



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 01:11 AM UTC

PDB ID : 6KWY / pdb_00006kwy
EMDB ID : EMD-0781
Title : human PA200-20S complex
Authors : Ouyang, S.; Hongxin, G.
Deposited on : 2019-09-09
Resolution : 2.72 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

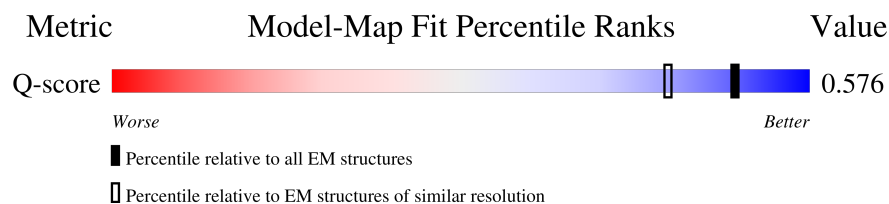
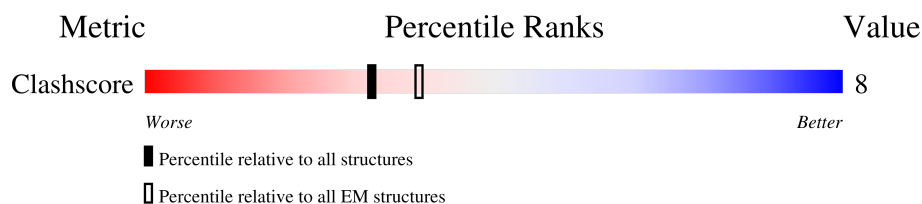
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

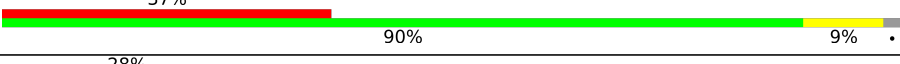
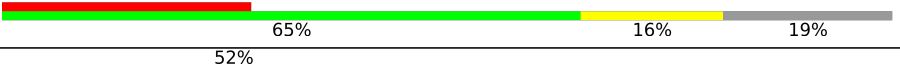
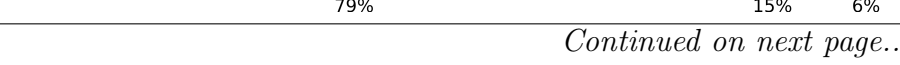
The reported resolution of this entry is 2.72 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Q-score	-	25397	10355 (2.22 - 3.22)

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

Mol	Chain	Length	Quality of chain
1	A	234	
1	O	234	
2	B	261	
2	P	261	
3	C	248	
3	Q	248	

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Mol	Chain	Length	Quality of chain
4	D	241	
4	R	241	
5	E	263	
5	S	263	
6	F	255	
6	T	255	
7	G	246	
7	U	246	
8	H	277	
8	V	277	
9	I	205	
9	W	205	
10	J	201	
10	X	201	
11	K	263	
11	Y	263	
12	L	241	
12	Z	241	
13	M	264	
13	a	264	
14	N	239	
14	b	239	
15	c	1878	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	IHP	c	1902	-	-	X	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 62505 atoms, of which 6 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	215	Total	C	N	O	S	0	0
			1671	1069	285	311	6		
1	O	230	Total	C	N	O	S	0	0
			1779	1136	301	336	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	212	Total	C	N	O	S	0	0
			1645	1040	277	319	9		
2	P	247	Total	C	N	O	S	2	0
			1919	1211	326	371	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	212	Total	C	N	O	S	0	0
			1641	1032	290	314	5		
3	Q	234	Total	C	N	O	S	0	0
			1817	1141	318	353	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	227	Total	C	N	O	S	0	0
			1741	1099	286	345	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	240	Total	C	N	O	S	0	0
			1881	1180	339	350	12		
5	S	238	Total	C	N	O	S	3	0
			1871	1173	338	349	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	245	Total	C	N	O	S	0	0
			1909	1210	326	361	12		
6	T	240	Total	C	N	O	S	1	0
			1867	1186	320	349	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	237	Total	C	N	O	S	1	0
			1860	1183	309	355	13		
7	U	244	Total	C	N	O	S	0	0
			1885	1196	316	360	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	220	Total	C	N	O	S	2	0
			1672	1053	286	320	13		
8	V	220	Total	C	N	O	S	2	0
			1655	1042	278	322	13		

- 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	6	0
			1633	1039	274	301	19		
9	W	204	Total	C	N	O	S	2	0
			1604	1021	269	295	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
			1561	1001	264	287	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	196	Total	C	N	O	S	1	0
			1574	1008	267	289	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	201	Total	C	N	O	S	0	0
			1543	974	267	293	9		
11	Y	199	Total	C	N	O	S	3	0
			1564	988	275	291	10		

- 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	2	0
			1656	1048	283	314	11		
12	Z	213	Total	C	N	O	S	1	0
			1644	1043	281	309	11		

- 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		
13	a	216	Total	C	N	O	S	1	0
			1688	1065	291	320	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	1	0
			1515	951	258	293	13		
14	b	203	Total	C	N	O	S	1	0
			1526	958	259	296	13		

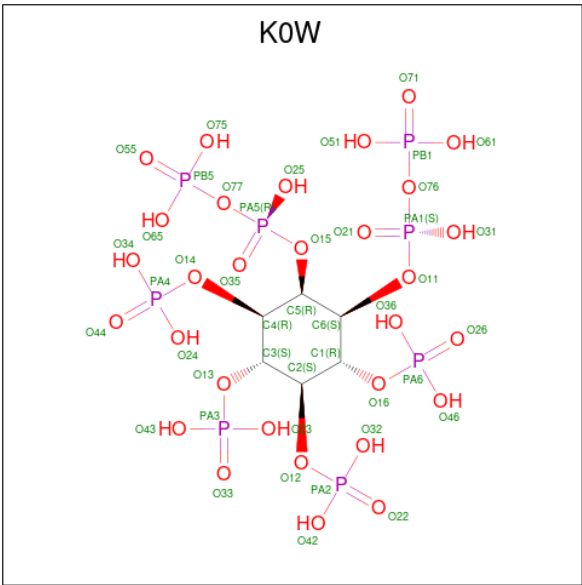
- Molecule 15 is a protein called Proteasome activator complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	c	1811	Total	C	N	O	S	0	0
			14643	9411	2500	2651	81		

There are 37 discrepancies between the modelled and reference sequences:

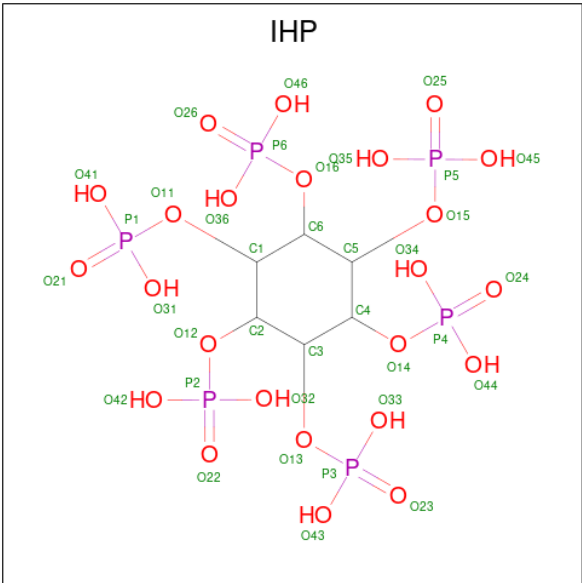
Chain	Residue	Modelled	Actual	Comment	Reference
c	-34	MET	-	initiating methionine	UNP Q14997
c	-33	GLY	-	expression tag	UNP Q14997
c	-32	THR	-	expression tag	UNP Q14997
c	-31	THR	-	expression tag	UNP Q14997
c	-30	ARG	-	expression tag	UNP Q14997
c	-29	SER	-	expression tag	UNP Q14997
c	-28	THR	-	expression tag	UNP Q14997
c	-27	MET	-	expression tag	UNP Q14997
c	-26	SER	-	expression tag	UNP Q14997
c	-25	TYR	-	expression tag	UNP Q14997
c	-24	TYR	-	expression tag	UNP Q14997
c	-23	HIS	-	expression tag	UNP Q14997
c	-22	HIS	-	expression tag	UNP Q14997
c	-21	HIS	-	expression tag	UNP Q14997
c	-20	HIS	-	expression tag	UNP Q14997
c	-19	HIS	-	expression tag	UNP Q14997
c	-18	HIS	-	expression tag	UNP Q14997
c	-17	ASP	-	expression tag	UNP Q14997
c	-16	TYR	-	expression tag	UNP Q14997
c	-15	ASP	-	expression tag	UNP Q14997
c	-14	ILE	-	expression tag	UNP Q14997
c	-13	PRO	-	expression tag	UNP Q14997
c	-12	THR	-	expression tag	UNP Q14997
c	-11	THR	-	expression tag	UNP Q14997
c	-10	GLU	-	expression tag	UNP Q14997
c	-9	ASN	-	expression tag	UNP Q14997
c	-8	LEU	-	expression tag	UNP Q14997
c	-7	TYR	-	expression tag	UNP Q14997
c	-6	PHE	-	expression tag	UNP Q14997
c	-5	GLN	-	expression tag	UNP Q14997
c	-4	GLY	-	expression tag	UNP Q14997
c	-3	ALA	-	expression tag	UNP Q14997
c	-2	MET	-	expression tag	UNP Q14997
c	-1	ASP	-	expression tag	UNP Q14997
c	0	PRO	-	expression tag	UNP Q14997
c	821	ILE	LEU	conflict	UNP Q14997
c	822	LEU	ILE	conflict	UNP Q14997

- Molecule 16 is [(1 {S},2 {R},3 {R},4 {S},5 {S},6 {R})-2-[oxidanyl(phosphonooxy)phosphoryl]oxy-3,4,5,6-tetrphosphonooxy-cyclohexyl] phosphono hydrogen phosphate (CCD ID: K0W) (formula: C₆H₂₀O₃₀P₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
16	c	1	Total	C	O	P	0
			44	6	30	8	

- Molecule 17 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).

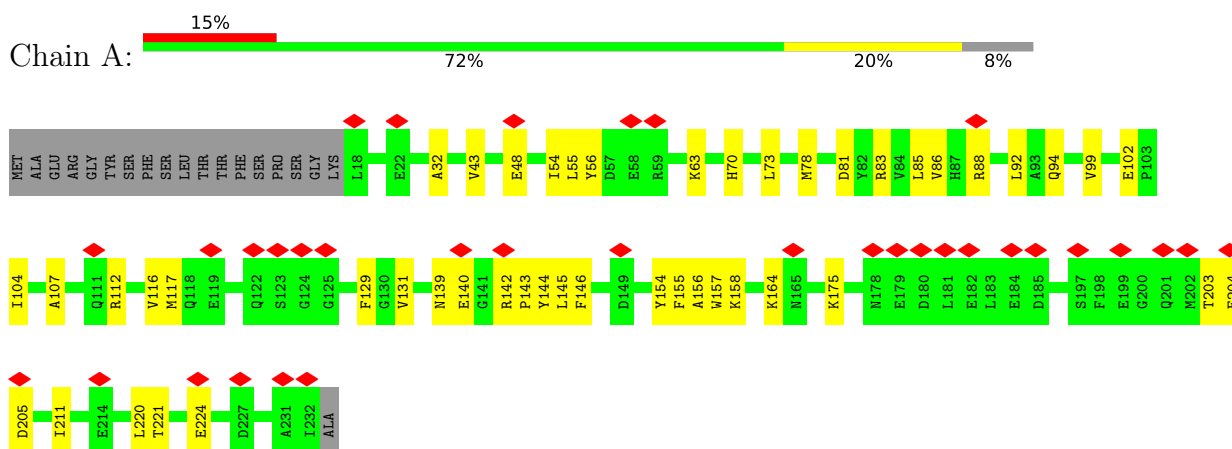


Mol	Chain	Residues	Atoms					AltConf
17	c	1	Total	C	H	O	P	0
			42	6	6	24	6	

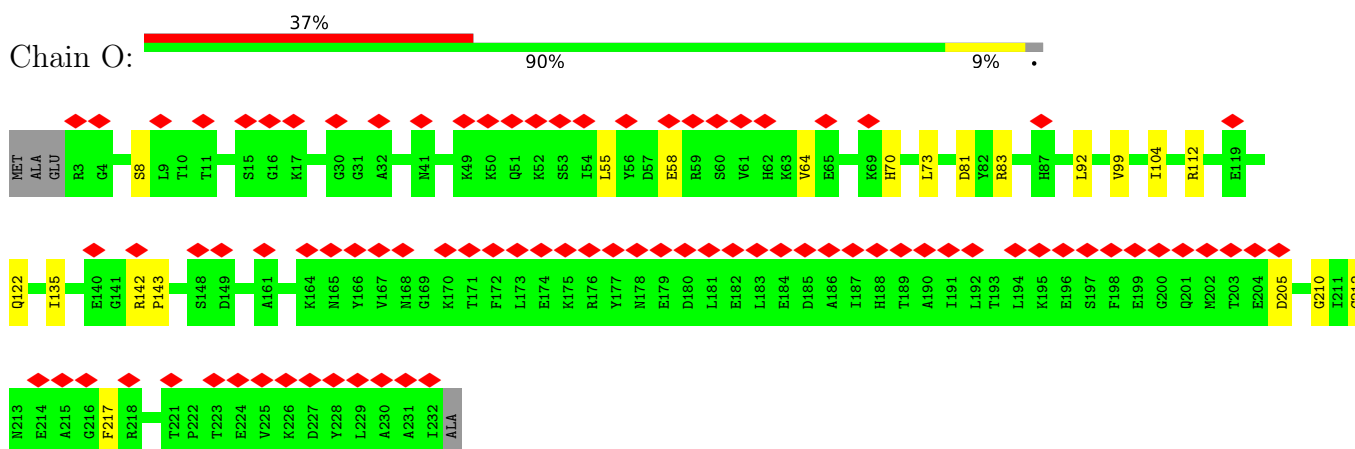
3 Residue-property plots

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

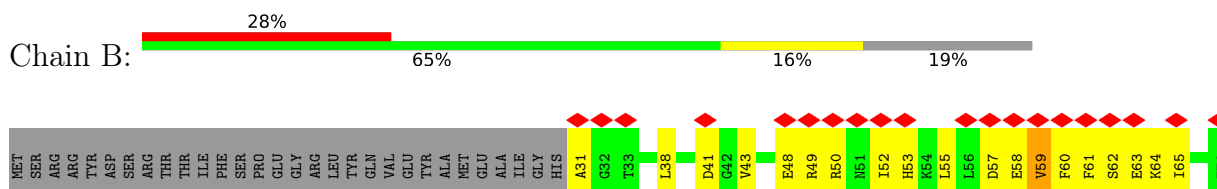
- Molecule 1: Proteasome subunit alpha type-2

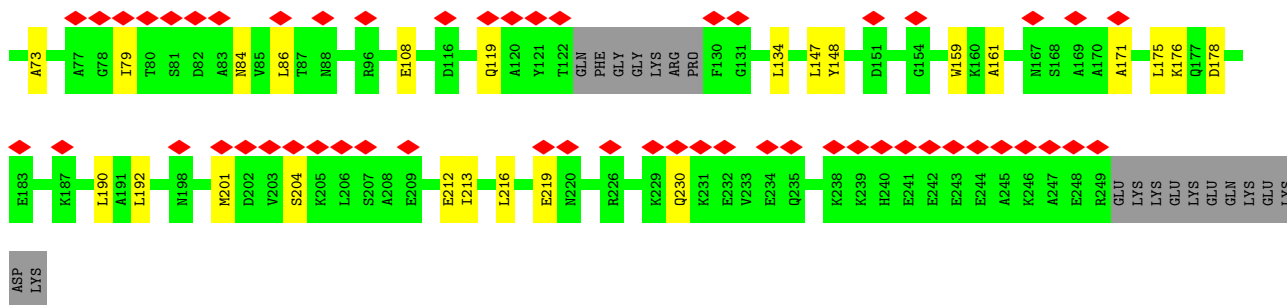


- Molecule 1: Proteasome subunit alpha type-2

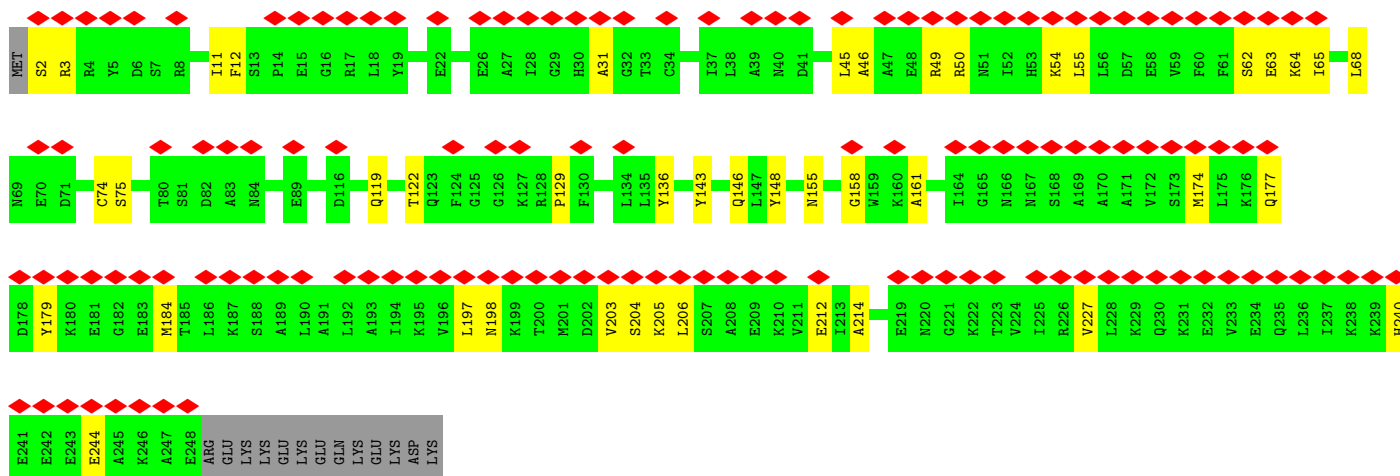
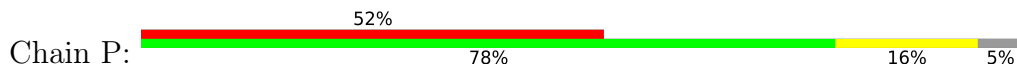


- Molecule 2: Proteasome subunit alpha type-4

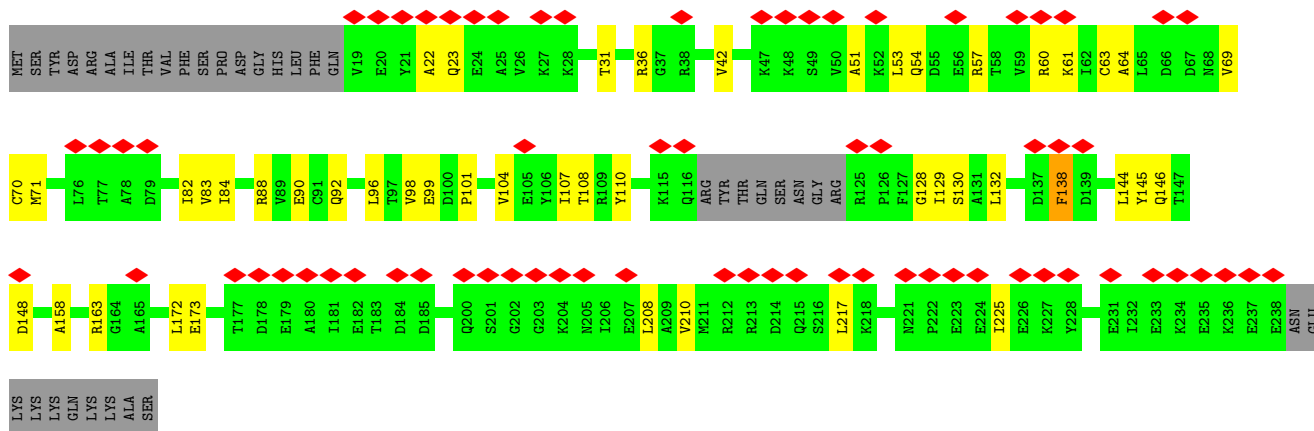




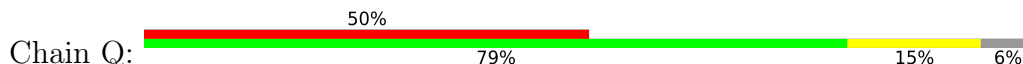
- Molecule 2: Proteasome subunit alpha type-4

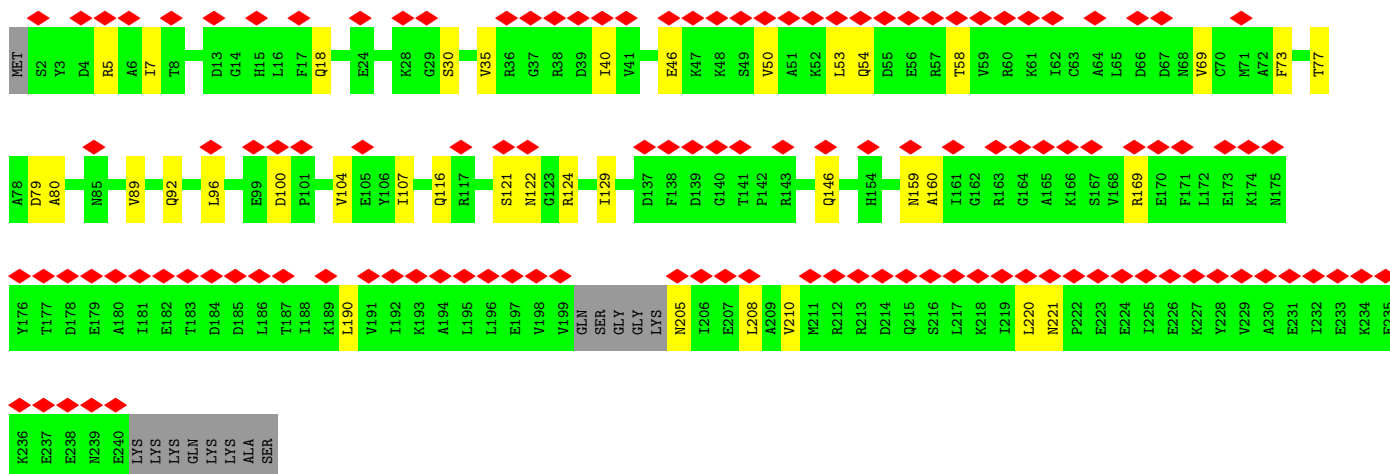


- Molecule 3: Proteasome subunit alpha type-7

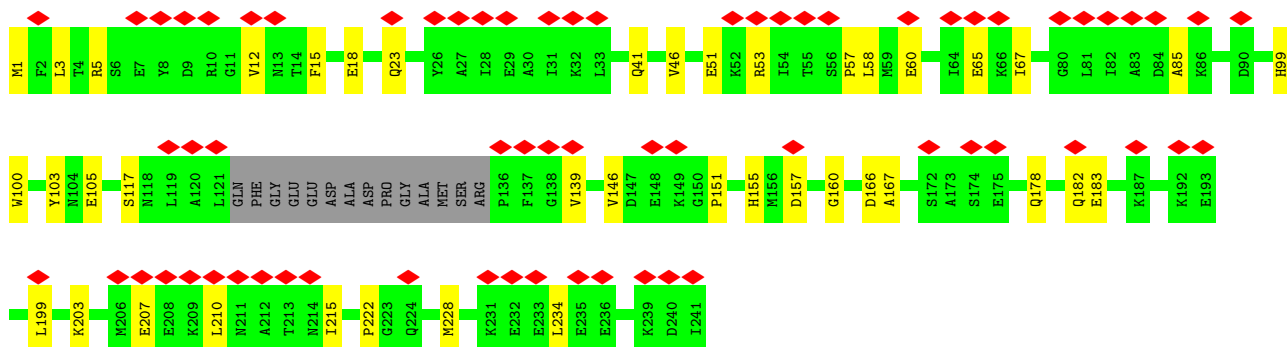
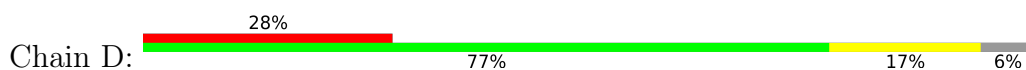


- Molecule 3: Proteasome subunit alpha type-7

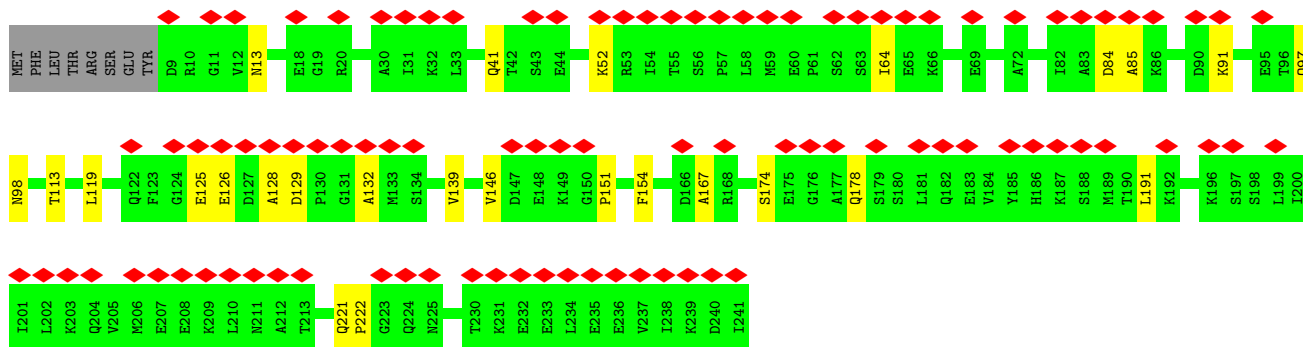
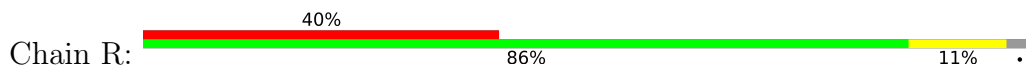




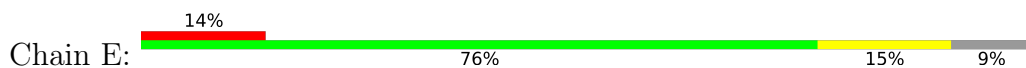
• Molecule 4: Proteasome subunit alpha type-5

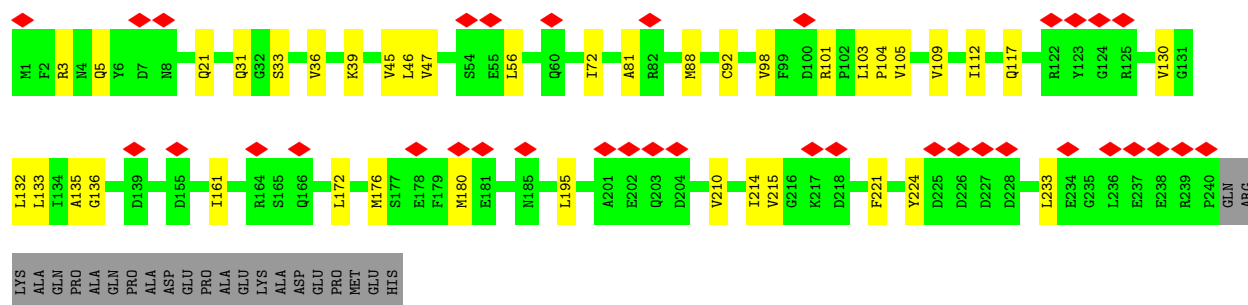


• Molecule 4: Proteasome subunit alpha type-5

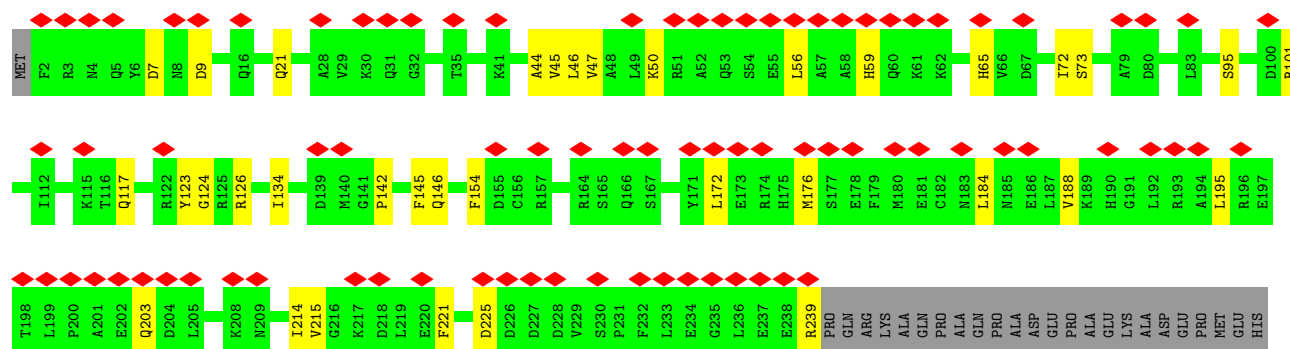
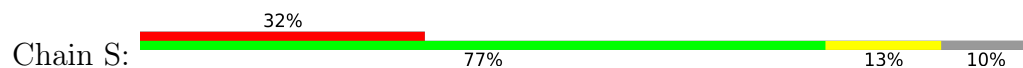


• Molecule 5: Proteasome subunit alpha type-1

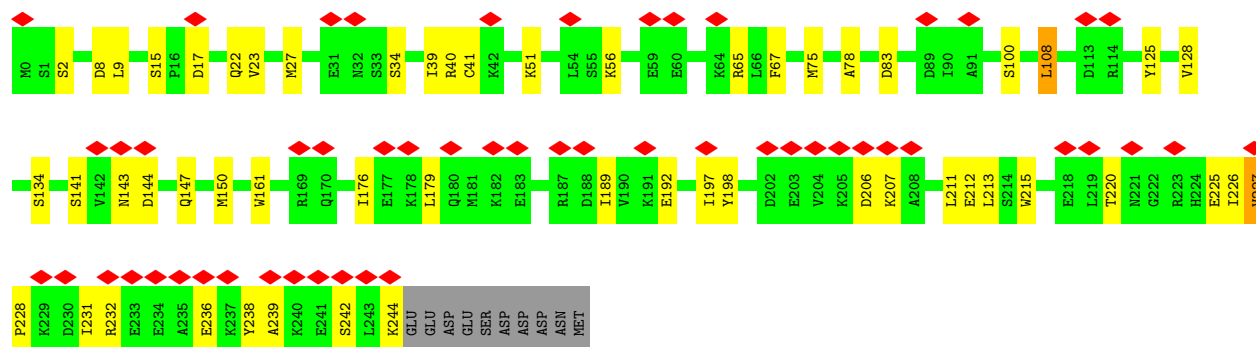
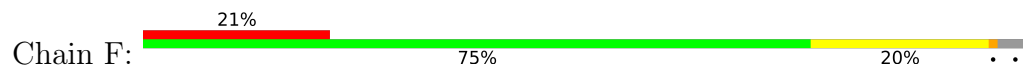




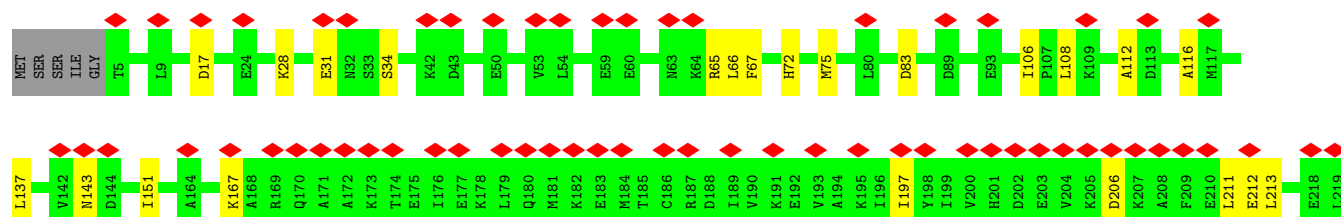
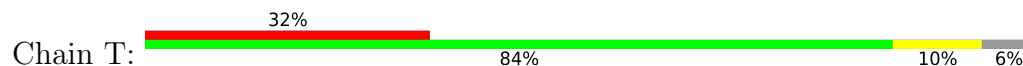
• Molecule 5: Proteasome subunit alpha type-1

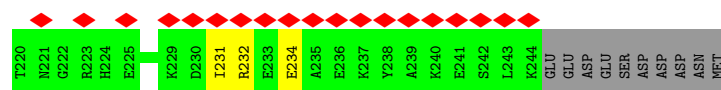


• Molecule 6: Proteasome subunit alpha type-3

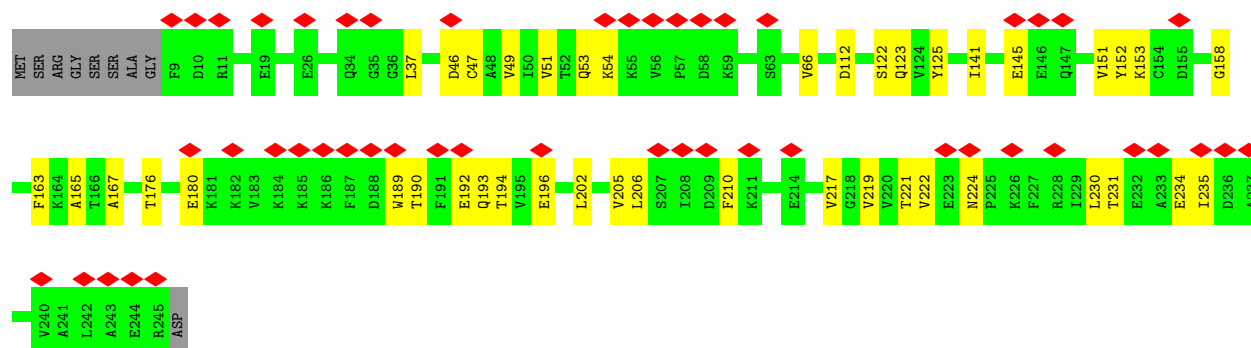
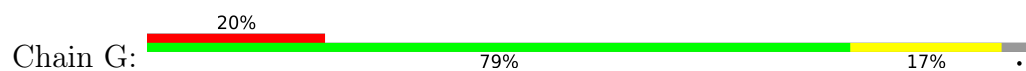


• Molecule 6: Proteasome subunit alpha type-3

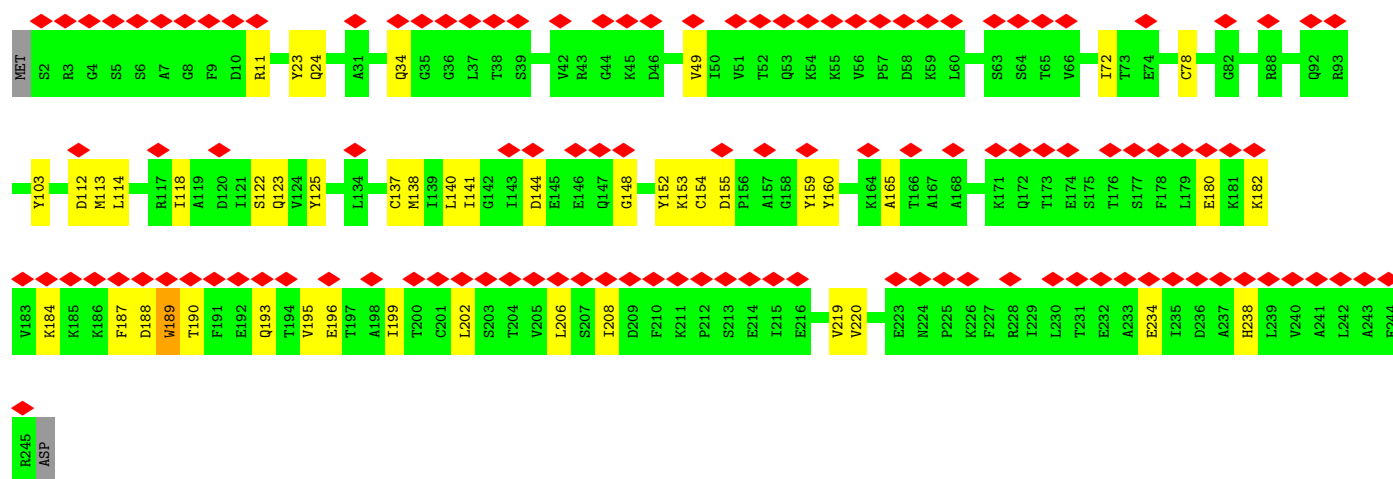
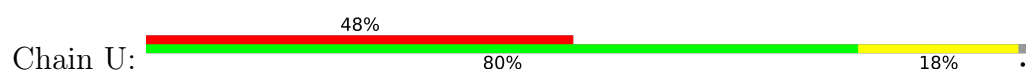




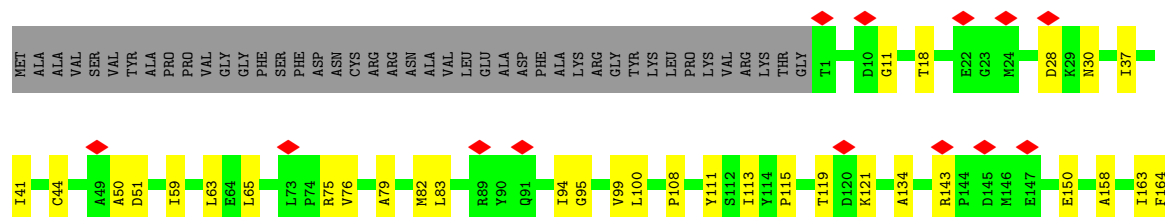
• Molecule 7: Proteasome subunit alpha type-6

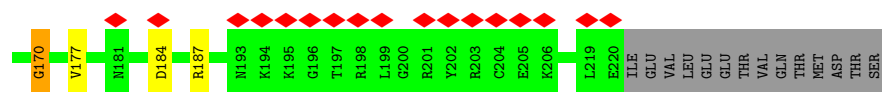


• Molecule 7: Proteasome subunit alpha type-6

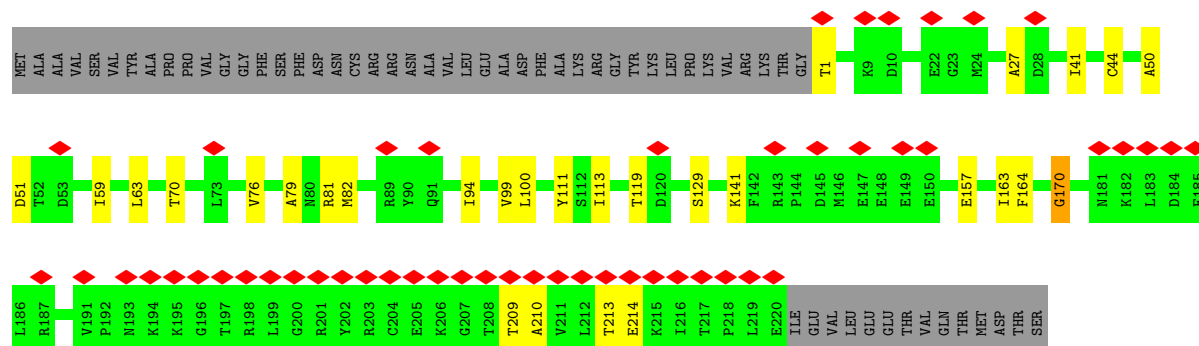


• Molecule 8: Proteasome subunit beta type-7

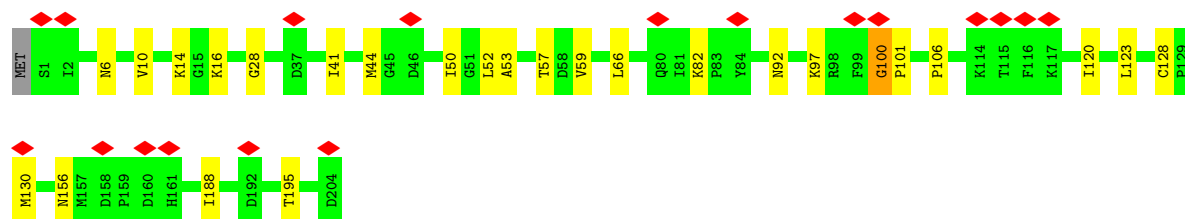
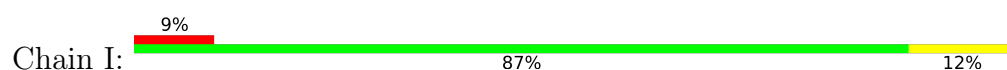




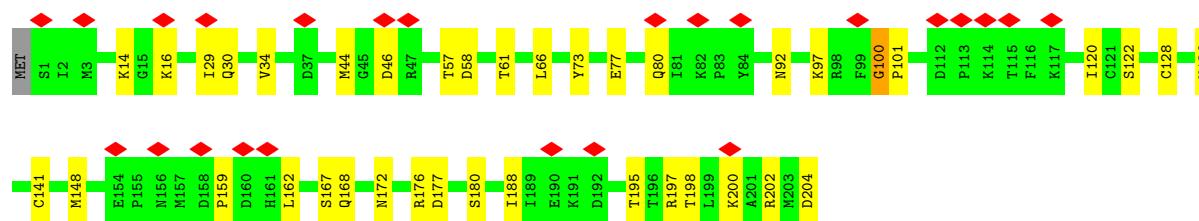
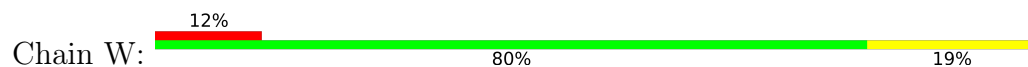
• Molecule 8: Proteasome subunit beta type-7



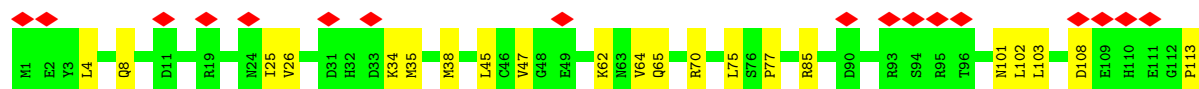
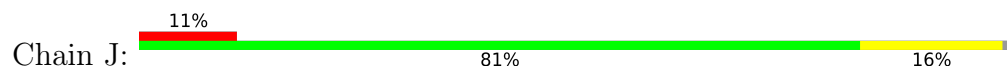
• Molecule 9: Proteasome subunit beta type-3

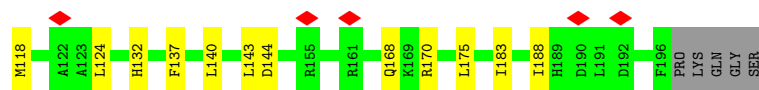


• Molecule 9: Proteasome subunit beta type-3

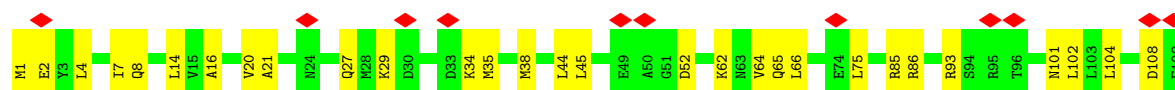
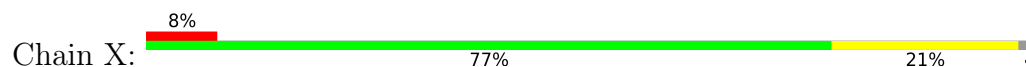


• Molecule 10: Proteasome subunit beta type-2

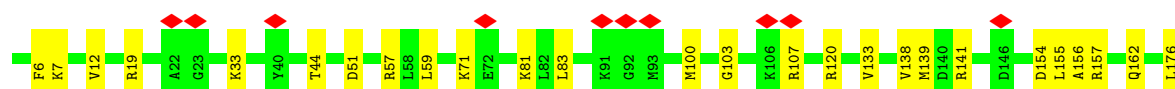
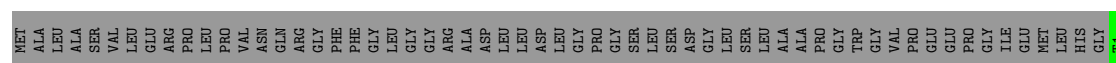




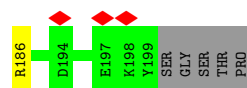
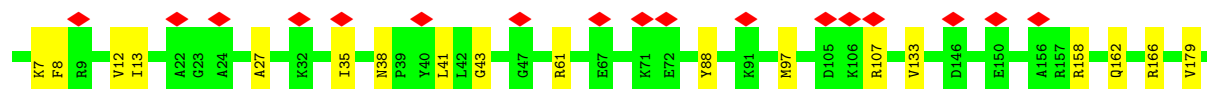
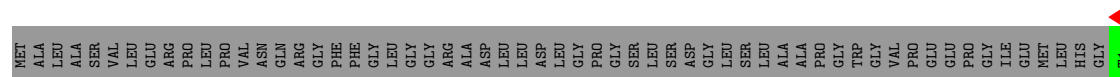
- Molecule 10: Proteasome subunit beta type-2



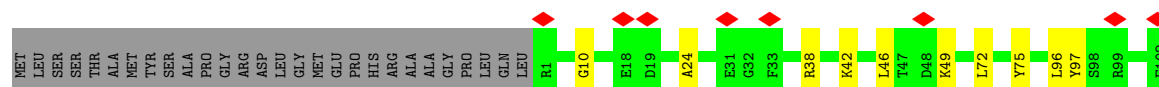
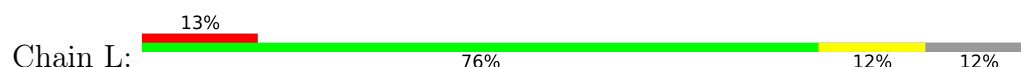
- Molecule 11: Proteasome subunit beta type-5

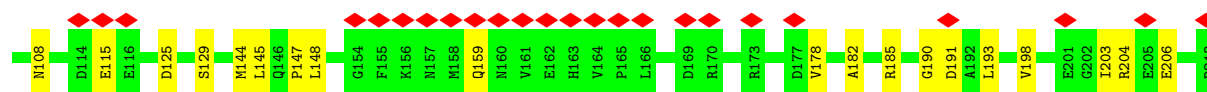


- Molecule 11: Proteasome subunit beta type-5

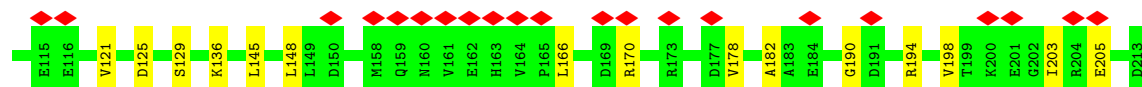
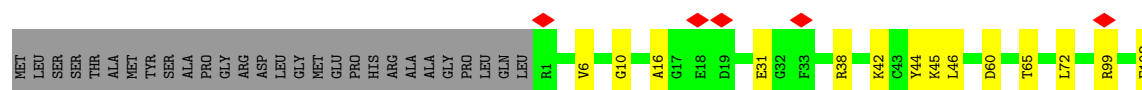
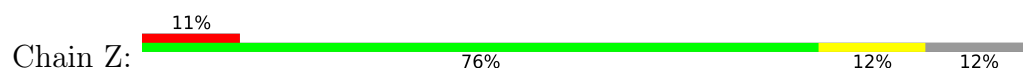


- Molecule 12: Proteasome subunit beta type-1

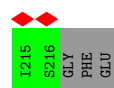
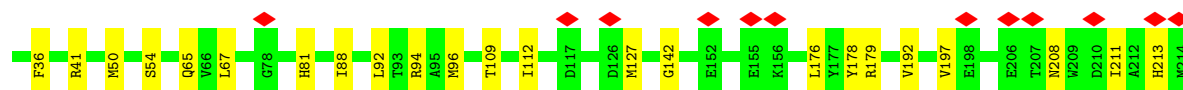
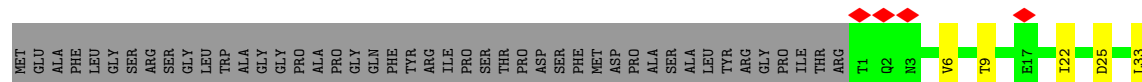




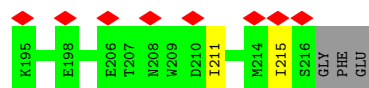
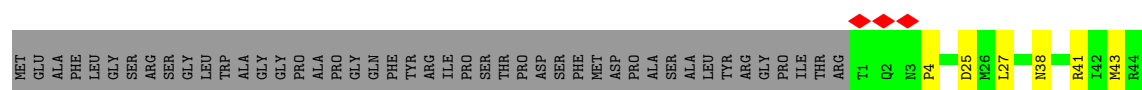
- Molecule 12: Proteasome subunit beta type-1



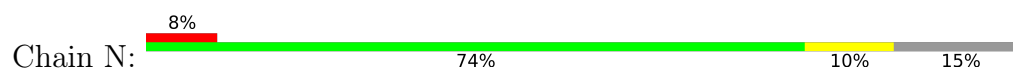
- Molecule 13: Proteasome subunit beta type-4

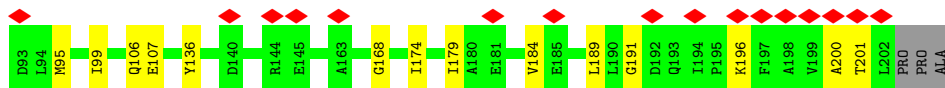


- Molecule 13: Proteasome subunit beta type-4

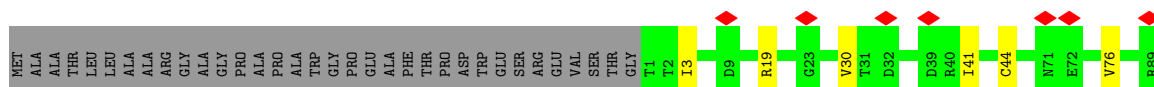
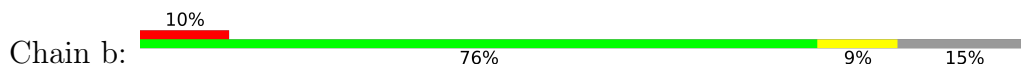


- Molecule 14: Proteasome subunit beta type-6

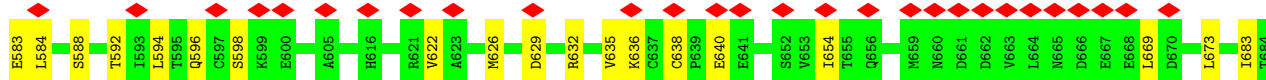
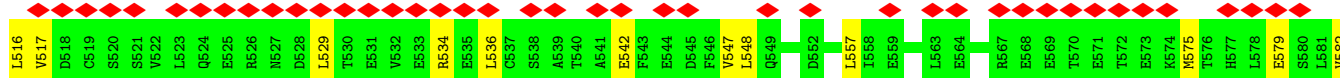
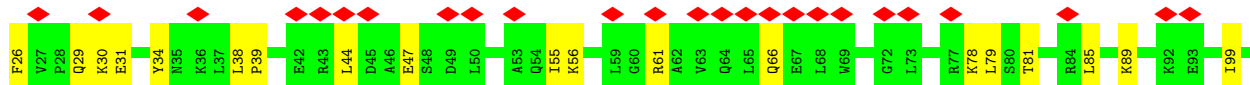
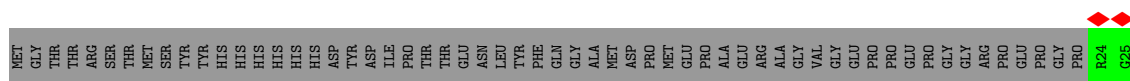




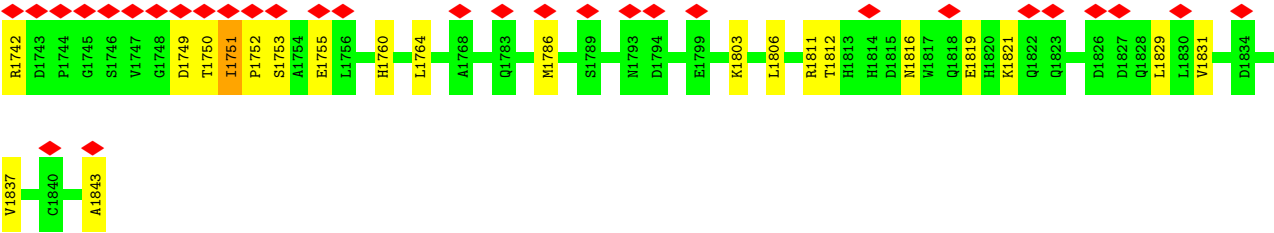
- Molecule 14: Proteasome subunit beta type-6



- Molecule 15: Proteasome activator complex subunit 4



L1665	Q1666	T1667	M1668	V1669	F1670	Y1671	T1672	L1673	F1674	L1677	M1678	N1679	E1680	D1685	I1686	R1687	V1690	L1693	E1697	Q1698	L1699	E1700	V1701	R1702	E1703	M1704	A1705	A1706	L1712	L1713	Q1714	T1719	M1720	D1721	S1722	P1723	M1724	Q1725	E1729	Q1730	L1731	C1732	T1733	A1734	K1735	A1650	L1736	P1737	K1738	K1739	R1740	K1741
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V1501	R1502	I1505	L1509	T1510	Y1511	L1512	F1513	D1516	V1517	S1518	L1519	P1520	M1521	L1538	E1539	K1540	L1541	K1542	P1543	L1544	M1545	D1546	V1547	D1548	E1549	E1550	T1551	Q1552	N1553	H1554	V1555	MET	GLU	GLU	ASN	GLY	ILE	GLY	GLU	D1565	E1566	R1567	T1568	Q1569	G1570	I1571	L1574	K1575	L1578	L1581	M1582	
E1403	C1406	L1409	R1410	N1415	E1419	C1427	S1431	C1432	E1433	S1434	R1435	K1439	L1440	L1443	F1444	E1445	L1446	L1447	L1448	E1449	S1450	P1451	L1452	S1453	G1454	E1455	G1456	G1457	D1461	A1462	L1468	Q1475	E1476	V1477	R1478	E1481	L1482	R1485	L1486	L1490	Q1496	A1499	N1500									
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E1403	C1406	L1409	R1410	N1415	E1419	C1427	S1431	C1432	E1433	S1434	R1435	K1439	L1440	L1443	F1444	E1445	L1446	L1447	L1448	E1449	S1450	P1451	L1452	S1453	G1454	E1455	G1456	G1457	D1461	A1462	L1468	Q1475	E1476	V1477	R1478	E1481	L1482	R1485	L1486	L1490	Q1496	A1499	N1500									
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V1501	R1502	I1505	L1509	T1510	Y1511	L1512	F1513	D1516	V1517	S1518	L1519	P1520	M1521	L1538	E1539	K1540	L1541	K1542	P1543	L1544	M1545	D1546	V1547	D1548	E1549	E1550	T1551	Q1552	N1553	H1554	V1555	MET	GLU	GLU	ASN	GLY	ILE	GLY	GLU	D1565	E1566	R1567	T1568	Q1569	G1570	I1571	L1574	K1575	L1578	L1581	M1582	
E1403	C1406	L1409	R1410	N1415	E1419	C1427	S1431	C1432	E1433	S1434	R1435	K1439	L1440	L1443	F1444	E1445	L1446	L1447	L1448	E1449	S1450	P1451	L1452	S1453	G1454	E1455	G1456	G1457	D1461	A1462	L1468	Q1475	E1476	V1477	R1478	E1481	L1482	R1485	L14													



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.179	Depositor
Minimum map value	-0.101	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	374.4, 374.4, 374.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: KOW, IHP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.48	0/1706	0.71	4/2314 (0.2%)
1	O	0.38	0/1818	0.59	0/2467
2	B	0.44	0/1666	0.71	3/2248 (0.1%)
2	P	0.38	0/1955	0.59	1/2642 (0.0%)
3	C	0.42	0/1660	0.81	3/2240 (0.1%)
3	Q	0.33	0/1842	0.65	2/2496 (0.1%)
4	D	0.45	0/1767	0.66	0/2386
4	R	0.38	0/1795	0.59	2/2424 (0.1%)
5	E	0.49	0/1917	0.69	0/2592
5	S	0.39	0/1915	0.61	2/2589 (0.1%)
6	F	0.45	0/1944	0.73	4/2617 (0.2%)
6	T	0.40	0/1905	0.64	0/2567
7	G	0.45	0/1897	0.72	1/2566 (0.0%)
7	U	0.37	0/1919	0.67	3/2596 (0.1%)
8	H	0.44	0/1705	0.66	2/2307 (0.1%)
8	V	0.41	0/1688	0.64	2/2288 (0.1%)
9	I	0.48	1/1668 (0.1%)	0.69	4/2247 (0.2%)
9	W	0.46	0/1636	0.74	7/2205 (0.3%)
10	J	0.44	0/1593	0.61	0/2156
10	X	0.44	0/1609	0.61	0/2176
11	K	0.46	0/1574	0.61	0/2128
11	Y	0.44	0/1604	0.64	0/2165
12	L	0.45	0/1692	0.66	2/2281 (0.1%)
12	Z	0.46	0/1677	0.67	2/2260 (0.1%)
13	M	0.47	0/1720	0.61	0/2328
13	a	0.48	0/1724	0.65	0/2334
14	N	0.45	0/1544	0.57	0/2090
14	b	0.45	0/1556	0.60	0/2107
15	c	0.46	0/14985	0.87	35/20326 (0.2%)
All	All	0.44	1/63681 (0.0%)	0.71	79/86142 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	41	ILE	C-N	5.86	1.43	1.33

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	c	303	THR	N-CA-C	12.09	124.46	111.28
7	U	189	TRP	N-CA-C	11.72	128.34	109.24
15	c	1270	GLU	N-CA-C	10.46	122.75	111.36
15	c	1112	ASN	CA-C-N	9.46	131.66	119.84
15	c	1112	ASN	C-N-CA	9.46	131.66	119.84
15	c	1125	ILE	N-CA-C	-9.00	103.92	112.83
9	I	41	ILE	CA-C-N	-7.31	106.84	123.15
9	I	41	ILE	C-N-CA	-7.31	106.84	123.15
9	W	16[A]	LYS	CA-C-N	7.20	132.89	121.08
9	W	16[A]	LYS	C-N-CA	7.20	132.89	121.08
9	W	16[B]	LYS	CA-C-N	7.20	132.89	121.08
9	W	16[B]	LYS	C-N-CA	7.20	132.89	121.08
15	c	1673	LEU	N-CA-C	7.05	118.97	111.28
2	B	59	VAL	N-CA-C	-6.92	103.73	110.72
15	c	1751	ILE	N-CA-C	-6.64	99.71	107.61
15	c	298	VAL	CA-C-N	6.64	126.42	119.05
15	c	298	VAL	C-N-CA	6.64	126.42	119.05
15	c	638	CYS	CA-C-N	6.62	126.06	118.85
15	c	638	CYS	C-N-CA	6.62	126.06	118.85
3	Q	221	ASN	CA-C-N	-6.53	112.90	119.56
3	Q	221	ASN	C-N-CA	-6.53	112.90	119.56
9	I	100	GLY	N-CA-C	-6.40	99.28	112.34
8	V	170	GLY	CA-C-N	6.33	133.62	121.54
8	V	170	GLY	C-N-CA	6.33	133.62	121.54
15	c	477	GLY	CA-C-N	6.21	125.94	119.05
15	c	477	GLY	C-N-CA	6.21	125.94	119.05
8	H	170	GLY	CA-C-N	6.20	133.37	121.54
8	H	170	GLY	C-N-CA	6.20	133.37	121.54
9	W	100	GLY	N-CA-C	-6.18	99.73	112.34
3	C	138	PHE	N-CA-C	6.09	117.92	111.28
15	c	1481	GLU	CA-C-N	6.08	133.16	121.54
15	c	1481	GLU	C-N-CA	6.08	133.16	121.54
7	G	192	GLU	N-CA-C	6.05	117.95	111.36
9	W	30	GLN	N-CA-C	-6.04	97.93	110.80
6	F	108	LEU	CA-C-N	6.01	133.01	121.54
6	F	108	LEU	C-N-CA	6.01	133.01	121.54
15	c	1671	TYR	N-CA-C	-5.92	100.35	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	c	1753	SER	N-CA-C	5.83	117.00	108.14
12	Z	190	GLY	CA-C-N	5.79	132.61	121.54
12	Z	190	GLY	C-N-CA	5.79	132.61	121.54
15	c	1091	GLY	N-CA-C	5.77	121.53	111.50
4	R	129	ASP	CA-C-N	-5.70	112.71	119.84
4	R	129	ASP	C-N-CA	-5.70	112.71	119.84
5	S	225	ASP	CA-C-N	5.61	129.24	120.82
5	S	225	ASP	C-N-CA	5.61	129.24	120.82
15	c	272	TRP	CA-C-N	5.60	127.09	120.09
15	c	272	TRP	C-N-CA	5.60	127.09	120.09
15	c	1742	ARG	CA-C-N	5.60	128.47	123.10
15	c	1742	ARG	C-N-CA	5.60	128.47	123.10
7	U	189	TRP	CA-C-N	5.58	132.37	122.45
7	U	189	TRP	C-N-CA	5.58	132.37	122.45
2	B	219	GLU	CA-C-N	5.55	130.28	122.46
2	B	219	GLU	C-N-CA	5.55	130.28	122.46
15	c	516	LEU	CA-CB-CG	5.48	135.49	116.30
2	P	205	LYS	N-CA-C	-5.45	102.21	110.28
15	c	1099	SER	N-CA-C	-5.45	108.41	114.62
15	c	1176	ARG	CA-C-N	5.40	136.01	126.45
15	c	1176	ARG	C-N-CA	5.40	136.01	126.45
15	c	1228	GLU	N-CA-C	-5.38	107.36	114.31
3	C	98	VAL	CA-C-N	5.36	131.78	121.54
3	C	98	VAL	C-N-CA	5.36	131.78	121.54
1	A	78	MET	CA-C-N	5.30	125.00	121.13
1	A	78	MET	C-N-CA	5.30	125.00	121.13
15	c	1734	THR	CA-C-N	5.30	131.66	121.54
15	c	1734	THR	C-N-CA	5.30	131.66	121.54
1	A	164	LYS	CA-C-N	5.29	131.65	121.54
1	A	164	LYS	C-N-CA	5.29	131.65	121.54
9	W	101	PRO	N-CA-C	5.26	123.30	112.47
6	F	227	VAL	CA-C-N	5.17	125.08	119.76
6	F	227	VAL	C-N-CA	5.17	125.08	119.76
15	c	304	ASN	N-CA-C	5.17	115.36	108.23
15	c	1004	ILE	N-CA-C	5.12	117.10	112.29
15	c	1468	LEU	CA-CB-CG	5.10	134.15	116.30
12	L	190	GLY	CA-C-N	5.10	131.27	121.54
12	L	190	GLY	C-N-CA	5.10	131.27	121.54
9	I	101	PRO	N-CA-C	5.03	122.83	112.47
15	c	750	TYR	CA-C-N	-5.03	115.90	122.74
15	c	750	TYR	C-N-CA	-5.03	115.90	122.74
15	c	972	LEU	N-CA-C	-5.03	105.80	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1671	0	1665	58	0
1	O	1779	0	1747	12	0
2	B	1645	0	1655	48	0
2	P	1919	0	1895	31	0
3	C	1641	0	1664	41	0
3	Q	1817	0	1786	34	0
4	D	1741	0	1738	37	0
4	R	1768	0	1756	27	0
5	E	1881	0	1862	27	0
5	S	1871	0	1855	22	0
6	F	1909	0	1900	66	0
6	T	1867	0	1847	15	0
7	G	1860	0	1866	41	0
7	U	1885	0	1881	35	0
8	H	1672	0	1703	23	0
8	V	1655	0	1661	20	0
9	I	1633	0	1660	15	0
9	W	1604	0	1626	29	0
10	J	1561	0	1558	25	0
10	X	1574	0	1578	32	0
11	K	1543	0	1495	25	0
11	Y	1564	0	1539	15	0
12	L	1656	0	1655	19	0
12	Z	1644	0	1644	17	0
13	M	1687	0	1666	19	0
13	a	1688	0	1666	18	0
14	N	1515	0	1492	16	0
14	b	1526	0	1503	15	0
15	c	14643	0	14837	428	0
16	c	44	0	0	15	0
17	c	36	6	6	12	0
All	All	62499	6	62406	1055	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 8.

All (1055) 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:c:972:LEU:HD11	15:c:1004:ILE:CD1	1.30	1.60
15:c:972:LEU:CD1	15:c:1004:ILE:HD11	1.34	1.52
15:c:300:ARG:NH1	15:c:1631:GLN:HG2	1.25	1.49
6:F:215:TRP:CZ2	6:F:227:VAL:HG13	1.48	1.47
6:F:215:TRP:NE1	6:F:227:VAL:HG22	1.36	1.36
15:c:298:VAL:CG2	15:c:299:PRO:HD3	1.57	1.34
1:A:146:PHE:HZ	2:B:60:PHE:CE2	1.46	1.34
6:F:215:TRP:CD1	6:F:227:VAL:HG22	1.62	1.32
15:c:324:LYS:O	15:c:326:VAL:N	1.63	1.29
1:A:146:PHE:HZ	2:B:60:PHE:CZ	1.49	1.28
6:F:215:TRP:CZ2	6:F:227:VAL:CG1	2.15	1.28
15:c:307:ASP:OD2	15:c:310:HIS:HD2	1.11	1.27
15:c:972:LEU:HD21	15:c:990:PHE:CE1	1.70	1.26
7:G:189:TRP:O	7:G:190:THR:HG23	1.28	1.25
7:G:189:TRP:O	7:G:190:THR:CG2	1.86	1.22
15:c:933:LYS:CG	16:c:1901:KOW:O71	1.87	1.22
15:c:300:ARG:NH1	15:c:1631:GLN:CG	2.04	1.19
15:c:1749:ASP:O	15:c:1750:THR:HG22	1.04	1.17
15:c:887:THR:O	15:c:891:PHE:CE2	1.96	1.17
1:A:146:PHE:CZ	2:B:60:PHE:CZ	2.33	1.16
6:F:244:LYS:HE2	6:F:244:LYS:HA	1.26	1.16
1:A:146:PHE:CZ	2:B:60:PHE:CE2	2.33	1.16
4:R:128:ALA:HB1	4:R:132:ALA:HB3	1.27	1.15
15:c:1749:ASP:O	15:c:1750:THR:CG2	1.93	1.15
15:c:1112:ASN:CB	15:c:1113:PRO:HD3	1.73	1.15
15:c:300:ARG:CZ	15:c:1631:GLN:HG2	1.78	1.14
15:c:375:LYS:HE3	15:c:375:LYS:H	1.14	1.13
15:c:298:VAL:HG23	15:c:299:PRO:CD	1.78	1.13
15:c:933:LYS:HG2	16:c:1901:KOW:O71	0.95	1.12
15:c:307:ASP:OD2	15:c:310:HIS:CD2	2.02	1.12
4:D:183:GLU:OE1	15:c:1751:ILE:O	1.67	1.11
4:R:128:ALA:CB	4:R:132:ALA:HB3	1.81	1.11
15:c:960:TYR:HE2	15:c:1003:ASP:OD2	1.32	1.11
6:F:215:TRP:CD1	6:F:227:VAL:CG2	2.35	1.10
15:c:972:LEU:CD2	15:c:990:PHE:CE1	2.33	1.10
1:A:145:LEU:HD12	1:A:157:TRP:HB2	1.13	1.09
15:c:297:LEU:HD13	15:c:1631:GLN:NE2	1.68	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:202:LEU:HD23	7:G:206:LEU:HD23	1.35	1.08
15:c:34:TYR:OH	15:c:933:LYS:CE	2.01	1.08
15:c:972:LEU:HD21	15:c:990:PHE:CZ	1.89	1.07
15:c:1112:ASN:HB2	15:c:1113:PRO:CD	1.85	1.06
15:c:887:THR:O	15:c:891:PHE:CD2	2.07	1.05
6:F:215:TRP:CE2	6:F:227:VAL:HG13	1.90	1.05
15:c:300:ARG:NH1	15:c:1631:GLN:O	1.91	1.03
3:C:138:PHE:CZ	11:K:107:ARG:NH2	2.26	1.02
3:C:138:PHE:CE1	11:K:107:ARG:NH2	2.25	1.02
7:G:202:LEU:HD22	7:G:210:PHE:HZ	1.17	1.02
2:B:62:SER:O	2:B:212:GLU:OE2	1.77	1.01
9:I:97:LYS:HB3	9:I:100:GLY:O	1.60	1.01
15:c:300:ARG:NH1	15:c:1631:GLN:C	2.19	1.00
15:c:34:TYR:OH	15:c:933:LYS:HE2	1.56	0.99
6:F:215:TRP:NE1	6:F:227:VAL:CG2	2.26	0.98
9:W:97:LYS:HB3	9:W:100:GLY:O	1.63	0.98
15:c:1271:LYS:HB2	15:c:1274:TRP:CD1	1.98	0.97
6:F:215:TRP:CE2	6:F:227:VAL:CG1	2.45	0.97
7:G:189:TRP:C	7:G:190:THR:HG22	1.88	0.96
7:G:189:TRP:C	7:G:190:THR:CG2	2.35	0.96
15:c:1271:LYS:O	15:c:1478:ARG:NH2	1.98	0.96
15:c:300:ARG:HH12	15:c:1631:GLN:CG	1.75	0.95
15:c:887:THR:O	15:c:891:PHE:HE2	1.47	0.95
15:c:933:LYS:NZ	16:c:1901:K0W:O61	2.00	0.94
1:A:158:LYS:HE3	2:B:57:ASP:HA	1.48	0.94
15:c:300:ARG:HH12	15:c:1631:GLN:HG2	1.26	0.93
15:c:208:GLN:NE2	15:c:251:TRP:HB3	1.83	0.93
15:c:131:GLU:HG3	15:c:379:LEU:CD1	1.97	0.93
6:F:215:TRP:CE2	6:F:227:VAL:HG22	2.04	0.92
4:D:183:GLU:CD	15:c:1751:ILE:O	2.12	0.92
15:c:1286:TYR:OH	17:c:1902:IHP:O42	1.87	0.91
15:c:933:LYS:HG2	16:c:1901:K0W:PB1	2.11	0.90
6:F:215:TRP:CE2	6:F:227:VAL:CG2	2.54	0.90
15:c:960:TYR:CE2	15:c:1003:ASP:OD2	2.24	0.89
1:A:142:ARG:NH2	2:B:59:VAL:HG21	1.86	0.89
7:G:202:LEU:HD22	7:G:210:PHE:CZ	2.08	0.89
6:F:227:VAL:HG12	6:F:228:PRO:HD2	1.55	0.89
3:Q:122:ASN:ND2	4:R:128:ALA:HB3	1.88	0.87
15:c:300:ARG:NH1	15:c:1631:GLN:CB	2.38	0.87
6:F:215:TRP:CZ2	6:F:227:VAL:HG11	2.10	0.87
15:c:1147:VAL:HG11	15:c:1182:PRO:HG2	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c:1213:LYS:NZ	17:c:1902:IHP:O33	2.07	0.86
7:U:180:GLU:O	7:U:184:LYS:HG3	1.75	0.86
6:F:215:TRP:CG	6:F:227:VAL:CG2	2.58	0.85
15:c:1181:LEU:HD12	15:c:1182:PRO:CD	2.05	0.85
15:c:1112:ASN:HB2	15:c:1113:PRO:HD3	0.89	0.85
4:D:183:GLU:OE1	15:c:1751:ILE:C	2.18	0.84
15:c:933:LYS:CG	16:c:1901:K0W:PB1	2.66	0.83
6:F:215:TRP:CG	6:F:227:VAL:HG21	2.14	0.83
1:A:144:TYR:CD1	2:B:60:PHE:HZ	1.97	0.82
15:c:131:GLU:HG3	15:c:379:LEU:HD11	1.62	0.82
15:c:1181:LEU:CD1	15:c:1182:PRO:HD2	2.09	0.82
15:c:375:LYS:HE3	15:c:375:LYS:N	1.93	0.81
15:c:297:LEU:HD13	15:c:1631:GLN:HE21	1.44	0.81
6:F:215:TRP:HZ2	6:F:227:VAL:HG13	1.41	0.81
15:c:298:VAL:HG23	15:c:299:PRO:HD3	0.84	0.81
6:F:227:VAL:CG1	6:F:228:PRO:HD2	2.09	0.81
15:c:56:LYS:NZ	15:c:1113:PRO:HD2	1.96	0.81
15:c:267:ILE:HD12	15:c:370:ARG:HH12	1.47	0.80
15:c:1181:LEU:HD12	15:c:1182:PRO:HD3	1.63	0.80
1:A:145:LEU:HD12	1:A:157:TRP:CB	2.07	0.80
15:c:131:GLU:HG3	15:c:379:LEU:HD13	1.64	0.78
15:c:929:LEU:HD13	15:c:929:LEU:O	1.84	0.78
6:F:215:TRP:CD2	6:F:227:VAL:HG21	2.19	0.78
15:c:1749:ASP:C	15:c:1750:THR:HG22	2.07	0.77
15:c:281:THR:OG1	15:c:1672:ASN:HA	1.84	0.77
1:A:142:ARG:HH22	2:B:59:VAL:HG21	1.47	0.76
15:c:291:VAL:CG1	15:c:1671:TYR:CE2	2.69	0.76
7:G:202:LEU:CD2	7:G:206:LEU:HD23	2.14	0.76
4:D:183:GLU:OE1	15:c:1752:PRO:HA	1.85	0.75
6:F:244:LYS:HA	6:F:244:LYS:CE	2.13	0.75
15:c:300:ARG:HH12	15:c:1631:GLN:C	1.93	0.74
3:Q:122:ASN:ND2	4:R:128:ALA:CB	2.50	0.74
15:c:1181:LEU:HG	15:c:1182:PRO:HD2	1.69	0.74
15:c:972:LEU:HD23	15:c:990:PHE:CE1	2.22	0.74
6:F:220:THR:HG22	6:F:225:GLU:OE1	1.88	0.73
15:c:373:TYR:CE2	15:c:929:LEU:HD11	2.23	0.73
15:c:1216:LYS:HA	15:c:1351:ASN:HD21	1.52	0.73
15:c:379:LEU:HD12	15:c:379:LEU:H	1.53	0.73
7:G:217:VAL:O	7:G:230:LEU:HD23	1.88	0.73
15:c:298:VAL:CG2	15:c:299:PRO:CD	2.52	0.73
1:A:144:TYR:CD1	2:B:60:PHE:CZ	2.76	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c:130:LYS:HG2	15:c:378:TRP:HZ3	1.54	0.73
15:c:56:LYS:HZ2	15:c:1113:PRO:HD2	1.54	0.72
15:c:297:LEU:H	15:c:297:LEU:HD23	1.53	0.72
15:c:1673:LEU:C	15:c:1673:LEU:HD23	2.14	0.72
15:c:300:ARG:HH12	15:c:1631:GLN:CA	2.03	0.72
15:c:887:THR:O	15:c:891:PHE:HD2	1.70	0.72
15:c:30:LYS:HE2	15:c:129:LYS:HD3	1.70	0.72
15:c:914:ARG:NH1	15:c:942:ASP:OD1	2.22	0.72
6:F:244:LYS:HE2	6:F:244:LYS:CA	2.13	0.72
3:Q:122:ASN:HD21	4:R:128:ALA:HB3	1.53	0.72
15:c:34:TYR:CZ	15:c:933:LYS:HE2	2.25	0.70
15:c:208:GLN:OE1	15:c:250:GLN:NE2	2.23	0.70
3:Q:122:ASN:HD21	4:R:128:ALA:CB	2.04	0.70
15:c:1181:LEU:CG	15:c:1182:PRO:HD2	2.21	0.70
1:A:144:TYR:HD1	2:B:60:PHE:CZ	2.10	0.70
6:F:215:TRP:CH2	6:F:227:VAL:HG11	2.27	0.70
15:c:297:LEU:HD13	15:c:1631:GLN:HE22	1.54	0.69
1:A:92:LEU:HD13	1:A:112:ARG:HB3	1.74	0.69
2:B:58:GLU:O	2:B:62:SER:HB2	1.91	0.69
15:c:933:LYS:CD	16:c:1901:K0W:PB1	2.80	0.69
15:c:1271:LYS:HB2	15:c:1274:TRP:NE1	2.07	0.69
4:D:183:GLU:OE2	15:c:1751:ILE:O	2.11	0.69
6:F:215:TRP:CD2	6:F:227:VAL:CG2	2.76	0.69
15:c:759:PRO:HB2	15:c:934:GLN:HB3	1.75	0.69
15:c:297:LEU:HD12	15:c:300:ARG:HG2	1.75	0.68
15:c:933:LYS:NZ	16:c:1901:K0W:PB1	2.66	0.67
15:c:300:ARG:HH12	15:c:1631:GLN:CB	2.03	0.67
15:c:324:LYS:O	15:c:325:LEU:C	2.38	0.67
15:c:1181:LEU:HD12	15:c:1182:PRO:HD2	1.71	0.67
7:U:118:ILE:HG21	7:U:138:MET:HE1	1.77	0.67
8:V:44:CYS:HB2	8:V:99:VAL:HB	1.76	0.67
15:c:910:GLU:O	15:c:914:ARG:HG3	1.94	0.67
6:F:227:VAL:CG1	6:F:228:PRO:CD	2.72	0.66
15:c:156:LYS:NZ	17:c:1902:IHP:O25	2.26	0.66
15:c:208:GLN:HE22	15:c:251:TRP:HB3	1.59	0.66
3:C:138:PHE:CD1	11:K:107:ARG:NH2	2.63	0.66
7:U:189:TRP:O	7:U:190:THR:HG23	1.95	0.66
15:c:933:LYS:HZ3	16:c:1901:K0W:PB1	2.19	0.66
1:A:145:LEU:CD1	1:A:157:TRP:HB2	2.07	0.66
15:c:371:GLU:HG2	15:c:382:VAL:HG21	1.78	0.66
15:c:150:GLU:OE2	15:c:209:LYS:CE	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c:1050:VAL:HG22	15:c:1146:LEU:HB2	1.78	0.66
12:Z:145:LEU:HD22	12:Z:178:VAL:HB	1.78	0.65
15:c:297:LEU:CD1	15:c:1631:GLN:NE2	2.56	0.65
15:c:718:CYS:SG	15:c:819:ASN:ND2	2.69	0.65
15:c:1109:GLN:O	15:c:1111:LYS:HD2	1.96	0.65
6:F:215:TRP:CH2	6:F:227:VAL:CG1	2.75	0.65
15:c:390:ASP:OD1	15:c:428:ARG:NH1	2.29	0.65
3:C:138:PHE:CE2	11:K:107:ARG:NH2	2.63	0.65
10:X:183:ILE:HG12	10:X:188:ILE:HG12	1.79	0.65
15:c:865:ARG:NH2	15:c:903:PHE:O	2.29	0.65
15:c:218:LEU:O	15:c:261:ARG:NH1	2.30	0.65
15:c:1662:LEU:HD13	15:c:1693:LEU:HD12	1.79	0.65
15:c:1720:MET:HE2	15:c:1725:GLN:HE21	1.62	0.65
1:A:142:ARG:HH21	2:B:59:VAL:HG11	1.62	0.65
15:c:933:LYS:HD2	16:c:1901:KOW:PB1	2.36	0.64
1:A:211:ILE:HG12	1:A:220:LEU:HD21	1.78	0.64
15:c:1216:LYS:HZ1	17:c:1902:IHP:P2	2.21	0.64
15:c:297:LEU:HD23	15:c:297:LEU:N	2.12	0.64
12:L:148:LEU:HD23	12:L:178:VAL:HG12	1.80	0.63
1:O:142:ARG:NH1	1:O:143:PRO:O	2.31	0.63
15:c:300:ARG:NH1	15:c:1631:GLN:CA	2.61	0.63
15:c:34:TYR:OH	15:c:933:LYS:HE3	1.93	0.63
15:c:1673:LEU:HD21	15:c:1677:LEU:CD1	2.29	0.63
15:c:887:THR:HG22	15:c:891:PHE:HE2	1.63	0.63
14:N:41:ILE:HG12	14:N:76:VAL:HG22	1.80	0.63
2:B:48:GLU:HG2	2:B:201:MET:HE3	1.79	0.63
2:P:3:ARG:NH2	5:S:9:ASP:OD1	2.32	0.63
3:Q:208:LEU:HD22	3:Q:220:LEU:HD12	1.81	0.63
15:c:1041:ALA:HA	15:c:1052:THR:HG21	1.80	0.63
6:F:227:VAL:HG12	6:F:228:PRO:CD	2.28	0.63
15:c:669:LEU:HD11	15:c:708:LEU:HD21	1.81	0.63
15:c:1216:LYS:NZ	17:c:1902:IHP:O12	2.32	0.63
15:c:379:LEU:HD12	15:c:379:LEU:N	2.14	0.62
10:J:183:ILE:HG12	10:J:188:ILE:HG12	1.80	0.62
15:c:1706:ALA:HB2	15:c:1764:LEU:HG	1.82	0.62
15:c:926:GLU:HG3	15:c:928:ARG:HG2	1.80	0.62
3:C:63:CYS:HB3	3:C:88:ARG:NH2	2.15	0.62
5:E:5:GLN:HE21	6:F:9:LEU:HD11	1.63	0.62
1:A:129:PHE:HB3	1:A:131:VAL:HG12	1.81	0.62
12:L:145:LEU:HD22	12:L:178:VAL:HB	1.82	0.62
4:D:1:MET:HE2	15:c:1666:GLN:HG3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:136:TYR:HB2	2:P:148:TYR:HB2	1.81	0.62
15:c:208:GLN:HA	15:c:208:GLN:HE21	1.64	0.62
5:E:46:LEU:HD13	5:E:135:ALA:HB2	1.80	0.62
10:X:8:GLN:HE21	10:X:113:PRO:HG2	1.65	0.62
12:Z:194:ARG:NH1	12:Z:205:GLU:OE2	2.33	0.61
15:c:1432:CYS:O	15:c:1475:GLN:NE2	2.32	0.61
15:c:575:MET:HE3	15:c:622:VAL:HG23	1.83	0.61
15:c:1004:ILE:HG12	15:c:1004:ILE:O	2.00	0.61
1:A:155:PHE:CD1	2:B:61:PHE:HZ	2.19	0.61
5:S:203:GLN:O	5:S:239:ARG:NH1	2.34	0.61
15:c:339:SER:OG	15:c:1714:GLN:NE2	2.33	0.61
15:c:972:LEU:HD21	15:c:990:PHE:HE1	1.56	0.61
15:c:972:LEU:CG	15:c:1004:ILE:HD11	2.24	0.61
6:F:8:ASP:O	6:F:22:GLN:NE2	2.34	0.61
7:U:49:VAL:HG23	7:U:219:VAL:HG12	1.80	0.61
15:c:56:LYS:NZ	15:c:1113:PRO:CD	2.64	0.61
15:c:478:PRO:HB2	15:c:536:LEU:HD11	1.82	0.61
15:c:972:LEU:CD2	15:c:990:PHE:CZ	2.71	0.61
1:A:83:ARG:NH2	7:G:158:GLY:O	2.34	0.60
15:c:367:ARG:NH1	15:c:371:GLU:OE2	2.34	0.60
7:U:188:ASP:O	7:U:193:GLN:HB3	2.00	0.60
7:U:138:MET:HE2	7:U:154:CYS:SG	2.40	0.60
15:c:61:ARG:HH11	15:c:1117:GLN:HB2	1.67	0.60
15:c:474:PHE:CE1	15:c:476:GLU:HG3	2.36	0.60
15:c:1326:LEU:O	15:c:1341:ARG:NH2	2.35	0.60
7:G:231:THR:O	7:G:235:ILE:HD12	2.02	0.60
9:I:57:THR:O	10:J:85:ARG:NH2	2.34	0.60
2:P:119:GLN:NE2	3:Q:79:ASP:OD1	2.35	0.60
9:W:57:THR:O	10:X:85:ARG:NH2	2.35	0.60
10:X:102:LEU:HB2	10:X:118:MET:HB3	1.83	0.60
12:Z:145:LEU:HD21	12:Z:182:ALA:HB2	1.82	0.60
15:c:324:LYS:N	15:c:324:LYS:HD2	2.16	0.60
6:F:2:SER:HB3	15:c:447:LEU:HA	1.84	0.60
5:S:146:GLN:HB3	5:S:154:PHE:HB2	1.84	0.60
1:A:158:LYS:HB2	2:B:55:LEU:HB2	1.82	0.59
14:N:174:ILE:HB	14:N:189:LEU:HB2	1.84	0.59
8:V:141:LYS:NZ	8:V:157:GLU:OE2	2.33	0.59
15:c:926:GLU:CG	15:c:928:ARG:HG2	2.33	0.59
9:W:188:ILE:HB	9:W:195:THR:HB	1.83	0.59
15:c:1760:HIS:O	15:c:1764:LEU:HB2	2.03	0.59
15:c:208:GLN:HE22	15:c:251:TRP:CA	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:208:LEU:HD12	3:C:225:ILE:HG12	1.84	0.59
15:c:61:ARG:HG2	15:c:1120:LEU:HD11	1.85	0.59
15:c:474:PHE:CE2	15:c:477:GLY:HA2	2.37	0.59
11:K:59:LEU:HD22	11:K:83:LEU:HB2	1.85	0.59
15:c:1271:LYS:HG3	15:c:1274:TRP:HE1	1.68	0.59
3:C:63:CYS:SG	3:C:84:ILE:HD13	2.42	0.59
4:D:53:ARG:NH1	15:c:1615:TYR:OH	2.36	0.59
14:b:179:ILE:HG12	14:b:184:VAL:HG22	1.84	0.59
4:D:100:TRP:O	11:K:57:ARG:NH2	2.35	0.58
7:G:54:LYS:NZ	7:G:66:VAL:O	2.35	0.58
15:c:1592:ALA:O	15:c:1638:GLN:NE2	2.36	0.58
15:c:1181:LEU:CD1	15:c:1182:PRO:CD	2.74	0.58
1:O:81:ASP:OD1	7:U:123:GLN:NE2	2.37	0.58
12:Z:148:LEU:HD23	12:Z:178:VAL:HG12	1.85	0.58
10:J:168:GLN:NE2	10:J:175:LEU:O	2.35	0.58
15:c:324:LYS:C	15:c:326:VAL:H	2.05	0.58
15:c:929:LEU:HD13	15:c:929:LEU:C	2.27	0.58
15:c:150:GLU:OE2	15:c:209:LYS:HE2	2.03	0.58
15:c:1402:TRP:HH2	15:c:1443:LEU:HD22	1.66	0.58
15:c:1663:THR:HG22	15:c:1704:MET:HE2	1.86	0.58
1:A:155:PHE:HD1	2:B:61:PHE:HZ	1.51	0.58
5:S:50:LYS:HB3	5:S:59:HIS:HB3	1.85	0.58
6:F:67:PHE:HB2	6:F:75:MET:HB3	1.85	0.58
11:K:157:ARG:HG3	11:K:176:LEU:HD22	1.85	0.58
15:c:968:ILE:O	15:c:972:LEU:HG	2.04	0.58
1:A:99:VAL:HG13	9:I:92:ASN:HD22	1.68	0.58
7:G:37:LEU:HA	7:G:53:GLN:HE21	1.68	0.58
4:R:41:GLN:NE2	4:R:151:PRO:O	2.36	0.58
5:S:45:VAL:HG21	5:S:188:VAL:HG22	1.85	0.58
15:c:933:LYS:NZ	16:c:1901:KOW:O71	2.36	0.58
4:D:183:GLU:OE1	15:c:1752:PRO:CA	2.52	0.58
15:c:298:VAL:N	15:c:299:PRO:CD	2.66	0.58
15:c:1271:LYS:CG	15:c:1274:TRP:HE1	2.17	0.58
9:I:14:LYS:HE3	9:I:120:ILE:HG12	1.86	0.58
6:F:213:LEU:O	6:F:226:ILE:O	2.22	0.57
8:H:59:ILE:HD12	8:H:82:MET:HB3	1.85	0.57
1:O:99:VAL:HG13	9:W:92:ASN:HD22	1.69	0.57
10:J:8:GLN:HE21	10:J:113:PRO:HG2	1.67	0.57
15:c:297:LEU:HB2	15:c:300:ARG:HB3	1.85	0.57
15:c:375:LYS:H	15:c:375:LYS:CE	2.02	0.57
15:c:1468:LEU:HD11	15:c:1486:LEU:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:143:ASN:OD1	14:b:106:GLN:NE2	2.38	0.57
15:c:767:ILE:HG12	15:c:941:ILE:HG12	1.86	0.57
15:c:1216:LYS:NZ	17:c:1902:IHP:O22	2.38	0.57
15:c:876:LEU:HD11	15:c:974:LEU:HD21	1.86	0.57
2:P:46:ALA:HB1	2:P:197:LEU:HD11	1.87	0.57
9:W:14:LYS:HE3	9:W:120:ILE:HG12	1.87	0.57
12:Z:10:GLY:HA3	12:Z:42:LYS:HE2	1.85	0.57
15:c:1323:ILE:HD13	15:c:1363:HIS:HB3	1.87	0.57
7:G:202:LEU:HD23	7:G:202:LEU:O	2.05	0.57
8:H:100:LEU:HB3	8:H:111:TYR:HB2	1.87	0.57
13:a:96:MET:HE3	13:a:127:MET:HA	1.86	0.57
15:c:102:LEU:HD22	15:c:122:LEU:HD22	1.87	0.57
15:c:912:ASP:O	15:c:916:LYS:HG3	2.05	0.57
2:P:68:LEU:HD11	2:P:74:CYS:HB3	1.86	0.57
10:X:35:MET:HG2	10:X:45:LEU:HG	1.86	0.57
7:G:190:THR:HG23	7:G:193:GLN:HB2	1.86	0.57
15:c:267:ILE:HG21	15:c:367:ARG:NH2	2.20	0.57
4:R:97:GLN:HB3	11:Y:61:ARG:HG2	1.86	0.56
12:Z:198:VAL:HG22	12:Z:203:ILE:HG12	1.87	0.56
15:c:1192:ASN:HB2	15:c:1195:HIS:HB2	1.87	0.56
15:c:1448:LEU:HD12	15:c:1468:LEU:HD21	1.86	0.56
7:G:122:SER:HA	7:G:125:TYR:HD2	1.69	0.56
15:c:108:ILE:HB	15:c:111:LEU:HB2	1.87	0.56
15:c:972:LEU:HD11	15:c:1004:ILE:CG1	2.25	0.56
15:c:1673:LEU:CD2	15:c:1677:LEU:HD12	2.35	0.56
4:D:65:GLU:OE1	11:K:71:LYS:NZ	2.38	0.56
2:P:2:SER:OG	3:Q:5:ARG:NH2	2.35	0.56
7:U:118:ILE:HG21	7:U:138:MET:CE	2.35	0.56
15:c:932:LYS:HB2	15:c:934:GLN:NE2	2.19	0.56
8:H:63:LEU:HD11	8:H:79:ALA:HB2	1.86	0.56
3:Q:208:LEU:CD2	3:Q:220:LEU:HD12	2.34	0.56
15:c:157:THR:OG1	15:c:163:ASN:ND2	2.39	0.56
6:F:197:ILE:HG21	6:F:211:LEU:HD13	1.87	0.56
15:c:478:PRO:O	15:c:481:MET:N	2.31	0.56
15:c:876:LEU:HD13	15:c:893:ILE:HG21	1.87	0.56
10:X:38:MET:O	10:X:65:GLN:NE2	2.39	0.56
15:c:373:TYR:HE2	15:c:929:LEU:HD11	1.69	0.56
7:U:137:CYS:SG	7:U:153:LYS:HD2	2.46	0.56
15:c:297:LEU:HB3	15:c:1631:GLN:HE22	1.69	0.56
12:Z:45:LYS:HE3	12:Z:203:ILE:HD12	1.88	0.56
15:c:334:PHE:O	15:c:338:THR:OG1	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c:1181:LEU:HB3	15:c:1186:ILE:HD11	1.86	0.56
15:c:1224:ILE:HG12	15:c:1285:VAL:HG22	1.87	0.56
5:E:215:VAL:HB	5:E:221:PHE:HD1	1.70	0.56
3:Q:80:ALA:HA	3:Q:129:ILE:HD13	1.88	0.56
5:S:117:GLN:NE2	6:T:83:ASP:OD1	2.38	0.56
9:W:73:TYR:O	9:W:77:GLU:CB	2.54	0.56
15:c:1667:THR:HG23	15:c:1671:TYR:CE2	2.41	0.56
15:c:267:ILE:CD1	15:c:370:ARG:HH12	2.15	0.55
15:c:379:LEU:CD1	15:c:379:LEU:H	2.17	0.55
15:c:529:LEU:HD13	15:c:534:ARG:HB2	1.88	0.55
3:C:99:GLU:OE1	11:K:120:ARG:NH2	2.39	0.55
5:E:3:ARG:NH2	15:c:409:PHE:O	2.38	0.55
12:L:204:ARG:NH1	12:L:206:GLU:OE2	2.38	0.55
15:c:596:GLN:HE22	15:c:738:SER:H	1.54	0.55
1:A:154:TYR:OH	2:B:84:ASN:ND2	2.38	0.55
2:B:43:VAL:HG23	2:B:216:LEU:HB3	1.89	0.55
12:L:38:ARG:NH2	8:V:164:PHE:O	2.40	0.55
15:c:56:LYS:HZ1	15:c:1113:PRO:CD	2.19	0.55
15:c:208:GLN:HE21	15:c:251:TRP:HB3	1.67	0.55
5:E:101:ARG:HH22	5:E:104:PRO:HD3	1.71	0.55
3:Q:208:LEU:HD22	3:Q:220:LEU:CD1	2.37	0.55
15:c:1749:ASP:O	15:c:1750:THR:CB	2.52	0.55
15:c:1357:LEU:HA	15:c:1360:LEU:HB2	1.89	0.55
11:K:197:GLU:OE2	9:W:200:LYS:NZ	2.40	0.55
11:Y:27:ALA:O	12:Z:136:LYS:NZ	2.39	0.55
15:c:1648:GLN:OE1	15:c:1651:ARG:NH2	2.40	0.55
1:A:175:LYS:NZ	15:c:885:ASP:OD1	2.37	0.55
4:D:167:ALA:HB3	5:E:56:LEU:HD13	1.89	0.55
5:E:39:LYS:HE3	5:E:180:MET:HE1	1.88	0.55
4:R:13:ASN:HB3	5:S:126:ARG:HB3	1.88	0.55
4:R:52:LYS:NZ	4:R:64:ILE:O	2.39	0.55
12:Z:125:ASP:OD1	12:Z:129:SER:N	2.36	0.55
15:c:373:TYR:CD2	15:c:929:LEU:CD1	2.90	0.55
6:F:23:VAL:HG12	6:F:27:MET:HE2	1.88	0.55
13:M:96:MET:HE3	13:M:127:MET:HA	1.87	0.55
5:E:47:VAL:HG12	5:E:195:LEU:HD22	1.88	0.55
15:c:482:LEU:HD11	15:c:542:GLU:HB3	1.89	0.55
15:c:788:LEU:HD11	15:c:868:ILE:HD11	1.89	0.55
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.89	0.54
15:c:208:GLN:HE22	15:c:251:TRP:CB	2.19	0.54
15:c:491:GLY:HA2	15:c:499:LYS:HE3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:95:SER:OG	5:S:101:ARG:NH2	2.41	0.54
7:G:49:VAL:HG12	7:G:219:VAL:HG12	1.88	0.54
3:Q:116:GLN:NE2	4:R:84:ASP:OD1	2.37	0.54
6:T:167:LYS:NZ	6:T:206:ASP:OD2	2.39	0.54
15:c:268:GLY:HA3	15:c:383:PRO:HG2	1.89	0.54
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.88	0.54
9:I:10[A]:VAL:HG23	9:I:53:ALA:HB2	1.88	0.54
15:c:1452:LEU:HD22	15:c:1461:ASP:HB3	1.89	0.54
7:U:180:GLU:HB3	7:U:184:LYS:HE2	1.89	0.54
11:Y:158:ARG:HE	11:Y:162:GLN:HE21	1.55	0.54
2:B:204:SER:HB2	15:c:1067:LEU:HD12	1.89	0.54
6:T:28:LYS:HA	6:T:31:GLU:HG2	1.89	0.54
15:c:635:VAL:HG12	15:c:686:VAL:HG21	1.89	0.54
9:I:6:ASN:HA	9:I:28:GLY:O	2.08	0.54
7:U:196:GLU:HA	7:U:199:ILE:HG22	1.90	0.54
13:a:67:LEU:HD11	13:a:88:ILE:HD12	1.88	0.54
14:b:167:ASP:HB3	14:b:170:SER:HB2	1.90	0.54
3:C:90:GLU:HG3	3:C:110:TYR:CZ	2.43	0.53
5:E:72:ILE:HG21	5:E:88:MET:HE1	1.91	0.53
2:B:171:ALA:O	2:B:175:LEU:HB2	2.08	0.53
2:P:155:ASN:OD1	3:Q:77:THR:OG1	2.26	0.53
4:D:51:GLU:OE2	4:D:53:ARG:NH2	2.41	0.53
6:F:2:SER:O	15:c:499:LYS:NZ	2.41	0.53
6:F:141:SER:OG	6:F:144:ASP:OD1	2.25	0.53
1:O:73:LEU:HD22	1:O:135:ILE:HG12	1.90	0.53
15:c:78:LYS:NZ	15:c:847:GLU:O	2.30	0.53
15:c:324:LYS:C	15:c:326:VAL:N	2.50	0.53
15:c:373:TYR:CE2	15:c:929:LEU:CD1	2.90	0.53
8:V:63:LEU:HD11	8:V:79:ALA:HB2	1.90	0.53
15:c:887:THR:HG22	15:c:891:PHE:CE2	2.42	0.53
15:c:1443:LEU:O	15:c:1447:LEU:HB3	2.08	0.53
7:U:206:LEU:HD23	7:U:208:ILE:HD12	1.91	0.53
11:Y:7:LYS:HG2	11:Y:12:VAL:HG22	1.90	0.53
13:a:86:ARG:NH1	13:a:133:GLU:OE2	2.42	0.53
15:c:188:ALA:HA	15:c:191:GLU:HG2	1.89	0.53
6:T:116:ALA:HB2	6:T:151:ILE:HG12	1.90	0.53
15:c:276:VAL:HG21	15:c:326:VAL:HG22	1.91	0.53
15:c:1216:LYS:NZ	17:c:1902:IHP:P2	2.82	0.53
15:c:1721:ASP:HB3	15:c:1723:PRO:HD2	1.91	0.53
15:c:286:SER:HB2	15:c:306:TYR:HB2	1.89	0.53
15:c:669:LEU:HD22	15:c:673:LEU:HD23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:141:ILE:HG22	7:G:151:VAL:HG22	1.90	0.53
6:T:108:LEU:HD11	6:T:137:LEU:HB3	1.90	0.53
8:V:213:THR:HG1	9:W:198:THR:HG1	1.53	0.53
15:c:478:PRO:O	15:c:479:THR:C	2.52	0.53
15:c:1056:ILE:HD11	15:c:1079:LEU:HD13	1.91	0.53
4:D:117:SER:OG	4:D:160:GLY:O	2.27	0.52
7:G:231:THR:OG1	7:G:234:GLU:HG3	2.09	0.52
8:H:177:VAL:HB	8:H:184:ASP:HB2	1.91	0.52
15:c:291:VAL:HG12	15:c:1671:TYR:CE2	2.44	0.52
15:c:1147:VAL:CG1	15:c:1182:PRO:HG2	2.36	0.52
3:C:101:PRO:HD2	3:C:138:PHE:HD1	1.73	0.52
5:E:81:ALA:HB2	5:E:130:VAL:HG21	1.91	0.52
8:H:18:THR:HB	8:H:30:ASN:HA	1.91	0.52
2:P:49:ARG:HE	2:P:212:GLU:HG3	1.74	0.52
15:c:267:ILE:HG22	15:c:267:ILE:O	2.09	0.52
15:c:863:ASN:HD22	15:c:864:HIS:N	2.07	0.52
7:G:153:LYS:NZ	7:G:167:ALA:O	2.41	0.52
15:c:512:THR:HG23	15:c:592:THR:HG23	1.92	0.52
15:c:1751:ILE:O	15:c:1751:ILE:HG13	2.07	0.52
4:D:12:VAL:HA	4:D:23:GLN:HG2	1.91	0.52
4:D:203:LYS:HB2	4:D:210:LEU:HD22	1.91	0.52
6:F:34:SER:OG	6:F:65:ARG:NH1	2.35	0.52
15:c:208:GLN:NE2	15:c:208:GLN:HA	2.23	0.52
3:C:36:ARG:NH2	4:D:60:GLU:OE2	2.41	0.52
7:G:221:THR:OG1	7:G:224:ASN:OD1	2.27	0.52
1:O:8:SER:OG	1:O:122:GLN:O	2.26	0.52
4:D:146:VAL:HG11	4:D:222:PRO:HA	1.92	0.52
4:D:207:GLU:OE2	15:c:1655:TRP:N	2.43	0.52
15:c:130:LYS:HG2	15:c:378:TRP:CZ3	2.41	0.52
15:c:949:GLU:O	15:c:953:LEU:HB2	2.10	0.52
15:c:1786:MET:HE1	15:c:1831:VAL:HG21	1.92	0.52
6:F:215:TRP:CE2	6:F:227:VAL:HG11	2.36	0.52
12:L:125:ASP:OD1	12:L:129:SER:N	2.40	0.52
15:c:908:LYS:HA	15:c:953:LEU:HD11	1.90	0.52
6:T:66:LEU:HD12	6:T:212:GLU:HG2	1.92	0.52
5:E:117:GLN:NE2	6:F:83:ASP:OD1	2.43	0.52
7:U:78:CYS:HB3	7:U:140:LEU:HD23	1.90	0.52
1:A:144:TYR:CE1	2:B:60:PHE:CZ	2.98	0.52
14:N:179:ILE:HG12	14:N:184:VAL:HG22	1.92	0.52
10:X:4:LEU:HD22	10:X:45:LEU:HB3	1.91	0.52
15:c:31:GLU:HG2	15:c:89:LYS:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c:1077:ASP:O	15:c:1081:GLU:HB2	2.10	0.51
8:H:164:PHE:O	12:Z:38:ARG:NH2	2.36	0.51
11:K:138:VAL:HG21	11:K:162:GLN:HG3	1.92	0.51
3:Q:35:VAL:HG11	3:Q:190:LEU:HD23	1.92	0.51
5:S:7:ASP:O	5:S:21:GLN:NE2	2.42	0.51
6:F:65:ARG:HH21	6:F:78:ALA:HA	1.74	0.51
7:G:153:LYS:HB3	7:G:163:PHE:HE2	1.74	0.51
9:W:29:ILE:HG12	9:W:34:VAL:HG21	1.91	0.51
15:c:1604:PHE:HD1	15:c:1660:THR:HG23	1.75	0.51
15:c:851:LEU:HD23	15:c:951:ARG:HG3	1.93	0.51
4:D:183:GLU:CD	15:c:1752:PRO:HA	2.36	0.51
8:H:143:ARG:NH1	8:H:150:GLU:OE1	2.43	0.51
6:T:197:ILE:HG21	6:T:211:LEU:HD13	1.93	0.51
15:c:286:SER:HB2	15:c:306:TYR:CB	2.41	0.51
15:c:304:ASN:O	15:c:305:ALA:HB3	2.11	0.51
15:c:858:ASP:OD2	15:c:861:ARG:NH1	2.43	0.51
15:c:918:PHE:CE1	15:c:943:ARG:HB2	2.45	0.51
15:c:1112:ASN:H	15:c:1113:PRO:CD	2.23	0.51
2:B:58:GLU:O	2:B:58:GLU:HG2	2.11	0.51
8:H:44:CYS:HB2	8:H:99:VAL:HB	1.93	0.51
3:C:22:ALA:HB1	3:C:128:GLY:HA2	1.93	0.51
13:a:25:ASP:OD1	13:a:41:ARG:NH2	2.41	0.51
2:B:86:LEU:HD13	2:B:134:LEU:HD11	1.93	0.51
11:Y:38:ASN:OD1	11:Y:41:LEU:N	2.44	0.51
15:c:297:LEU:HB3	15:c:1631:GLN:NE2	2.26	0.51
3:C:23:GLN:NE2	3:C:148:ASP:OD2	2.43	0.51
9:W:73:TYR:O	9:W:77:GLU:HB2	2.10	0.51
14:b:190:LEU:H	14:b:193:GLN:HB2	1.76	0.50
15:c:933:LYS:CD	16:c:1901:K0W:O71	2.56	0.50
15:c:1816:ASN:ND2	15:c:1819:GLU:OE2	2.43	0.50
3:C:60:ARG:O	3:C:61:LYS:HB2	2.10	0.50
3:C:101:PRO:HD2	3:C:138:PHE:CD1	2.46	0.50
5:E:98:VAL:HA	13:M:94:ARG:HG3	1.93	0.50
15:c:1462:ALA:HB2	15:c:1501:VAL:HG22	1.92	0.50
4:D:18:GLU:O	5:E:31:GLN:NE2	2.45	0.50
4:D:41:GLN:NE2	4:D:151:PRO:O	2.43	0.50
15:c:818:HIS:O	15:c:822:LEU:HB2	2.11	0.50
1:A:81:ASP:OD1	7:G:123:GLN:NE2	2.43	0.50
10:J:35:MET:HG2	10:J:45:LEU:HG	1.94	0.50
15:c:1112:ASN:N	15:c:1113:PRO:CD	2.74	0.50
15:c:1486:LEU:HD22	15:c:1512:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:LEU:HA	2:B:43:VAL:HG12	1.94	0.50
4:R:91:LYS:HG2	4:R:119:LEU:HD11	1.93	0.50
15:c:496:ASP:HB2	15:c:499:LYS:HG2	1.94	0.50
15:c:1350:ARG:O	15:c:1350:ARG:HG2	2.12	0.50
1:A:142:ARG:NH2	2:B:59:VAL:HG11	2.26	0.50
9:W:29:ILE:HG12	9:W:34:VAL:CG2	2.42	0.50
3:C:173:GLU:HG2	4:D:57:PRO:HG2	1.94	0.50
2:P:63:GLU:HG2	2:P:64:LYS:HG3	1.93	0.50
3:Q:208:LEU:CD2	3:Q:220:LEU:CD1	2.89	0.50
15:c:297:LEU:N	15:c:297:LEU:CD2	2.75	0.50
15:c:1435:ARG:HH22	17:c:1902:IHP:P4	2.34	0.50
1:A:144:TYR:CE1	2:B:60:PHE:HZ	2.28	0.50
6:F:238:TYR:O	6:F:242:SER:HB3	2.12	0.50
14:N:3:ILE:HB	14:N:44:CYS:HB3	1.92	0.50
1:A:54:ILE:HG22	7:G:180:GLU:HG3	1.93	0.49
7:U:11:ARG:HG2	7:U:23:TYR:HD2	1.76	0.49
8:V:41:ILE:HG12	8:V:76:VAL:HG22	1.94	0.49
15:c:1176:ARG:HG3	15:c:1178:ASP:H	1.77	0.49
15:c:1662:LEU:HD21	15:c:1705:ALA:HB2	1.94	0.49
6:F:198:TYR:OH	6:F:236:GLU:OE1	2.18	0.49
6:F:228:PRO:HG2	6:F:231:ILE:HD12	1.93	0.49
13:M:25:ASP:OD1	13:M:41:ARG:NH2	2.43	0.49
2:P:158:GLY:O	3:Q:54:GLN:NE2	2.45	0.49
4:R:126:GLU:HG3	5:S:123:TYR:O	2.11	0.49
15:c:936:ILE:HD11	15:c:939:LEU:HD23	1.92	0.49
15:c:1154:VAL:HG21	15:c:1168:ILE:HG13	1.94	0.49
3:C:42:VAL:HG22	3:C:210:VAL:HG12	1.94	0.49
3:C:96:LEU:HB2	10:J:62:LYS:HG3	1.93	0.49
13:M:9:THR:O	13:M:41:ARG:NH1	2.42	0.49
15:c:547:VAL:HG23	15:c:548:LEU:HD12	1.94	0.49
15:c:1803:LYS:HG2	15:c:1837:VAL:HA	1.94	0.49
12:L:96:LEU:HD11	12:L:108:ASN:HD22	1.77	0.49
15:c:1082:LYS:HG3	15:c:1085:ARG:HH21	1.78	0.49
7:G:189:TRP:O	7:G:190:THR:HG22	1.80	0.49
14:N:191:GLY:O	14:N:196:LYS:NZ	2.46	0.49
14:b:19:ARG:NH1	14:b:168:GLY:O	2.43	0.49
3:Q:89:VAL:HG22	10:X:66:LEU:HD21	1.94	0.49
10:J:144:ASP:OD2	11:Y:166:ARG:NE	2.42	0.49
2:P:174:MET:HA	2:P:177:GLN:HG2	1.95	0.49
15:c:1009:LEU:HD21	15:c:1052:THR:HA	1.95	0.49
15:c:1406:CYS:HA	15:c:1446:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c:1669:VAL:O	15:c:1673:LEU:HA	2.13	0.49
3:C:138:PHE:CE2	11:K:107:ARG:NE	2.81	0.49
6:F:238:TYR:O	6:F:242:SER:CB	2.60	0.49
8:V:100:LEU:HB3	8:V:111:TYR:HB2	1.93	0.49
9:W:141:CYS:HB3	9:W:177:ASP:HB2	1.95	0.49
2:B:52:ILE:HD12	2:B:53:HIS:HB2	1.94	0.49
2:B:190:LEU:HD11	2:B:213:ILE:HG21	1.95	0.49
15:c:1183:LEU:HD11	15:c:1308:ILE:HD11	1.94	0.49
1:A:48:GLU:O	1:A:63:LYS:NZ	2.45	0.49
1:A:203:THR:HG23	1:A:205:ASP:H	1.78	0.49
10:J:85:ARG:HG3	10:J:124:LEU:HB2	1.94	0.49
6:T:17:ASP:O	7:U:34:GLN:NE2	2.45	0.49
12:Z:99:ARG:HH21	12:Z:102:PHE:HD2	1.61	0.49
15:c:124:ILE:HG13	15:c:176:LEU:HD23	1.95	0.49
15:c:1667:THR:HG23	15:c:1671:TYR:HE2	1.78	0.49
4:D:67:ILE:HB	4:D:228:MET:HE1	1.94	0.48
6:F:206:ASP:OD1	6:F:206:ASP:N	2.45	0.48
4:R:128:ALA:CA	4:R:132:ALA:HB3	2.43	0.48
8:V:51:ASP:HB3	8:V:94:ILE:HG23	1.93	0.48
15:c:1138:ASP:HA	15:c:1141:ARG:HB2	1.93	0.48
1:A:43:VAL:HG23	1:A:143:PRO:HB2	1.95	0.48
1:A:221:THR:HG23	1:A:224:GLU:H	1.78	0.48
7:G:217:VAL:C	7:G:230:LEU:HD23	2.38	0.48
10:J:25:ILE:HG13	10:J:26:VAL:HG13	1.95	0.48
3:Q:121:SER:HB2	3:Q:124:ARG:HD2	1.94	0.48
8:V:209:THR:HG21	9:W:167:SER:HB3	1.96	0.48
5:E:33:SER:H	15:c:1843:ALA:HB2	1.79	0.48
9:I:16[B]:LYS:HB2	9:I:156:ASN:HA	1.95	0.48
14:N:44:CYS:HB2	14:N:99:ILE:HB	1.96	0.48
3:Q:160:ALA:O	3:Q:169:ARG:NH2	2.46	0.48
5:S:72:ILE:HG22	5:S:134:ILE:HG12	1.94	0.48
12:Z:166:LEU:HD12	12:Z:170:ARG:HE	1.77	0.48
12:L:49:LYS:NZ	12:L:115:GLU:OE2	2.46	0.48
15:c:929:LEU:C	15:c:929:LEU:CD1	2.86	0.48
1:A:142:ARG:HH21	2:B:59:VAL:HG21	1.76	0.48
6:F:239:ALA:HA	6:F:242:SER:OG	2.14	0.48
13:M:54:SER:HB2	13:M:109:THR:HB	1.94	0.48
4:R:146:VAL:HG11	4:R:222:PRO:HA	1.95	0.48
14:b:44:CYS:HB2	14:b:99:ILE:HB	1.96	0.48
15:c:26:PHE:HB3	15:c:1112:ASN:HB3	1.94	0.48
15:c:1737:PRO:HG3	15:c:1755:GLU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:GLN:HE21	3:C:82:ILE:HD12	1.79	0.48
4:D:105:GLU:OE2	12:L:75:TYR:OH	2.23	0.48
10:J:77:PRO:HD2	10:J:108:ASP:HB2	1.95	0.48
15:c:1182:PRO:O	15:c:1186:ILE:HG12	2.14	0.48
2:B:31:ALA:HB3	2:B:50:ARG:HH21	1.77	0.48
4:D:41:GLN:HB3	4:D:166:ASP:HA	1.96	0.48
13:a:111:VAL:HG13	13:a:137:LEU:HD12	1.94	0.48
15:c:112:GLU:OE2	15:c:1044:HIS:NE2	2.46	0.48
11:K:44:THR:HG21	11:K:100:MET:HE3	1.96	0.48
4:R:128:ALA:HB2	4:R:132:ALA:HB3	1.88	0.48
7:U:141:ILE:HD12	7:U:220:VAL:HG22	1.96	0.48
9:W:29:ILE:HD11	10:X:117:TYR:HE2	1.78	0.48
15:c:1380:ALA:HB1	15:c:1427:CYS:HB2	1.96	0.48
4:R:167:ALA:HB3	5:S:56:LEU:HD13	1.96	0.48
1:A:144:TYR:HB3	1:A:146:PHE:CE2	2.48	0.48
15:c:1181:LEU:CG	15:c:1182:PRO:CD	2.91	0.48
15:c:1269:VAL:HG12	15:c:1478:ARG:HH22	1.79	0.48
15:c:1608:PRO:HD3	15:c:1619:LYS:HB3	1.94	0.48
2:B:63:GLU:O	2:B:64:LYS:HD2	2.14	0.47
6:F:227:VAL:HG13	6:F:228:PRO:HD2	1.93	0.47
2:P:161:ALA:HB3	3:Q:53:LEU:HD22	1.95	0.47
1:A:220:LEU:N	1:A:220:LEU:HD22	2.28	0.47
4:D:41:GLN:HA	4:D:46:VAL:HG12	1.95	0.47
10:J:140:LEU:HD23	10:J:143:LEU:HD12	1.96	0.47
5:S:46:LEU:HD13	5:S:73[B]:SER:HB3	1.97	0.47
8:V:214:GLU:HG3	9:W:197:ARG:HG2	1.96	0.47
9:W:202:ARG:NH2	9:W:204:ASP:OD2	2.45	0.47
4:R:174:SER:O	4:R:178:GLN:HB2	2.14	0.47
7:U:103:TYR:O	8:V:81:ARG:NH1	2.47	0.47
8:V:59:ILE:HD12	8:V:82:MET:HB3	1.95	0.47
15:c:1821:LYS:HB2	15:c:1829:LEU:HD21	1.95	0.47
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.96	0.47
11:K:141:ARG:NH1	10:X:166:GLU:OE1	2.47	0.47
3:Q:40:ILE:HD11	3:Q:210:VAL:HB	1.96	0.47
3:C:51:ALA:HB3	3:C:54:GLN:HB2	1.95	0.47
8:H:51:ASP:HB3	8:H:94:ILE:HG23	1.95	0.47
15:c:949:GLU:HA	15:c:952:THR:HG22	1.97	0.47
15:c:1702:ARG:HB3	15:c:1764:LEU:HD21	1.97	0.47
7:G:145:GLU:OE1	8:H:75:ARG:NH2	2.46	0.47
6:T:34:SER:OG	6:T:65:ARG:NH1	2.47	0.47
15:c:299:PRO:HB2	15:c:1628:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c:579:GLU:HA	15:c:582:VAL:HG22	1.96	0.47
8:H:50:ALA:HB2	9:I:128:CYS:HB2	1.97	0.47
10:J:4:LEU:HD22	10:J:45:LEU:HD23	1.97	0.47
10:J:118:MET:HE2	10:J:124:LEU:HD13	1.96	0.47
12:L:159:GLN:HG3	8:V:210:ALA:HB2	1.97	0.47
14:N:201:THR:HG23	13:a:38:ASN:HD21	1.79	0.47
2:P:143:TYR:HB2	2:P:146:GLN:NE2	2.30	0.47
15:c:238:LEU:HG	15:c:255:LEU:HD11	1.97	0.47
15:c:933:LYS:CG	16:c:1901:KOW:O51	2.63	0.47
15:c:1541:LEU:HD11	15:c:1574:LEU:HB2	1.96	0.47
2:P:11:ILE:HG22	3:Q:7:ILE:HG23	1.96	0.47
15:c:478:PRO:O	15:c:480:HIS:N	2.47	0.47
6:F:41:CYS:HB3	6:F:189:ILE:HG13	1.97	0.47
3:Q:50:VAL:HG21	3:Q:205:ASN:HD22	1.79	0.47
5:S:47:VAL:HG12	5:S:195:LEU:HD22	1.96	0.47
15:c:1502:ARG:HH12	15:c:1575:LYS:HD3	1.79	0.47
15:c:1806:LEU:HB2	15:c:1837:VAL:HG11	1.97	0.47
13:a:92:LEU:HD22	13:a:110:MET:HE1	1.97	0.47
15:c:1346:LYS:NZ	17:c:1902:IHP:O43	2.41	0.47
7:G:153:LYS:HB3	7:G:163:PHE:CE2	2.50	0.46
11:K:51:ASP:OD1	12:L:97:TYR:OH	2.28	0.46
14:b:3:ILE:HB	14:b:44:CYS:HB3	1.96	0.46
15:c:1181:LEU:HG	15:c:1182:PRO:CD	2.44	0.46
15:c:1181:LEU:HB3	15:c:1186:ILE:CD1	2.45	0.46
11:K:7:LYS:HG2	11:K:12:VAL:HB	1.98	0.46
3:Q:69:VAL:HG22	3:Q:104:VAL:HG22	1.96	0.46
15:c:517:VAL:HG22	15:c:598:SER:HB3	1.98	0.46
1:A:55:LEU:HD22	7:G:165:ALA:HB3	1.97	0.46
3:C:92:GLN:HB3	10:J:62:LYS:HB3	1.96	0.46
6:F:220:THR:CG2	6:F:225:GLU:OE1	2.61	0.46
14:N:30:VAL:HG11	13:a:211:ILE:HG13	1.98	0.46
2:P:3:ARG:NH1	4:R:125:GLU:OE2	2.48	0.46
1:A:220:LEU:N	1:A:220:LEU:CD2	2.78	0.46
5:E:45:VAL:HG22	5:E:214:ILE:HG12	1.97	0.46
8:H:59:ILE:HG21	8:H:83:LEU:HG	1.98	0.46
10:J:25:ILE:HD11	11:K:133:VAL:HG11	1.97	0.46
3:Q:146:GLN:OE1	3:Q:159:ASN:ND2	2.42	0.46
7:U:49:VAL:HG21	7:U:195:VAL:HG23	1.98	0.46
15:c:39:PRO:HG3	15:c:769:TRP:CG	2.51	0.46
6:F:143:ASN:OD1	14:N:106:GLN:NE2	2.49	0.46
2:P:54:LYS:HG3	2:P:55:LEU:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:203:VAL:O	2:P:204:SER:HB3	2.16	0.46
7:U:234:GLU:O	7:U:238:HIS:ND1	2.48	0.46
1:A:144:TYR:HB3	1:A:146:PHE:HE2	1.81	0.46
3:C:138:PHE:CE2	11:K:107:ARG:CZ	2.99	0.46
11:Y:97[B]:MET:HB3	11:Y:97[B]:MET:HE2	1.77	0.46
15:c:297:LEU:HD12	15:c:300:ARG:CG	2.44	0.46
15:c:358:GLN:HB3	15:c:416:GLU:HB3	1.98	0.46
13:M:22:ILE:HG23	13:M:50:MET:HE3	1.97	0.46
3:Q:100:ASP:OD1	11:Y:107:ARG:NH2	2.46	0.46
15:c:30:LYS:CE	15:c:129:LYS:HD3	2.42	0.46
15:c:55:ILE:HG21	15:c:79:LEU:HD13	1.98	0.46
15:c:460:VAL:HA	15:c:463:VAL:HG12	1.98	0.46
3:C:173:GLU:HG3	4:D:58:LEU:HG	1.98	0.46
10:J:38:MET:O	10:J:65:GLN:NE2	2.42	0.46
7:U:155:ASP:OD1	7:U:159:TYR:N	2.49	0.46
10:X:38:MET:HE3	10:X:44:LEU:HB3	1.96	0.46
13:a:142:GLY:HA2	13:a:176:LEU:HD21	1.96	0.46
15:c:208:GLN:HE21	15:c:208:GLN:CA	2.26	0.46
2:B:65:ILE:HD11	2:B:73:ALA:HB1	1.98	0.46
5:E:214:ILE:HD12	5:E:224:TYR:HE2	1.81	0.46
7:G:193:GLN:O	7:G:196:GLU:HB3	2.16	0.46
8:V:209:THR:OG1	9:W:168:GLN:NE2	2.41	0.46
15:c:1183:LEU:HD11	15:c:1308:ILE:CD1	2.45	0.46
4:D:178:GLN:HE21	4:D:182:GLN:HE21	1.64	0.46
5:E:104:PRO:HB3	13:M:81:HIS:CD2	2.50	0.46
15:c:324:LYS:N	15:c:324:LYS:CD	2.79	0.46
15:c:368:LEU:HD11	15:c:393:VAL:HG21	1.98	0.46
3:C:69:VAL:HG22	3:C:104:VAL:HG22	1.98	0.45
15:c:478:PRO:C	15:c:480:HIS:N	2.72	0.45
15:c:640:GLU:HG2	15:c:690:LYS:HD2	1.98	0.45
4:D:3:LEU:HD11	4:D:5:ARG:HH11	1.82	0.45
7:G:112:ASP:HB3	7:G:152:TYR:CZ	2.52	0.45
10:X:20:VAL:O	10:X:34:LYS:NZ	2.46	0.45
10:X:108:ASP:HB3	10:X:111:GLU:HB2	1.97	0.45
15:c:1490:LEU:HD21	15:c:1505:ILE:HG23	1.98	0.45
10:J:45:LEU:HB2	10:J:103:LEU:HB2	1.99	0.45
13:M:67:LEU:HD11	13:M:88:ILE:HD12	1.98	0.45
2:P:240:HIS:NE2	2:P:244:GLU:OE2	2.50	0.45
10:X:52:ASP:OD1	11:Y:88:TYR:OH	2.31	0.45
13:a:27:LEU:HD22	13:a:184:TYR:HB2	1.98	0.45
14:b:174:ILE:HB	14:b:189:LEU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c:123:LEU:HD23	15:c:176:LEU:HD21	1.98	0.45
15:c:629:ASP:HA	15:c:632:ARG:HG2	1.98	0.45
15:c:891:PHE:HD1	15:c:985:LYS:HD2	1.81	0.45
15:c:1574:LEU:O	15:c:1578:LEU:HB2	2.16	0.45
3:C:63:CYS:HB3	3:C:88:ARG:HH22	1.80	0.45
6:F:227:VAL:HG13	6:F:228:PRO:CD	2.46	0.45
8:H:134:ALA:HB1	8:H:158:ALA:HB1	1.98	0.45
10:J:170:ARG:NH1	10:X:27:GLN:O	2.45	0.45
15:c:1271:LYS:CB	15:c:1274:TRP:NE1	2.77	0.45
15:c:1811:ARG:HG3	15:c:1812:THR:HG23	1.98	0.45
1:O:64:VAL:HG11	1:O:210:GLY:HA3	1.98	0.45
3:Q:92:GLN:HG3	10:X:66:LEU:HB2	1.99	0.45
7:U:187:PHE:HB2	7:U:189:TRP:CD1	2.52	0.45
15:c:636:LYS:HA	15:c:686:VAL:HG23	1.98	0.45
15:c:1271:LYS:HB2	15:c:1274:TRP:HD1	1.73	0.45
15:c:1649:THR:HG23	15:c:1661:VAL:HG11	1.99	0.45
8:H:95:GLY:HA2	8:H:115:PRO:HB3	1.99	0.45
9:I:44:MET:HE3	9:I:66:LEU:HD23	1.99	0.45
12:L:24:ALA:HB1	12:L:193:LEU:HD11	1.99	0.45
1:O:83:ARG:HD3	7:U:160:TYR:HE1	1.82	0.45
15:c:1272:THR:O	15:c:1477:TRP:NE1	2.42	0.45
15:c:1698:GLN:HB3	15:c:1701:VAL:HG22	1.99	0.45
4:R:85:ALA:HB2	4:R:139:VAL:HG11	1.97	0.45
7:U:182:LYS:HE3	7:U:188:ASP:OD2	2.17	0.45
7:U:189:TRP:O	7:U:190:THR:CG2	2.65	0.45
15:c:56:LYS:NZ	15:c:1113:PRO:HG2	2.32	0.45
15:c:891:PHE:O	15:c:894:ILE:HB	2.16	0.45
15:c:1085:ARG:HE	15:c:1086:GLN:HG3	1.82	0.45
1:A:85:LEU:HD22	1:A:117:MET:HE3	1.99	0.45
8:H:121:LYS:NZ	13:a:215:ILE:O	2.42	0.45
7:U:11:ARG:O	7:U:24:GLN:NE2	2.49	0.45
7:U:118:ILE:HG13	7:U:138:MET:HE1	1.98	0.45
15:c:1393:TRP:HB2	15:c:1398:VAL:HG13	1.98	0.45
15:c:1482:LEU:HA	15:c:1485:ARG:HB2	1.98	0.45
1:A:145:LEU:HD13	1:A:145:LEU:C	2.41	0.45
12:L:185:ARG:NH1	8:V:27:ALA:O	2.47	0.45
6:T:112:ALA:HB1	6:T:151:ILE:HD11	1.98	0.45
12:Z:60:ASP:OD1	13:a:97:TYR:OH	2.32	0.45
15:c:925:MET:SD	15:c:936:ILE:HD13	2.57	0.45
15:c:936:ILE:CD1	15:c:939:LEU:HD23	2.47	0.45
15:c:1194:ASN:HD22	15:c:1321:GLN:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c:1673:LEU:HD21	15:c:1677:LEU:HD11	1.98	0.45
1:A:70:HIS:NE2	1:A:104:ILE:O	2.38	0.45
2:P:198:ASN:HA	2:P:206:LEU:HD22	1.99	0.45
15:c:402:GLN:O	15:c:406:LEU:HB2	2.17	0.45
15:c:762:LEU:HD13	15:c:940:LEU:HD11	1.99	0.45
15:c:1435:ARG:NH1	17:c:1902:IHP:O34	2.49	0.45
7:U:72:ILE:HG21	7:U:114:LEU:HD21	1.99	0.44
15:c:1019:VAL:HG23	15:c:1020:THR:H	1.82	0.44
15:c:1077:ASP:OD1	15:c:1162:LYS:NZ	2.50	0.44
15:c:1673:LEU:CD2	15:c:1677:LEU:CD1	2.94	0.44
3:C:130:SER:OG	3:C:146:GLN:OE1	2.34	0.44
3:C:138:PHE:CZ	11:K:107:ARG:CZ	2.98	0.44
6:F:179:LEU:HD11	6:F:192:GLU:HB3	1.98	0.44
7:G:230:LEU:N	7:G:230:LEU:HD22	2.31	0.44
12:L:145:LEU:HD21	12:L:182:ALA:HB2	1.98	0.44
13:M:211:ILE:HG13	14:b:30:VAL:HG11	2.00	0.44
2:P:45:LEU:HD13	2:P:75:SER:HB2	1.99	0.44
3:Q:96:LEU:HB2	10:X:62:LYS:HG3	1.98	0.44
10:X:101:ASN:HB3	10:X:132:HIS:CD2	2.52	0.44
15:c:429:PRO:HD2	15:c:473:TRP:HE1	1.82	0.44
15:c:933:LYS:HD2	16:c:1901:K0W:O61	2.18	0.44
5:E:210:VAL:HG11	5:E:233:LEU:HD11	2.00	0.44
9:I:106:PRO:HD2	9:I:123:LEU:HB2	1.99	0.44
12:L:38:ARG:NH1	12:L:191:ASP:OD1	2.49	0.44
10:X:7:ILE:N	10:X:14:LEU:O	2.43	0.44
6:F:213:LEU:HD13	6:F:232:ARG:HG3	1.98	0.44
13:M:50:MET:HE2	13:M:192:VAL:HG12	1.99	0.44
15:c:729:THR:HG23	15:c:827:LEU:HG	1.98	0.44
15:c:1054:PRO:HA	15:c:1057:VAL:HG12	1.99	0.44
15:c:1216:LYS:CE	17:c:1902:IHP:O22	2.65	0.44
3:C:108:THR:HG21	3:C:145:TYR:HB3	1.99	0.44
6:F:15:SER:OG	6:F:17:ASP:OD1	2.34	0.44
6:F:125:TYR:HB2	6:F:128:VAL:HG22	1.98	0.44
12:L:198:VAL:HG22	12:L:203:ILE:HG12	1.99	0.44
2:P:49:ARG:HH21	2:P:212:GLU:HG2	1.83	0.44
8:V:113:ILE:HG12	8:V:119:THR:HG22	2.00	0.44
15:c:129:LYS:NZ	16:c:1901:K0W:O44	2.47	0.44
15:c:728:THR:HG21	15:c:779:PHE:HD2	1.82	0.44
15:c:933:LYS:HD2	16:c:1901:K0W:O51	2.17	0.44
7:G:37:LEU:HD22	7:G:53:GLN:HG3	2.00	0.44
10:X:118:MET:HE2	10:X:124:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:4:PRO:HG3	13:a:107:TRP:CE2	2.52	0.44
15:c:298:VAL:N	15:c:299:PRO:HD2	2.32	0.44
15:c:862:GLU:OE2	15:c:867:VAL:HG21	2.17	0.44
15:c:972:LEU:CD2	15:c:990:PHE:HE1	2.16	0.44
6:T:67:PHE:HB2	6:T:75:MET:HB3	2.00	0.44
6:F:144:ASP:OD1	6:F:144:ASP:N	2.50	0.44
12:L:10:GLY:HA3	12:L:42:LYS:HE2	2.00	0.44
9:W:73:TYR:O	9:W:77:GLU:HB3	2.18	0.44
14:b:90:TYR:HB3	14:b:93:ASP:HB2	1.99	0.44
15:c:436:VAL:O	15:c:440:THR:OG1	2.26	0.44
15:c:737:CYS:SG	15:c:738:SER:N	2.91	0.44
1:A:203:THR:OG1	1:A:204:GLU:OE1	2.36	0.44
2:P:179:TYR:CE1	2:P:184:MET:HG3	2.53	0.44
7:U:190:THR:OG1	7:U:193:GLN:N	2.39	0.44
10:X:85:ARG:HG3	10:X:124:LEU:HB2	1.98	0.44
15:c:785:ASP:OD1	15:c:789:GLN:NE2	2.51	0.44
15:c:990:PHE:HZ	15:c:1004:ILE:HD13	1.82	0.44
15:c:1510:THR:HG21	15:c:1587:ARG:HD2	1.98	0.44
15:c:1665:LEU:HD21	15:c:1686:ILE:HG23	2.00	0.44
15:c:1673:LEU:HD23	15:c:1673:LEU:O	2.18	0.44
10:X:64:VAL:HG22	10:X:75:LEU:HD12	1.99	0.43
15:c:34:TYR:OH	15:c:933:LYS:NZ	2.50	0.43
15:c:1112:ASN:CB	15:c:1113:PRO:CD	2.59	0.43
1:A:156:ALA:HB3	2:B:60:PHE:HB2	2.01	0.43
5:S:134:ILE:HB	5:S:145:PHE:HB2	2.01	0.43
9:W:148:MET:HE2	9:W:172:ASN:HB2	2.00	0.43
15:c:213:TYR:O	15:c:217:PHE:HB2	2.18	0.43
1:A:94:GLN:HG3	8:H:65:LEU:HD22	2.00	0.43
5:E:105:VAL:HG21	5:E:136:GLY:HA3	2.00	0.43
8:H:41:ILE:HG12	8:H:76:VAL:HG22	2.00	0.43
3:Q:122:ASN:HD22	4:R:128:ALA:HB3	1.78	0.43
10:X:44:LEU:HD11	10:X:102:LEU:HD22	1.99	0.43
15:c:267:ILE:HD12	15:c:370:ARG:NH1	2.24	0.43
15:c:1050:VAL:HG21	15:c:1142:ASN:HB3	2.00	0.43
6:F:134:SER:OG	6:F:150:MET:SD	2.76	0.43
15:c:85:LEU:HD11	15:c:951:ARG:HA	1.99	0.43
15:c:685:ARG:HB3	15:c:723:HIS:HB3	2.00	0.43
2:B:49:ARG:HH22	2:B:230:GLN:HE22	1.65	0.43
3:C:158:ALA:HB1	3:C:172:LEU:HD13	2.00	0.43
5:E:36:VAL:HG13	5:E:172:LEU:HD11	1.99	0.43
9:I:188:ILE:HB	9:I:195:THR:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:46:LEU:HB3	12:L:72:LEU:HD11	1.99	0.43
5:S:172:LEU:O	5:S:176:MET:HB3	2.18	0.43
15:c:1034:ASN:O	15:c:1082:LYS:NZ	2.40	0.43
10:J:64:VAL:HG22	10:J:75:LEU:HD12	2.01	0.43
11:K:6:PHE:HE1	11:K:156:ALA:HB2	1.84	0.43
2:P:62:SER:OG	2:P:65:ILE:O	2.37	0.43
12:Z:44:TYR:CD2	12:Z:65:THR:HG21	2.54	0.43
15:c:29:GLN:HG2	15:c:132:LEU:HD22	1.99	0.43
15:c:286:SER:CB	15:c:306:TYR:CB	2.95	0.43
15:c:635:VAL:HG21	15:c:683:ILE:HG13	2.01	0.43
15:c:980:SER:HA	15:c:983:ARG:HE	1.82	0.43
15:c:990:PHE:CZ	15:c:1004:ILE:HD13	2.54	0.43
5:S:215:VAL:HB	5:S:221:PHE:HD1	1.84	0.43
10:X:16:ALA:HB2	10:X:160:LEU:HD21	2.01	0.43
15:c:66:GLN:HA	15:c:1096:ILE:HD12	2.00	0.43
15:c:1053:TRP:CD2	15:c:1170:LEU:HD12	2.54	0.43
15:c:1435:ARG:HH12	17:c:1902:IHP:P4	2.42	0.43
15:c:1509:LEU:HD12	15:c:1513:PHE:CE2	2.53	0.43
15:c:1673:LEU:C	15:c:1673:LEU:CD2	2.85	0.43
4:D:1:MET:HE1	15:c:1712:LEU:HD22	2.01	0.43
4:D:166:ASP:OD1	4:D:166:ASP:N	2.51	0.43
4:D:215:ILE:HD11	4:D:234:LEU:HD21	2.00	0.43
9:I:50:ILE:HD11	9:I:106:PRO:HB3	2.00	0.43
13:M:92:LEU:HD23	13:M:112:ILE:HD11	1.99	0.43
9:W:46:ASP:OD2	9:W:80:GLN:NE2	2.52	0.43
13:a:56:ASP:O	13:a:108:ASN:ND2	2.47	0.43
15:c:99:ILE:HG23	15:c:127:LEU:HD11	2.00	0.43
15:c:594:LEU:HA	15:c:594:LEU:HD12	1.83	0.43
15:c:936:ILE:HG12	15:c:939:LEU:HD23	2.00	0.43
15:c:1016:ARG:HH11	15:c:1019:VAL:HG12	1.83	0.43
15:c:1109:GLN:O	15:c:1111:LYS:CD	2.64	0.43
15:c:1270:GLU:OE2	15:c:1439:LYS:CD	2.67	0.43
15:c:1383:ILE:HG21	15:c:1409:LEU:HD21	2.01	0.43
2:B:161:ALA:HB3	3:C:53:LEU:HD23	2.01	0.43
7:G:231:THR:OG1	7:G:234:GLU:CG	2.66	0.43
13:M:178:TYR:OH	13:M:208:ASN:N	2.42	0.43
15:c:891:PHE:HA	15:c:894:ILE:HD12	1.99	0.43
15:c:932:LYS:HB2	15:c:934:GLN:HE21	1.82	0.43
15:c:1450:SER:HB3	15:c:1453:SER:HB3	2.01	0.43
12:L:147:PRO:HG3	9:W:176:ARG:HG3	2.01	0.43
14:N:106:GLN:HG2	14:N:107:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:122:THR:HG22	2:P:129:PRO:HB3	2.01	0.43
15:c:959:GLU:HB3	15:c:961:LYS:HE3	1.99	0.43
15:c:1582:MET:HE1	15:c:1624:LEU:HB3	2.00	0.43
4:D:199:LEU:HD12	4:D:210:LEU:HD21	2.00	0.42
8:H:37:ILE:HG22	8:H:63:LEU:HD12	2.01	0.42
7:U:202:LEU:O	7:U:206:LEU:HB2	2.19	0.42
15:c:99:ILE:HG21	15:c:138:LEU:HD21	2.00	0.42
5:E:3:ARG:HG2	15:c:451:HIS:CD2	2.54	0.42
1:O:212:CYS:HB2	1:O:217:PHE:HD1	1.84	0.42
2:P:214:ALA:HA	2:P:227:VAL:HA	2.00	0.42
1:A:73:LEU:HD21	1:A:86:VAL:HG22	2.01	0.42
4:D:155:HIS:CE1	4:D:157:ASP:HB3	2.55	0.42
2:P:31:ALA:O	2:P:50:ARG:NH2	2.52	0.42
9:W:177:ASP:HB3	9:W:180:SER:HB2	2.02	0.42
12:Z:46:LEU:HB3	12:Z:72:LEU:HD11	2.01	0.42
15:c:1440:LEU:HD12	15:c:1443:LEU:HD23	2.02	0.42
15:c:1650:ALA:HB1	15:c:1693:LEU:HD21	2.00	0.42
3:C:70:CYS:SG	3:C:71:MET:N	2.92	0.42
4:D:15:PHE:H	5:E:21:GLN:HE22	1.67	0.42
4:R:98:ASN:OD1	11:Y:61:ARG:NH2	2.48	0.42
11:Y:35:ILE:N	11:Y:43:GLY:O	2.51	0.42
15:c:298:VAL:HG22	15:c:299:PRO:HD3	1.82	0.42
1:A:145:LEU:HB3	1:A:157:TRP:O	2.19	0.42
5:E:72:ILE:HD12	5:E:132:LEU:HD22	2.01	0.42
6:F:40:ARG:HG2	6:F:161:TRP:HA	2.01	0.42
7:G:205:VAL:HG23	7:G:206:LEU:HD22	2.01	0.42
8:H:11:GLY:HA2	8:H:108:PRO:HB3	2.02	0.42
2:P:12:PHE:H	3:Q:18:GLN:HE22	1.67	0.42
15:c:880:LEU:CD2	15:c:890:LEU:HD11	2.49	0.42
15:c:1674:PHE:O	15:c:1678:ASN:N	2.44	0.42
1:A:32:ALA:HB1	1:A:48:GLU:HB3	2.01	0.42
1:A:56:TYR:HA	7:G:163:PHE:HD1	1.84	0.42
7:G:46:ASP:HB2	7:G:222:VAL:HB	2.01	0.42
3:Q:30:SER:HB3	3:Q:46:GLU:HB3	2.01	0.42
9:W:44:MET:HE3	9:W:66:LEU:HD23	2.02	0.42
10:X:44:LEU:HD13	10:X:104:LEU:HD12	2.02	0.42
13:a:50:MET:HE2	13:a:192:VAL:HG12	2.02	0.42
15:c:368:LEU:HB3	15:c:929:LEU:HD21	2.02	0.42
15:c:1236:THR:OG1	15:c:1237:GLN:N	2.47	0.42
2:B:147:LEU:HD12	2:B:159:TRP:HB2	2.01	0.42
5:E:109:VAL:HA	5:E:112:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:58:GLU:HG3	1:O:205:ASP:HB3	2.01	0.42
15:c:204:ASP:OD1	15:c:204:ASP:N	2.51	0.42
15:c:836:VAL:HG11	15:c:960:TYR:HD2	1.85	0.42
15:c:1444:PHE:HB3	15:c:1482:LEU:HD21	2.00	0.42
11:K:19:ARG:O	11:K:33:LYS:NZ	2.35	0.42
1:O:70:HIS:NE2	1:O:104:ILE:O	2.47	0.42
2:P:198:ASN:CA	2:P:206:LEU:HD22	2.50	0.42
4:R:91:LYS:HE3	4:R:119:LEU:HD21	2.01	0.42
15:c:1073:VAL:HG23	15:c:1162:LYS:HE3	2.01	0.42
1:A:107:ALA:HB2	2:B:60:PHE:HE2	1.84	0.42
2:B:178:ASP:HB3	2:B:192:LEU:HD11	2.02	0.42
10:J:137:PHE:HB3	11:Y:133:VAL:HG21	2.01	0.42
13:M:192:VAL:HB	13:M:197:VAL:HG22	2.02	0.42
3:Q:73:PHE:HE2	3:Q:77:THR:HG22	1.85	0.42
4:R:191:LEU:HD23	4:R:221:GLN:HE21	1.85	0.42
6:T:231:ILE:HA	6:T:234:GLU:HG2	2.02	0.42
15:c:134:SER:O	15:c:134:SER:OG	2.34	0.42
15:c:437:LEU:HA	15:c:440:THR:HB	2.01	0.42
15:c:921:VAL:HG12	15:c:939:LEU:HD22	2.02	0.42
1:A:139:ASN:HD22	1:A:140:GLU:H	1.67	0.42
15:c:238:LEU:HD12	15:c:238:LEU:HA	1.92	0.42
15:c:282:ARG:HB3	15:c:306:TYR:OH	2.20	0.42
15:c:1731:LEU:O	15:c:1734:THR:OG1	2.37	0.42
6:F:51:LYS:HE2	6:F:51:LYS:HB3	1.94	0.41
6:F:215:TRP:CE2	6:F:227:VAL:CB	3.03	0.41
8:H:28:ASP:HB2	9:I:130:MET:SD	2.60	0.41
10:J:101:ASN:HB3	10:J:132:HIS:CE1	2.54	0.41
2:P:198:ASN:HD22	2:P:240:HIS:CD2	2.38	0.41
15:c:38:LEU:HD12	15:c:44:LEU:HD11	2.02	0.41
15:c:848:GLU:HB3	15:c:958:CYS:HA	2.02	0.41
15:c:1065:MET:HE1	15:c:1067:LEU:HG	2.02	0.41
3:C:132:LEU:HD22	3:C:144:LEU:HD11	2.02	0.41
9:I:52:LEU:HB2	9:I:59:VAL:HG13	2.01	0.41
14:N:48:SER:HB2	14:N:95:MET:HE2	2.02	0.41
2:P:158:GLY:N	3:Q:58:THR:OG1	2.42	0.41
11:Y:186[A]:ARG:HE	11:Y:186[A]:ARG:HB2	1.43	0.41
15:c:47:GLU:CD	15:c:951:ARG:HH12	2.28	0.41
15:c:297:LEU:HB2	15:c:300:ARG:CB	2.49	0.41
15:c:1402:TRP:CH2	15:c:1443:LEU:HD22	2.51	0.41
1:A:145:LEU:HD13	1:A:146:PHE:N	2.35	0.41
1:A:146:PHE:CE1	2:B:60:PHE:CE2	3.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:99:HIS:O	4:D:103:TYR:HB2	2.19	0.41
5:E:133:LEU:HD12	5:E:161:ILE:HG12	2.01	0.41
7:G:47:CYS:SG	7:G:194:THR:HG21	2.60	0.41
4:R:128:ALA:CB	4:R:132:ALA:CB	2.74	0.41
7:U:11:ARG:HG2	7:U:23:TYR:CD2	2.54	0.41
7:U:122:SER:HA	7:U:125:TYR:HD2	1.84	0.41
9:W:61:THR:OG1	10:X:85:ARG:NH2	2.51	0.41
13:a:41:ARG:HH11	13:a:41:ARG:HD2	1.74	0.41
13:a:43:MET:HE2	13:a:45:VAL:HA	2.01	0.41
2:B:41:ASP:OD1	2:B:41:ASP:N	2.53	0.41
3:C:83:VAL:HG11	3:C:129:ILE:HD11	2.02	0.41
6:F:108:LEU:HD12	6:F:147:GLN:HB3	2.01	0.41
5:S:44:ALA:HB2	5:S:142:PRO:HB3	2.02	0.41
6:T:213:LEU:HD12	6:T:232:ARG:HG3	2.02	0.41
11:Y:8:PHE:CE1	11:Y:13:ILE:HG12	2.55	0.41
15:c:972:LEU:HD23	15:c:990:PHE:CD1	2.56	0.41
11:K:139:MET:HA	11:K:155:LEU:HD11	2.02	0.41
12:L:144:MET:HE2	12:L:144:MET:HB3	1.78	0.41
14:N:7:GLN:HA	14:N:12:VAL:HG12	2.01	0.41
12:Z:16:ALA:HB2	12:Z:121:VAL:HG23	2.03	0.41
15:c:461:ILE:HG21	15:c:505:GLN:HE22	1.85	0.41
6:F:100:SER:HA	13:M:65:GLN:HE21	1.84	0.41
10:J:34:LYS:HD3	10:J:47:VAL:HG12	2.02	0.41
13:M:179:ARG:HA	13:M:179:ARG:HD3	1.93	0.41
6:T:72:HIS:NE2	6:T:106:ILE:O	2.42	0.41
7:U:113:MET:HG3	8:V:70:THR:HG22	2.03	0.41
8:V:1:THR:O	8:V:129:SER:N	2.53	0.41
15:c:297:LEU:HG	15:c:297:LEU:O	2.20	0.41
15:c:494:PRO:HG3	15:c:557:LEU:HA	2.02	0.41
1:A:88:ARG:HD3	1:A:116:VAL:HG11	2.02	0.41
4:R:126:GLU:HG3	5:S:124:GLY:HA3	2.03	0.41
12:Z:6:VAL:HG21	12:Z:31:GLU:HG3	2.03	0.41
15:c:375:LYS:N	15:c:375:LYS:CE	2.73	0.41
15:c:880:LEU:HD21	15:c:890:LEU:HD11	2.03	0.41
15:c:1187:ARG:HG2	15:c:1308:ILE:HG12	2.02	0.41
1:A:102:GLU:OE2	9:I:82:LYS:NZ	2.48	0.41
6:F:39:ILE:HD11	6:F:176:ILE:HG12	2.03	0.41
14:N:200:ALA:HB1	14:b:124:SER:HB2	2.03	0.41
2:P:214:ALA:HB2	2:P:227:VAL:HG22	2.03	0.41
7:U:112:ASP:HB3	7:U:152:TYR:CZ	2.56	0.41
15:c:339:SER:O	15:c:345:ASN:ND2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c:583:GLU:HB3	15:c:626:MET:HG2	2.03	0.41
15:c:1674:PHE:O	15:c:1677:LEU:N	2.54	0.41
1:A:55:LEU:HD12	7:G:176:THR:HG23	2.03	0.41
1:A:146:PHE:CZ	2:B:60:PHE:CE1	3.02	0.41
2:B:79:ILE:H	2:B:79:ILE:HG13	1.54	0.41
6:F:228:PRO:CG	6:F:231:ILE:HD12	2.51	0.41
7:G:51:VAL:HG22	7:G:217:VAL:HG22	2.03	0.41
10:J:4:LEU:HD22	10:J:45:LEU:HB3	2.02	0.41
14:N:19:ARG:NH1	14:N:168:GLY:O	2.47	0.41
1:O:55:LEU:HD22	7:U:165:ALA:HB3	2.02	0.41
4:R:113:THR:HG21	4:R:154:PHE:HB3	2.03	0.41
5:S:50:LYS:O	5:S:59:HIS:ND1	2.54	0.41
8:V:50:ALA:HB2	9:W:128:CYS:HB2	2.03	0.41
9:W:58:ASP:CG	10:X:93:ARG:HH22	2.29	0.41
10:X:2:GLU:HB3	10:X:34:LYS:HE2	2.01	0.41
11:Y:12:VAL:HB	11:Y:179:VAL:HB	2.03	0.41
15:c:1502:ARG:HA	15:c:1505:ILE:HB	2.03	0.41
5:E:92:CYS:HA	5:E:103:LEU:HD23	2.02	0.41
1:O:92:LEU:HD13	1:O:112:ARG:HB3	2.02	0.41
3:Q:69:VAL:HG11	3:Q:107:ILE:HG21	2.02	0.41
13:a:63:LEU:HD11	13:a:106:LEU:HD13	2.03	0.41
15:c:78:LYS:HA	15:c:81:THR:HG22	2.03	0.41
15:c:191:GLU:HA	15:c:194:GLU:HG3	2.03	0.41
15:c:401:ILE:HD12	15:c:432:VAL:HG22	2.03	0.41
15:c:654:ILE:HG23	15:c:673:LEU:HD11	2.02	0.41
15:c:719:ASN:HA	15:c:722:HIS:HB3	2.03	0.41
15:c:828:LEU:H	15:c:828:LEU:HG	1.51	0.41
15:c:1353:ASP:HB2	15:c:1393:TRP:CZ2	2.56	0.41
2:B:176:LYS:HG2	3:C:53:LEU:HD13	2.02	0.40
3:C:64:ALA:HB2	3:C:217:LEU:HD12	2.02	0.40
6:F:207:LYS:HD2	6:F:207:LYS:H	1.86	0.40
8:H:30:ASN:O	8:H:187[A]:ARG:NH2	2.53	0.40
11:K:103:GLY:HA2	11:K:179:VAL:HG11	2.03	0.40
11:K:154:ASP:OD1	11:K:157:ARG:NH2	2.54	0.40
14:N:136:TYR:HB3	14:b:166:ARG:HG3	2.03	0.40
15:c:282:ARG:HD3	15:c:306:TYR:OH	2.21	0.40
15:c:584:LEU:O	15:c:588:SER:HB2	2.21	0.40
2:B:108:GLU:HB2	2:B:148:TYR:HH	1.85	0.40
3:C:99:GLU:HB2	11:K:81:LYS:HG2	2.03	0.40
4:D:85:ALA:HA	4:D:139:VAL:HG21	2.03	0.40
5:S:65[A]:HIS:HD2	5:S:221:PHE:HD2	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c:961:LYS:O	15:c:963:ILE:N	2.54	0.40
15:c:1581:LEU:HD22	15:c:1603:PHE:HE2	1.85	0.40
15:c:1668:MET:HE2	15:c:1668:MET:HB3	1.99	0.40
3:C:69:VAL:HG11	3:C:107:ILE:HG21	2.04	0.40
3:C:88:ARG:HH11	10:J:70:ARG:HA	1.86	0.40
6:F:51:LYS:NZ	6:F:212:GLU:OE2	2.47	0.40
10:J:102:LEU:HB2	10:J:118:MET:HB3	2.02	0.40
13:M:33:LEU:HD13	14:b:134:TYR:CE1	2.57	0.40
5:S:184:LEU:HD11	5:S:214:ILE:HD13	2.04	0.40
7:U:144:ASP:N	7:U:148:GLY:O	2.43	0.40
9:W:61:THR:HG23	10:X:86:ARG:HH12	1.86	0.40
9:W:122:SER:HB3	9:W:136:VAL:HB	2.03	0.40
10:X:181:ARG:NE	10:X:190:ASP:OD1	2.54	0.40
15:c:724:LEU:O	15:c:728:THR:OG1	2.24	0.40
15:c:1299:ARG:HH22	15:c:1307:GLN:NE2	2.20	0.40
5:E:176:MET:HE1	6:F:56:LYS:HG2	2.04	0.40
7:G:202:LEU:HD23	7:G:202:LEU:C	2.46	0.40
13:M:6:VAL:HG11	13:M:36:PHE:HD2	1.87	0.40
10:X:21:ALA:HB3	10:X:29:LYS:HB3	2.02	0.40
15:c:1349:PHE:CZ	15:c:1386:LEU:HD12	2.57	0.40
15:c:1687:ARG:HA	15:c:1690:VAL:HG12	2.03	0.40
1:A:156:ALA:HB2	2:B:60:PHE:CG	2.57	0.40
2:B:148:TYR:OH	3:C:57:ARG:NH2	2.54	0.40
3:C:31:THR:OG1	3:C:163:ARG:O	2.28	0.40
13:M:142:GLY:HA2	13:M:176:LEU:HD21	2.03	0.40
13:M:213:HIS:HE1	14:b:190:LEU:HD21	1.87	0.40
14:N:86[B]:MET:HE3	14:N:86[B]:MET:HB2	1.84	0.40
3:Q:107:ILE:HD12	3:Q:107:ILE:HA	1.93	0.40
9:W:159:PRO:HA	9:W:162:LEU:HB3	2.04	0.40
10:X:1:MET:HG2	10:X:134:TYR:H	1.87	0.40
14:b:41:ILE:HG12	14:b:76:VAL:HG22	2.04	0.40
15:c:61:ARG:NH2	15:c:1124:LYS:HZ1	2.20	0.40
15:c:291:VAL:CG1	15:c:1671:TYR:HE2	2.30	0.40
15:c:967:MET:O	15:c:971:LEU:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
17	IHP	c	1902	-	36,36,36	0.72	0	60,60,60	0.96	0
16	K0W	c	1901	-	42,44,44	1.77	7 (16%)	68,74,74	1.15	6 (8%)

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
17	IHP	c	1902	-	-	2/30/54/54	0/1/1/1
16	K0W	c	1901	-	-	9/42/66/66	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	c	1901	K0W	PA5-O77	5.82	1.65	1.59
16	c	1901	K0W	PA1-O76	5.30	1.65	1.59
16	c	1901	K0W	PA3-O13	3.59	1.65	1.59
16	c	1901	K0W	PA6-O16	3.02	1.64	1.59
16	c	1901	K0W	PA4-O14	2.86	1.64	1.59
16	c	1901	K0W	PA2-O12	2.83	1.64	1.59
16	c	1901	K0W	PA5-O15	2.03	1.65	1.59

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	c	1901	K0W	C5-C6-C1	3.35	117.78	110.43
16	c	1901	K0W	C5-C4-C3	2.77	116.50	110.43
16	c	1901	K0W	C4-C3-C2	2.60	116.12	110.43
16	c	1901	K0W	C6-C1-C2	2.37	115.63	110.43
16	c	1901	K0W	PA6-O16-C1	-2.06	117.93	123.43
16	c	1901	K0W	O51-PB1-O76	2.00	111.35	104.64

There are no chirality outliers.

All (11) torsion outliers are listed below:

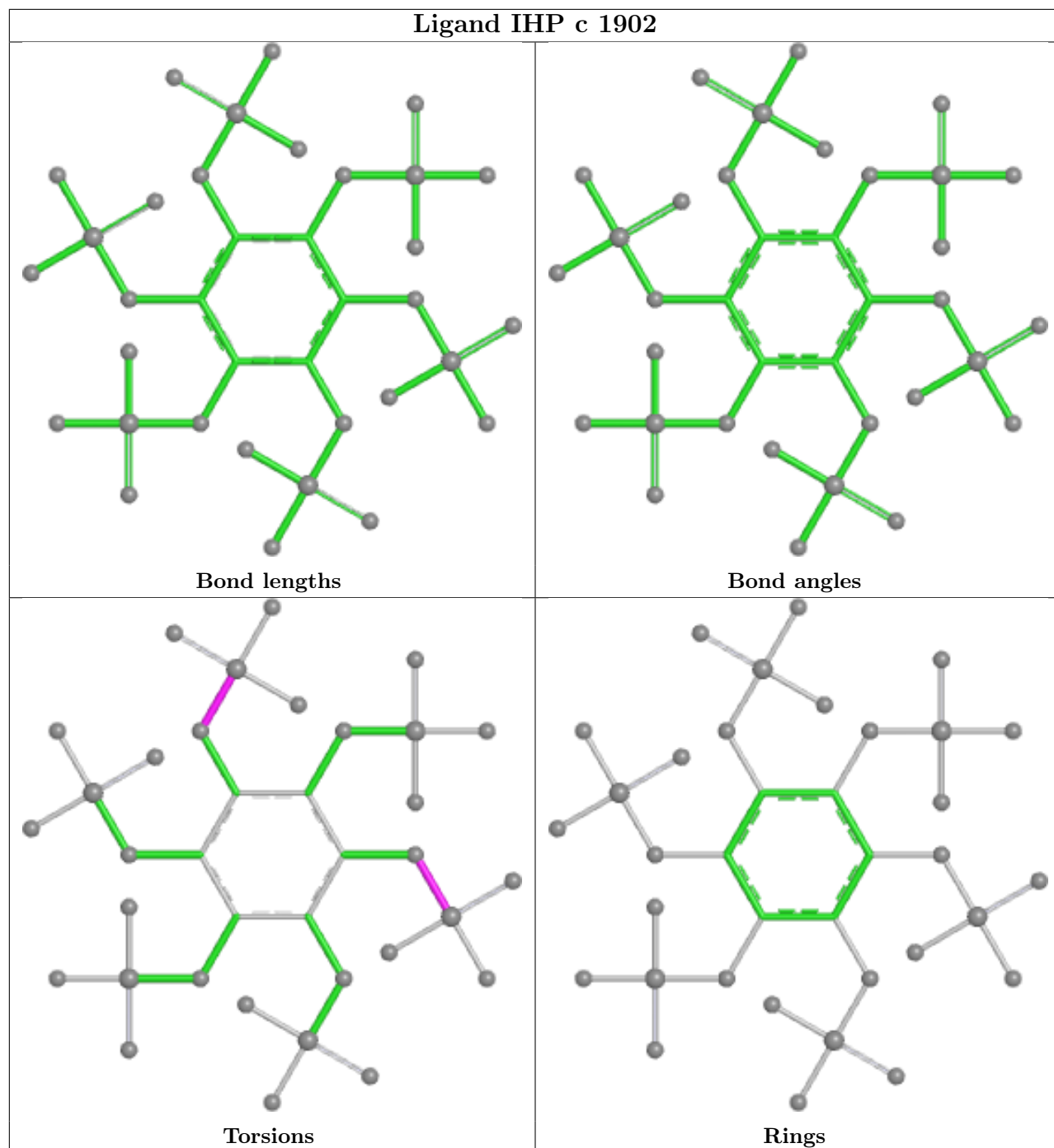
Mol	Chain	Res	Type	Atoms
16	c	1901	K0W	C4-C3-O13-PA3
16	c	1901	K0W	C6-O11-PA1-O76
16	c	1901	K0W	C3-O13-PA3-O23
17	c	1902	IHP	C3-O13-P3-O43
16	c	1901	K0W	C2-C3-O13-PA3
16	c	1901	K0W	C2-O12-PA2-O22
16	c	1901	K0W	C2-O12-PA2-O32
16	c	1901	K0W	C4-O14-PA4-O24
17	c	1902	IHP	C5-O15-P5-O45
16	c	1901	K0W	C1-O16-PA6-O26
16	c	1901	K0W	PB5-O77-PA5-O25

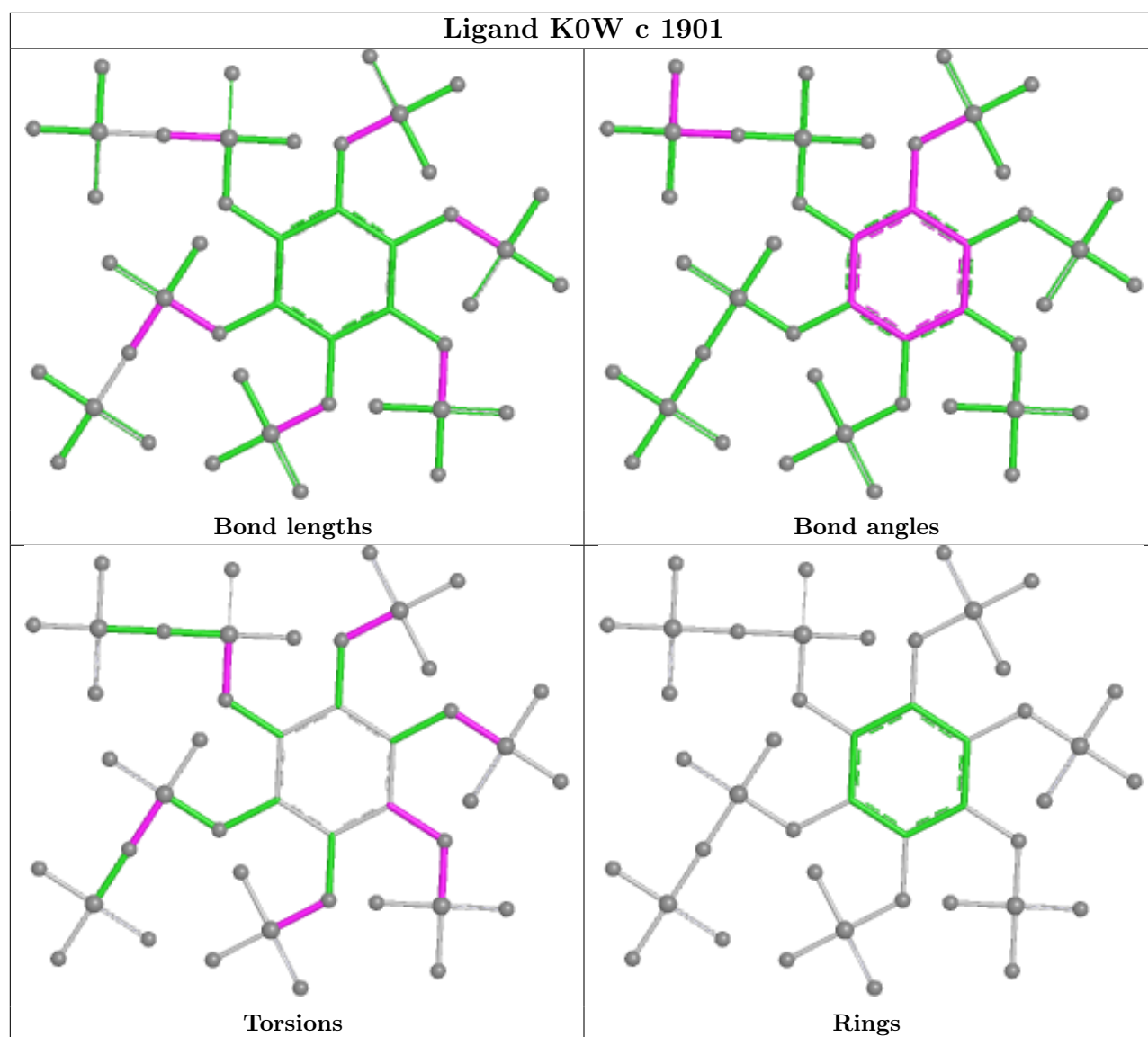
There are no ring outliers.

2 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	c	1902	IHP	12	0
16	c	1901	KOW	15	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

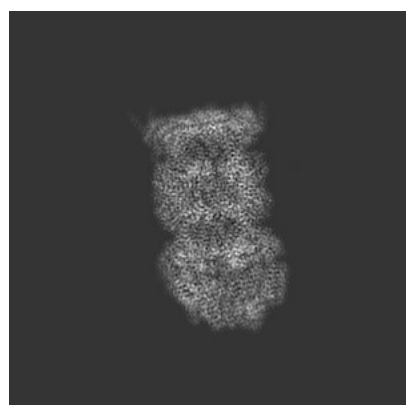
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0781. These allow visual inspection of the internal detail of the map and identification of artifacts.

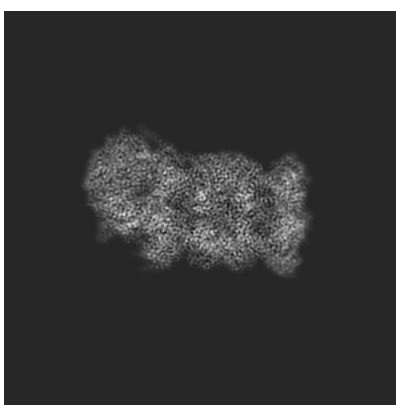
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

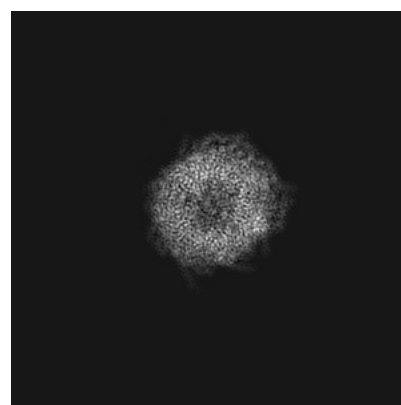
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

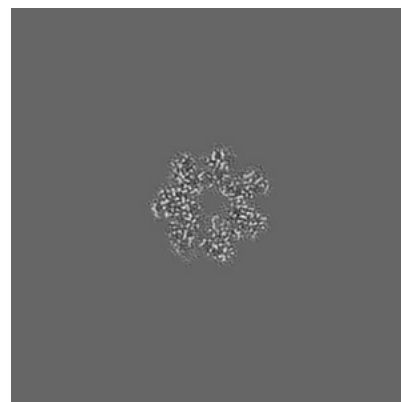
6.2.1 Primary map



X Index: 180



Y Index: 180

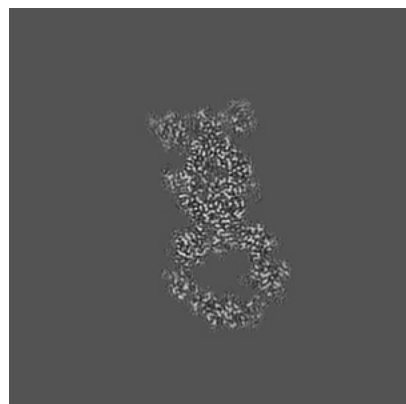


Z Index: 180

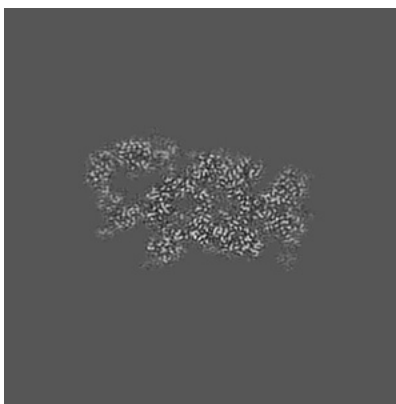
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

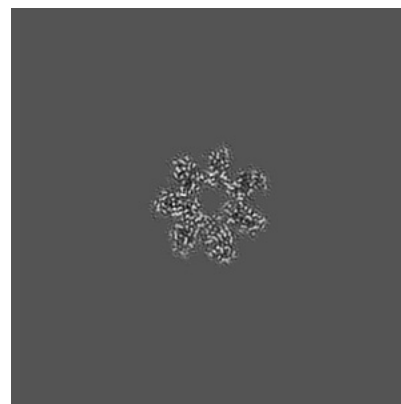
6.3.1 Primary map



X Index: 207



Y Index: 208

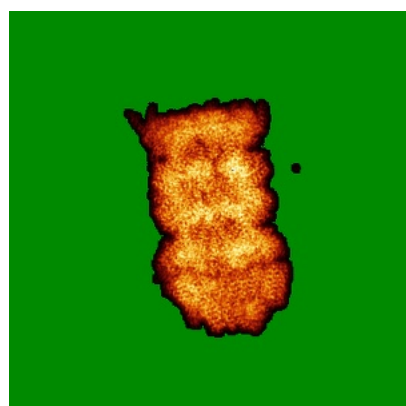


Z Index: 177

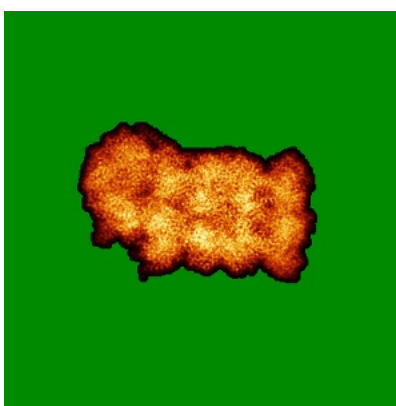
The images above show the largest variance slices of the map in three orthogonal directions.

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

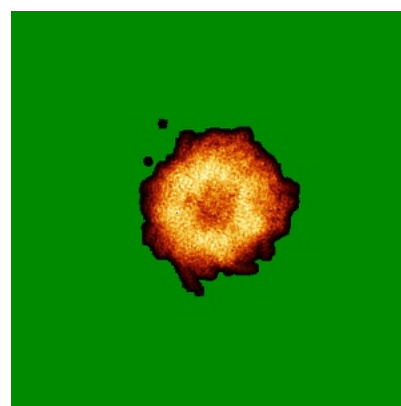
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

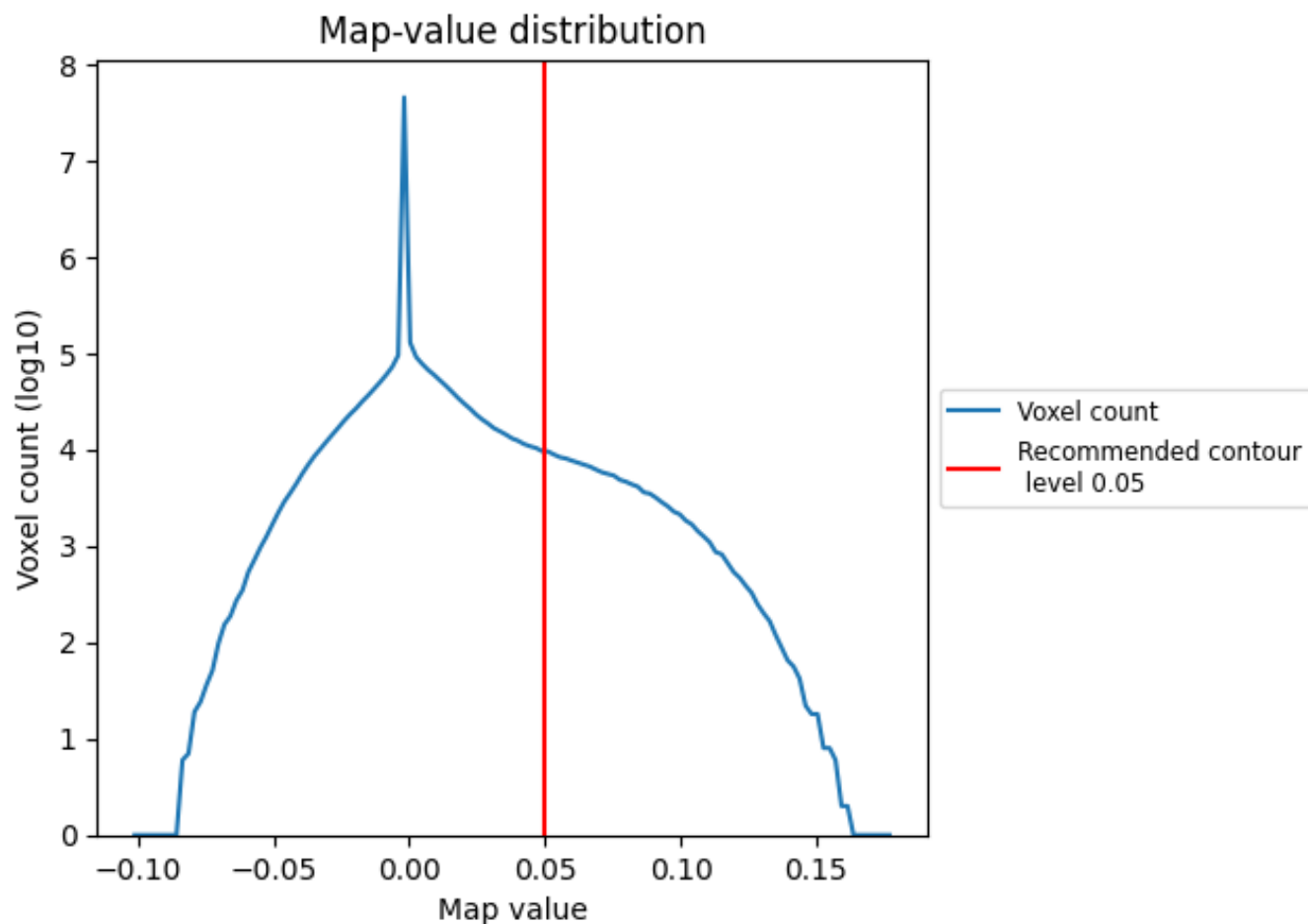
6.6 Mask visualisation

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

7 Map analysis [i](#)

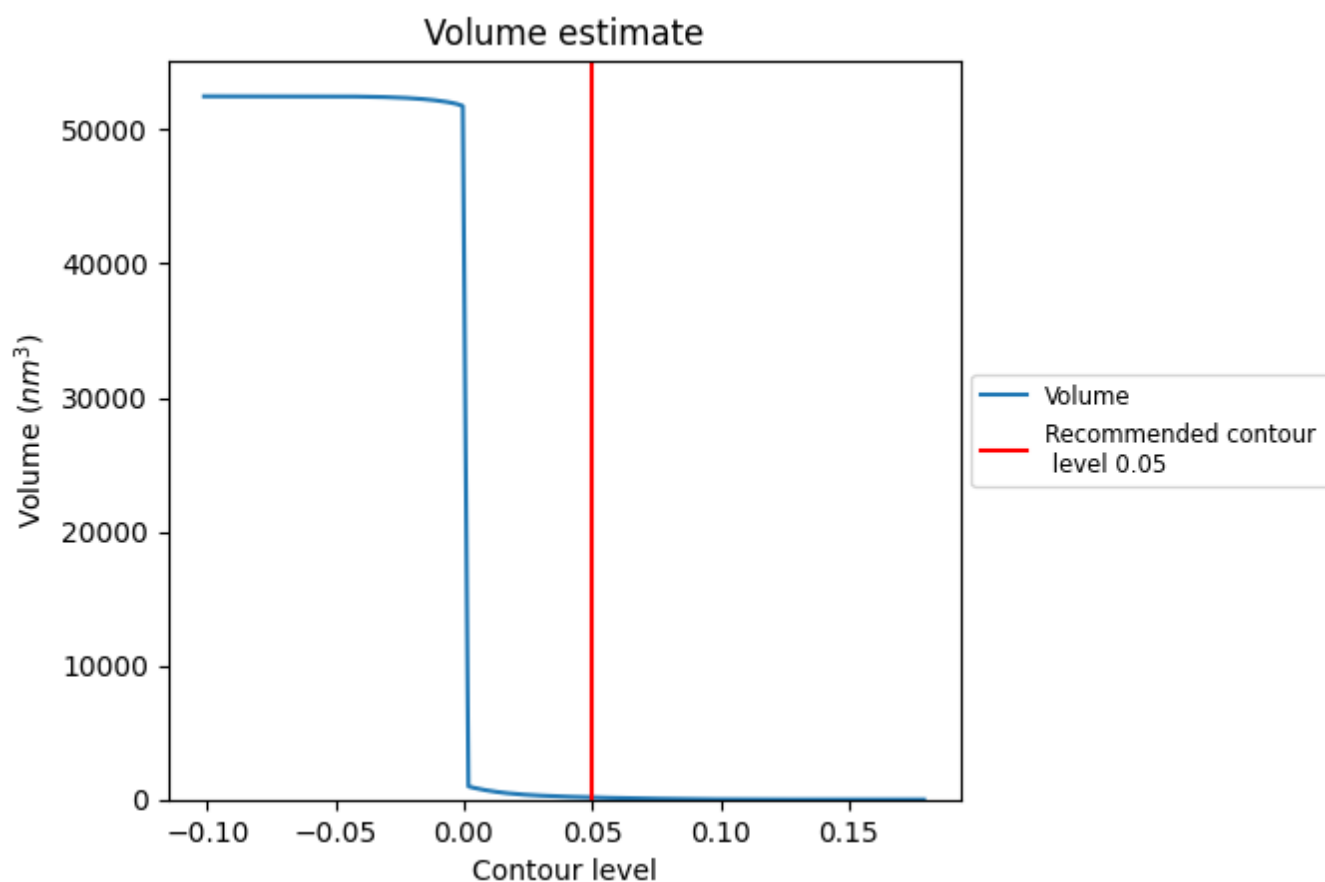
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

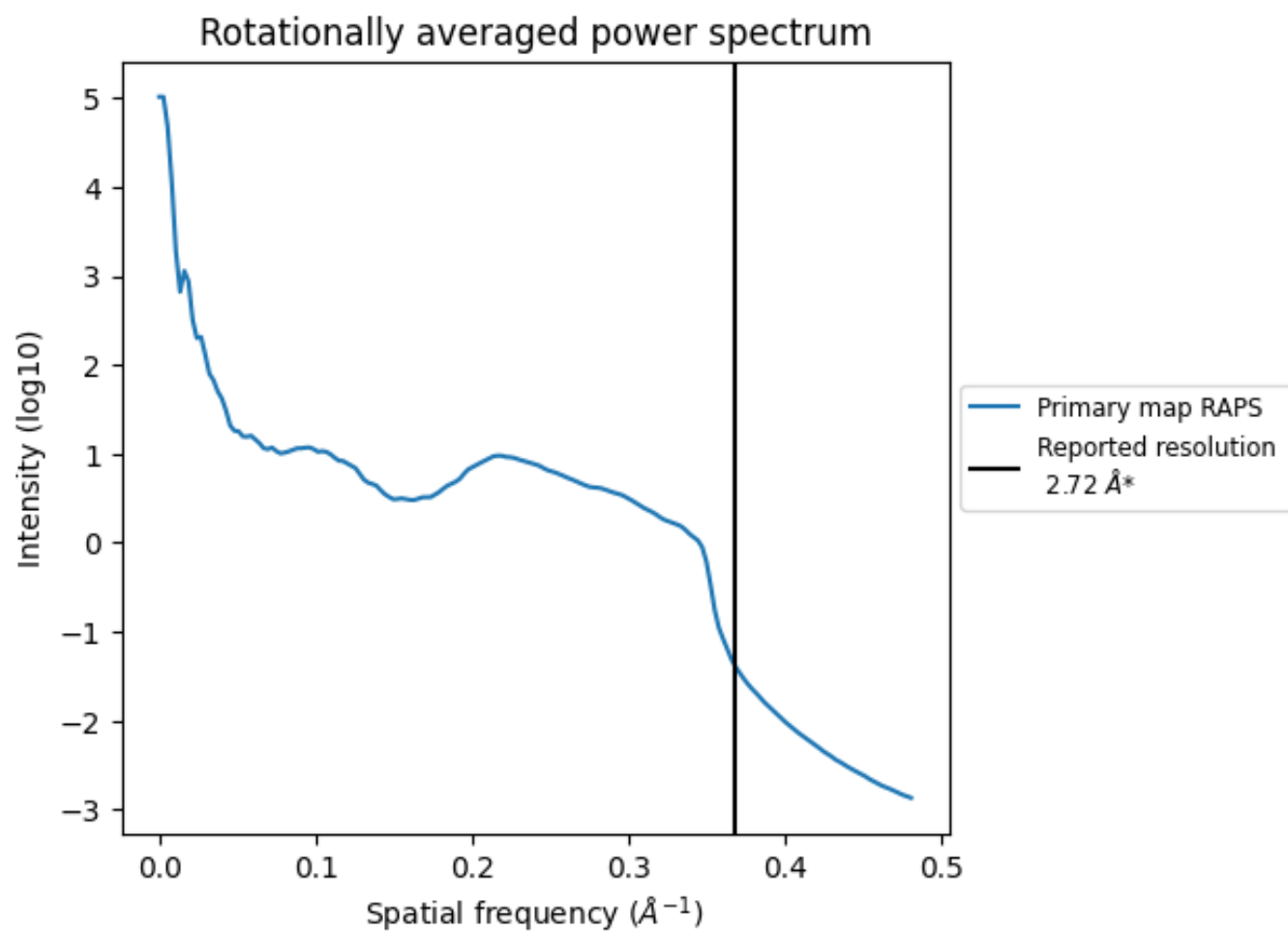
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 159 nm³; this corresponds to an approximate mass of 144 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

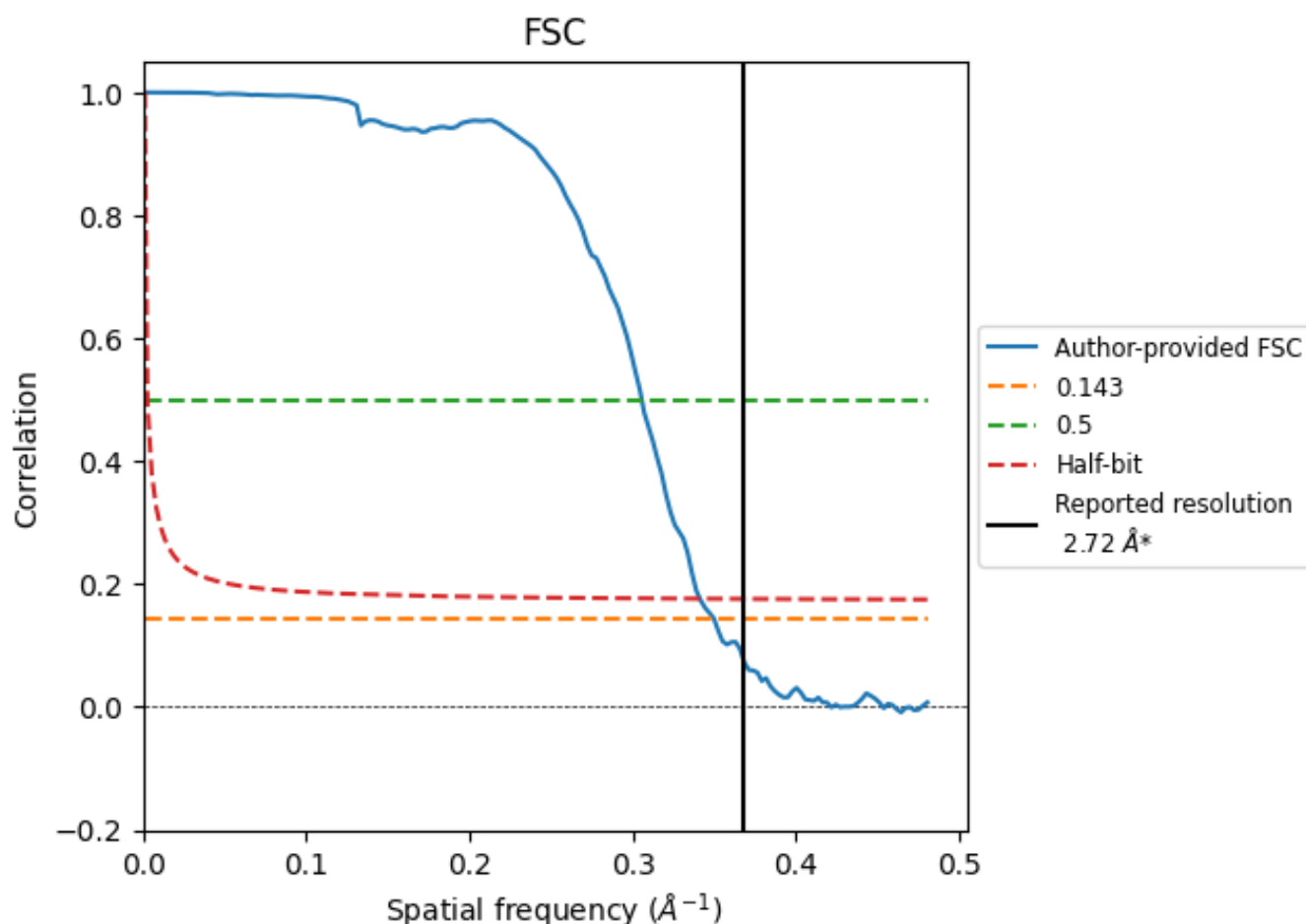


*Reported resolution corresponds to spatial frequency of 0.368 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.368 Å⁻¹

8.2 Resolution estimates [i](#)

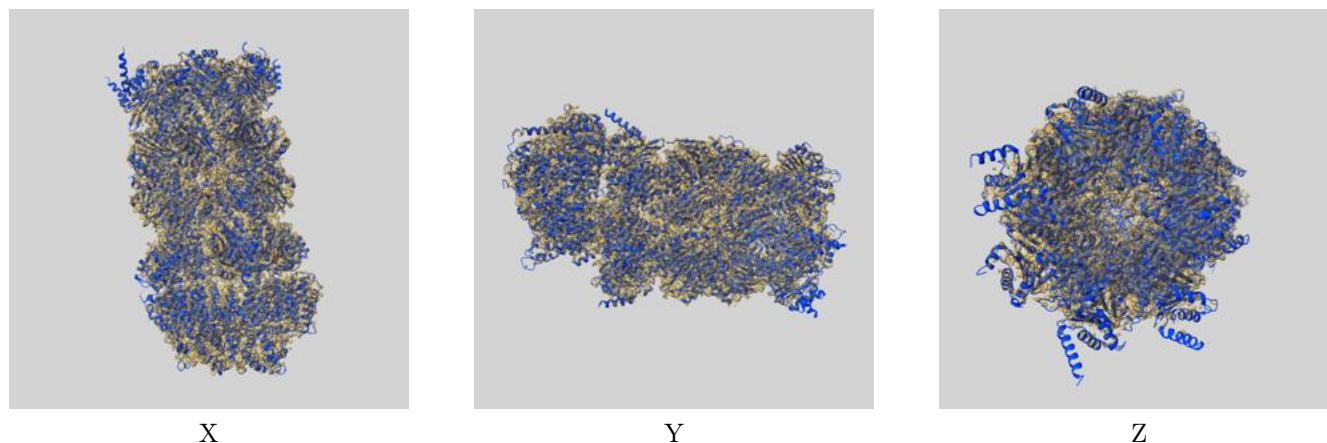
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	2.86	3.27	2.93
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

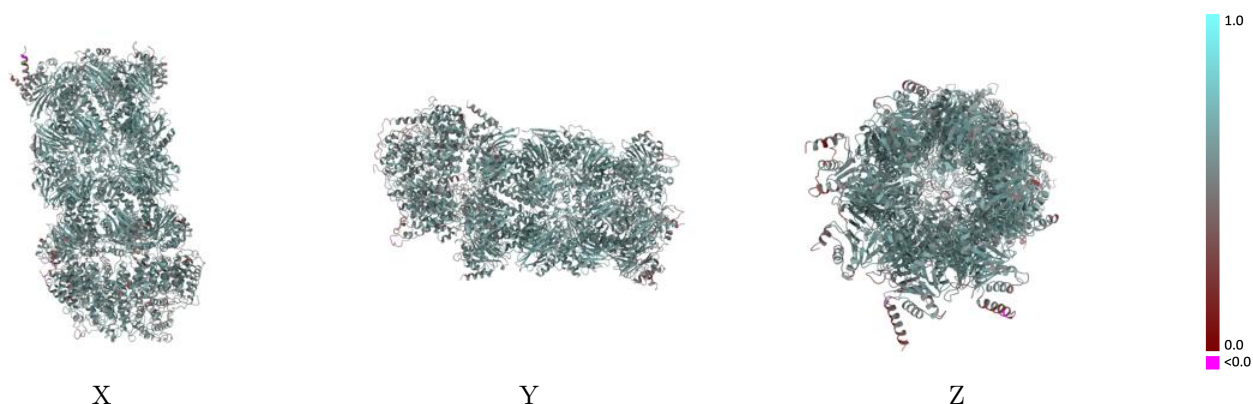
This section contains information regarding the fit between EMDB map EMD-0781 and PDB model 6KWY. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

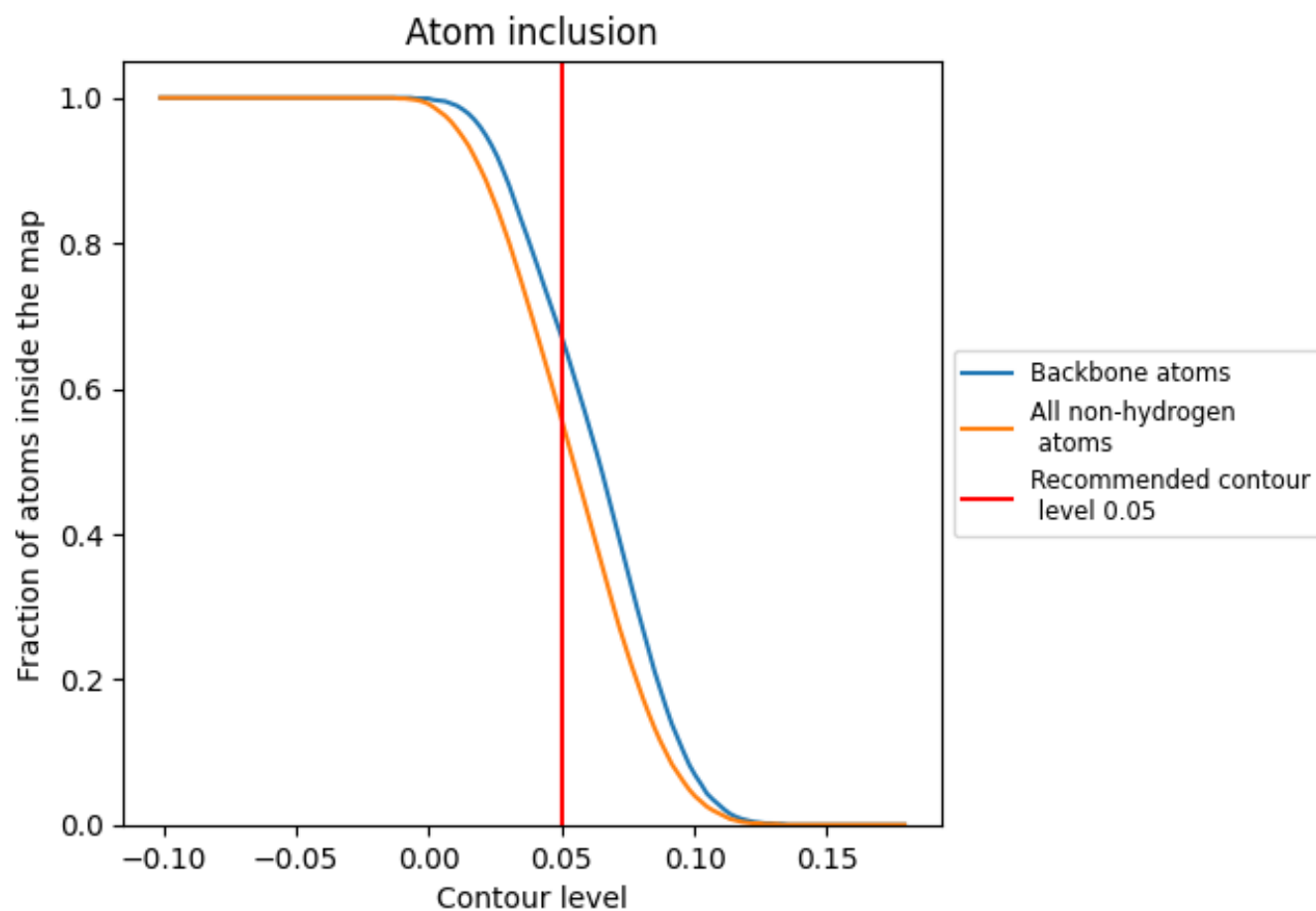


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5570	 0.5760
A	 0.6300	 0.5930
B	 0.5170	 0.5580
C	 0.5130	 0.5580
D	 0.5360	 0.5700
E	 0.6560	 0.5960
F	 0.5950	 0.5860
G	 0.5860	 0.5790
H	 0.6530	 0.6070
I	 0.6750	 0.6190
J	 0.6810	 0.6120
K	 0.6970	 0.6150
L	 0.6160	 0.5970
M	 0.6840	 0.6110
N	 0.7030	 0.6210
O	 0.4510	 0.5560
P	 0.3660	 0.5440
Q	 0.3640	 0.5450
R	 0.4600	 0.5740
S	 0.4930	 0.5700
T	 0.5090	 0.5630
U	 0.3960	 0.5460
V	 0.5760	 0.5770
W	 0.6500	 0.6110
X	 0.6730	 0.6090
Y	 0.6800	 0.6150
Z	 0.6350	 0.6100
a	 0.6790	 0.6120
b	 0.6680	 0.6120
c	 0.4890	 0.5400

