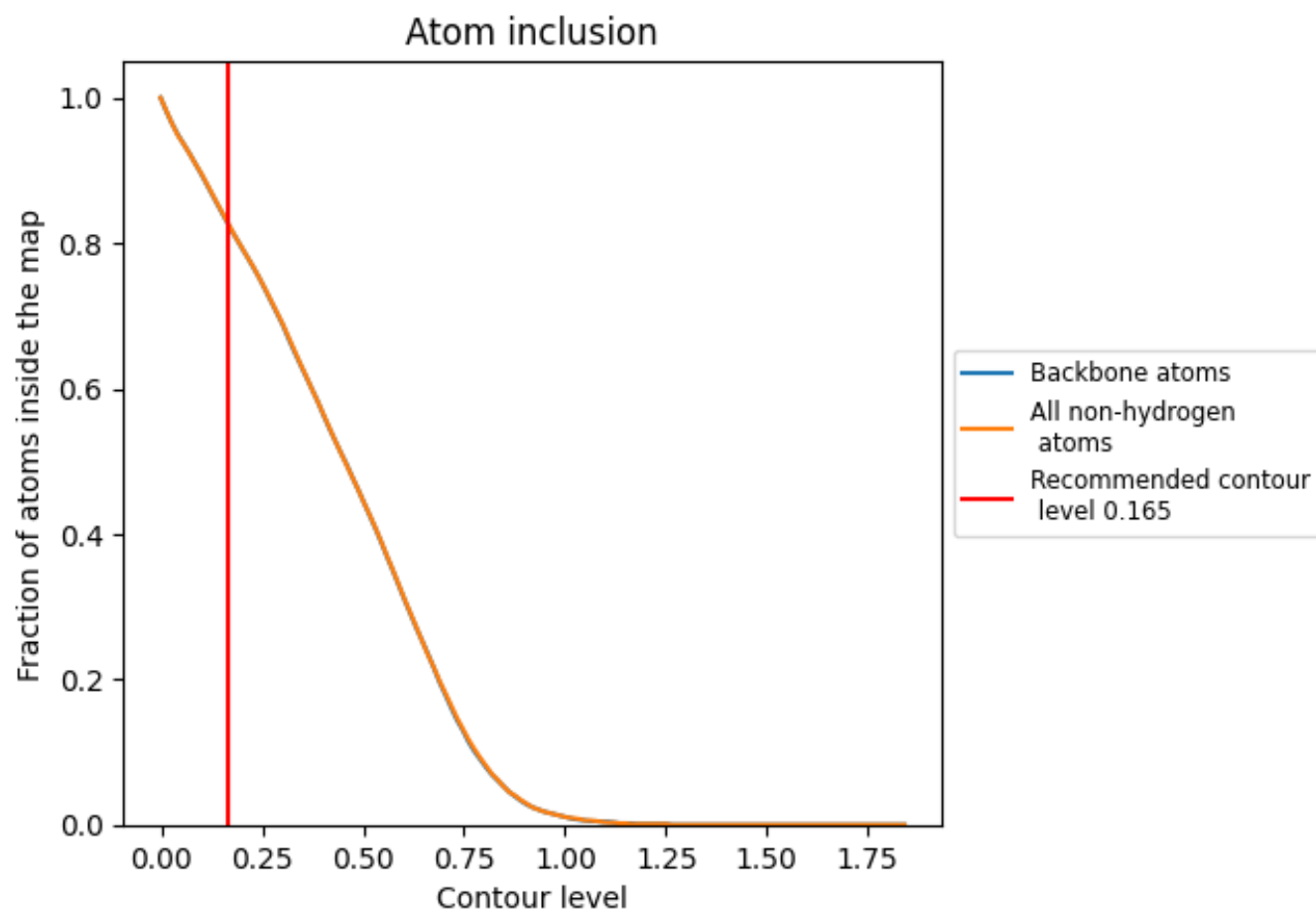
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.165).

9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 83% 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 (0.165) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8280	 0.5380
A	 0.7770	 0.5170
B	 0.7490	 0.4880
C	 0.6640	 0.4600
D	 0.7560	 0.5130
E	 0.7290	 0.4830
F	 0.6850	 0.4650
G	 0.9820	 0.5920
H	 0.9880	 0.6080
I	 0.9750	 0.5990
J	 0.9910	 0.6040
K	 0.9750	 0.5990
L	 0.9890	 0.6110
M	 0.9790	 0.5980
N	 0.9840	 0.6290
O	 0.9910	 0.6290
P	 0.9930	 0.6330
Q	 0.9900	 0.6440
R	 0.9900	 0.6410
S	 0.9900	 0.6380
T	 0.9880	 0.6360
U	 0.7370	 0.4920
V	 0.6700	 0.4490
W	 0.6890	 0.4730
X	 0.6390	 0.4240
Y	 0.7080	 0.4690
Z	 0.7310	 0.4960
a	 0.6640	 0.4240
b	 0.6630	 0.4240
c	 0.7740	 0.5340
d	 0.5960	 0.3690
e	 0.5250	 0.3600
f	 0.7610	 0.4760
g	 0.9780	 0.6250
h	 0.9880	 0.6330



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Chain	Atom inclusion	Q-score
i	 0.9770	 0.6200
j	 0.9880	 0.6120
k	 0.9660	 0.6140
l	 0.9890	 0.6230
m	 0.9740	 0.6220
n	 0.9850	 0.6360
o	 0.9940	 0.6360
p	 0.9890	 0.6390
q	 0.9880	 0.6410
r	 0.9850	 0.6410
s	 0.9880	 0.6340
t	 0.9900	 0.6280
v	 0.8000	 0.5970
z	 0.6120	 0.4320