



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 3, 2019 – 08:38 PM EST

PDB ID : 5M32  
EMDB ID: : EMD-4146  
Title : Human 26S proteasome in complex with Oprozomib  
Authors : Haselbach, D.; Schrader, J.; Lambrecht, F.; Henneberg, F.; Chari, A.; Stark, H.  
Deposited on : 2016-10-14  
Resolution : 3.80 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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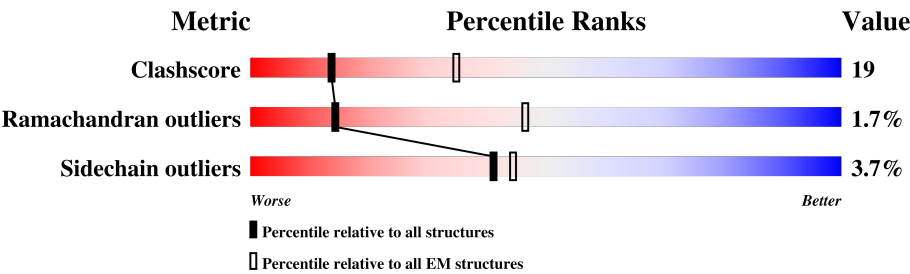
MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	234	73% 24% . .
1	O	234	74% 23% . .
2	B	261	68% 18% . 10%
2	P	261	70% 19% . . 7%
3	C	234	74% 23% . .
4	D	241	78% 17% . .
4	R	241	78% 17% . .
5	E	234	78% 19% .
6	F	255	68% 21% . 9%



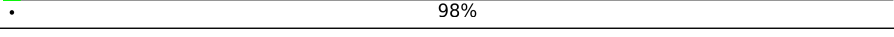
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Mol	Chain	Length	Quality of chain
6	T	255	 70% 22% • 6%
7	G	246	 71% 22% • 5%
7	U	246	 74% 22% • •
8	H	277	 60% 19% • 20%
8	V	277	 61% 17% • 21%
9	I	205	 71% 28%
9	W	205	 74% 25%
10	J	196	 77% 22% •
10	X	196	 79% 20% •
11	K	204	 76% 22% •
11	Y	204	 74% 25% •
12	L	241	 63% 25% 12%
12	Z	241	 63% 25% 12%
13	M	264	 63% 18% • 18%
13	a	264	 79% • 18%
14	N	239	 68% 17% 15%
14	b	239	 84% 15%
15	Q	235	 67% 27% • •
16	S	238	 79% 18% •
17	c	433	 73% 6% • 20%
18	d	428	 64% 11% • 22%
19	e	418	 78% 7% • 14%
20	f	379	 85% 6% • 8%
21	g	439	 77% 5% • 17%
22	h	355	 81% 11% • 6%

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Mol	Chain	Length	Quality of chain
23	i	953	
24	j	534	
25	k	456	
26	l	422	
27	m	389	
28	n	324	
29	o	376	
30	p	377	
31	q	310	
32	r	350	
33	s	70	
34	t	4	
34	u	4	

## 2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 76085 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	230	Total	C	N	O	S	0	0
			1763	1132	297	328	6		
1	O	230	Total	C	N	O	S	0	0
			1764	1126	301	331	6		

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	234	Total	C	N	O	S	0	0
			1836	1164	315	348	9		
2	P	244	Total	C	N	O	S	0	0
			1875	1187	323	355	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	234	Total	C	N	O	S	0	0
			1771	1107	315	344	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	48	ALA	LYS	conflict	UNP O14818
C	179	ASP	GLU	conflict	UNP O14818
C	200	GLU	GLN	conflict	UNP O14818

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	233	Total	C	N	O	S	0	0
			1757	1103	290	353	11		
4	R	233	Total	C	N	O	S	0	0
			1768	1112	294	351	11		

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	234	Total	C	N	O	S	0	0
			1805	1133	321	340	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	185	ASP	ASN	conflict	UNP P25786
E	234	ASP	GLU	conflict	UNP P25786

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	232	Total	C	N	O	S	0	0
			1818	1153	310	344	11		
6	T	240	Total	C	N	O	S	0	0
			1877	1190	320	356	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	233	Total	C	N	O	S	0	0
			1806	1147	301	345	13		
7	U	241	Total	C	N	O	S	0	0
			1841	1168	308	352	13		

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	221	Total	C	N	O	S	0	0
			1663	1047	283	321	12		
8	V	220	Total	C	N	O	S	1	0
			1627	1025	273	318	11		

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	204	Total	C	N	O	S	0	0
			1590	1013	265	293	19		
9	W	204	Total	C	N	O	S	0	0
			1586	1010	263	294	19		

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	196	Total	C	N	O	S	0	0
			1560	1001	266	284	9		
10	X	196	Total	C	N	O	S	0	0
			1563	1002	267	285	9		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	182	VAL	ILE	conflict	UNP P49721
J	186	ASP	ASN	conflict	UNP P49721
J	190	ASN	ASP	conflict	UNP P49721
J	192	GLU	ASP	conflict	UNP P49721
J	195	ALA	SER	conflict	UNP P49721
X	182	VAL	ILE	conflict	UNP P49721
X	186	ASP	ASN	conflict	UNP P49721
X	190	ASN	ASP	conflict	UNP P49721
X	192	GLU	ASP	conflict	UNP P49721
X	195	ALA	SER	conflict	UNP P49721

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	200	Total	C	N	O	S	0	0
			1545	974	269	293	9		
11	Y	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	213	Total	C	N	O	S	1	0
			1637	1038	277	312	10		
12	Z	213	Total	C	N	O	S	0	0
			1642	1040	281	311	10		

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	216	Total	C	N	O	S	0	0
			1687	1064	291	320	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	216	Total	C	N	O	S	0	0
			1679	1059	290	318	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	202	Total	C	N	O	S	0	0
			1513	948	258	295	12		
14	b	203	Total	C	N	O	S	0	0
			1519	952	259	296	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	235	Total	C	N	O	S	0	0
			1785	1118	318	344	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	179	ASP	GLU	conflict	UNP O14818

- Molecule 16 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	238	Total	C	N	O	S	0	0
			1834	1147	329	347	11		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	2	ALA	PHE	conflict	UNP P25786
S	3	ALA	ARG	conflict	UNP P25786
S	185	ASP	ASN	conflict	UNP P25786
S	234	ASP	GLU	conflict	UNP P25786

- Molecule 17 is a protein called 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	c	347	Total	C	N	O	S	0	0
			2728	1722	485	503	18		



- Molecule 18 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	d	333	Total	C	N	O	S	0	0
			2560	1614	433	501	12		

- Molecule 19 is a protein called 26S protease regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	361	Total	C	N	O	S	0	0
			2776	1752	488	525	11		

- Molecule 20 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	f	348	Total	C	N	O	S	0	0
			2692	1692	483	501	16		

- Molecule 21 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	g	363	Total	C	N	O	S	0	0
			2777	1753	480	529	15		

- Molecule 22 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	h	332	Total	C	N	O	S	0	0
			2518	1589	447	466	16		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	i	230	Total	C	N	O	0	0
			1145	685	230	230		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	j	155	Total	C	N	O	0	0
			779	470	155	154		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	k	364	Total	C	N	O	0	0
			1819	1092	364	363		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	l	415	Total	C	N	O	S	0	0
			2572	1598	474	494	6		

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	m	375	Total	C	N	O	S	0	0
			2421	1513	434	468	6		

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	n	206	Total	C	N	O	0	0
			1030	618	206	206		

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	o	75	Total	C	N	O	0	0
			377	227	75	75		

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	p	101	Total	C	N	O	0	0
			504	303	101	100		

- Molecule 31 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	q	259	Total	C	N	O	0	0
			1311	789	261	261		

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	r	8	Total	C	N	O	0	0
			40	25	8	7		

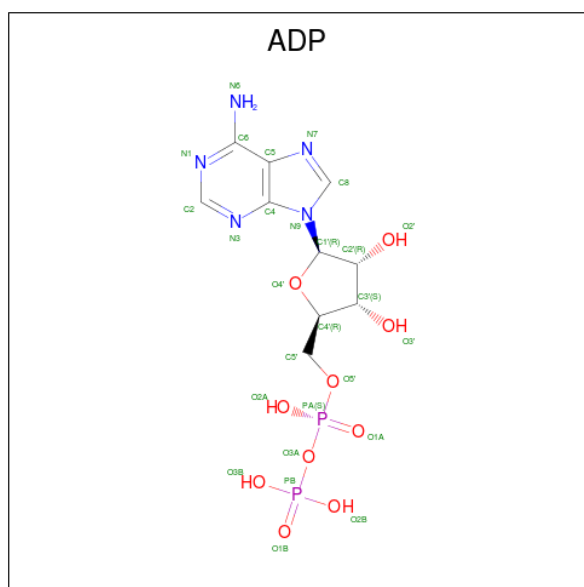
- Molecule 33 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	s	26	Total	C	N	O	0	0
			130	79	26	25		

- Molecule 34 is a protein called bound Oprozomib.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	t	4	Total	C	N	O	S	0	0
			37	25	4	7	1		
34	u	4	Total	C	N	O	S	0	0
			37	25	4	7	1		

- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



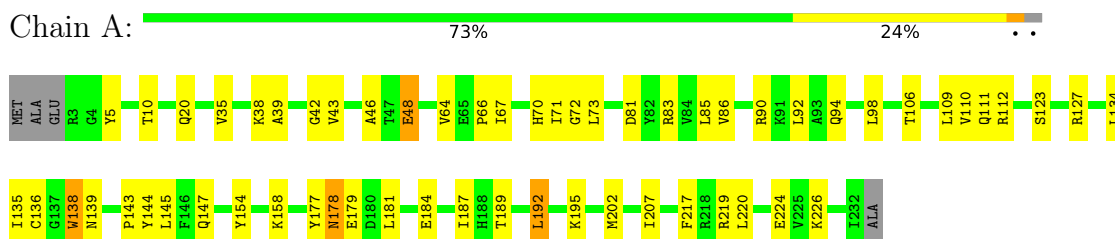
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Mol	Chain	Residues	Atoms					AltConf
35	g	1	Total	C	N	O	P	0
			54	20	10	20	4	
35	g	1	Total	C	N	O	P	0
			54	20	10	20	4	
35	h	1	Total	C	N	O	P	0
			27	10	5	10	2	

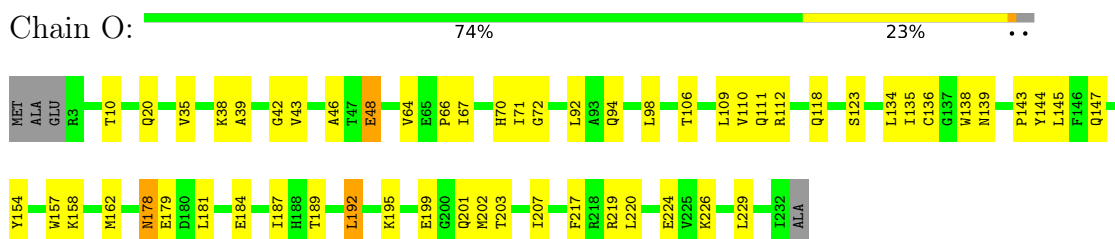
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

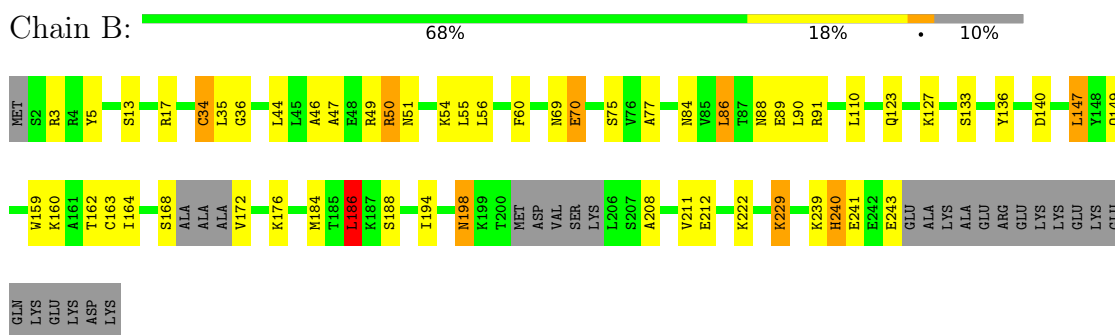
- Molecule 1: Proteasome subunit alpha type-2



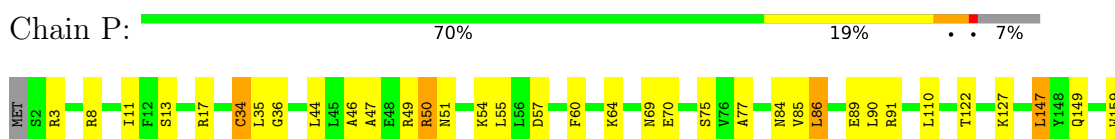
- Molecule 1: Proteasome subunit alpha type-2

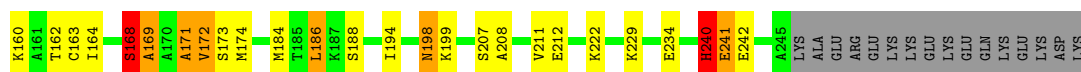


- Molecule 2: Proteasome subunit alpha type-4



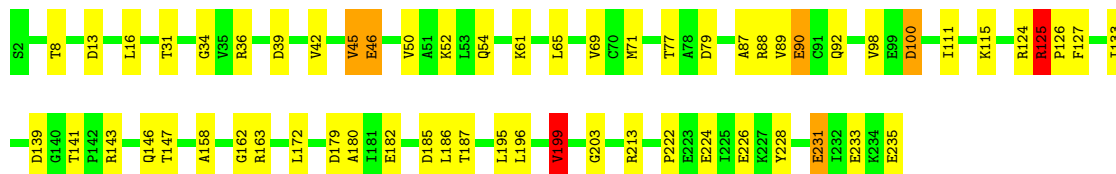
- Molecule 2: Proteasome subunit alpha type-4





• Molecule 3: Proteasome subunit alpha type-7

Chain C: 74% 23% ..



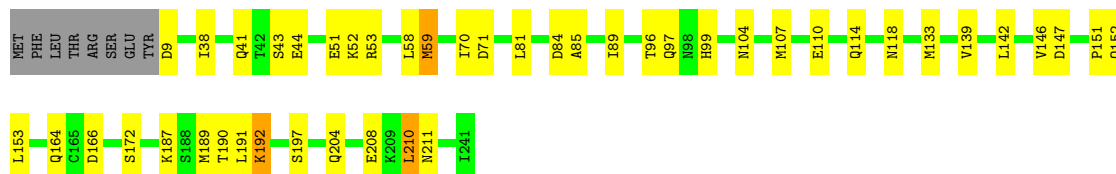
• Molecule 4: Proteasome subunit alpha type-5

Chain D: 78% 17% ..



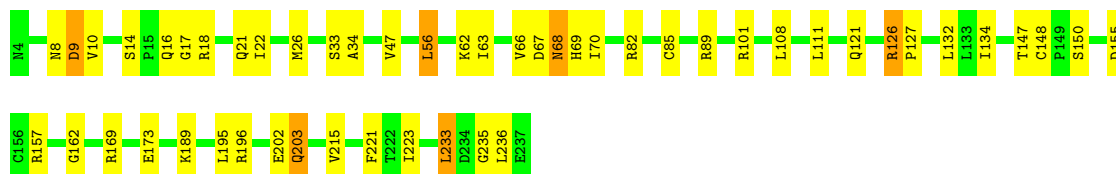
• Molecule 4: Proteasome subunit alpha type-5

Chain R: 78% 17% ..



• Molecule 5: Proteasome subunit alpha type-1

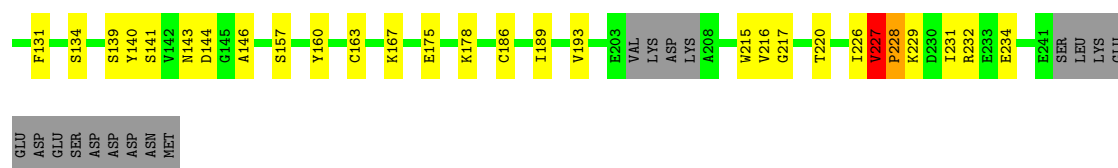
Chain E: 78% 19% .



• Molecule 6: Proteasome subunit alpha type-3

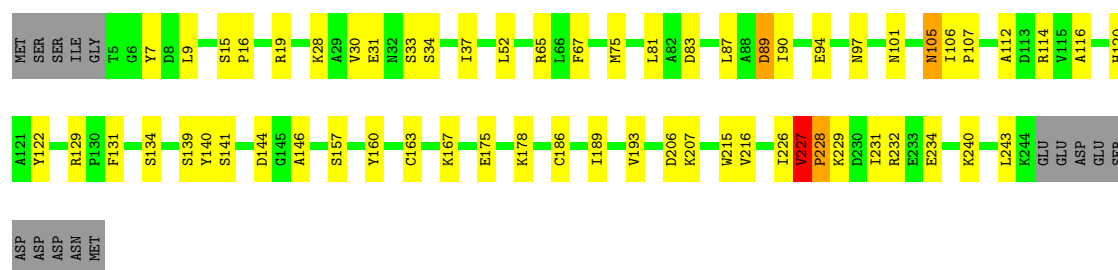
Chain F: 68% 21% 9%





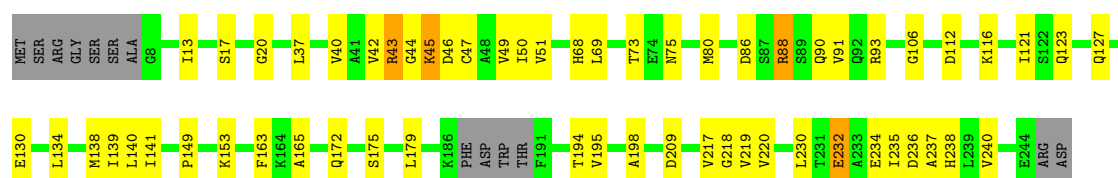
• Molecule 6: Proteasome subunit alpha type-3

Chain T: 70% 22% 6%



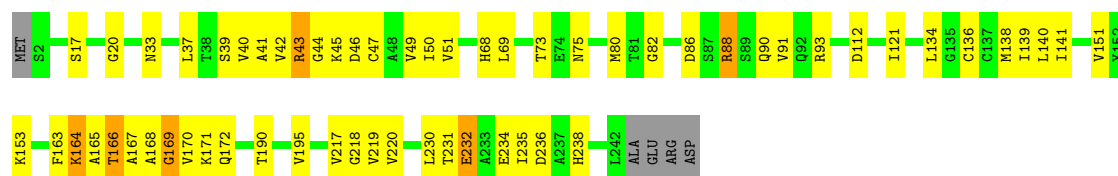
• Molecule 7: Proteasome subunit alpha type-6

Chain G: 71% 22% 5%



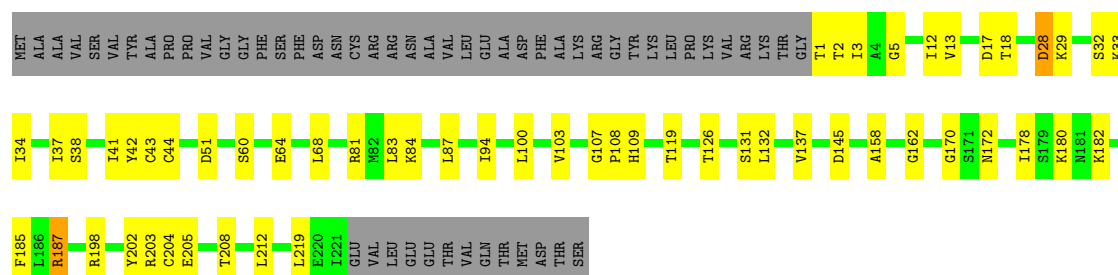
• Molecule 7: Proteasome subunit alpha type-6

Chain U: 74% 22% . .

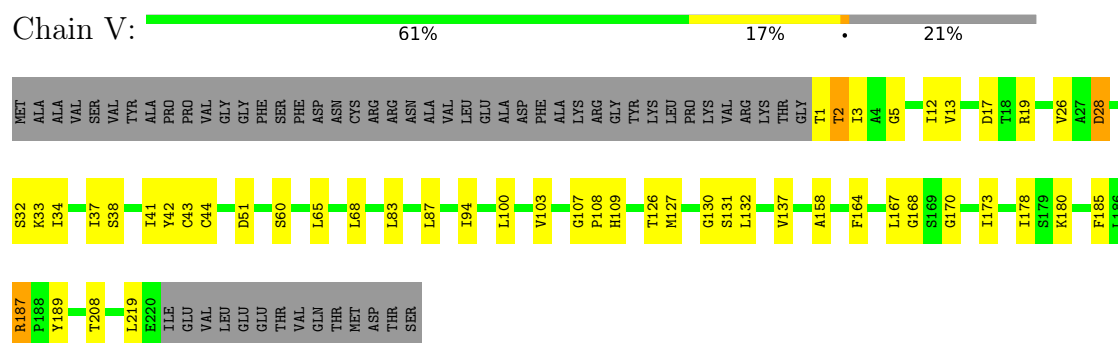


• Molecule 8: Proteasome subunit beta type-7

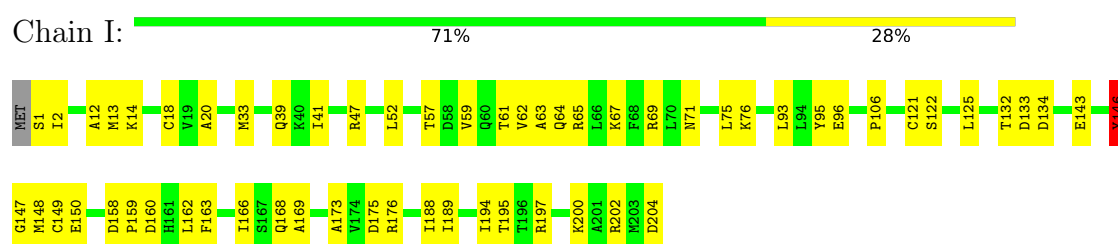
Chain H: 60% 19% 20%



- Molecule 8: Proteasome subunit beta type-7



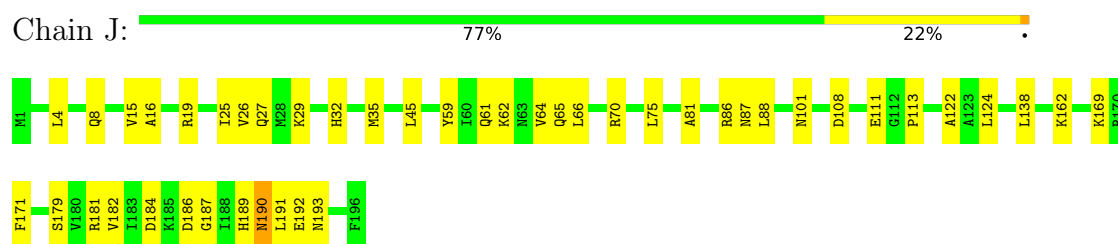
- Molecule 9: Proteasome subunit beta type-3



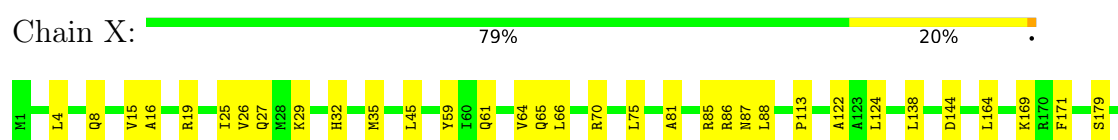
- Molecule 9: Proteasome subunit beta type-3



- Molecule 10: Proteasome subunit beta type-2



- Molecule 10: Proteasome subunit beta type-2







- Molecule 11: Proteasome subunit beta type-5

Chain K: 76% 22%



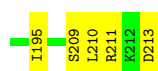
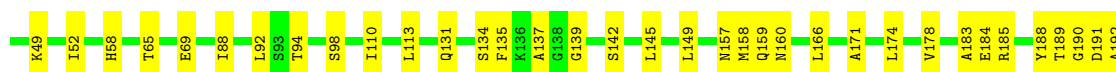
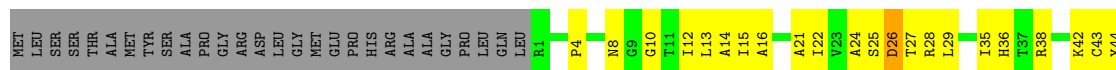
- Molecule 11: Proteasome subunit beta type-5

Chain Y: 74% 25%



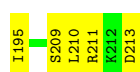
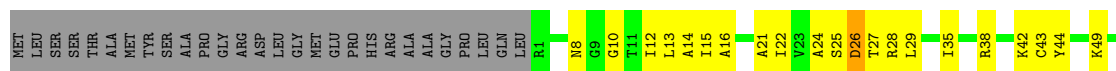
- Molecule 12: Proteasome subunit beta type-1

Chain L: 63% 25% 12%



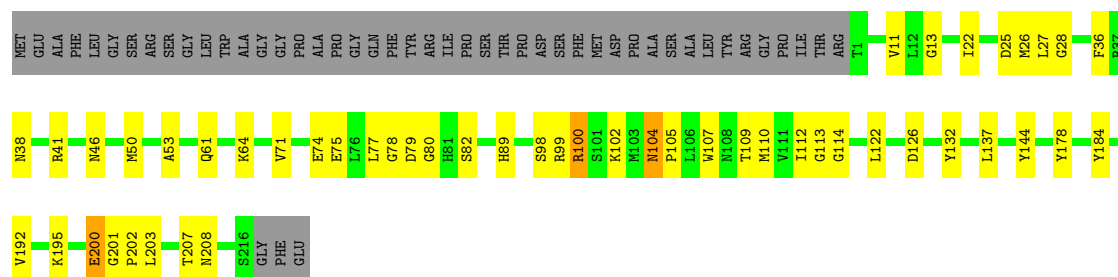
- Molecule 12: Proteasome subunit beta type-1

Chain Z: 63% 25% 12%




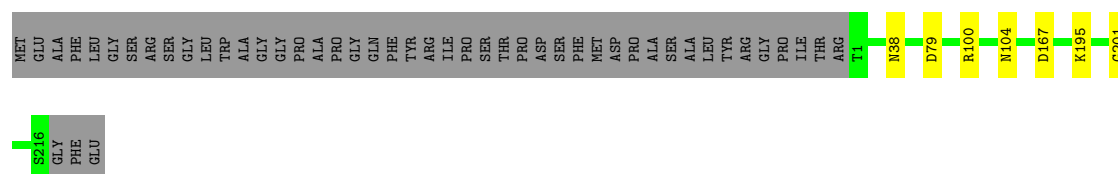
- Molecule 13: Proteasome subunit beta type-4

Chain M: 



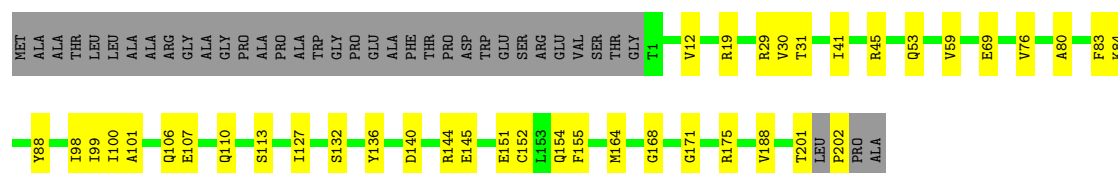
- Molecule 13: Proteasome subunit beta type-4

Chain a: 




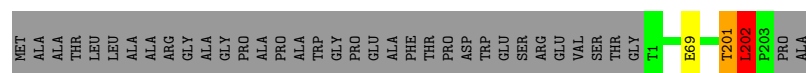
- Molecule 14: Proteasome subunit beta type-6

Chain N: 



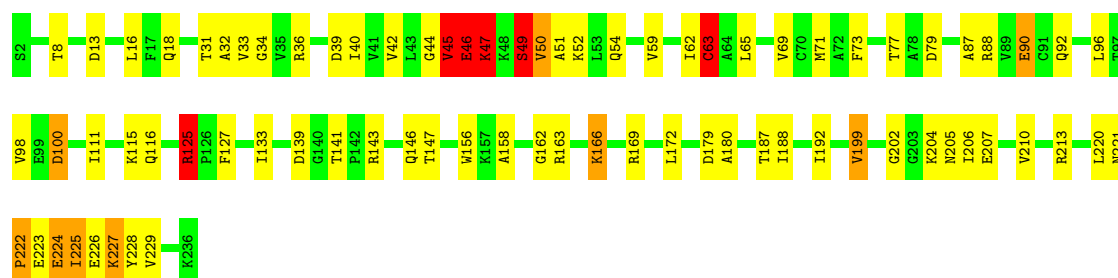
- Molecule 14: Proteasome subunit beta type-6

Chain b: 

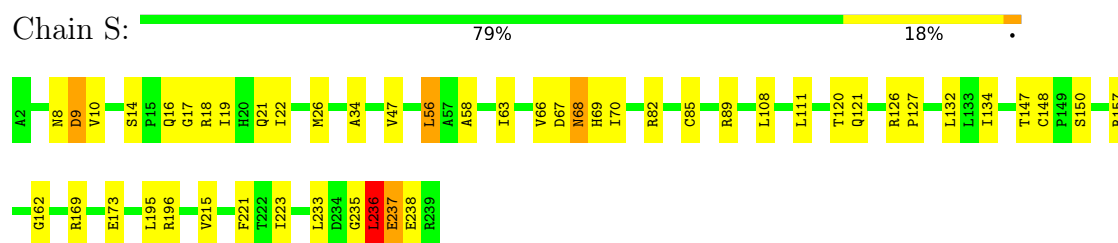


- Molecule 15: Proteasome subunit alpha type-7

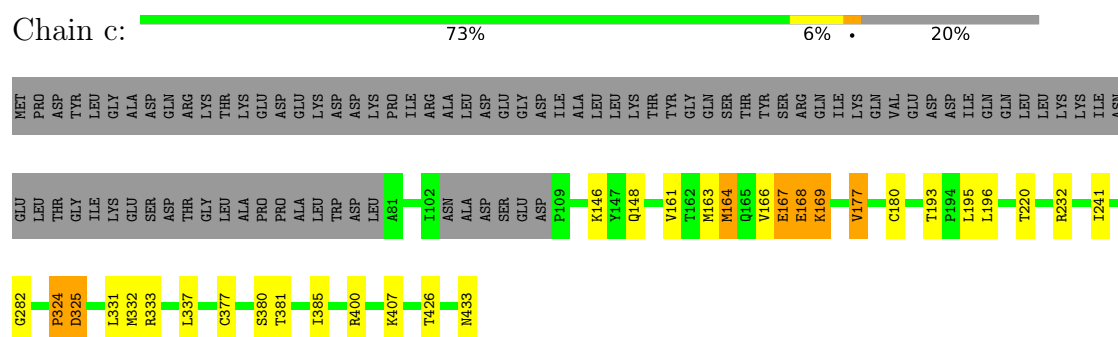
Chain Q: 



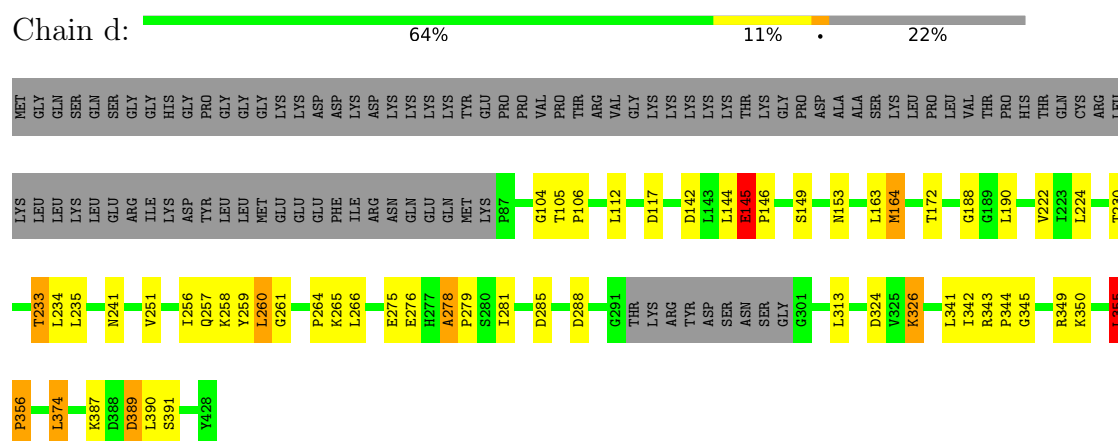
- Molecule 16: Proteasome subunit alpha type-1



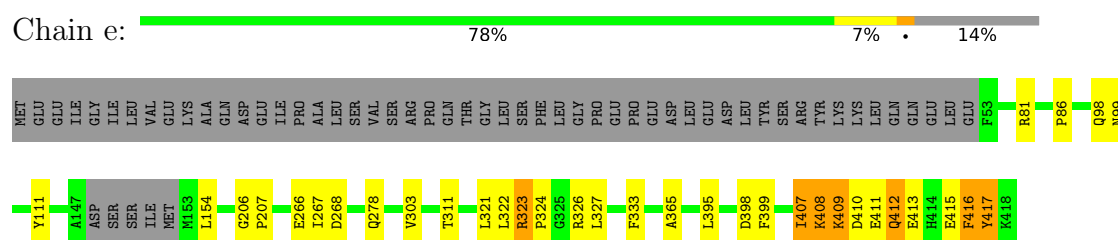
- Molecule 17: 26S protease regulatory subunit 7



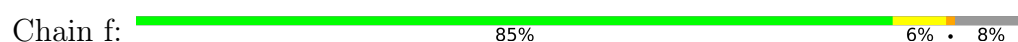
- Molecule 18: 26S protease regulatory subunit 4

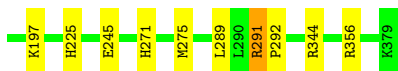


- Molecule 19: 26S protease regulatory subunit 6B



- Molecule 20: 26S protease regulatory subunit 10B

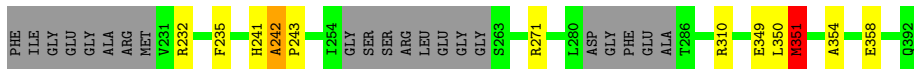




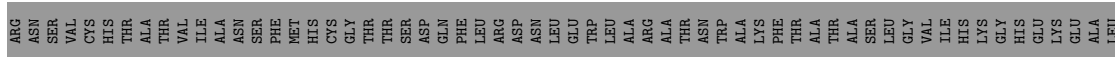
- Chain g:  77% 5% • 17%



- Chain h:  81% 11% 6%



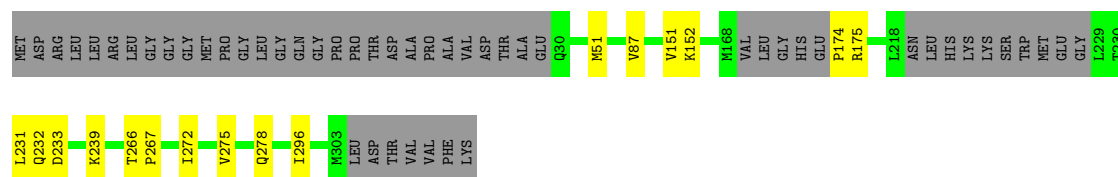
- Chain i:  22% 76%



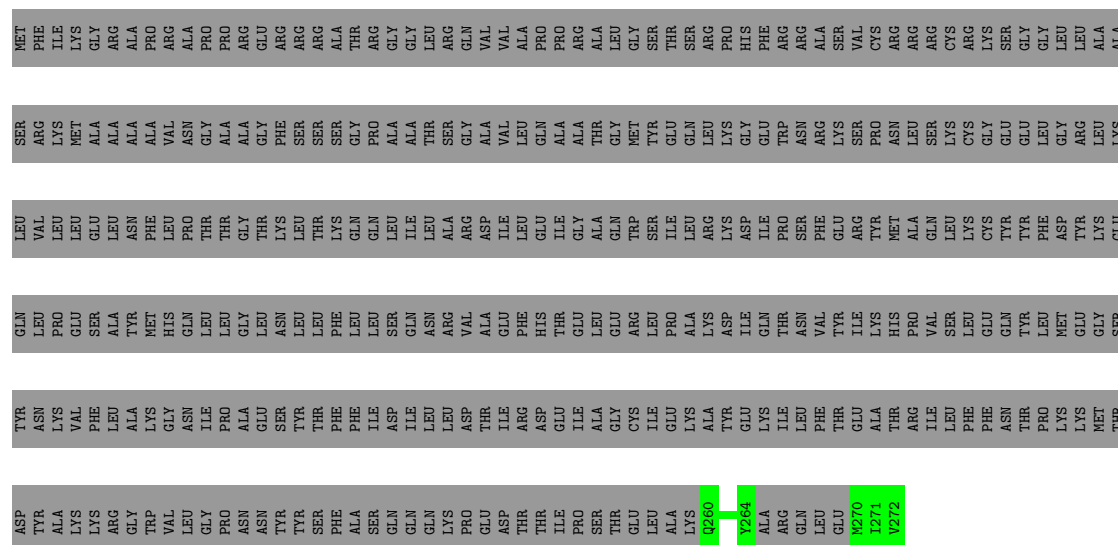




- Molecule 31: 26S proteasome non-ATPase regulatory subunit 14



- Molecule 32: 26S proteasome non-ATPase regulatory subunit 8



- Molecule 33: 26S proteasome complex subunit SEM1



MET	SER	GLU	LYS	LYS	GLN	PRO	VAL	ASP	LEU	GLY	LEU	LEU	GLU	GLU	ASP	ASP	GLU	PHE	GLU	PHE	PRO	ALA	GLU	ASP	TRP	ALA	GLY	LEU	ASP	GLU	ASP	GLU	ASP	ALA	HIS	VAL	HIS	GLY	TYR	LYS	MET	GLU	THR	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 34: bound Oprozomib

Chain t:  100%

There are no outlier residues recorded for this chain.

- Molecule 34: bound Oprozomib

Chain u:  100%

There are no outlier residues recorded for this chain.



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	233000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	2	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	8400	Depositor
Magnification	110236	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 7C9, 6VA, 6V9, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 2$	RMSZ	# $ Z  > 2$
1	A	0.40	0/1802	0.69	4/2446 (0.2%)
1	O	0.41	0/1802	0.70	5/2446 (0.2%)
10	J	0.39	0/1592	0.62	0/2153
10	X	0.39	0/1595	0.62	0/2157
11	K	0.44	0/1576	0.65	0/2131
11	Y	0.44	0/1590	0.65	0/2147
12	L	0.40	0/1670	0.73	4/2254 (0.2%)
12	Z	0.40	0/1672	0.73	4/2253 (0.2%)
13	M	0.42	0/1720	0.70	1/2328 (0.0%)
13	a	0.43	0/1712	0.68	0/2319
14	N	0.43	0/1539	0.62	0/2082
14	b	0.43	0/1546	0.69	2/2094 (0.1%)
15	Q	0.85	2/1810 (0.1%)	0.85	8/2456 (0.3%)
16	S	0.43	0/1868	0.85	8/2531 (0.3%)
17	c	0.37	0/2774	0.72	1/3739 (0.0%)
18	d	0.40	0/2597	1.00	14/3514 (0.4%)
19	e	0.36	0/2818	0.83	4/3812 (0.1%)
2	B	0.37	0/1864	0.77	4/2513 (0.2%)
2	P	0.38	0/1904	0.83	7/2573 (0.3%)
20	f	0.36	0/2734	0.70	4/3690 (0.1%)
21	g	0.37	0/2815	0.79	2/3804 (0.1%)
22	h	0.35	0/2550	0.75	2/3442 (0.1%)
23	i	0.30	0/1150	0.74	2/1599 (0.1%)
24	j	0.32	0/780	0.72	0/1086
25	k	0.28	0/1819	0.66	2/2536 (0.1%)
26	l	0.33	0/2601	0.68	2/3569 (0.1%)
27	m	0.34	0/2450	0.74	4/3356 (0.1%)
28	n	0.30	0/1032	0.74	1/1438 (0.1%)
29	o	0.30	0/378	0.62	0/528
3	C	0.41	0/1796	0.69	2/2438 (0.1%)
30	p	0.26	0/501	0.52	0/691
31	q	0.31	0/1318	0.78	2/1836 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
32	r	0.26	0/38	0.60	0/50
33	s	0.33	0/129	0.69	0/179
4	D	0.36	0/1784	0.68	1/2416 (0.0%)
4	R	0.36	0/1795	0.68	1/2424 (0.0%)
5	E	0.42	0/1839	0.84	8/2492 (0.3%)
6	F	0.44	0/1852	0.73	2/2494 (0.1%)
6	T	0.43	0/1912	0.74	3/2576 (0.1%)
7	G	0.39	0/1836	0.70	1/2481 (0.0%)
7	U	0.39	0/1875	0.67	1/2542 (0.0%)
8	H	0.42	0/1690	0.74	2/2289 (0.1%)
8	V	0.42	0/1657	0.73	2/2252 (0.1%)
9	I	0.40	0/1619	0.68	2/2184 (0.1%)
9	W	0.40	0/1614	0.68	2/2176 (0.1%)
All	All	0.40	2/77015 (0.0%)	0.73	114/104516 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	O	0	1
10	J	0	1
10	X	0	1
13	a	0	1
14	b	0	2
15	Q	0	4
16	S	0	5
17	c	0	7
18	d	0	12
19	e	0	4
2	B	0	4
2	P	0	10
20	f	0	3
21	g	0	3
22	h	0	4
23	i	0	4
24	j	0	4
25	k	0	8
26	l	0	7
27	m	0	8

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Mol	Chain	#Chirality outliers	#Planarity outliers
28	n	0	9
29	o	0	1
3	C	0	1
30	p	0	1
31	q	0	6
4	D	0	1
4	R	0	1
5	E	0	4
6	F	0	3
6	T	0	3
7	G	0	3
7	U	0	2
8	H	0	1
8	V	0	1
9	I	0	2
9	W	0	2
All	All	0	136

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Q	45	VAL	C-N	-30.59	0.63	1.34
15	Q	63	CYS	C-N	9.29	1.55	1.34

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	e	323	ARG	C-N-CD	-26.33	62.68	120.60
18	d	145	GLU	C-N-CD	-25.89	63.65	120.60
21	g	228	PRO	C-N-CD	-22.40	71.32	120.60
15	Q	63	CYS	O-C-N	-14.91	98.84	122.70
31	q	266	THR	C-N-CD	-14.89	87.84	120.60
7	G	209	ASP	CB-CG-OD1	11.77	128.90	118.30
23	i	629	THR	C-N-CD	-11.14	96.10	120.60
8	H	28	ASP	CB-CG-OD1	10.95	128.16	118.30
8	V	28	ASP	CB-CG-OD1	10.87	128.08	118.30
14	b	202	LEU	C-N-CD	-10.57	97.35	120.60
18	d	278	ALA	C-N-CD	-10.38	97.77	120.60
4	R	210	LEU	CA-CB-CG	9.43	136.99	115.30
4	D	210	LEU	CA-CB-CG	9.42	136.97	115.30
2	P	186	LEU	CA-CB-CG	9.29	136.68	115.30
2	B	186	LEU	CA-CB-CG	9.28	136.65	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	89	ASP	CB-CG-OD1	9.16	126.55	118.30
6	T	89	ASP	CB-CG-OD1	9.11	126.50	118.30
15	Q	62	ILE	O-C-N	8.84	136.85	122.70
12	Z	26	ASP	CB-CG-OD1	8.54	125.99	118.30
12	L	26	ASP	CB-CG-OD1	8.53	125.98	118.30
2	B	147	LEU	CA-CB-CG	8.45	134.73	115.30
2	P	147	LEU	CA-CB-CG	8.45	134.73	115.30
13	M	201	GLY	C-N-CD	-8.38	102.17	120.60
20	f	291	ARG	C-N-CD	-8.25	102.45	120.60
15	Q	45	VAL	CA-C-N	-8.07	99.45	117.20
18	d	374	LEU	CA-CB-CG	8.06	133.85	115.30
2	P	168	SER	O-C-N	-8.01	109.89	122.70
15	Q	49	SER	N-CA-C	-7.83	89.85	111.00
18	d	261	GLY	N-CA-C	-7.75	93.73	113.10
18	d	224	LEU	CA-CB-CG	7.65	132.89	115.30
21	g	437	TYR	C-N-CA	-7.46	103.05	121.70
2	P	171	ALA	C-N-CA	-7.21	103.66	121.70
5	E	56	LEU	CA-CB-CG	7.00	131.40	115.30
16	S	56	LEU	CA-CB-CG	6.99	131.37	115.30
1	O	48	GLU	CA-CB-CG	6.87	128.50	113.40
1	A	48	GLU	CA-CB-CG	6.86	128.49	113.40
18	d	233	THR	N-CA-CB	6.78	123.18	110.30
6	F	9	LEU	CA-CB-CG	6.74	130.81	115.30
6	T	9	LEU	CA-CB-CG	6.74	130.81	115.30
16	S	236	LEU	CA-C-N	-6.68	102.51	117.20
3	C	90	GLU	CA-CB-CG	6.66	128.05	113.40
15	Q	90	GLU	CA-CB-CG	6.65	128.04	113.40
2	P	240	HIS	CA-C-N	-6.62	102.63	117.20
16	S	233	LEU	CA-CB-CG	6.61	130.51	115.30
15	Q	62	ILE	CA-C-N	-6.61	102.67	117.20
5	E	233	LEU	CA-CB-CG	6.59	130.45	115.30
18	d	326	LYS	CB-CA-C	6.58	123.55	110.40
3	C	13	ASP	CB-CG-OD1	6.57	124.21	118.30
15	Q	13	ASP	CB-CG-OD1	6.55	124.20	118.30
18	d	343	ARG	N-CA-C	-6.53	93.36	111.00
5	E	9	ASP	N-CA-C	6.33	128.09	111.00
16	S	9	ASP	N-CA-C	6.33	128.08	111.00
23	i	665	ASN	N-CA-C	6.31	128.03	111.00
15	Q	45	VAL	C-N-CA	-6.30	105.95	121.70
20	f	85	ARG	C-N-CA	6.30	137.45	121.70
22	h	242	ALA	C-N-CD	-6.27	106.82	120.60
2	P	34	CYS	CA-CB-SG	6.17	125.10	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	34	CYS	CA-CB-SG	6.16	125.09	114.00
9	W	175	ASP	CB-CG-OD1	6.09	123.78	118.30
9	I	175	ASP	CB-CG-OD1	6.05	123.74	118.30
1	A	181	LEU	CA-CB-CG	5.94	128.96	115.30
1	O	181	LEU	CA-CB-CG	5.93	128.93	115.30
18	d	190	LEU	CA-CB-CG	5.82	128.68	115.30
7	U	169	GLY	N-CA-C	-5.80	98.60	113.10
27	m	66	ASP	N-CA-C	5.75	126.54	111.00
26	l	166	LEU	CA-CB-CG	5.69	128.40	115.30
19	e	206	GLY	C-N-CD	-5.69	108.08	120.60
18	d	163	LEU	CB-CG-CD1	5.69	120.67	111.00
28	n	70	LEU	CB-CA-C	5.62	120.88	110.20
27	m	215	ASP	CB-CG-OD1	5.62	123.36	118.30
14	b	201	THR	CA-C-N	-5.61	104.86	117.20
5	E	203	GLN	N-CA-C	5.60	126.11	111.00
18	d	112	LEU	CA-CB-CG	5.54	128.04	115.30
19	e	111	TYR	CA-CB-CG	5.51	123.87	113.40
27	m	95	LEU	CA-CB-CG	5.47	127.89	115.30
20	f	138	LEU	CA-CB-CG	5.41	127.75	115.30
18	d	234	LEU	CA-CB-CG	5.36	127.62	115.30
12	Z	174	LEU	CA-CB-CG	5.35	127.60	115.30
27	m	138	LEU	CA-CB-CG	5.34	127.58	115.30
12	L	174	LEU	CA-CB-CG	5.33	127.57	115.30
6	T	206	ASP	CB-CG-OD1	5.33	123.10	118.30
5	E	68	ASN	C-N-CA	5.28	134.89	121.70
20	f	86	GLN	CA-CB-CG	5.27	125.00	113.40
16	S	68	ASN	C-N-CA	5.25	134.83	121.70
16	S	111	LEU	CA-CB-CG	5.24	127.35	115.30
1	O	192	LEU	CA-CB-CG	5.24	127.34	115.30
5	E	111	LEU	CA-CB-CG	5.23	127.32	115.30
1	A	192	LEU	CA-CB-CG	5.22	127.31	115.30
1	O	199	GLU	CA-CB-CG	5.21	124.86	113.40
5	E	108	LEU	CA-CB-CG	5.20	127.26	115.30
17	c	196	LEU	CA-CB-CG	5.20	127.26	115.30
31	q	87	VAL	C-N-CA	5.20	134.69	121.70
16	S	108	LEU	CA-CB-CG	5.19	127.24	115.30
26	l	239	TYR	N-CA-C	-5.17	97.03	111.00
12	Z	29	LEU	CA-CB-CG	5.17	127.19	115.30
12	L	29	LEU	CA-CB-CG	5.17	127.19	115.30
25	k	197	LYS	C-N-CA	5.16	134.60	121.70
9	I	95	TYR	C-N-CA	5.16	134.59	121.70
9	W	95	TYR	C-N-CA	5.14	134.55	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	26	ASP	CB-CA-C	5.13	120.65	110.40
12	Z	26	ASP	CB-CA-C	5.12	120.65	110.40
25	k	373	ILE	C-N-CA	5.10	134.46	121.70
1	A	98	LEU	CA-CB-CG	5.08	126.99	115.30
22	h	86	LEU	CA-CB-CG	5.07	126.97	115.30
18	d	355	LEU	CA-CB-CG	5.06	126.94	115.30
1	O	98	LEU	CA-CB-CG	5.05	126.92	115.30
8	H	28	ASP	CB-CG-OD2	-5.05	113.76	118.30
16	S	134	ILE	CG1-CB-CG2	-5.04	100.32	111.40
5	E	134	ILE	CG1-CB-CG2	-5.03	100.33	111.40
19	e	395	LEU	CA-CB-CG	5.02	126.84	115.30
2	P	86	LEU	CA-CB-CG	5.01	126.82	115.30
18	d	313	LEU	CA-CB-CG	5.01	126.82	115.30
2	B	86	LEU	CA-CB-CG	5.01	126.82	115.30
8	V	28	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

All (136) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	TRP	Peptide
1	A	139	ASN	Peptide
2	B	229	LYS	Peptide
2	B	240	HIS	Peptide
2	B	54	LYS	Peptide
2	B	60	PHE	Peptide
3	C	199	VAL	Mainchain
4	D	58	LEU	Peptide
5	E	202	GLU	Peptide
5	E	203	GLN	Peptide
5	E	66	VAL	Peptide
5	E	8	ASN	Peptide
6	F	226	ILE	Peptide
6	F	227	VAL	Peptide
6	F	228	PRO	Peptide
7	G	163	PHE	Peptide
7	G	37	LEU	Peptide
7	G	68	HIS	Peptide
8	H	187	ARG	Peptide
9	I	146	TYR	Mainchain
9	I	96	GLU	Peptide
10	J	32	HIS	Peptide

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Mol	Chain	Res	Type	Group
1	O	139	ASN	Peptide
2	P	168	SER	Mainchain,Peptide
2	P	169	ALA	Peptide
2	P	171	ALA	Peptide
2	P	229	LYS	Peptide
2	P	240	HIS	Mainchain,Peptide
2	P	241	GLU	Peptide
2	P	54	LYS	Peptide
2	P	60	PHE	Peptide
15	Q	199	VAL	Mainchain
15	Q	45	VAL	Mainchain
15	Q	49	SER	Peptide
15	Q	63	CYS	Mainchain
4	R	58	LEU	Peptide
16	S	236	LEU	Mainchain,Peptide
16	S	237	GLU	Peptide
16	S	66	VAL	Peptide
16	S	8	ASN	Peptide
6	T	226	ILE	Peptide
6	T	227	VAL	Peptide
6	T	228	PRO	Peptide
7	U	37	LEU	Peptide
7	U	68	HIS	Peptide
8	V	187	ARG	Peptide
9	W	146	TYR	Mainchain
9	W	96	GLU	Peptide
10	X	32	HIS	Peptide
13	a	201	GLY	Peptide
14	b	201	THR	Mainchain
14	b	202	LEU	Peptide
17	c	193	THR	Peptide
17	c	241	ILE	Peptide
17	c	282	GLY	Peptide
17	c	324	PRO	Peptide
17	c	325	ASP	Peptide
17	c	377	CYS	Peptide
17	c	426	THR	Peptide
18	d	117	ASP	Peptide
18	d	164	MET	Peptide
18	d	172	THR	Peptide
18	d	222	VAL	Peptide
18	d	241	ASN	Peptide

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Mol	Chain	Res	Type	Group
18	d	278	ALA	Peptide
18	d	288	ASP	Peptide
18	d	324	ASP	Peptide
18	d	326	LYS	Mainchain,Peptide
18	d	355	LEU	Peptide
18	d	356	PRO	Peptide
19	e	278	GLN	Peptide
19	e	333	PHE	Peptide
19	e	365	ALA	Peptide
19	e	407	ILE	Peptide
20	f	116	ASP	Peptide
20	f	117	PRO	Peptide
20	f	245	GLU	Peptide
21	g	279	ALA	Peptide
21	g	299	GLU	Peptide
21	g	349	ASP	Peptide
22	h	242	ALA	Peptide
22	h	351	MET	Peptide
22	h	83	LYS	Peptide
22	h	92	GLU	Peptide
23	i	538	GLU	Peptide
23	i	661	ALA	Peptide
23	i	770	TRP	Peptide
23	i	773	PHE	Peptide
24	j	193	ILE	Peptide
24	j	194	PRO	Peptide
24	j	207	SER	Peptide
24	j	209	MET	Peptide
25	k	121	LYS	Peptide
25	k	170	GLN	Peptide
25	k	195	ALA	Peptide
25	k	196	VAL	Peptide
25	k	198	ASP	Peptide
25	k	340	VAL	Peptide
25	k	341	PHE	Peptide
25	k	412	ILE	Peptide
26	l	180	LEU	Peptide
26	l	185	LYS	Peptide
26	l	250	SER	Peptide
26	l	370	LEU	Peptide
26	l	372	LYS	Peptide
26	l	74	ARG	Peptide

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Mol	Chain	Res	Type	Group
26	l	75	PRO	Peptide
27	m	134	LEU	Peptide
27	m	169	GLU	Peptide
27	m	174	TRP	Peptide
27	m	216	TYR	Peptide
27	m	288	PHE	Peptide
27	m	30	GLU	Peptide
27	m	36	ALA	Peptide
27	m	65	ILE	Peptide
28	n	114	ARG	Peptide
28	n	162	ILE	Peptide
28	n	178	ASP	Peptide
28	n	183	THR	Peptide
28	n	45	LYS	Peptide
28	n	49	ASP	Peptide
28	n	60	GLU	Peptide
28	n	61	ASP	Peptide
28	n	70	LEU	Peptide
29	o	123	THR	Peptide
30	p	57	ASP	Peptide
31	q	151	VAL	Peptide
31	q	152	LYS	Peptide
31	q	174	PRO	Peptide
31	q	239	LYS	Peptide
31	q	278	GLN	Peptide
31	q	296	ILE	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1763	0	1741	42	0
1	O	1764	0	1732	33	0
2	B	1836	0	1838	40	0
2	P	1875	0	1865	35	0
3	C	1771	0	1712	56	0
4	D	1757	0	1713	33	0
4	R	1768	0	1756	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1805	0	1765	28	0
6	F	1818	0	1792	37	0
6	T	1877	0	1857	35	0
7	G	1806	0	1816	44	0
7	U	1841	0	1809	69	0
8	H	1663	0	1681	55	0
8	V	1627	0	1608	46	0
9	I	1590	0	1612	41	0
9	W	1586	0	1607	32	0
10	J	1560	0	1561	40	0
10	X	1563	0	1565	33	0
11	K	1545	0	1495	29	0
11	Y	1559	0	1520	35	0
12	L	1637	0	1620	39	0
12	Z	1642	0	1630	40	0
13	M	1687	0	1666	35	0
13	a	1679	0	1651	0	0
14	N	1513	0	1483	23	0
14	b	1519	0	1487	0	0
15	Q	1785	0	1734	142	0
16	S	1834	0	1788	29	0
17	c	2728	0	2775	0	0
18	d	2560	0	2556	0	0
19	e	2776	0	2740	0	0
20	f	2692	0	2696	0	0
21	g	2777	0	2782	0	0
22	h	2518	0	2530	0	0
23	i	1145	0	592	0	0
24	j	779	0	366	0	0
25	k	1819	0	809	0	0
26	l	2572	0	1980	0	0
27	m	2421	0	1885	0	0
28	n	1030	0	474	0	0
29	o	377	0	173	0	0
30	p	504	0	238	0	0
31	q	1311	0	656	0	0
32	r	40	0	17	0	0
33	s	130	0	56	0	0
34	t	37	0	0	0	0
34	u	37	0	0	0	0
35	c	27	0	11	0	0
35	d	27	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	e	27	0	12	0	0
35	g	54	0	24	0	0
35	h	27	0	12	0	0
All	All	76085	0	70499	1007	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 19.

All (1007) 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)
15:Q:192:ILE:CD1	15:Q:228:TYR:HB3	1.27	1.61
7:U:163:PHE:CD2	7:U:166:THR:HG21	1.37	1.57
15:Q:188:ILE:CG2	15:Q:228:TYR:CZ	1.79	1.56
3:C:50:VAL:HA	3:C:54:GLN:CG	1.29	1.56
15:Q:192:ILE:HD13	15:Q:228:TYR:CB	1.17	1.54
15:Q:220:LEU:CD2	15:Q:224:GLU:HG3	1.37	1.54
3:C:50:VAL:CA	3:C:54:GLN:CG	1.84	1.53
3:C:50:VAL:CB	3:C:54:GLN:HG3	1.07	1.52
15:Q:32:ALA:HA	15:Q:45:VAL:CG1	1.42	1.49
15:Q:206:ILE:HG23	15:Q:225:ILE:CG2	1.45	1.44
7:U:40:VAL:HA	7:U:167:ALA:CB	1.45	1.44
15:Q:220:LEU:HB3	15:Q:224:GLU:CB	1.46	1.43
15:Q:188:ILE:HG21	15:Q:228:TYR:CZ	0.91	1.43
15:Q:220:LEU:HD22	15:Q:224:GLU:CG	1.47	1.42
3:C:50:VAL:CB	3:C:54:GLN:CG	1.96	1.40
7:U:163:PHE:CD2	7:U:166:THR:CG2	2.05	1.37
8:V:3:ILE:CD1	8:V:44:CYS:HB3	1.51	1.37
3:C:50:VAL:CA	3:C:54:GLN:HG3	1.49	1.34
2:P:168:SER:C	2:P:172:VAL:H	1.32	1.32
15:Q:188:ILE:CG2	15:Q:228:TYR:CE1	2.11	1.32
8:V:3:ILE:HD11	8:V:44:CYS:CB	1.61	1.31
15:Q:32:ALA:CA	15:Q:45:VAL:CG1	2.08	1.30
15:Q:206:ILE:CG2	15:Q:225:ILE:HG22	1.59	1.30
7:U:39:SER:O	7:U:167:ALA:HB1	1.27	1.28
15:Q:188:ILE:HD13	15:Q:228:TYR:OH	1.13	1.27
15:Q:188:ILE:HG21	15:Q:228:TYR:CE1	1.69	1.27
7:U:163:PHE:CE2	7:U:166:THR:HG21	1.70	1.26
15:Q:206:ILE:CG2	15:Q:225:ILE:CG2	2.10	1.26
3:C:50:VAL:CA	3:C:54:GLN:HG2	1.51	1.25
7:U:43:ARG:CG	7:U:164:LYS:O	1.87	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:188:ILE:HG21	15:Q:228:TYR:CE2	1.79	1.16
8:H:1:THR:HG22	8:H:33:LYS:HZ1	1.12	1.15
15:Q:192:ILE:HD12	15:Q:228:TYR:C	1.66	1.14
15:Q:188:ILE:HG21	15:Q:228:TYR:OH	1.46	1.14
15:Q:192:ILE:CD1	15:Q:228:TYR:C	2.16	1.14
15:Q:188:ILE:CG2	15:Q:228:TYR:CE2	2.31	1.13
15:Q:32:ALA:CA	15:Q:45:VAL:HG12	1.70	1.12
2:P:240:HIS:C	2:P:242:GLU:H	1.37	1.11
8:H:1:THR:HG22	8:H:33:LYS:NZ	1.63	1.11
15:Q:206:ILE:HG23	15:Q:225:ILE:HG21	1.24	1.09
2:B:240:HIS:CE1	2:B:243:GLU:OE1	2.04	1.09
16:S:236:LEU:C	16:S:238:GLU:H	1.38	1.08
2:B:176:LYS:HD2	3:C:52:LYS:HG2	1.34	1.07
7:U:40:VAL:CA	7:U:167:ALA:HB2	1.84	1.07
2:B:240:HIS:HE1	2:B:243:GLU:OE1	1.35	1.07
7:U:43:ARG:HG3	7:U:164:LYS:O	0.90	1.07
4:D:20:ARG:HD3	4:D:25:GLU:OE1	1.53	1.06
15:Q:192:ILE:CD1	15:Q:228:TYR:CA	2.32	1.06
15:Q:32:ALA:HA	15:Q:45:VAL:HG13	1.08	1.06
8:H:3:ILE:HD11	8:H:44:CYS:HB3	1.32	1.06
15:Q:188:ILE:CD1	15:Q:228:TYR:OH	2.02	1.06
7:U:40:VAL:CA	7:U:167:ALA:CB	2.34	1.05
15:Q:188:ILE:HG22	15:Q:228:TYR:CE1	1.91	1.05
8:H:1:THR:CG2	8:H:33:LYS:NZ	2.20	1.04
8:H:3:ILE:CD1	8:H:44:CYS:HB3	1.86	1.04
7:U:40:VAL:HA	7:U:167:ALA:HB2	1.08	1.03
15:Q:32:ALA:HA	15:Q:45:VAL:HG12	1.26	1.02
3:C:46:GLU:OE1	3:C:199:VAL:CB	2.09	1.01
15:Q:220:LEU:HB3	15:Q:224:GLU:HB2	1.03	1.01
7:U:163:PHE:CG	7:U:166:THR:CG2	2.42	1.01
8:V:3:ILE:HD11	8:V:44:CYS:HB3	1.14	1.00
4:D:18:GLU:OE1	4:D:20:ARG:CZ	2.09	1.00
10:J:181:ARG:HG2	10:J:190:ASN:HB3	1.44	1.00
2:B:168:SER:C	2:B:172:VAL:N	2.15	1.00
15:Q:220:LEU:CB	15:Q:224:GLU:CB	2.40	1.00
16:S:236:LEU:C	16:S:238:GLU:N	2.13	0.99
7:U:41:ALA:O	7:U:165:ALA:HB1	1.61	0.99
2:B:176:LYS:HD2	3:C:52:LYS:CG	1.86	0.99
15:Q:32:ALA:N	15:Q:45:VAL:HG12	1.77	0.99
2:P:34:CYS:HA	2:P:46:ALA:O	1.62	0.99
15:Q:220:LEU:CG	15:Q:224:GLU:HG3	1.92	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:42:VAL:HG22	7:U:49:VAL:O	1.63	0.98
2:P:168:SER:C	2:P:172:VAL:N	2.15	0.98
2:B:34:CYS:HA	2:B:46:ALA:O	1.62	0.97
15:Q:192:ILE:HD13	15:Q:228:TYR:CA	1.92	0.97
8:H:1:THR:CB	8:H:33:LYS:NZ	2.28	0.96
4:D:18:GLU:OE1	4:D:20:ARG:NH1	1.80	0.96
15:Q:220:LEU:CB	15:Q:224:GLU:HB2	1.96	0.96
7:U:42:VAL:CG2	7:U:49:VAL:O	2.13	0.96
15:Q:47:LYS:HA	15:Q:207:GLU:OE1	1.65	0.95
7:U:163:PHE:CG	7:U:166:THR:HG22	2.02	0.94
3:C:50:VAL:O	3:C:54:GLN:HB2	1.66	0.94
15:Q:32:ALA:CB	15:Q:45:VAL:CG1	2.44	0.94
15:Q:32:ALA:CA	15:Q:45:VAL:HG13	1.87	0.94
2:P:240:HIS:C	2:P:242:GLU:N	2.13	0.94
8:V:3:ILE:CD1	8:V:44:CYS:CB	2.31	0.93
15:Q:206:ILE:CG2	15:Q:225:ILE:HG21	1.88	0.93
14:N:201:THR:C	14:N:202:PRO:N	2.23	0.92
7:U:163:PHE:CD2	7:U:166:THR:HG22	2.01	0.91
7:U:39:SER:O	7:U:167:ALA:CB	2.17	0.91
15:Q:220:LEU:HB3	15:Q:224:GLU:CG	2.00	0.91
15:Q:188:ILE:HD13	15:Q:228:TYR:HH	1.12	0.90
7:U:40:VAL:HA	7:U:167:ALA:HB3	1.54	0.89
15:Q:47:LYS:HG3	15:Q:206:ILE:O	1.68	0.89
8:H:1:THR:CG2	8:H:33:LYS:HZ1	1.81	0.89
4:D:20:ARG:CD	4:D:25:GLU:OE1	2.22	0.88
15:Q:32:ALA:HB2	15:Q:45:VAL:HG11	1.54	0.87
8:V:3:ILE:HD11	8:V:44:CYS:SG	2.14	0.87
15:Q:192:ILE:CD1	15:Q:228:TYR:CB	2.03	0.87
8:H:1:THR:HB	8:H:33:LYS:HZ3	1.40	0.86
15:Q:206:ILE:HG21	15:Q:225:ILE:HG22	1.56	0.85
15:Q:188:ILE:HG22	15:Q:228:TYR:CD1	2.12	0.85
15:Q:192:ILE:HD13	15:Q:228:TYR:CG	2.12	0.84
1:O:39:ALA:HB3	1:O:42:GLY:O	1.77	0.84
3:C:45:VAL:HG21	3:C:61:LYS:HG3	1.57	0.84
7:G:44:GLY:O	7:G:46:ASP:N	2.10	0.84
8:H:1:THR:CB	8:H:33:LYS:HZ3	1.86	0.84
15:Q:221:ASN:O	15:Q:223:GLU:N	2.11	0.83
2:B:176:LYS:CD	3:C:52:LYS:HG2	2.06	0.83
2:B:194:ILE:O	2:B:198:ASN:HB2	1.79	0.83
1:A:39:ALA:HB3	1:A:42:GLY:O	1.77	0.83
8:H:1:THR:CG2	8:H:33:LYS:HZ3	1.89	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:39:SER:C	7:U:167:ALA:HB1	2.00	0.82
2:P:194:ILE:O	2:P:198:ASN:HB2	1.79	0.81
8:H:145:ASP:OD1	8:H:145:ASP:N	4.38	0.81
3:C:222:PRO:O	3:C:226:GLU:HG2	1.80	0.80
8:H:1:THR:HB	8:H:33:LYS:NZ	1.94	0.80
7:U:164:LYS:NZ	7:U:164:LYS:HB2	1.96	0.80
8:V:3:ILE:HD12	8:V:44:CYS:HB3	1.64	0.80
3:C:50:VAL:CB	3:C:54:GLN:CB	2.59	0.79
10:X:182:VAL:CG2	10:X:191:LEU:HD11	2.13	0.79
7:U:42:VAL:CG2	7:U:49:VAL:C	2.49	0.78
15:Q:221:ASN:HB2	15:Q:222:PRO:HD2	1.67	0.77
13:M:71:VAL:O	13:M:75:GLU:HB2	1.84	0.77
15:Q:220:LEU:HB3	15:Q:224:GLU:HB3	1.63	0.77
10:X:182:VAL:HG21	10:X:191:LEU:HD11	1.68	0.76
15:Q:192:ILE:CD1	15:Q:228:TYR:O	2.33	0.75
10:J:187:GLY:O	10:J:189:HIS:CE1	2.39	0.75
15:Q:220:LEU:CB	15:Q:224:GLU:CG	2.65	0.75
15:Q:192:ILE:HD11	15:Q:228:TYR:O	1.87	0.74
15:Q:192:ILE:HG21	15:Q:228:TYR:CB	2.16	0.74
7:U:163:PHE:CB	7:U:166:THR:HG22	2.17	0.74
10:J:191:LEU:HD23	10:J:191:LEU:N	2.02	0.74
15:Q:32:ALA:HB2	15:Q:45:VAL:CG1	2.13	0.74
8:V:2:THR:OG1	8:V:130:GLY:C	2.25	0.74
15:Q:31:THR:C	15:Q:45:VAL:HG12	2.08	0.74
15:Q:49:SER:O	15:Q:204:LYS:NZ	2.21	0.73
15:Q:192:ILE:CG1	15:Q:228:TYR:HB3	2.18	0.73
10:J:187:GLY:O	10:J:189:HIS:ND1	2.22	0.73
4:D:20:ARG:HD3	4:D:25:GLU:CD	2.10	0.72
8:H:17:ASP:O	8:H:33:LYS:HD2	1.89	0.72
15:Q:220:LEU:HD13	15:Q:224:GLU:HB3	1.71	0.72
8:V:1:THR:N	8:V:168:GLY:O	2.23	0.72
10:J:182:VAL:O	10:J:189:HIS:O	2.08	0.72
7:U:164:LYS:HZ3	7:U:164:LYS:HB2	1.53	0.71
8:H:3:ILE:HD11	8:H:44:CYS:CB	2.18	0.71
4:R:110:GLU:O	4:R:114:GLN:HB2	1.90	0.71
7:U:163:PHE:HB3	7:U:166:THR:HG22	1.73	0.71
3:C:50:VAL:O	3:C:54:GLN:CB	2.37	0.71
12:L:8:ASN:HD22	12:L:58:HIS:H	1.38	0.71
2:P:47:ALA:HB3	2:P:212:GLU:O	1.91	0.71
12:Z:8:ASN:HD22	12:Z:58:HIS:H	1.38	0.71
15:Q:192:ILE:HG21	15:Q:228:TYR:HB3	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:ALA:HB3	2:B:212:GLU:O	1.91	0.70
4:D:110:GLU:O	4:D:114:GLN:HB2	1.90	0.70
9:W:69:ARG:HH12	9:W:93:LEU:HD13	1.56	0.69
15:Q:50:VAL:HA	15:Q:204:LYS:CD	2.11	0.69
8:H:208:THR:HG23	12:Z:158:MET:HG3	1.73	0.69
7:G:50:ILE:O	7:G:217:VAL:HA	1.91	0.69
15:Q:188:ILE:HG22	15:Q:228:TYR:CZ	2.08	0.69
7:U:50:ILE:O	7:U:217:VAL:HA	1.92	0.69
9:I:69:ARG:HH12	9:I:93:LEU:HD13	1.56	0.69
15:Q:206:ILE:HG22	15:Q:225:ILE:CG2	2.21	0.68
15:Q:192:ILE:HD11	15:Q:228:TYR:C	2.14	0.68
7:U:232:GLU:O	7:U:236:ASP:HB2	1.94	0.68
4:D:20:ARG:CZ	4:D:25:GLU:OE1	2.20	0.68
12:Z:12:ILE:HG22	12:Z:25:SER:HA	1.76	0.68
12:L:12:ILE:HG22	12:L:25:SER:HA	1.76	0.67
7:G:232:GLU:O	7:G:236:ASP:HB2	1.94	0.67
8:H:3:ILE:HD13	8:H:44:CYS:HB3	1.76	0.67
6:T:52:LEU:HD22	6:T:207:LYS:HD2	1.76	0.67
15:Q:220:LEU:CD2	15:Q:224:GLU:CG	2.31	0.66
2:P:90:LEU:HD13	2:P:110:LEU:HD21	1.78	0.66
2:B:90:LEU:HD13	2:B:110:LEU:HD21	1.78	0.66
9:W:159:PRO:O	9:W:163:PHE:HB2	1.96	0.66
7:U:42:VAL:HG23	7:U:49:VAL:O	1.96	0.66
15:Q:192:ILE:HD12	15:Q:229:VAL:N	2.11	0.65
9:I:159:PRO:O	9:I:163:PHE:HB2	1.96	0.65
15:Q:226:GLU:OE1	15:Q:226:GLU:HA	1.95	0.65
10:J:108:ASP:HB3	10:J:111:GLU:HG2	1.78	0.65
10:J:190:ASN:OD1	10:J:190:ASN:N	2.28	0.65
9:I:132:THR:HG22	9:I:134:ASP:H	1.60	0.65
8:H:219:LEU:HD21	9:I:194:ILE:HG12	1.79	0.65
9:I:33:MET:O	11:Y:166:ARG:NH1	2.30	0.65
10:X:190:ASN:N	10:X:190:ASN:OD1	2.28	0.65
6:F:157:SER:H	7:G:88:ARG:HH22	1.45	0.64
3:C:31:THR:HA	3:C:162:GLY:HA3	1.80	0.64
8:H:2:THR:HG21	8:H:162:GLY:HA3	1.78	0.64
15:Q:224:GLU:HA	15:Q:224:GLU:OE1	1.97	0.64
15:Q:220:LEU:CB	15:Q:224:GLU:HG3	2.26	0.64
2:B:240:HIS:ND1	2:B:243:GLU:HB3	2.13	0.64
9:W:132:THR:HG22	9:W:134:ASP:H	1.61	0.64
11:K:164:THR:HG22	11:K:170:SER:HB3	1.80	0.64
3:C:50:VAL:HA	3:C:54:GLN:HG2	0.66	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:51:ASP:HB3	8:V:94:ILE:HG23	1.80	0.64
8:H:119:THR:H	14:N:53:GLN:HE22	1.45	0.64
12:L:14:ALA:HA	12:L:22:ILE:O	1.98	0.63
15:Q:192:ILE:HD12	15:Q:228:TYR:HB3	1.66	0.63
8:V:3:ILE:HG23	8:V:127:MET:H	1.63	0.63
14:N:175:ARG:HG2	14:N:188:VAL:HG12	1.80	0.63
12:Z:14:ALA:HA	12:Z:22:ILE:O	1.98	0.63
2:B:91:ARG:HD3	9:I:75:LEU:HB3	1.81	0.63
14:N:45:ARG:HA	14:N:98:ILE:HG22	1.79	0.63
15:Q:31:THR:HA	15:Q:162:GLY:HA3	1.80	0.63
8:H:208:THR:O	9:I:168:GLN:NE2	2.32	0.63
7:U:51:VAL:HG12	7:U:217:VAL:HG22	1.81	0.63
8:V:17:ASP:HB2	8:V:170:GLY:HA3	1.81	0.63
10:J:25:ILE:HG23	10:J:26:VAL:HG13	1.81	0.63
12:L:38:ARG:NH2	8:V:164:PHE:O	2.32	0.62
4:D:20:ARG:CD	4:D:20:ARG:H	2.10	0.62
11:Y:164:THR:HG22	11:Y:170:SER:HB3	1.80	0.62
10:X:25:ILE:HG23	10:X:26:VAL:HG13	1.81	0.62
1:A:5:TYR:CZ	7:G:130:GLU:HB3	2.35	0.62
8:H:51:ASP:HB3	8:H:94:ILE:HG23	1.80	0.62
3:C:100:ASP:OD1	3:C:100:ASP:N	2.31	0.62
12:L:183:ALA:HB2	12:L:210:LEU:HD23	1.82	0.62
15:Q:100:ASP:N	15:Q:100:ASP:OD1	2.31	0.62
15:Q:220:LEU:HD22	15:Q:224:GLU:HG3	0.68	0.62
12:Z:183:ALA:HB2	12:Z:210:LEU:HD23	1.82	0.62
6:T:139:SER:HA	6:T:216:VAL:HG11	1.82	0.61
8:V:103:VAL:HG22	8:V:108:PRO:HB3	1.82	0.61
8:H:17:ASP:HB2	8:H:170:GLY:HA3	1.81	0.61
15:Q:220:LEU:HD22	15:Q:224:GLU:CD	2.19	0.61
7:G:51:VAL:HG12	7:G:217:VAL:HG22	1.81	0.61
1:O:38:LYS:HA	1:O:43:VAL:HG12	1.83	0.61
15:Q:188:ILE:CB	15:Q:228:TYR:CE1	2.83	0.61
14:N:41:ILE:HG12	14:N:76:VAL:HG22	1.82	0.61
11:Y:173:ALA:HA	11:Y:191:ASN:HA	1.83	0.61
7:G:44:GLY:N	7:G:47:CYS:O	2.33	0.61
11:K:11:GLY:HA3	11:K:179:VAL:O	2.01	0.61
7:G:42:VAL:HG21	7:G:194:THR:HG21	1.83	0.60
8:H:103:VAL:HG22	8:H:108:PRO:HB3	1.82	0.60
13:M:26:MET:HE2	13:M:202:PRO:HB3	1.83	0.60
15:Q:192:ILE:HD12	15:Q:228:TYR:CB	2.25	0.60
7:U:42:VAL:HG23	7:U:49:VAL:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:88:ARG:HA	7:U:91:VAL:HG12	1.83	0.60
6:F:65:ARG:HG2	6:F:81:LEU:HD11	1.83	0.60
7:U:44:GLY:O	7:U:46:ASP:N	2.34	0.60
5:E:67:ASP:OD1	5:E:67:ASP:N	2.33	0.60
6:F:120:HIS:NE2	7:G:86:ASP:OD1	2.23	0.60
11:K:173:ALA:HA	11:K:191:ASN:HA	1.83	0.60
12:L:135:PHE:HB2	12:L:149:LEU:HD13	1.83	0.60
16:S:67:ASP:OD1	16:S:67:ASP:N	2.33	0.60
1:A:81:ASP:OD1	7:G:123:GLN:NE2	2.31	0.60
8:H:219:LEU:HG	9:I:47:ARG:HE	1.66	0.60
12:Z:92:LEU:HD13	12:Z:110:ILE:HD11	1.84	0.60
13:M:28:GLY:HA3	13:M:36:PHE:HB2	1.83	0.60
15:Q:206:ILE:O	15:Q:225:ILE:HD12	2.00	0.60
6:T:65:ARG:HG2	6:T:81:LEU:HD11	1.83	0.60
9:W:64:GLN:OE1	10:X:86:ARG:NH2	2.34	0.60
1:A:38:LYS:HA	1:A:43:VAL:HG12	1.83	0.60
9:I:121:CYS:SG	9:I:122:SER:N	2.75	0.60
11:Y:11:GLY:HA3	11:Y:179:VAL:O	2.01	0.60
12:Z:135:PHE:HB2	12:Z:149:LEU:HD13	1.83	0.60
3:C:46:GLU:CD	3:C:199:VAL:CB	2.70	0.59
7:G:44:GLY:C	7:G:46:ASP:N	2.53	0.59
8:H:103:VAL:HG11	8:H:180:LYS:HA	1.84	0.59
2:B:136:TYR:O	2:B:140:ASP:HB2	12.94	0.59
4:R:164:GLN:HB3	16:S:58:ALA:H	1.66	0.59
10:X:193:ASN:N	10:X:193:ASN:HD22	2.00	0.59
7:G:88:ARG:HA	7:G:91:VAL:HG12	1.84	0.59
6:T:240:LYS:HA	6:T:243:LEU:HB2	1.84	0.59
9:W:121:CYS:SG	9:W:122:SER:N	2.75	0.59
5:E:155:ASP:HB3	6:F:62:SER:HA	1.85	0.59
10:X:182:VAL:HG23	10:X:191:LEU:CD1	2.33	0.59
10:X:19:ARG:NH1	10:X:193:ASN:OD1	2.36	0.59
7:G:44:GLY:C	7:G:46:ASP:H	2.06	0.59
8:V:103:VAL:HG11	8:V:180:LYS:HA	1.84	0.59
10:J:186:ASP:HB2	10:J:189:HIS:CE1	2.37	0.59
4:D:20:ARG:NE	4:D:25:GLU:OE1	2.36	0.59
6:F:139:SER:HA	6:F:216:VAL:HG11	1.84	0.59
9:I:64:GLN:OE1	10:J:86:ARG:NH2	2.36	0.59
3:C:65:LEU:HB2	3:C:69:VAL:HG23	1.85	0.58
12:L:92:LEU:HD13	12:L:110:ILE:HD11	1.84	0.58
5:E:189:LYS:HE3	5:E:233:LEU:H	1.67	0.58
7:G:90:GLN:HE21	7:G:134:LEU:HD11	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:136:TYR:O	14:N:140:ASP:HB2	2.02	0.58
15:Q:33:VAL:HG12	15:Q:44:GLY:O	2.03	0.58
5:E:101:ARG:NH1	13:M:74:GLU:OE2	2.37	0.58
1:O:111:GLN:NE2	1:O:154:TYR:OH	2.36	0.58
15:Q:51:ALA:HA	15:Q:54:GLN:CG	2.33	0.58
3:C:45:VAL:HG22	3:C:45:VAL:O	2.04	0.58
13:M:41:ARG:NH1	13:M:53:ALA:O	2.36	0.58
8:V:219:LEU:HG	9:W:47:ARG:HE	1.68	0.58
12:L:157:ASN:HD21	9:W:202:ARG:HG2	1.69	0.58
6:T:97:ASN:O	6:T:101:ASN:HB2	2.04	0.58
7:U:90:GLN:HE21	7:U:134:LEU:HD11	1.68	0.58
10:X:182:VAL:HG23	10:X:191:LEU:HG	1.86	0.58
10:J:27:GLN:NE2	10:X:169:LYS:O	2.37	0.57
11:K:155:LEU:O	11:K:159:ALA:HB2	2.04	0.57
15:Q:65:LEU:HB2	15:Q:69:VAL:HG23	1.85	0.57
3:C:50:VAL:CA	3:C:54:GLN:CB	2.76	0.57
12:L:28:ARG:NH2	12:L:213:ASP:OXT	2.37	0.57
1:O:123:SER:HA	2:P:127:LYS:HE3	1.85	0.57
6:F:97:ASN:O	6:F:101:ASN:HB2	2.04	0.57
8:H:1:THR:HG22	8:H:33:LYS:CE	2.34	0.57
1:O:42:GLY:H	1:O:143:PRO:HG3	1.70	0.57
11:Y:155:LEU:O	11:Y:159:ALA:HB2	2.04	0.57
5:E:10:VAL:HB	5:E:21:GLN:HE21	1.69	0.57
9:I:188:ILE:HB	9:I:195:THR:HB	1.87	0.57
4:R:118:ASN:OD1	16:S:82:ARG:NH1	2.37	0.57
1:A:43:VAL:HG21	1:A:136:CYS:HB2	1.85	0.57
15:Q:92:GLN:O	15:Q:96:LEU:CB	3.67	0.57
7:U:42:VAL:HG22	7:U:49:VAL:C	2.17	0.57
4:D:97:GLN:HB3	11:K:61:ARG:HG3	1.87	0.57
10:J:8:GLN:NE2	10:J:113:PRO:O	2.38	0.57
7:U:44:GLY:O	7:U:45:LYS:C	2.41	0.57
9:W:188:ILE:HB	9:W:195:THR:HB	1.87	0.57
11:Y:177:TYR:OH	11:Y:186:ARG:NH2	2.38	0.57
8:V:3:ILE:HD13	8:V:44:CYS:HB3	1.73	0.57
4:D:20:ARG:H	4:D:20:ARG:HD2	1.70	0.56
1:O:43:VAL:HG21	1:O:136:CYS:HB2	1.85	0.56
11:K:177:TYR:OH	11:K:186:ARG:NH2	2.38	0.56
15:Q:220:LEU:CG	15:Q:224:GLU:CG	2.75	0.56
1:A:42:GLY:H	1:A:143:PRO:HG3	1.70	0.56
1:A:144:TYR:HB3	8:H:132:LEU:HB3	53.89	0.56
10:J:193:ASN:N	10:J:193:ASN:HD22	2.02	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:8:GLN:NE2	10:X:113:PRO:O	2.38	0.56
10:J:16:ALA:HA	10:J:179:SER:O	2.05	0.56
14:N:164:MET:HB2	14:N:171:GLY:HA2	1.87	0.56
11:K:13:ILE:HA	11:K:177:TYR:O	2.06	0.56
16:S:10:VAL:HB	16:S:21:GLN:HE21	1.69	0.56
3:C:182:GLU:OE2	3:C:186:LEU:N	2.33	0.56
10:X:16:ALA:HA	10:X:179:SER:O	2.05	0.56
2:P:184:MET:O	2:P:188:SER:OG	2.24	0.56
7:G:80:MET:SD	7:G:80:MET:N	2.79	0.56
9:I:39:GLN:NE2	9:I:41:ILE:O	2.39	0.56
7:U:41:ALA:HB1	7:U:151:VAL:HG21	1.88	0.56
13:M:144:TYR:HB3	8:V:132:LEU:HB3	1.87	0.56
8:H:12:ILE:HD11	8:H:178:ILE:HD12	1.88	0.55
2:B:184:MET:O	2:B:188:SER:OG	2.24	0.55
7:U:232:GLU:HA	7:U:235:ILE:HG22	1.88	0.55
9:W:13:MET:HG3	9:W:162:LEU:HD11	1.87	0.55
5:E:121:GLN:NE2	6:F:83:ASP:OD1	2.40	0.55
9:W:39:GLN:NE2	9:W:41:ILE:O	2.39	0.55
4:R:97:GLN:HB3	11:Y:61:ARG:HG3	1.89	0.55
16:S:22:ILE:HG22	16:S:127:PRO:HG3	1.89	0.55
11:Y:13:ILE:HA	11:Y:177:TYR:O	2.06	0.55
9:I:13:MET:HG3	9:I:162:LEU:HD11	1.87	0.55
10:X:182:VAL:HG23	10:X:191:LEU:HD11	1.88	0.55
13:M:25:ASP:OD1	13:M:41:ARG:NH2	2.40	0.55
8:V:12:ILE:HD11	8:V:178:ILE:HD12	1.88	0.55
6:F:37:ILE:HD11	6:F:193:VAL:HG13	1.89	0.55
12:L:28:ARG:HH11	12:L:35:ILE:HG21	1.72	0.55
1:O:92:LEU:HD13	1:O:112:ARG:HB3	1.89	0.55
7:G:232:GLU:HA	7:G:235:ILE:HG22	1.88	0.54
15:Q:206:ILE:HG23	15:Q:225:ILE:HG22	1.26	0.54
7:U:80:MET:SD	7:U:80:MET:N	2.79	0.54
6:T:157:SER:H	7:U:88:ARG:HH22	1.55	0.54
13:M:89:HIS:HB2	13:M:112:ILE:HD11	1.89	0.54
6:T:215:TRP:HZ3	6:T:227:VAL:HG23	1.73	0.54
6:T:37:ILE:HD11	6:T:193:VAL:HG13	1.89	0.54
10:J:182:VAL:HG21	10:J:191:LEU:HD11	1.89	0.54
6:T:227:VAL:HG11	6:T:232:ARG:HG2	1.90	0.54
4:D:20:ARG:C	4:D:20:ARG:HD2	2.27	0.54
5:E:22:ILE:HG22	5:E:127:PRO:HG3	1.88	0.54
6:F:186:CYS:HA	6:F:189:ILE:HG12	1.90	0.54
14:N:19:ARG:NH1	14:N:168:GLY:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:2:THR:OG1	8:V:130:GLY:HA3	2.07	0.54
5:E:215:VAL:HB	5:E:221:PHE:HD1	1.73	0.54
13:M:109:THR:HG23	13:M:126:ASP:HA	1.89	0.54
2:B:88:ASN:HD21	9:I:76:LYS:HE2	1.73	0.54
8:H:1:THR:CB	8:H:33:LYS:HZ1	2.09	0.54
2:P:169:ALA:HA	2:P:173:SER:H	1.73	0.54
7:G:44:GLY:O	7:G:45:LYS:C	2.44	0.54
6:F:215:TRP:HZ3	6:F:227:VAL:HG23	1.73	0.54
12:L:13:LEU:O	12:L:24:ALA:N	2.39	0.54
1:A:127:ARG:O	7:G:127:GLN:NE2	2.41	0.54
6:F:227:VAL:HG11	6:F:232:ARG:HG2	1.89	0.54
13:M:105:PRO:HG2	13:M:107:TRP:HE1	1.73	0.54
9:W:146:TYR:O	9:W:149:CYS:N	2.41	0.54
1:A:111:GLN:NE2	1:A:154:TYR:OH	2.36	0.54
1:A:92:LEU:HD13	1:A:112:ARG:HB3	1.89	0.54
16:S:215:VAL:HB	16:S:221:PHE:HD1	1.73	0.54
3:C:233:GLU:HA	3:C:233:GLU:OE1	2.08	0.53
12:Z:28:ARG:NH2	12:Z:213:ASP:OXT	2.37	0.53
12:Z:28:ARG:HH11	12:Z:35:ILE:HG21	1.72	0.53
15:Q:47:LYS:CA	15:Q:207:GLU:OE1	2.50	0.53
9:I:146:TYR:O	9:I:149:CYS:N	2.41	0.53
12:L:166:LEU:HD23	12:L:171:ALA:HB2	1.91	0.53
1:A:67:ILE:N	1:A:71:ILE:O	2.34	0.53
2:B:49:ARG:NH1	2:B:211:VAL:O	2.41	0.53
5:E:34:ALA:HA	5:E:162:GLY:HA3	1.90	0.53
7:G:40:VAL:O	7:G:51:VAL:CG2	2.57	0.53
7:U:168:ALA:HB2	7:U:172:GLN:NE2	2.24	0.53
4:D:20:ARG:N	4:D:20:ARG:HD2	2.24	0.53
1:O:118:GLN:HE21	2:P:85:VAL:HG21	1.73	0.53
7:U:139:ILE:HD13	7:U:153:LYS:HB2	1.91	0.53
11:Y:73:ARG:NH2	11:Y:104:TRP:O	2.42	0.53
6:T:186:CYS:HA	6:T:189:ILE:HG12	1.90	0.53
11:K:166:ARG:NH2	10:X:144:ASP:OD1	2.34	0.53
5:E:9:ASP:N	5:E:9:ASP:OD1	2.41	0.53
12:L:88:ILE:HG22	12:L:110:ILE:HD13	1.91	0.53
13:M:13:GLY:HA3	13:M:22:ILE:HG22	1.91	0.53
15:Q:158:ALA:HB1	15:Q:172:LEU:HD13	1.90	0.53
4:D:41:GLN:HB3	4:D:166:ASP:HA	1.91	0.53
15:Q:46:GLU:O	15:Q:47:LYS:C	2.46	0.53
8:V:2:THR:OG1	8:V:130:GLY:CA	2.57	0.53
8:V:2:THR:CB	8:V:130:GLY:HA3	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:52:LEU:HG	9:I:106:PRO:HB3	1.91	0.53
2:P:49:ARG:NH1	2:P:211:VAL:O	2.41	0.53
4:D:189:MET:HG3	4:D:191:LEU:H	1.74	0.52
9:W:52:LEU:HG	9:W:106:PRO:HB3	1.91	0.52
12:Z:166:LEU:HD23	12:Z:171:ALA:HB2	1.91	0.52
11:K:73:ARG:NH2	11:K:104:TRP:O	2.42	0.52
16:S:121:GLN:NE2	6:T:83:ASP:OD1	2.43	0.52
4:D:81:LEU:HD12	4:D:84:ASP:HB2	1.91	0.52
15:Q:221:ASN:O	15:Q:222:PRO:C	2.46	0.52
7:G:139:ILE:HD13	7:G:153:LYS:HB2	1.91	0.52
14:N:12:VAL:HG21	14:N:101:ALA:HB1	1.91	0.52
15:Q:221:ASN:C	15:Q:223:GLU:N	2.63	0.52
3:C:158:ALA:HB1	3:C:172:LEU:HD13	1.90	0.52
15:Q:31:THR:O	15:Q:45:VAL:HA	2.10	0.52
12:Z:43:CYS:HA	12:Z:52:ILE:O	2.10	0.52
3:C:45:VAL:HG11	3:C:61:LYS:HB2	1.92	0.52
3:C:98:VAL:HG23	11:K:78:ALA:HB2	1.92	0.52
10:J:88:LEU:HD22	10:J:122:ALA:HB2	1.91	0.52
15:Q:98:VAL:HG23	11:Y:78:ALA:HB2	1.92	0.52
4:R:81:LEU:HD12	4:R:84:ASP:HB2	1.91	0.52
12:Z:88:ILE:HG22	12:Z:110:ILE:HD13	1.91	0.52
6:F:94:GLU:OE2	6:F:114:ARG:NH1	2.43	0.52
12:L:27:THR:OG1	12:L:192:ALA:O	2.28	0.52
13:M:46:ASN:ND2	13:M:82:SER:OG	2.42	0.52
15:Q:192:ILE:HD11	15:Q:228:TYR:CA	2.35	0.52
6:T:94:GLU:OE2	6:T:114:ARG:NH1	2.43	0.52
12:Z:10:GLY:HA3	12:Z:42:LYS:HE3	1.92	0.52
12:L:10:GLY:HA3	12:L:42:LYS:HE3	1.92	0.52
14:N:31:THR:O	14:N:175:ARG:NH1	2.42	0.52
1:O:110:VAL:HG22	1:O:135:ILE:HG13	1.92	0.52
15:Q:87:ALA:HB2	15:Q:111:ILE:HD11	1.92	0.52
15:Q:116:GLN:NE2	4:R:84:ASP:OD1	2.42	0.52
8:V:2:THR:HG1	8:V:130:GLY:C	2.10	0.52
15:Q:49:SER:O	15:Q:50:VAL:CB	2.56	0.51
16:S:34:ALA:HA	16:S:162:GLY:HA3	1.90	0.51
8:V:3:ILE:HG21	8:V:127:MET:HB2	1.92	0.51
12:Z:13:LEU:O	12:Z:24:ALA:N	2.39	0.51
7:G:42:VAL:CG2	7:G:194:THR:HG21	2.40	0.51
12:L:43:CYS:HA	12:L:52:ILE:O	2.10	0.51
13:M:11:VAL:HG21	13:M:53:ALA:H	1.75	0.51
2:P:49:ARG:NH2	2:P:212:GLU:OE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:188:ILE:HG23	15:Q:228:TYR:CE2	2.40	0.51
10:X:88:LEU:HD22	10:X:122:ALA:HB2	1.91	0.51
1:A:110:VAL:HG22	1:A:135:ILE:HG13	1.92	0.51
10:J:19:ARG:NH1	10:J:193:ASN:OD1	2.43	0.51
12:L:139:GLY:N	12:L:142:SER:OG	2.36	0.51
15:Q:46:GLU:O	15:Q:47:LYS:O	2.28	0.51
7:U:230:LEU:HD22	7:U:234:GLU:HG3	1.93	0.51
3:C:87:ALA:HB2	3:C:111:ILE:HD11	1.92	0.51
7:U:44:GLY:C	7:U:46:ASP:N	2.62	0.51
3:C:50:VAL:C	3:C:54:GLN:CG	2.74	0.51
15:Q:206:ILE:HG22	15:Q:225:ILE:HG21	1.86	0.51
1:O:38:LYS:HE3	1:O:143:PRO:HG2	1.93	0.51
15:Q:50:VAL:HA	15:Q:204:LYS:HD3	1.92	0.51
4:R:51:GLU:OE1	4:R:204:GLN:NE2	2.44	0.51
16:S:9:ASP:OD1	16:S:9:ASP:N	2.41	0.51
11:K:127:SER:O	11:K:132:SER:OG	2.29	0.51
15:Q:51:ALA:HA	15:Q:54:GLN:HG2	1.92	0.51
3:C:39:ASP:OD1	3:C:213:ARG:NE	2.43	0.51
8:H:29:LYS:NZ	9:I:150:GLU:OE2	2.32	0.51
15:Q:192:ILE:CG2	15:Q:228:TYR:HB3	2.40	0.51
4:R:41:GLN:HB3	4:R:166:ASP:HA	1.91	0.51
10:X:182:VAL:HG23	10:X:191:LEU:CG	2.41	0.51
12:Z:139:GLY:N	12:Z:142:SER:OG	2.36	0.51
2:P:162:THR:HA	2:P:172:VAL:HG21	1.93	0.50
15:Q:188:ILE:HG22	15:Q:228:TYR:CG	2.46	0.50
12:L:13:LEU:HB3	12:L:24:ALA:HB3	1.93	0.50
13:M:114:GLY:HA2	13:M:192:VAL:HG11	1.92	0.50
1:O:35:VAL:HG12	1:O:46:ALA:HB3	1.94	0.50
15:Q:32:ALA:CB	15:Q:45:VAL:HG13	2.27	0.50
4:R:189:MET:HG3	4:R:191:LEU:H	1.74	0.50
7:G:40:VAL:O	7:G:51:VAL:HG22	2.10	0.50
12:L:13:LEU:HD13	12:L:137:ALA:HB2	1.94	0.50
1:A:123:SER:HA	2:B:127:LYS:HE3	1.93	0.50
4:D:146:VAL:HG23	4:D:151:PRO:HG3	1.94	0.50
4:D:51:GLU:OE1	4:D:204:GLN:NE2	2.44	0.50
16:S:85:CYS:O	16:S:89:ARG:HB2	2.11	0.50
13:M:98:SER:O	13:M:102:LYS:NZ	2.41	0.50
14:N:84:LYS:O	14:N:88:TYR:CB	2.60	0.50
12:L:185:ARG:HD3	8:V:26:VAL:HG13	1.94	0.50
15:Q:220:LEU:CD1	15:Q:228:TYR:HE2	2.23	0.50
4:R:146:VAL:HG23	4:R:151:PRO:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:16:GLN:HG2	5:E:17:GLY:H	1.77	0.50
16:S:132:LEU:HB2	16:S:147:THR:HG22	1.94	0.50
16:S:16:GLN:HG2	16:S:17:GLY:H	1.77	0.50
12:Z:13:LEU:HD13	12:Z:137:ALA:HB2	1.94	0.50
6:T:67:PHE:HB2	6:T:75:MET:HB2	1.94	0.50
7:G:230:LEU:HD22	7:G:234:GLU:HG3	1.93	0.50
14:N:151:GLU:HA	14:N:154:GLN:HG2	1.93	0.50
2:P:49:ARG:NH1	2:P:208:ALA:O	2.45	0.50
4:R:147:ASP:OD2	4:R:152:GLN:NE2	2.45	0.50
7:U:170:VAL:O	7:U:171:LYS:CB	2.59	0.50
10:X:4:LEU:HD22	10:X:45:LEU:HD23	1.94	0.50
7:U:232:GLU:O	7:U:236:ASP:CB	2.59	0.50
4:D:121:LEU:HD23	5:E:126:ARG:HH21	1.76	0.50
15:Q:188:ILE:HG21	15:Q:228:TYR:HH	1.68	0.50
7:U:49:VAL:HG23	7:U:219:VAL:HG12	1.93	0.50
2:B:49:ARG:NH2	2:B:212:GLU:OE1	2.44	0.49
2:B:49:ARG:NH1	2:B:208:ALA:O	2.45	0.49
5:E:85:CYS:O	5:E:89:ARG:HB2	2.11	0.49
8:H:198:ARG:NH1	9:I:150:GLU:O	2.45	0.49
12:Z:13:LEU:HB3	12:Z:24:ALA:HB3	1.93	0.49
6:F:227:VAL:HG13	6:F:229:LYS:HA	1.94	0.49
7:G:73:THR:HG23	7:G:75:ASN:H	1.78	0.49
8:H:32:SER:HB3	8:H:187:ARG:HH12	1.77	0.49
14:N:144:ARG:HG3	14:N:145:GLU:H	1.77	0.49
1:O:201:GLN:OE1	1:O:203:THR:OG1	2.28	0.49
15:Q:192:ILE:HG21	15:Q:228:TYR:CG	2.47	0.49
8:V:43:CYS:HA	8:V:100:LEU:HA	1.94	0.49
11:Y:127:SER:O	11:Y:132:SER:OG	2.29	0.49
7:G:49:VAL:HG23	7:G:219:VAL:HG12	1.93	0.49
6:T:227:VAL:HG13	6:T:229:LYS:HA	1.94	0.49
12:Z:15:ILE:O	12:Z:21:ALA:HA	2.12	0.49
10:J:193:ASN:ND2	10:J:193:ASN:N	2.60	0.49
1:A:38:LYS:HE3	1:A:143:PRO:HG2	1.93	0.49
5:E:132:LEU:HB2	5:E:147:THR:HG22	1.94	0.49
10:J:4:LEU:HD22	10:J:45:LEU:HD23	1.94	0.49
2:B:13:SER:OG	2:B:17:ARG:N	2.46	0.49
4:D:110:GLU:O	4:D:114:GLN:CB	2.59	0.49
1:O:184:GLU:HG3	1:O:187:ILE:HD12	1.94	0.49
7:U:43:ARG:HD3	7:U:151:VAL:HG12	1.93	0.49
11:K:166:ARG:NH1	9:W:33:MET:O	2.40	0.49
1:O:106:THR:HB	1:O:144:TYR:HD2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:GLU:HG3	1:A:187:ILE:HD12	1.94	0.49
1:A:35:VAL:HG12	1:A:46:ALA:HB3	1.93	0.49
8:H:38:SER:HB3	8:H:41:ILE:HB	1.95	0.49
8:V:32:SER:HB3	8:V:187:ARG:HH12	1.77	0.49
1:A:70:HIS:HA	1:A:217:PHE:H	1.78	0.49
4:D:147:ASP:OD2	4:D:152:GLN:NE2	2.45	0.49
6:F:140:TYR:HB3	6:F:146:ALA:HA	1.94	0.49
7:G:165:ALA:HB1	7:G:179:LEU:HD13	1.95	0.49
8:H:119:THR:H	14:N:53:GLN:NE2	2.11	0.49
10:J:59:TYR:HE2	10:J:87:ASN:HD21	1.59	0.49
14:N:29:ARG:HG3	14:N:30:VAL:HG22	1.95	0.49
8:V:37:ILE:HG23	8:V:60:SER:HA	1.95	0.49
3:C:34:GLY:HA2	3:C:42:VAL:O	2.13	0.49
5:E:67:ASP:OD2	5:E:70:ILE:N	2.46	0.49
6:F:67:PHE:HB2	6:F:75:MET:HB2	1.94	0.49
8:H:37:ILE:HG23	8:H:60:SER:HA	1.95	0.49
7:U:73:THR:HG23	7:U:75:ASN:H	1.77	0.49
9:W:59:VAL:O	9:W:63:ALA:HB2	2.13	0.49
10:X:59:TYR:HE2	10:X:87:ASN:HD21	1.59	0.49
9:I:59:VAL:O	9:I:63:ALA:HB2	2.13	0.48
2:P:13:SER:OG	2:P:17:ARG:N	2.46	0.48
15:Q:47:LYS:HG2	15:Q:205:ASN:N	2.04	0.48
16:S:67:ASP:HB2	16:S:70:ILE:H	1.78	0.48
9:W:12:ALA:HA	9:W:20:ALA:O	2.13	0.48
10:X:164:LEU:HD12	10:X:194:ILE:HD12	1.95	0.48
12:Z:27:THR:OG1	12:Z:192:ALA:O	2.28	0.48
12:Z:44:TYR:HB2	12:Z:52:ILE:HG22	1.95	0.48
9:I:12:ALA:HA	9:I:20:ALA:O	2.13	0.48
12:L:28:ARG:NH2	12:L:189:THR:OG1	2.46	0.48
15:Q:34:GLY:HA2	15:Q:42:VAL:O	2.13	0.48
7:U:44:GLY:HA3	7:U:47:CYS:O	2.12	0.48
3:C:115:LYS:HG2	3:C:127:PHE:HD2	1.78	0.48
8:H:43:CYS:HA	8:H:100:LEU:HA	1.94	0.48
12:L:15:ILE:O	12:L:21:ALA:HA	2.13	0.48
2:B:162:THR:HA	2:B:172:VAL:HG21	1.93	0.48
9:I:146:TYR:O	9:I:148:MET:N	2.46	0.48
9:I:150:GLU:OE1	12:Z:185:ARG:NE	2.46	0.48
10:J:182:VAL:CG2	10:J:191:LEU:HD11	2.43	0.48
1:O:134:LEU:HB3	1:O:162:MET:HE1	1.94	0.48
6:T:160:TYR:CG	6:T:163:CYS:HB3	2.49	0.48
9:W:146:TYR:O	9:W:148:MET:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:28:ARG:NH2	12:Z:189:THR:OG1	2.46	0.48
5:E:67:ASP:HB2	5:E:70:ILE:H	1.79	0.48
15:Q:115:LYS:HG2	15:Q:127:PHE:HD2	1.78	0.48
15:Q:192:ILE:HD13	15:Q:228:TYR:HB3	0.50	0.48
3:C:89:VAL:HG22	10:J:66:LEU:HD11	1.95	0.48
4:D:85:ALA:HB2	4:D:139:VAL:HG21	1.95	0.48
4:R:99:HIS:CD2	4:R:107:MET:HG2	2.49	0.48
10:X:193:ASN:N	10:X:193:ASN:ND2	2.60	0.48
9:I:202:ARG:HG2	12:Z:157:ASN:HD21	1.76	0.48
3:C:141:THR:HG22	3:C:143:ARG:HG3	1.96	0.48
13:M:122:LEU:HG	13:M:137:LEU:HD12	1.96	0.48
14:N:152:CYS:HA	14:N:155:PHE:HB3	1.96	0.48
1:O:70:HIS:HA	1:O:217:PHE:H	1.78	0.48
15:Q:188:ILE:CD1	15:Q:228:TYR:HH	2.02	0.48
15:Q:39:ASP:OD1	15:Q:213:ARG:NE	2.43	0.48
4:R:110:GLU:O	4:R:114:GLN:CB	2.59	0.48
16:S:85:CYS:O	16:S:89:ARG:CB	2.62	0.48
11:Y:19:ARG:NH1	11:Y:170:SER:O	2.47	0.48
11:Y:157:ARG:NH1	11:Y:190:ASP:OD2	2.47	0.48
7:U:112:ASP:N	7:U:112:ASP:OD1	2.46	0.48
4:D:99:HIS:CD2	4:D:107:MET:HG2	2.48	0.48
6:F:141:SER:HB2	6:F:144:ASP:HB2	1.96	0.48
16:S:67:ASP:OD2	16:S:70:ILE:N	2.46	0.48
8:V:107:GLY:O	8:V:109:HIS:ND1	2.46	0.48
8:H:204:CYS:SG	8:H:205:GLU:N	2.86	0.48
4:R:85:ALA:HB2	4:R:139:VAL:HG21	1.95	0.48
6:F:160:TYR:CG	6:F:163:CYS:HB3	2.49	0.48
15:Q:221:ASN:HB2	15:Q:222:PRO:CD	2.42	0.48
6:T:141:SER:HB2	6:T:144:ASP:HB2	1.96	0.48
10:X:182:VAL:CG2	10:X:191:LEU:CD1	2.87	0.48
8:V:38:SER:HB3	8:V:41:ILE:HB	1.95	0.47
1:A:106:THR:HB	1:A:144:TYR:HD2	1.78	0.47
2:B:34:CYS:SG	2:B:75:SER:OG	2.67	0.47
3:C:50:VAL:C	3:C:54:GLN:HG2	2.29	0.47
5:E:85:CYS:O	5:E:89:ARG:CB	2.62	0.47
6:T:140:TYR:HB3	6:T:146:ALA:HA	1.94	0.47
12:Z:16:ALA:HB3	12:Z:134:SER:HA	1.96	0.47
11:K:157:ARG:NH1	11:K:190:ASP:OD2	2.47	0.47
15:Q:47:LYS:H	15:Q:47:LYS:HD2	1.78	0.47
8:V:137:VAL:HG21	8:V:158:ALA:HA	1.97	0.47
10:J:186:ASP:HB2	10:J:189:HIS:NE2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:19:ARG:NH1	11:K:170:SER:O	2.47	0.47
12:L:16:ALA:HB3	12:L:134:SER:HA	1.96	0.47
12:L:36:HIS:HB3	13:M:132:TYR:CZ	2.49	0.47
6:F:157:SER:H	7:G:88:ARG:NH2	2.12	0.47
7:G:42:VAL:HG11	7:G:198:ALA:HA	1.96	0.47
12:L:28:ARG:HG2	12:L:38:ARG:HG2	1.96	0.47
12:L:65:THR:O	12:L:69:GLU:HB2	2.14	0.47
15:Q:141:THR:HG22	15:Q:143:ARG:HG3	1.96	0.47
4:R:142:LEU:HD13	4:R:153:LEU:HD13	1.97	0.47
10:X:186:ASP:HB2	10:X:189:HIS:HE1	1.80	0.47
4:D:71:ASP:HB2	4:D:96:THR:HG21	1.96	0.47
12:L:44:TYR:HB2	12:L:52:ILE:HG22	1.95	0.47
1:O:157:TRP:HA	2:P:57:ASP:H	1.79	0.47
7:G:232:GLU:O	7:G:236:ASP:CB	2.59	0.47
10:J:81:ALA:HB1	10:J:124:LEU:HD11	1.97	0.47
2:P:86:LEU:HA	2:P:89:GLU:HB2	1.97	0.47
4:R:71:ASP:HB2	4:R:96:THR:HG21	1.96	0.47
7:U:40:VAL:C	7:U:167:ALA:HB2	2.33	0.47
6:F:87:LEU:HA	6:F:90:ILE:HG13	1.96	0.47
7:G:17:SER:OG	7:G:20:GLY:O	2.32	0.47
6:T:175:GLU:HA	6:T:178:LYS:HG2	1.97	0.47
6:F:97:ASN:O	6:F:101:ASN:CB	2.63	0.47
12:Z:24:ALA:HA	12:Z:195:ILE:HG22	1.96	0.47
12:Z:65:THR:O	12:Z:69:GLU:HB2	2.14	0.47
2:B:50:ARG:NH1	2:B:51:ASN:OD1	2.48	0.47
15:Q:180:ALA:HB1	15:Q:187:THR:HG22	1.97	0.47
11:Y:84:ALA:O	11:Y:88:TYR:HB2	2.15	0.47
6:F:175:GLU:HA	6:F:178:LYS:HG2	1.97	0.47
15:Q:220:LEU:CD1	15:Q:224:GLU:HB3	2.41	0.46
6:F:112:ALA:O	6:F:116:ALA:HB2	2.15	0.46
6:F:143:ASN:HD21	14:N:106:GLN:HG3	1.79	0.46
11:K:84:ALA:O	11:K:88:TYR:HB2	2.15	0.46
13:M:110:MET:SD	13:M:110:MET:N	2.87	0.46
6:T:87:LEU:HA	6:T:90:ILE:HG13	1.97	0.46
9:W:57:THR:O	9:W:61:THR:OG1	2.25	0.46
2:B:123:GLN:NE2	3:C:124:ARG:O	2.47	0.46
4:D:208:GLU:OE2	4:D:211:ASN:ND2	2.49	0.46
5:E:14:SER:HB2	5:E:18:ARG:HB3	1.98	0.46
6:F:15:SER:OG	6:F:19:ARG:N	2.48	0.46
12:L:24:ALA:HA	12:L:195:ILE:HG22	1.96	0.46
13:M:26:MET:CE	13:M:202:PRO:HG3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:14:SER:HB2	16:S:18:ARG:HB3	1.98	0.46
6:T:97:ASN:O	6:T:101:ASN:CB	2.63	0.46
2:P:34:CYS:SG	2:P:75:SER:OG	2.67	0.46
12:L:94:THR:O	12:L:98:SER:HB3	2.16	0.46
15:Q:202:GLY:H	15:Q:229:VAL:HG21	1.81	0.46
2:B:240:HIS:CE1	2:B:243:GLU:HB3	2.49	0.46
4:D:142:LEU:HD13	4:D:153:LEU:HD13	1.97	0.46
7:G:112:ASP:OD1	7:G:112:ASP:N	2.46	0.46
2:P:50:ARG:NH1	2:P:51:ASN:OD1	2.48	0.46
2:B:86:LEU:HA	2:B:89:GLU:HB2	1.97	0.46
9:I:163:PHE:O	9:I:197:ARG:NH2	2.49	0.46
3:C:92:GLN:HB3	10:J:62:LYS:HG3	1.97	0.46
6:T:15:SER:OG	6:T:19:ARG:N	2.48	0.46
8:V:3:ILE:CG2	8:V:127:MET:HB2	2.45	0.46
9:W:163:PHE:O	9:W:197:ARG:NH2	2.49	0.46
12:Z:94:THR:O	12:Z:98:SER:HB3	2.16	0.46
4:R:38:ILE:HD13	4:R:197:SER:HB2	1.98	0.46
1:A:134:LEU:HA	1:A:147:GLN:HA	1.98	0.46
6:F:28:LYS:HD3	6:F:31:GLU:HB2	1.98	0.46
8:H:1:THR:CA	8:H:33:LYS:NZ	2.79	0.46
9:I:14:LYS:HE3	9:I:133:ASP:HA	1.98	0.46
16:S:169:ARG:O	16:S:173:GLU:N	2.48	0.46
3:C:180:ALA:HB1	3:C:187:THR:HG22	1.97	0.46
9:I:1:SER:OG	9:I:2:ILE:N	2.48	0.46
15:Q:146:GLN:NE2	15:Q:147:THR:O	2.49	0.46
6:T:112:ALA:O	6:T:116:ALA:HB2	2.15	0.46
9:I:169:ALA:O	9:I:173:ALA:CB	2.64	0.46
1:O:67:ILE:N	1:O:71:ILE:O	2.34	0.46
9:W:14:LYS:HE3	9:W:133:ASP:HA	1.98	0.46
9:W:1:SER:OG	9:W:2:ILE:N	2.48	0.46
12:Z:28:ARG:HG2	12:Z:38:ARG:HG2	1.96	0.46
16:S:14:SER:N	16:S:18:ARG:O	2.43	0.45
16:S:121:GLN:HB3	6:T:122:TYR:OH	2.15	0.45
7:U:17:SER:OG	7:U:20:GLY:O	2.32	0.45
9:I:204:ASP:HB3	11:Y:192:VAL:HG11	1.99	0.45
10:J:64:VAL:HG13	10:J:75:LEU:HD12	1.98	0.45
15:Q:63:CYS:HG	15:Q:73:PHE:HE1	1.63	0.45
7:U:141:ILE:HD12	7:U:220:VAL:HG22	1.98	0.45
10:X:66:LEU:O	10:X:70:ARG:HB2	2.17	0.45
6:T:30:VAL:HG11	6:T:134:SER:H	1.81	0.45
9:I:18:CYS:HA	9:I:189:ILE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:127:ILE:HG12	14:N:132:SER:HB2	1.98	0.45
1:O:134:LEU:HA	1:O:147:GLN:HA	1.98	0.45
15:Q:188:ILE:HG22	15:Q:228:TYR:CE2	2.41	0.45
9:I:146:TYR:HB3	12:Z:185:ARG:HG2	1.97	0.45
10:X:64:VAL:HG13	10:X:75:LEU:HD12	1.98	0.45
6:F:105:ASN:HD22	6:F:106:ILE:H	1.64	0.45
6:F:34:SER:HG	6:F:65:ARG:HH12	1.59	0.45
8:H:107:GLY:O	8:H:109:HIS:ND1	2.46	0.45
8:H:137:VAL:HG21	8:H:158:ALA:HA	1.97	0.45
11:K:97:MET:H	11:K:116:SER:HB2	1.82	0.45
12:L:145:LEU:HD22	12:L:178:VAL:HB	1.98	0.45
1:O:202:MET:HE3	1:O:207:ILE:HG12	1.98	0.45
9:W:169:ALA:O	9:W:173:ALA:CB	2.64	0.45
10:X:81:ALA:HB1	10:X:124:LEU:HD11	1.97	0.45
3:C:146:GLN:NE2	3:C:147:THR:O	2.49	0.45
15:Q:79:ASP:HB3	15:Q:127:PHE:HD1	1.82	0.45
6:T:28:LYS:HD3	6:T:31:GLU:HB2	1.98	0.45
11:Y:97:MET:H	11:Y:116:SER:HB2	1.82	0.45
1:A:202:MET:HE3	1:A:207:ILE:HG12	1.99	0.45
4:D:38:ILE:HD13	4:D:197:SER:HB2	1.98	0.45
5:E:196:ARG:HH22	5:E:235:GLY:HA3	1.81	0.45
6:F:106:ILE:HD12	6:F:107:PRO:HD2	1.98	0.45
6:F:30:VAL:HG11	6:F:134:SER:H	1.81	0.45
7:G:141:ILE:HD12	7:G:220:VAL:HG22	1.98	0.45
12:L:191:ASP:O	12:L:210:LEU:N	2.49	0.45
12:L:4:PRO:O	13:M:100:ARG:NH2	2.37	0.45
13:M:207:THR:HG22	13:M:207:THR:O	4.98	0.45
14:N:84:LYS:O	14:N:88:TYR:HB2	2.16	0.45
6:T:105:ASN:HD22	6:T:106:ILE:H	1.64	0.45
7:U:164:LYS:CB	7:U:164:LYS:NZ	2.73	0.45
12:Z:191:ASP:O	12:Z:210:LEU:N	2.49	0.45
4:D:18:GLU:CD	4:D:20:ARG:CZ	2.73	0.45
11:K:18:SER:OG	11:K:173:ALA:N	2.46	0.45
4:R:114:GLN:OE1	16:S:82:ARG:NH1	2.50	0.45
12:L:188:TYR:HE1	8:V:167:LEU:HD13	1.82	0.45
1:O:220:LEU:HD12	1:O:224:GLU:HG2	1.99	0.45
1:A:220:LEU:HD12	1:A:224:GLU:HG2	1.99	0.45
12:L:158:MET:HG3	8:V:208:THR:HG23	1.98	0.45
4:R:208:GLU:OE2	4:R:211:ASN:ND2	2.49	0.45
1:O:178:ASN:HD22	1:O:179:GLU:H	1.64	0.45
3:C:79:ASP:HB3	3:C:127:PHE:HD1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:50:VAL:CB	3:C:54:GLN:HB2	2.42	0.44
11:K:157:ARG:O	11:K:161:TYR:HB2	2.17	0.44
1:O:192:LEU:HA	1:O:195:LYS:HB3	1.98	0.44
7:U:40:VAL:CA	7:U:167:ALA:HB1	2.38	0.44
9:W:67:LYS:O	9:W:71:ASN:HB2	2.17	0.44
1:A:70:HIS:HD2	1:A:138:TRP:H	1.65	0.44
4:D:41:GLN:NE2	4:D:151:PRO:O	2.50	0.44
11:K:84:ALA:O	11:K:88:TYR:CB	2.65	0.44
13:M:99:ARG:HG3	13:M:105:PRO:HA	2.00	0.44
2:P:8:ARG:HH22	4:R:9:ASP:N	2.15	0.44
1:A:178:ASN:HD22	1:A:179:GLU:H	1.64	0.44
3:C:224:GLU:O	3:C:228:TYR:CD1	2.70	0.44
8:H:84:LYS:HA	8:H:84:LYS:HD2	4.68	0.44
13:M:99:ARG:NE	13:M:104:ASN:O	2.50	0.44
1:O:94:GLN:HG3	8:V:65:LEU:HD12	1.99	0.44
8:V:68:LEU:HD23	8:V:68:LEU:HA	1.83	0.44
10:X:138:LEU:HD21	10:X:171:PHE:HB2	1.99	0.44
15:Q:222:PRO:HA	15:Q:225:ILE:HG13	2.00	0.44
7:U:168:ALA:HA	7:U:172:GLN:HG3	1.98	0.44
5:E:169:ARG:O	5:E:173:GLU:N	2.48	0.44
13:M:26:MET:HE2	13:M:202:PRO:HG3	1.99	0.44
2:P:50:ARG:NH1	2:P:51:ASN:O	2.51	0.44
16:S:196:ARG:HH22	16:S:235:GLY:HA3	1.83	0.44
9:W:18:CYS:HA	9:W:189:ILE:O	2.16	0.44
11:Y:84:ALA:O	11:Y:88:TYR:CB	2.65	0.44
10:J:66:LEU:O	10:J:70:ARG:HB2	2.17	0.44
13:M:26:MET:CE	13:M:202:PRO:CG	2.95	0.44
2:P:174:MET:SD	2:P:199:LYS:NZ	2.73	0.44
6:T:106:ILE:HD12	6:T:107:PRO:HD2	1.98	0.44
2:B:50:ARG:NH1	2:B:51:ASN:O	2.51	0.44
13:M:178:TYR:OH	13:M:208:ASN:N	2.46	0.44
16:S:63:ILE:HD11	16:S:223:ILE:HG23	2.00	0.44
11:Y:148:GLU:HG2	11:Y:151:GLN:HE22	1.83	0.44
1:A:192:LEU:HA	1:A:195:LYS:HB3	1.98	0.44
1:A:85:LEU:HD23	1:A:85:LEU:HA	1.86	0.44
2:B:239:LYS:HA	2:B:239:LYS:HD2	1.55	0.44
9:W:143:GLU:HA	9:W:146:TYR:HB2	2.00	0.44
12:Z:139:GLY:H	12:Z:142:SER:HG	1.61	0.44
1:O:189:THR:HA	1:O:192:LEU:HG	2.00	0.44
12:Z:145:LEU:HD22	12:Z:178:VAL:HB	1.98	0.44
8:H:126:THR:HB	8:H:131:SER:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:61:GLN:O	10:J:65:GLN:HB2	2.18	0.44
15:Q:51:ALA:HA	15:Q:54:GLN:HG3	1.98	0.44
4:R:41:GLN:NE2	4:R:151:PRO:O	2.50	0.44
9:W:59:VAL:O	9:W:63:ALA:CB	2.66	0.44
2:P:91:ARG:HD3	9:W:75:LEU:HB3	2.00	0.44
9:I:59:VAL:O	9:I:63:ALA:CB	2.66	0.44
8:V:2:THR:HB	8:V:130:GLY:HA3	2.00	0.44
6:F:83:ASP:HB3	6:F:131:PHE:HD1	1.83	0.43
8:H:42:TYR:HE2	8:H:185:PHE:HB2	1.83	0.43
9:W:13:MET:HG2	9:W:166:ILE:HD12	2.00	0.43
1:A:38:LYS:HB3	1:A:158:LYS:HA	2.00	0.43
4:D:60:GLU:OE2	4:D:62:SER:OG	2.28	0.43
9:I:176:ARG:HA	11:Y:26:ILE:HD11	1.99	0.43
6:T:83:ASP:HB3	6:T:131:PHE:HD1	1.83	0.43
1:A:158:LYS:HB3	1:A:177:TYR:CZ	2.54	0.43
7:U:93:ARG:HE	7:U:121:ILE:HG21	1.84	0.43
9:W:169:ALA:O	9:W:173:ALA:HB2	2.19	0.43
3:C:139:ASP:OD1	3:C:139:ASP:N	2.52	0.43
9:I:67:LYS:O	9:I:71:ASN:HB2	2.17	0.43
10:J:184:ASP:OD1	10:J:189:HIS:ND1	2.52	0.43
14:N:107:GLU:HG2	14:N:110:GLN:HE21	1.83	0.43
2:P:122:THR:HG23	15:Q:125:ARG:HH22	1.82	0.43
16:S:47:VAL:HG12	16:S:195:LEU:HD22	2.01	0.43
7:U:41:ALA:N	7:U:167:ALA:HB2	2.32	0.43
9:I:169:ALA:O	9:I:173:ALA:HB2	2.19	0.43
15:Q:139:ASP:N	15:Q:139:ASP:OD1	2.52	0.43
16:S:120:THR:HG22	6:T:129:ARG:HH21	1.83	0.43
1:A:189:THR:HA	1:A:192:LEU:HG	2.00	0.43
2:B:149:GLN:HB3	2:B:159:TRP:CD1	2.54	0.43
5:E:236:LEU:HD12	5:E:236:LEU:C	2.38	0.43
9:I:143:GLU:HA	9:I:146:TYR:HB2	2.00	0.43
11:K:148:GLU:HG2	11:K:151:GLN:HE22	1.83	0.43
11:K:157:ARG:O	11:K:161:TYR:CB	2.67	0.43
1:O:38:LYS:HB3	1:O:158:LYS:HA	2.00	0.43
1:O:64:VAL:HG23	1:O:219:ARG:HE	1.84	0.43
2:P:77:ALA:HB2	2:P:164:ILE:HD12	2.00	0.43
4:R:43:SER:OG	4:R:44:GLU:OE1	2.32	0.43
7:U:195:VAL:HG12	7:U:238:HIS:CD2	2.53	0.43
8:V:42:TYR:HE2	8:V:185:PHE:HB2	1.83	0.43
1:A:83:ARG:HD2	7:G:116:LYS:HG3	2.01	0.43
5:E:63:ILE:HD11	5:E:223:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:195:VAL:HG12	7:G:238:HIS:CD2	2.53	0.43
9:I:160:ASP:O	9:I:163:PHE:HB3	2.18	0.43
14:N:80:ALA:HB2	14:N:100:ILE:HD11	2.00	0.43
11:Y:157:ARG:O	11:Y:161:TYR:HB2	2.17	0.43
6:F:231:ILE:HA	6:F:234:GLU:HB3	2.01	0.43
10:J:138:LEU:HD21	10:J:171:PHE:HB2	1.99	0.43
1:O:70:HIS:HD2	1:O:138:TRP:H	1.65	0.43
1:O:134:LEU:HD12	1:O:145:LEU:HD21	2.01	0.43
10:X:61:GLN:O	10:X:65:GLN:HB2	2.18	0.43
9:W:158:ASP:OD1	9:W:158:ASP:N	2.52	0.43
11:Y:18:SER:OG	11:Y:173:ALA:N	2.46	0.43
13:M:61:GLN:HA	13:M:64:LYS:HG2	2.01	0.43
12:Z:184:GLU:OE2	12:Z:211:ARG:NH1	2.51	0.43
3:C:50:VAL:O	3:C:54:GLN:N	2.47	0.43
5:E:148:CYS:SG	5:E:150:SER:OG	2.64	0.43
7:G:93:ARG:HE	7:G:121:ILE:HG21	1.84	0.43
11:K:160:ILE:HA	11:K:163:ALA:HB3	2.01	0.43
15:Q:188:ILE:CG2	15:Q:228:TYR:CD2	2.96	0.43
10:X:29:LYS:HD3	11:Y:123:GLY:HA2	2.01	0.43
15:Q:88:ARG:HH11	10:X:70:ARG:HG3	1.84	0.43
4:D:114:GLN:OE1	5:E:82:ARG:NH1	2.51	0.43
3:C:88:ARG:HH11	10:J:70:ARG:HG3	1.83	0.43
12:L:184:GLU:OE2	12:L:211:ARG:NH1	2.52	0.43
15:Q:45:VAL:O	15:Q:47:LYS:N	2.40	0.43
8:V:173:ILE:O	8:V:189:TYR:N	2.43	0.43
9:W:57:THR:O	10:X:85:ARG:NH2	2.52	0.43
11:Y:160:ILE:HA	11:Y:163:ALA:HB3	2.01	0.43
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.19	0.43
1:A:10:THR:HG23	1:A:20:GLN:HB2	2.01	0.42
2:B:77:ALA:HB2	2:B:164:ILE:HD12	2.00	0.42
10:J:169:LYS:O	10:X:27:GLN:NE2	2.51	0.42
12:Z:49:LYS:HD3	12:Z:113:LEU:HD11	2.01	0.42
4:R:53:ARG:NH2	4:R:172:SER:OG	2.52	0.42
2:P:149:GLN:HB3	2:P:159:TRP:CD1	2.54	0.42
7:U:44:GLY:C	7:U:46:ASP:H	2.22	0.42
7:U:40:VAL:HB	7:U:51:VAL:HG23	2.01	0.42
1:A:220:LEU:HA	1:A:220:LEU:HD13	1.92	0.42
10:X:35:MET:HG2	10:X:45:LEU:HG	2.01	0.42
15:Q:188:ILE:HB	15:Q:228:TYR:CE1	2.54	0.42
3:C:125:ARG:HA	3:C:126:PRO:HD2	1.91	0.42
9:I:13:MET:HG2	9:I:166:ILE:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:189:THR:OG1	12:L:190:GLY:N	2.53	0.42
16:S:148:CYS:HG	16:S:150:SER:HG	1.57	0.42
7:U:50:ILE:HB	7:U:218:GLY:O	2.20	0.42
11:Y:157:ARG:O	11:Y:161:TYR:CB	2.67	0.42
9:W:160:ASP:O	9:W:163:PHE:HB3	2.18	0.42
11:Y:98:GLY:HA2	11:Y:115:ASP:HA	2.02	0.42
1:A:195:LYS:HE3	1:A:195:LYS:HB2	4.50	0.42
1:A:64:VAL:HG23	1:A:219:ARG:HE	1.84	0.42
1:A:94:GLN:NE2	8:H:64:GLU:OE2	2.53	0.42
11:K:5:ALA:HA	11:K:13:ILE:O	2.19	0.42
11:K:58:LEU:HD11	11:K:61:ARG:HH21	1.84	0.42
3:C:195:LEU:HB3	3:C:196:LEU:H	3.81	0.42
8:H:1:THR:CA	8:H:33:LYS:HZ1	2.32	0.42
9:I:158:ASP:OD1	9:I:158:ASP:N	2.52	0.42
2:P:86:LEU:O	2:P:89:GLU:HB2	2.20	0.42
15:Q:220:LEU:CD1	15:Q:228:TYR:CE2	3.02	0.42
15:Q:8:THR:HG22	15:Q:16:LEU:HD11	2.02	0.42
8:H:202:TYR:OH	12:Z:177:ASP:OD2	2.38	0.42
12:Z:210:LEU:HB3	12:Z:211:ARG:H	1.71	0.42
1:O:10:THR:HG23	1:O:20:GLN:HB2	2.01	0.42
2:P:208:ALA:HA	2:P:211:VAL:HG12	2.02	0.42
5:E:47:VAL:HG12	5:E:195:LEU:HD22	2.01	0.42
5:E:33:SER:HB3	5:E:62:LYS:HZ3	1.85	0.42
13:M:78:GLY:O	13:M:80:GLY:N	2.53	0.42
1:O:229:LEU:HD23	1:O:229:LEU:HA	1.89	0.42
6:T:120:HIS:NE2	7:U:86:ASP:OD1	2.42	0.42
12:Z:159:GLN:HB3	12:Z:160:ASN:H	1.70	0.42
1:A:71:ILE:HG21	1:A:109:LEU:HD23	2.02	0.42
2:B:36:GLY:HA2	2:B:44:LEU:O	2.19	0.42
3:C:231:GLU:OE1	3:C:231:GLU:N	2.53	0.42
10:J:35:MET:HG2	10:J:45:LEU:HG	2.01	0.42
7:U:138:MET:HB3	7:U:140:LEU:HD23	2.02	0.42
1:A:134:LEU:HD12	1:A:145:LEU:HD21	2.01	0.42
3:C:182:GLU:OE2	3:C:185:ASP:N	2.53	0.42
11:K:98:GLY:HA2	11:K:115:ASP:HA	2.02	0.42
13:M:26:MET:HE2	13:M:202:PRO:CB	2.49	0.42
15:Q:227:LYS:HB3	15:Q:227:LYS:HE2	1.50	0.42
15:Q:156:TRP:CD1	4:R:59:MET:HB2	2.55	0.42
12:Z:189:THR:OG1	12:Z:190:GLY:N	2.53	0.42
2:B:86:LEU:O	2:B:89:GLU:HB2	2.20	0.41
3:C:50:VAL:C	3:C:54:GLN:HB2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:26:MET:SD	5:E:148:CYS:HB2	2.60	0.41
1:A:90:ARG:NH2	8:H:68:LEU:O	2.53	0.41
2:P:36:GLY:HA2	2:P:44:LEU:O	2.19	0.41
16:S:26:MET:SD	16:S:148:CYS:HB2	2.60	0.41
6:T:157:SER:H	7:U:88:ARG:NH2	2.18	0.41
11:Y:58:LEU:HD11	11:Y:61:ARG:HH21	1.84	0.41
7:G:50:ILE:HB	7:G:218:GLY:O	2.20	0.41
15:Q:71:MET:HB3	15:Q:133:ILE:HD13	2.02	0.41
15:Q:225:ILE:H	15:Q:225:ILE:HG12	1.42	0.41
2:B:176:LYS:CD	3:C:52:LYS:CG	2.68	0.41
9:I:62:VAL:HA	9:I:65:ARG:HB3	2.03	0.41
6:T:7:TYR:CD2	6:T:16:PRO:HD3	2.55	0.41
7:U:33:ASN:ND2	7:U:169:GLY:O	2.53	0.41
1:A:5:TYR:HA	1:A:5:TYR:HD1	1.76	0.41
3:C:203:GLY:HA2	3:C:226:GLU:OE2	2.21	0.41
5:E:14:SER:N	5:E:18:ARG:O	2.43	0.41
12:L:49:LYS:HD3	12:L:113:LEU:HD11	2.01	0.41
13:M:200:GLU:O	13:M:203:LEU:CD1	2.68	0.41
13:M:74:GLU:HA	13:M:77:LEU:HD23	2.02	0.41
6:T:231:ILE:HA	6:T:234:GLU:HB3	2.01	0.41
8:V:126:THR:HB	8:V:131:SER:HA	2.00	0.41
8:V:5:GLY:HA2	8:V:13:VAL:O	2.21	0.41
11:Y:21:THR:HG22	11:Y:26:ILE:HG22	2.02	0.41
11:Y:19:ARG:NH2	11:Y:26:ILE:HG21	2.36	0.41
11:Y:155:LEU:O	11:Y:159:ALA:CB	2.68	0.41
1:O:71:ILE:HG21	1:O:109:LEU:HD23	2.02	0.41
4:R:187:LYS:HD2	4:R:192:LYS:HZ3	1.85	0.41
2:B:208:ALA:HA	2:B:211:VAL:HG12	2.02	0.41
1:A:158:LYS:NZ	2:B:56:LEU:H	2.18	0.41
3:C:71:MET:HB3	3:C:133:ILE:HD13	2.03	0.41
3:C:88:ARG:NH1	10:J:70:ARG:O	2.53	0.41
4:D:232:GLU:HA	4:D:235:GLU:HG2	2.02	0.41
7:G:172:GLN:O	7:G:175:SER:OG	2.36	0.41
8:H:5:GLY:HA2	8:H:13:VAL:O	2.21	0.41
16:S:19:ILE:H	16:S:19:ILE:HG22	1.59	0.41
1:A:66:PRO:HB3	1:A:217:PHE:HD2	1.86	0.41
2:B:70:GLU:H	2:B:70:GLU:HG3	1.71	0.41
10:J:66:LEU:O	10:J:70:ARG:CB	2.69	0.41
12:L:159:GLN:HB3	12:L:160:ASN:H	1.70	0.41
13:M:50:MET:N	13:M:113:GLY:O	2.44	0.41
14:N:59:VAL:HG21	14:N:83:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:33:SER:O	6:T:167:LYS:N	2.54	0.41
7:U:82:GLY:HA3	7:U:136:CYS:HA	2.03	0.41
8:V:3:ILE:HG22	8:V:127:MET:O	2.21	0.41
12:Z:209:SER:OG	12:Z:210:LEU:N	2.54	0.41
1:A:73:LEU:HD11	1:A:86:VAL:HG22	2.03	0.41
6:F:217:GLY:H	6:F:220:THR:HG1	1.66	0.41
7:G:138:MET:HB3	7:G:140:LEU:HD23	2.02	0.41
8:H:83:LEU:O	8:H:87:LEU:CB	2.69	0.41
10:J:162:LYS:HB3	11:Y:141:ARG:HD3	2.02	0.41
11:K:19:ARG:NH2	11:K:26:ILE:HG21	2.36	0.41
14:N:99:ILE:HG22	14:N:113:SER:HA	2.02	0.41
1:O:66:PRO:HA	1:O:72:GLY:HA2	2.03	0.41
4:R:190:THR:HG1	4:R:192:LYS:HZ2	1.62	0.41
2:P:11:ILE:HG23	15:Q:18:GLN:HE22	1.85	0.41
3:C:8:THR:HG22	3:C:16:LEU:HD11	2.02	0.41
6:F:7:TYR:CD2	6:F:16:PRO:HD3	2.55	0.41
7:G:40:VAL:HB	7:G:51:VAL:HG23	2.01	0.41
10:J:101:ASN:OD1	10:J:101:ASN:N	2.54	0.41
12:L:209:SER:OG	12:L:210:LEU:N	2.54	0.41
4:R:70:ILE:HD11	4:R:89:ILE:HD12	2.03	0.41
11:Y:130:SER:OG	11:Y:131:GLY:N	2.53	0.41
2:B:136:TYR:O	2:B:140:ASP:CB	12.05	0.41
7:G:106:GLY:HA2	8:H:81:ARG:HE	1.85	0.41
2:P:163:CYS:SG	2:P:164:ILE:N	2.94	0.41
8:V:34:ILE:HB	8:V:185:PHE:HE1	1.86	0.41
7:U:231:THR:N	7:U:234:GLU:OE2	2.46	0.41
12:Z:113:LEU:HA	12:Z:119:GLY:HA2	2.03	0.41
13:M:71:VAL:O	13:M:75:GLU:CB	2.64	0.41
15:Q:221:ASN:C	15:Q:223:GLU:H	2.25	0.41
6:F:105:ASN:HD22	6:F:106:ILE:N	2.19	0.41
6:F:120:HIS:CE1	7:G:86:ASP:HA	2.56	0.41
6:T:34:SER:OG	6:T:65:ARG:NH1	2.33	0.40
1:A:66:PRO:HA	1:A:72:GLY:HA2	2.03	0.40
2:B:163:CYS:SG	2:B:164:ILE:N	2.94	0.40
4:D:70:ILE:HD11	4:D:89:ILE:HD12	2.03	0.40
6:F:33:SER:O	6:F:167:LYS:N	2.54	0.40
8:H:18:THR:OG1	8:H:172:ASN:OD1	2.38	0.40
8:H:34:ILE:HB	8:H:185:PHE:HE1	1.86	0.40
8:H:83:LEU:O	8:H:87:LEU:HB3	2.20	0.40
9:I:57:THR:O	9:I:61:THR:OG1	2.25	0.40
15:Q:40:ILE:HD11	15:Q:210:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:59:VAL:O	15:Q:59:VAL:HG13	2.20	0.40
7:U:42:VAL:HG23	7:U:49:VAL:H	1.86	0.40
8:V:19:ARG:H	8:V:33:LYS:HZ1	1.68	0.40
8:V:1:THR:OG1	8:V:1:THR:O	2.32	0.40
8:H:1:THR:HA	8:H:33:LYS:HZ1	1.85	0.40
8:H:212:LEU:HD12	9:I:200:LYS:HB2	2.03	0.40
13:M:26:MET:HE2	13:M:202:PRO:CG	2.50	0.40
2:P:207:SER:OG	2:P:234:GLU:OE2	2.36	0.40
8:V:83:LEU:O	8:V:87:LEU:HB3	2.20	0.40
9:W:164:GLU:O	9:W:167:SER:OG	2.29	0.40
11:Y:4:LEU:HD12	11:Y:135:ALA:HB1	2.04	0.40
8:V:83:LEU:O	8:V:87:LEU:CB	2.69	0.40
7:G:43:ARG:NH1	7:G:149:PRO:O	2.53	0.40
11:K:130:SER:OG	11:K:131:GLY:N	2.53	0.40
15:Q:51:ALA:O	15:Q:54:GLN:HG2	2.21	0.40
15:Q:220:LEU:CB	15:Q:224:GLU:HB3	2.35	0.40
2:B:133:SER:HA	2:B:136:TYR:CE2	7.71	0.40
2:B:5:TYR:CG	7:G:13:ILE:HD11	2.56	0.40
10:J:181:ARG:HG2	10:J:190:ASN:CB	2.31	0.40
10:J:15:VAL:HG21	10:J:45:LEU:HD11	2.03	0.40
10:J:29:LYS:HD3	11:K:123:GLY:HA2	2.03	0.40
13:M:27:LEU:HD13	13:M:184:TYR:HB2	2.04	0.40
2:P:47:ALA:HB1	2:P:64:LYS:HG2	2.04	0.40
15:Q:221:ASN:O	15:Q:224:GLU:N	2.54	0.40
15:Q:31:THR:HB	15:Q:46:GLU:CG	2.51	0.40
11:Y:103:GLY:HA2	11:Y:179:VAL:HG21	2.03	0.40
11:Y:115:ASP:OD2	11:Y:119:ASN:ND2	2.55	0.40
10:X:15:VAL:HG21	10:X:45:LEU:HD11	2.03	0.40
3:C:182:GLU:HG2	3:C:186:LEU:HD23	2.04	0.40
6:F:112:ALA:O	6:F:116:ALA:CB	2.70	0.40
7:G:237:ALA:HA	7:G:240:VAL:HG22	2.04	0.40
11:K:21:THR:HG22	11:K:26:ILE:HG22	2.02	0.40
15:Q:166:LYS:HA	15:Q:169:ARG:HG2	2.04	0.40
7:U:45:LYS:HD3	7:U:190:THR:HB	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	228/234 (97%)	197 (86%)	31 (14%)	0	100	100
1	O	228/234 (97%)	197 (86%)	31 (14%)	0	100	100
2	B	228/261 (87%)	195 (86%)	30 (13%)	3 (1%)	13	54
2	P	242/261 (93%)	203 (84%)	35 (14%)	4 (2%)	10	49
3	C	232/234 (99%)	191 (82%)	38 (16%)	3 (1%)	13	54
4	D	231/241 (96%)	199 (86%)	32 (14%)	0	100	100
4	R	231/241 (96%)	199 (86%)	32 (14%)	0	100	100
5	E	232/234 (99%)	190 (82%)	41 (18%)	1 (0%)	36	75
6	F	228/255 (89%)	195 (86%)	31 (14%)	2 (1%)	19	60
6	T	238/255 (93%)	202 (85%)	34 (14%)	2 (1%)	21	62
7	G	229/246 (93%)	206 (90%)	21 (9%)	2 (1%)	19	60
7	U	239/246 (97%)	213 (89%)	25 (10%)	1 (0%)	36	75
8	H	219/277 (79%)	208 (95%)	11 (5%)	0	100	100
8	V	219/277 (79%)	208 (95%)	11 (5%)	0	100	100
9	I	202/205 (98%)	182 (90%)	18 (9%)	2 (1%)	17	58
9	W	202/205 (98%)	182 (90%)	18 (9%)	2 (1%)	17	58
10	J	194/196 (99%)	175 (90%)	19 (10%)	0	100	100
10	X	194/196 (99%)	175 (90%)	19 (10%)	0	100	100
11	K	198/204 (97%)	174 (88%)	24 (12%)	0	100	100
11	Y	199/204 (98%)	175 (88%)	24 (12%)	0	100	100
12	L	212/241 (88%)	184 (87%)	28 (13%)	0	100	100
12	Z	211/241 (88%)	184 (87%)	27 (13%)	0	100	100
13	M	214/264 (81%)	192 (90%)	21 (10%)	1 (0%)	31	71
13	a	214/264 (81%)	192 (90%)	21 (10%)	1 (0%)	31	71
14	N	199/239 (83%)	179 (90%)	20 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	b	201/239 (84%)	179 (89%)	21 (10%)	1 (0%)	31	71
15	Q	233/235 (99%)	186 (80%)	38 (16%)	9 (4%)	3	33
16	S	236/238 (99%)	195 (83%)	39 (16%)	2 (1%)	21	62
17	c	343/433 (79%)	256 (75%)	74 (22%)	13 (4%)	3	34
18	d	329/428 (77%)	251 (76%)	59 (18%)	19 (6%)	2	25
19	e	355/418 (85%)	279 (79%)	63 (18%)	13 (4%)	4	34
20	f	346/379 (91%)	285 (82%)	51 (15%)	10 (3%)	5	40
21	g	359/439 (82%)	292 (81%)	60 (17%)	7 (2%)	9	48
22	h	324/355 (91%)	248 (76%)	59 (18%)	17 (5%)	2	27
23	i	224/953 (24%)	173 (77%)	31 (14%)	20 (9%)	1	14
24	j	147/534 (28%)	111 (76%)	32 (22%)	4 (3%)	5	41
25	k	354/456 (78%)	272 (77%)	77 (22%)	5 (1%)	12	52
26	l	411/422 (97%)	341 (83%)	62 (15%)	8 (2%)	9	48
27	m	373/389 (96%)	318 (85%)	51 (14%)	4 (1%)	16	57
28	n	200/324 (62%)	147 (74%)	46 (23%)	7 (4%)	4	36
29	o	73/376 (19%)	56 (77%)	12 (16%)	5 (7%)	1	21
30	p	90/377 (24%)	78 (87%)	11 (12%)	1 (1%)	16	57
31	q	253/310 (82%)	191 (76%)	54 (21%)	8 (3%)	4	38
32	r	4/350 (1%)	4 (100%)	0	0	100	100
33	s	24/70 (34%)	19 (79%)	5 (21%)	0	100	100
All	All	10342/13680 (76%)	8678 (84%)	1487 (14%)	177 (2%)	14	49

All (177) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	69	HIS
6	F	227	VAL
6	F	228	PRO
7	G	69	LEU
13	M	79	ASP
2	P	241	GLU
15	Q	47	LYS
15	Q	50	VAL
15	Q	222	PRO
16	S	69	HIS

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Mol	Chain	Res	Type
16	S	237	GLU
6	T	227	VAL
6	T	228	PRO
7	U	69	LEU
13	a	79	ASP
14	b	202	LEU
17	c	164	MET
17	c	167	GLU
17	c	337	LEU
17	c	385	ILE
18	d	146	PRO
18	d	149	SER
18	d	233	THR
18	d	251	VAL
18	d	260	LEU
18	d	279	PRO
18	d	344	PRO
18	d	349	ARG
19	e	207	PRO
19	e	324	PRO
19	e	408	LYS
19	e	409	LYS
19	e	412	GLN
19	e	413	GLU
19	e	416	PHE
20	f	64	LEU
20	f	65	THR
20	f	129	ASN
21	g	229	PRO
21	g	345	SER
21	g	425	LEU
22	h	84	LYS
22	h	117	ARG
22	h	131	VAL
22	h	133	PRO
22	h	142	LYS
22	h	243	PRO
22	h	354	ALA
23	i	506	ALA
23	i	540	GLN
23	i	586	VAL
23	i	614	VAL

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Mol	Chain	Res	Type
23	i	625	ILE
23	i	626	LEU
23	i	630	PRO
23	i	631	GLU
23	i	666	LYS
23	i	680	VAL
24	j	208	LEU
24	j	340	MET
25	k	413	ILE
26	l	241	SER
26	l	244	SER
26	l	370	LEU
26	l	407	MET
27	m	18	ARG
28	n	243	GLN
28	n	264	SER
29	o	106	ALA
29	o	124	VAL
31	q	51	MET
31	q	232	GLN
31	q	233	ASP
31	q	267	PRO
2	B	55	LEU
3	C	77	THR
7	G	45	LYS
9	I	146	TYR
9	I	147	GLY
2	P	55	LEU
15	Q	49	SER
15	Q	52	LYS
15	Q	77	THR
9	W	146	TYR
9	W	147	GLY
17	c	166	VAL
17	c	168	GLU
17	c	180	CYS
17	c	325	ASP
18	d	389	ASP
18	d	391	SER
19	e	98	GLN
19	e	99	ASN
19	e	268	ASP

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Mol	Chain	Res	Type
20	f	66	GLU
20	f	128	GLY
20	f	271	HIS
22	h	108	VAL
22	h	129	ASN
22	h	358	GLU
23	i	560	MET
23	i	567	ILE
25	k	119	PRO
26	l	369	ILE
26	l	404	ILE
27	m	48	ASN
28	n	114	ARG
28	n	179	ILE
31	q	231	LEU
31	q	275	VAL
17	c	169	LYS
17	c	380	SER
18	d	106	PRO
18	d	264	PRO
18	d	285	ASP
20	f	86	GLN
20	f	123	SER
20	f	292	PRO
21	g	349	ASP
22	h	138	MET
23	i	521	LEU
23	i	538	GLU
23	i	661	ALA
26	l	82	LYS
28	n	178	ASP
29	o	101	THR
30	p	56	ASN
15	Q	46	GLU
18	d	104	GLY
18	d	145	GLU
18	d	188	GLY
18	d	355	LEU
19	e	417	TYR
22	h	106	ASN
23	i	543	LYS
23	i	549	ALA

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Mol	Chain	Res	Type
23	i	627	PHE
24	j	262	SER
27	m	206	SER
28	n	177	ARG
29	o	107	ASN
31	q	175	ARG
2	P	160	LYS
2	P	172	VAL
17	c	324	PRO
22	h	66	LEU
22	h	121	TYR
25	k	200	ILE
26	l	395	LYS
29	o	123	THR
2	B	160	LYS
2	B	186	LEU
3	C	199	VAL
17	c	195	LEU
20	f	61	LEU
21	g	399	VAL
22	h	105	ILE
23	i	568	GLU
25	k	198	ASP
27	m	205	VAL
31	q	272	ILE
18	d	345	GLY
18	d	356	PRO
22	h	195	GLY
22	h	351	MET
24	j	193	ILE
25	k	412	ILE
3	C	125	ARG
15	Q	125	ARG
21	g	228	PRO
23	i	550	VAL
28	n	184	VAL
15	Q	199	VAL
17	c	177	VAL
19	e	303	VAL
21	g	280	PRO
19	e	86	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	181/191 (95%)	178 (98%)	3 (2%)	63	84
1	O	181/191 (95%)	178 (98%)	3 (2%)	63	84
2	B	195/221 (88%)	183 (94%)	12 (6%)	20	56
2	P	194/221 (88%)	184 (95%)	10 (5%)	25	62
3	C	179/197 (91%)	169 (94%)	10 (6%)	23	60
4	D	189/203 (93%)	182 (96%)	7 (4%)	37	69
4	R	192/203 (95%)	186 (97%)	6 (3%)	43	72
5	E	192/200 (96%)	188 (98%)	4 (2%)	56	80
6	F	190/212 (90%)	188 (99%)	2 (1%)	76	88
6	T	197/212 (93%)	195 (99%)	2 (1%)	78	89
7	G	197/210 (94%)	194 (98%)	3 (2%)	67	85
7	U	196/210 (93%)	191 (97%)	5 (3%)	49	76
8	H	181/228 (79%)	178 (98%)	3 (2%)	63	84
8	V	173/228 (76%)	171 (99%)	2 (1%)	74	88
9	I	173/174 (99%)	172 (99%)	1 (1%)	87	94
9	W	172/174 (99%)	171 (99%)	1 (1%)	87	94
10	J	163/166 (98%)	161 (99%)	2 (1%)	74	88
10	X	164/166 (99%)	162 (99%)	2 (1%)	74	88
11	K	154/159 (97%)	150 (97%)	4 (3%)	49	76
11	Y	156/159 (98%)	152 (97%)	4 (3%)	49	76
12	L	175/199 (88%)	173 (99%)	2 (1%)	76	88
12	Z	175/199 (88%)	173 (99%)	2 (1%)	76	88
13	M	179/215 (83%)	174 (97%)	5 (3%)	47	74
13	a	177/215 (82%)	172 (97%)	5 (3%)	47	74
14	N	157/181 (87%)	156 (99%)	1 (1%)	87	94
14	b	157/181 (87%)	156 (99%)	1 (1%)	87	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	Q	182/199 (92%)	169 (93%)	13 (7%)	16	52
16	S	194/202 (96%)	190 (98%)	4 (2%)	56	80
17	c	297/372 (80%)	279 (94%)	18 (6%)	20	57
18	d	281/375 (75%)	256 (91%)	25 (9%)	11	43
19	e	289/366 (79%)	268 (93%)	21 (7%)	15	51
20	f	287/331 (87%)	273 (95%)	14 (5%)	27	62
21	g	291/379 (77%)	274 (94%)	17 (6%)	22	59
22	h	266/307 (87%)	237 (89%)	29 (11%)	7	34
23	i	8/816 (1%)	8 (100%)	0	100	100
24	j	5/460 (1%)	5 (100%)	0	100	100
25	k	5/416 (1%)	5 (100%)	0	100	100
26	l	148/362 (41%)	142 (96%)	6 (4%)	33	66
27	m	154/344 (45%)	143 (93%)	11 (7%)	16	52
28	n	5/295 (2%)	5 (100%)	0	100	100
29	o	2/336 (1%)	2 (100%)	0	100	100
30	p	3/312 (1%)	3 (100%)	0	100	100
31	q	14/268 (5%)	14 (100%)	0	100	100
32	r	1/294 (0%)	1 (100%)	0	100	100
All	All	7071/11549 (61%)	6811 (96%)	260 (4%)	41	69

All (260) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	A	178	ASN
1	A	226	LYS
2	B	3	ARG
2	B	35	LEU
2	B	50	ARG
2	B	69	ASN
2	B	70	GLU
2	B	84	ASN
2	B	147	LEU
2	B	186	LEU
2	B	198	ASN
2	B	222	LYS

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Mol	Chain	Res	Type
2	B	229	LYS
2	B	241	GLU
3	C	36	ARG
3	C	45	VAL
3	C	46	GLU
3	C	90	GLU
3	C	100	ASP
3	C	125	ARG
3	C	163	ARG
3	C	179	ASP
3	C	231	GLU
3	C	235	GLU
4	D	20	ARG
4	D	52	LYS
4	D	59	MET
4	D	104	ASN
4	D	133	MET
4	D	192	LYS
4	D	210	LEU
5	E	56	LEU
5	E	68	ASN
5	E	126	ARG
5	E	157	ARG
6	F	89	ASP
6	F	105	ASN
7	G	43	ARG
7	G	88	ARG
7	G	232	GLU
8	H	28	ASP
8	H	182	LYS
8	H	203	ARG
9	I	125	LEU
10	J	190	ASN
10	J	192	GLU
11	K	72	GLU
11	K	100	MET
11	K	120	ARG
11	K	180	ARG
12	L	26	ASP
12	L	131	GLN
13	M	38	ASN
13	M	100	ARG

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Mol	Chain	Res	Type
13	M	104	ASN
13	M	195	LYS
13	M	200	GLU
14	N	69	GLU
1	O	48	GLU
1	O	178	ASN
1	O	226	LYS
2	P	3	ARG
2	P	35	LEU
2	P	50	ARG
2	P	69	ASN
2	P	70	GLU
2	P	84	ASN
2	P	147	LEU
2	P	186	LEU
2	P	198	ASN
2	P	222	LYS
15	Q	36	ARG
15	Q	45	VAL
15	Q	46	GLU
15	Q	47	LYS
15	Q	90	GLU
15	Q	100	ASP
15	Q	125	ARG
15	Q	163	ARG
15	Q	166	LYS
15	Q	179	ASP
15	Q	224	GLU
15	Q	225	ILE
15	Q	227	LYS
4	R	52	LYS
4	R	59	MET
4	R	104	ASN
4	R	133	MET
4	R	192	LYS
4	R	210	LEU
16	S	56	LEU
16	S	68	ASN
16	S	126	ARG
16	S	157	ARG
6	T	89	ASP
6	T	105	ASN

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Mol	Chain	Res	Type
7	U	43	ARG
7	U	88	ARG
7	U	164	LYS
7	U	166	THR
7	U	232	GLU
8	V	2	THR
8	V	28	ASP
9	W	125	LEU
10	X	190	ASN
10	X	192	GLU
11	Y	72	GLU
11	Y	100	MET
11	Y	120	ARG
11	Y	180	ARG
12	Z	26	ASP
12	Z	131	GLN
13	a	38	ASN
13	a	100	ARG
13	a	104	ASN
13	a	167	ASP
13	a	195	LYS
14	b	69	GLU
17	c	146	LYS
17	c	148	GLN
17	c	161	VAL
17	c	163	MET
17	c	164	MET
17	c	167	GLU
17	c	168	GLU
17	c	169	LYS
17	c	177	VAL
17	c	220	THR
17	c	232	ARG
17	c	331	LEU
17	c	332	MET
17	c	333	ARG
17	c	381	THR
17	c	400	ARG
17	c	407	LYS
17	c	433	ASN
18	d	105	THR
18	d	142	ASP

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Mol	Chain	Res	Type
18	d	144	LEU
18	d	145	GLU
18	d	153	ASN
18	d	164	MET
18	d	230	THR
18	d	235	LEU
18	d	256	ILE
18	d	257	GLN
18	d	258	LYS
18	d	259	TYR
18	d	260	LEU
18	d	265	LYS
18	d	266	LEU
18	d	275	GLU
18	d	276	GLU
18	d	281	ILE
18	d	341	LEU
18	d	342	ILE
18	d	350	LYS
18	d	374	LEU
18	d	387	LYS
18	d	389	ASP
18	d	390	LEU
19	e	81	ARG
19	e	154	LEU
19	e	266	GLU
19	e	267	ILE
19	e	311	THR
19	e	321	LEU
19	e	322	LEU
19	e	323	ARG
19	e	326	ARG
19	e	327	LEU
19	e	398	ASP
19	e	399	PHE
19	e	407	ILE
19	e	408	LYS
19	e	409	LYS
19	e	410	ASP
19	e	411	GLU
19	e	412	GLN
19	e	415	GLU

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Mol	Chain	Res	Type
19	e	416	PHE
19	e	417	TYR
20	f	63	GLN
20	f	64	LEU
20	f	66	GLU
20	f	68	LYS
20	f	91	LYS
20	f	182	LEU
20	f	185	ARG
20	f	197	LYS
20	f	225	HIS
20	f	275	MET
20	f	289	LEU
20	f	291	ARG
20	f	344	ARG
20	f	356	ARG
21	g	175	MET
21	g	238	ARG
21	g	263	ASP
21	g	277	GLU
21	g	323	ASN
21	g	332	THR
21	g	342	LEU
21	g	343	LEU
21	g	347	ARG
21	g	348	LEU
21	g	396	CYS
21	g	397	LYS
21	g	430	LYS
21	g	431	LYS
21	g	432	LYS
21	g	436	GLN
21	g	437	TYR
22	h	63	LEU
22	h	69	GLN
22	h	92	GLU
22	h	94	LYS
22	h	105	ILE
22	h	106	ASN
22	h	107	ASP
22	h	112	CYS
22	h	113	ARG

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Mol	Chain	Res	Type
22	h	114	VAL
22	h	116	LEU
22	h	118	ASN
22	h	127	LEU
22	h	130	LYS
22	h	135	VAL
22	h	140	VAL
22	h	142	LYS
22	h	145	ASP
22	h	178	LEU
22	h	180	ILE
22	h	196	LYS
22	h	232	ARG
22	h	235	PHE
22	h	241	HIS
22	h	271	ARG
22	h	310	ARG
22	h	349	GLU
22	h	350	LEU
22	h	351	MET
26	l	157	LEU
26	l	160	MET
26	l	163	LYS
26	l	165	LEU
26	l	240	ASP
26	l	242	ILE
27	m	137	ARG
27	m	138	LEU
27	m	141	VAL
27	m	167	LEU
27	m	169	GLU
27	m	199	GLU
27	m	202	LEU
27	m	204	THR
27	m	207	THR
27	m	208	PHE
27	m	233	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN

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Mol	Chain	Res	Type
1	A	70	HIS
1	A	95	GLN
1	A	108	GLN
1	A	111	GLN
1	A	178	ASN
2	B	69	ASN
2	B	84	ASN
2	B	88	ASN
2	B	240	HIS
3	C	23	GLN
3	C	120	GLN
3	C	205	ASN
4	D	99	HIS
4	D	104	ASN
4	D	204	GLN
5	E	21	GLN
5	E	31	GLN
5	E	68	ASN
5	E	166	GLN
6	F	105	ASN
6	F	201	HIS
8	H	66	HIS
9	I	172	ASN
10	J	71	ASN
12	L	8	ASN
12	L	157	ASN
13	M	38	ASN
13	M	47	ASN
13	M	104	ASN
14	N	53	GLN
1	O	70	HIS
1	O	95	GLN
1	O	108	GLN
1	O	111	GLN
1	O	118	GLN
1	O	178	ASN
2	P	69	ASN
2	P	84	ASN
15	Q	23	GLN
15	Q	122	ASN
4	R	99	HIS
4	R	204	GLN

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Mol	Chain	Res	Type
16	S	21	GLN
16	S	59	HIS
16	S	68	ASN
16	S	166	GLN
6	T	22	GLN
6	T	105	ASN
7	U	12	HIS
7	U	33	ASN
10	X	71	ASN
12	Z	8	ASN
12	Z	157	ASN
13	a	47	ASN
13	a	104	ASN
17	c	91	GLN
17	c	293	ASN
17	c	433	ASN
18	d	153	ASN
18	d	195	GLN
19	e	412	GLN
20	f	194	ASN
20	f	254	GLN
20	f	316	HIS
21	g	130	GLN
21	g	321	GLN
21	g	434	ASN
22	h	106	ASN
22	h	332	HIS
22	h	337	ASN
26	l	170	GLN
26	l	218	HIS
27	m	178	ASN
27	m	184	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
34	6V9	t	1	34	6,8,9	0.75	0	3,10,12	5.13	3 (100%)
34	7C9	t	2	34	6,6,7	0.44	0	2,6,8	1.39	0
34	7C9	t	3	34	6,6,7	0.52	0	2,6,8	1.57	1 (50%)
34	6V9	u	1	34	6,8,9	0.65	0	3,10,12	4.97	3 (100%)
34	7C9	u	2	34	6,6,7	0.52	0	2,6,8	1.34	0
34	7C9	u	3	34	6,6,7	0.55	0	2,6,8	1.77	1 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	6V9	t	1	34	-	0/0/2/4	0/1/1/1
34	7C9	t	2	34	-	2/3/5/7	-
34	7C9	t	3	34	-	0/3/5/7	-
34	6V9	u	1	34	-	0/0/2/4	0/1/1/1
34	7C9	u	2	34	-	2/3/5/7	-
34	7C9	u	3	34	-	0/3/5/7	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	t	1	6V9	O1-C4-C3	-6.91	118.73	124.39
34	u	1	6V9	O1-C4-C3	-6.57	119.02	124.39
34	t	1	6V9	C2-C1-N1	4.53	133.54	121.74
34	u	1	6V9	C2-C1-N1	4.48	133.42	121.74
34	u	1	6V9	C2-C1-S	-3.30	115.67	120.12
34	t	1	6V9	C2-C1-S	-3.28	115.70	120.12
34	u	3	7C9	O18-C05-C04	-2.48	118.33	124.98
34	t	3	7C9	O18-C05-C04	-2.21	119.04	124.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	u	2	7C9	N03-C04-C19-O20
34	t	2	7C9	N03-C04-C19-O20
34	u	2	7C9	C05-C04-C19-O20
34	t	2	7C9	C05-C04-C19-O20

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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	ADP	c	501	-	24,29,29	0.94	1 (4%)	25,45,45	1.59	3 (12%)
35	ADP	d	501	-	24,29,29	0.98	1 (4%)	25,45,45	1.54	3 (12%)
35	ADP	e	501	-	24,29,29	1.02	1 (4%)	25,45,45	1.51	3 (12%)
35	ADP	g	501	-	24,29,29	0.94	1 (4%)	25,45,45	1.66	3 (12%)
35	ADP	g	502	-	24,29,29	0.92	1 (4%)	25,45,45	1.68	3 (12%)
35	ADP	h	401	-	24,29,29	0.91	1 (4%)	25,45,45	1.60	3 (12%)

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	ADP	c	501	-	-	4/12/32/32	0/3/3/3
35	ADP	d	501	-	-	2/12/32/32	0/3/3/3
35	ADP	e	501	-	-	5/12/32/32	0/3/3/3
35	ADP	g	501	-	-	4/12/32/32	0/3/3/3
35	ADP	g	502	-	-	2/12/32/32	0/3/3/3
35	ADP	h	401	-	-	1/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	e	501	ADP	C5-C4	3.11	1.47	1.40
35	d	501	ADP	C5-C4	2.90	1.47	1.40
35	g	501	ADP	C5-C4	2.86	1.47	1.40
35	h	401	ADP	C5-C4	2.82	1.46	1.40
35	c	501	ADP	C5-C4	2.74	1.46	1.40
35	g	502	ADP	C5-C4	2.71	1.46	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	g	502	ADP	PA-O3A-PB	-5.64	114.66	132.57
35	g	501	ADP	PA-O3A-PB	-5.33	115.64	132.57
35	h	401	ADP	PA-O3A-PB	-4.92	116.94	132.57
35	c	501	ADP	PA-O3A-PB	-4.58	118.01	132.57
35	d	501	ADP	PA-O3A-PB	-4.42	118.54	132.57
35	e	501	ADP	PA-O3A-PB	-3.81	120.46	132.57
35	g	501	ADP	N3-C2-N1	-3.12	123.65	128.68
35	e	501	ADP	N3-C2-N1	-3.08	123.72	128.68
35	h	401	ADP	N3-C2-N1	-3.04	123.78	128.68
35	g	502	ADP	N3-C2-N1	-3.02	123.82	128.68
35	d	501	ADP	C4-C5-N7	-2.98	106.30	109.40
35	d	501	ADP	N3-C2-N1	-2.97	123.89	128.68
35	c	501	ADP	C4-C5-N7	-2.90	106.38	109.40
35	c	501	ADP	N3-C2-N1	-2.83	124.11	128.68
35	e	501	ADP	C4-C5-N7	-2.66	106.63	109.40
35	g	502	ADP	C4-C5-N7	-2.51	106.78	109.40
35	h	401	ADP	C4-C5-N7	-2.49	106.81	109.40
35	g	501	ADP	C4-C5-N7	-2.42	106.88	109.40

There are no chirality outliers.

All (18) torsion outliers are listed below:

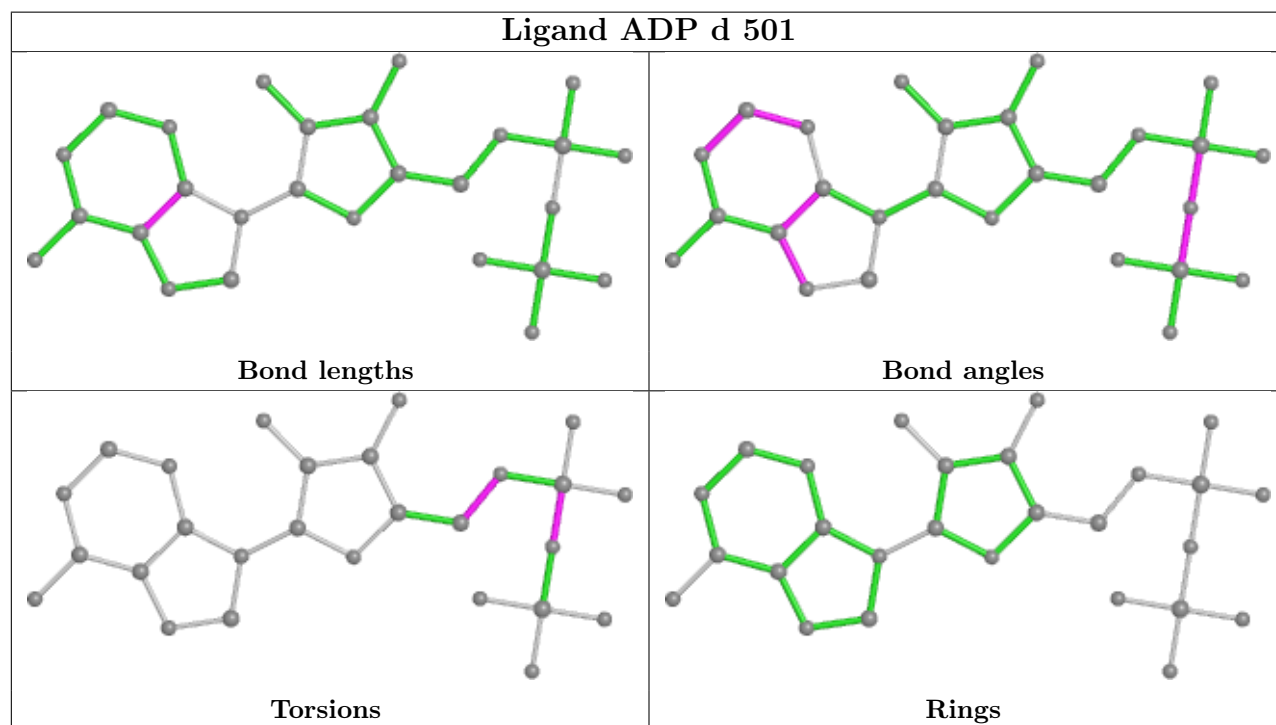
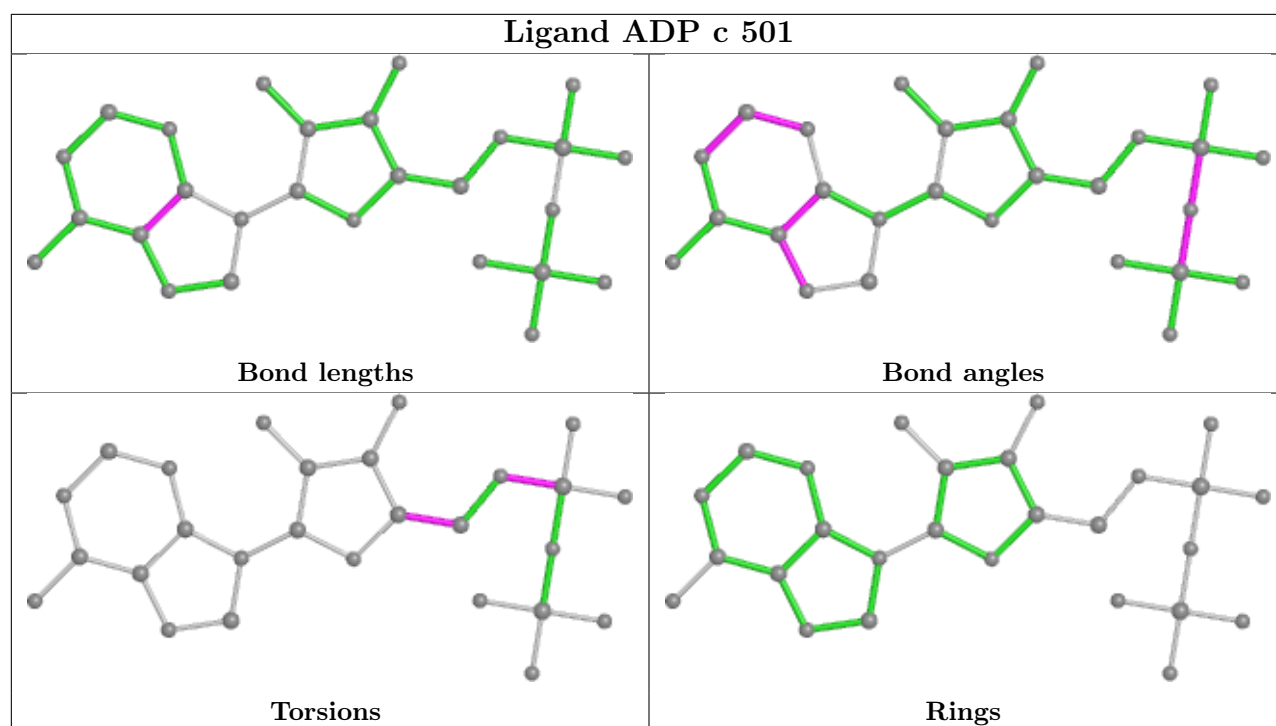
Mol	Chain	Res	Type	Atoms
35	c	501	ADP	C5'-O5'-PA-O1A
35	c	501	ADP	C3'-C4'-C5'-O5'
35	h	401	ADP	C5'-O5'-PA-O1A
35	e	501	ADP	C5'-O5'-PA-O1A
35	e	501	ADP	C5'-O5'-PA-O2A
35	d	501	ADP	C4'-C5'-O5'-PA
35	g	502	ADP	C5'-O5'-PA-O2A
35	g	502	ADP	C5'-O5'-PA-O3A
35	g	501	ADP	C5'-O5'-PA-O1A
35	e	501	ADP	O4'-C4'-C5'-O5'
35	c	501	ADP	O4'-C4'-C5'-O5'
35	g	501	ADP	C4'-C5'-O5'-PA
35	e	501	ADP	C3'-C4'-C5'-O5'
35	g	501	ADP	PB-O3A-PA-O1A
35	g	501	ADP	PB-O3A-PA-O2A
35	c	501	ADP	C5'-O5'-PA-O3A
35	e	501	ADP	C5'-O5'-PA-O3A
35	d	501	ADP	PB-O3A-PA-O2A

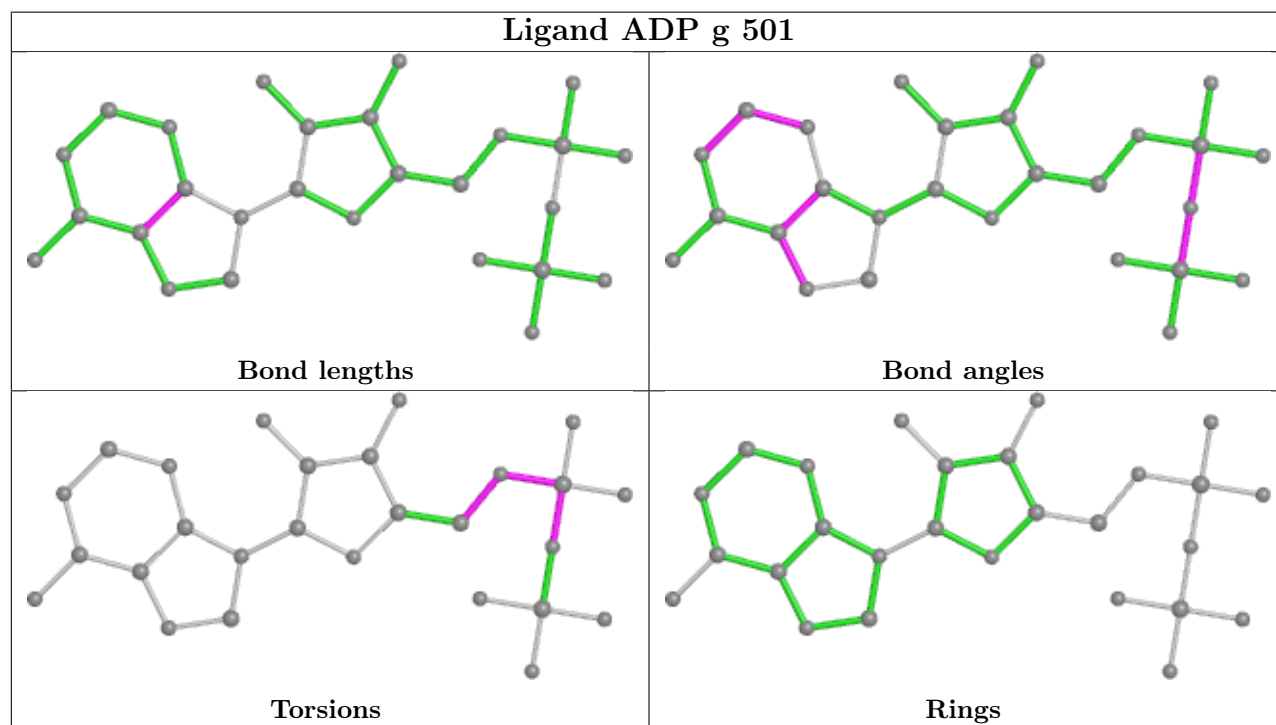
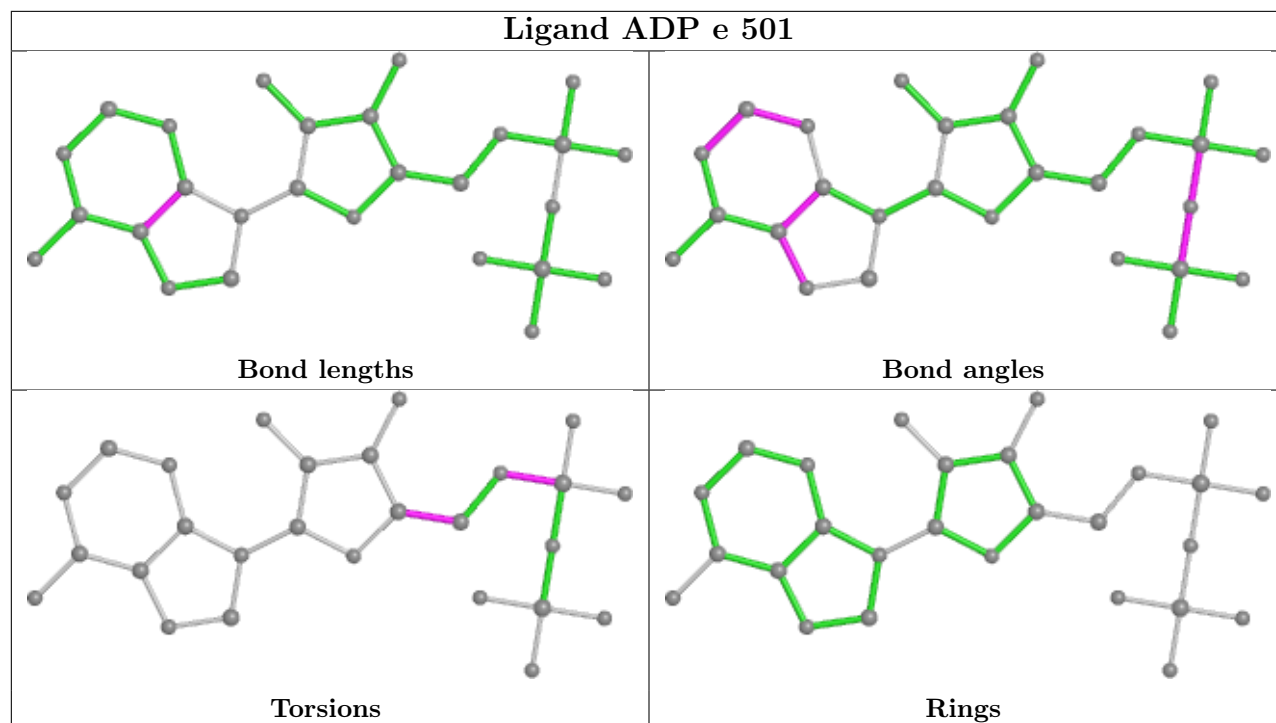
There are no ring outliers.

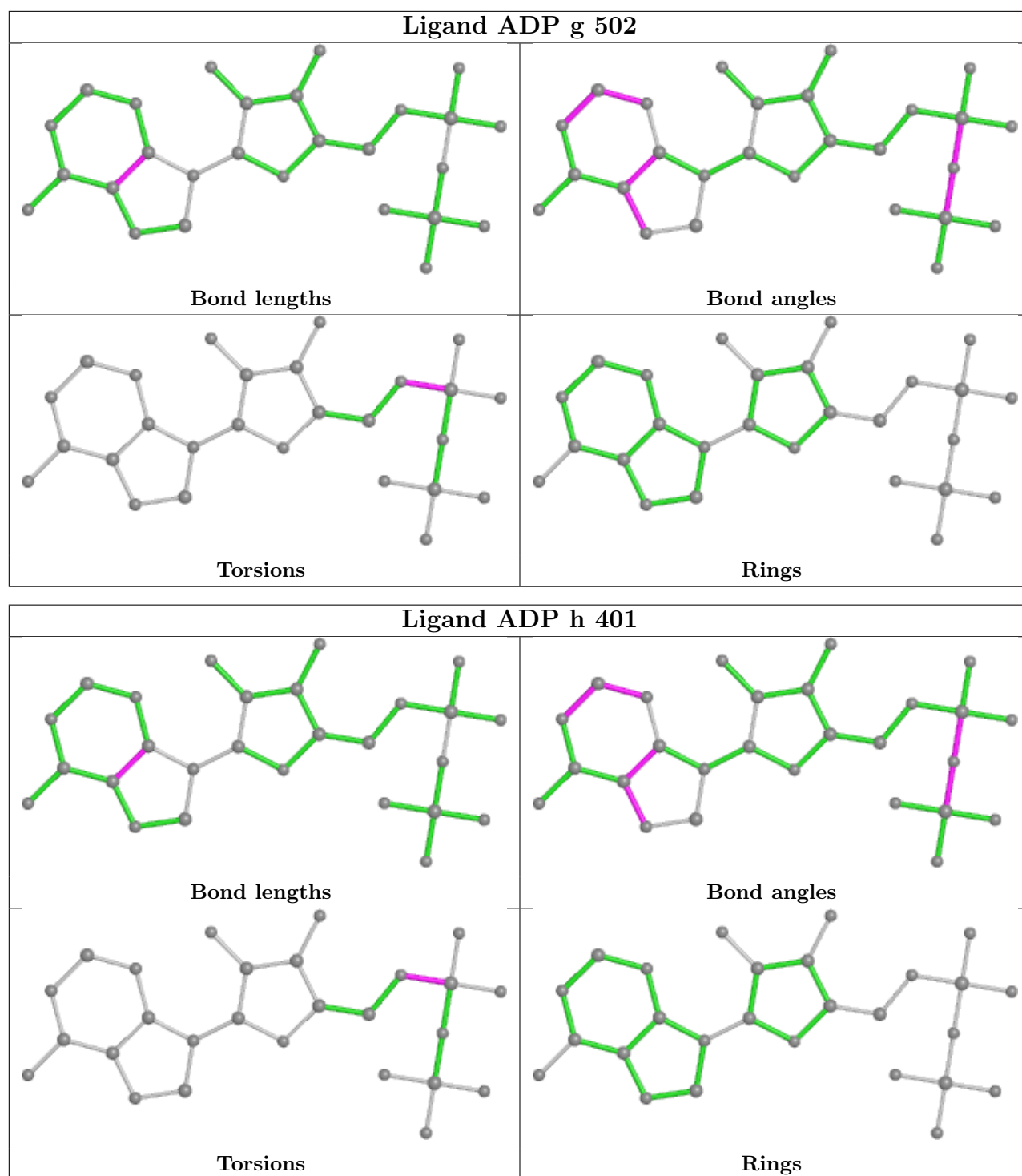
No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
15	Q	1
19	e	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	e	414:HIS	C	415:GLU	N	4.11
1	Q	45:VAL	C	46:GLU	N	0.63