Full wwPDB EM Validation Report ⓘ

Jul 24, 2024 – 04:25 PM JST

PDB ID	:	8YVP
EMDB ID	:	EMD-39612
Title	:	canine immunoproteasome 20S subunit in complex with compound 1
Authors	:	Kashima, A.; Arai, Y.
Deposited on	:	2024-03-29
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

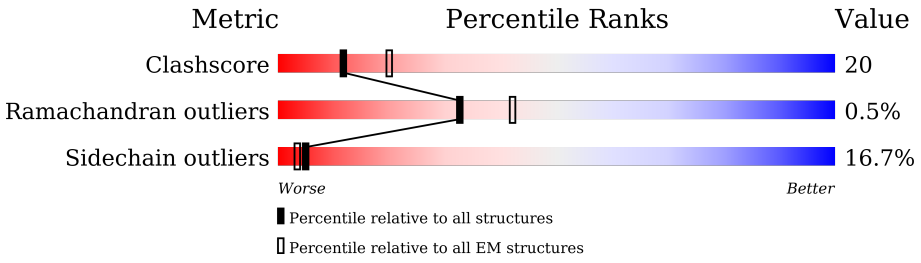
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	B	234	53% 36% 5% 6%
1	E	234	54% 35% 5% 6%
2	C	204	68% 25%
2	D	204	68% 25%
3	P	234	50% 41% 6%
3	b	234	83% 14%
4	J	255	5% 53% 33% 6% 8%
4	Q	255	5% 54% 31% 7% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	K	246	7% 57% 32% 7%
5	R	246	7% 56% 33% 7%
6	A	204	69% 26%
6	F	204	67% 28%
7	S	240	60% 24% 12%
7	X	240	60% 24% 12%
8	U	205	61% 36%
8	Y	205	60% 38%
9	W	264	49% 28% 19%
9	a	264	70% 11% 19%
10	H	241	5% 54% 39%
10	M	241	6% 54% 38%
11	T	201	71% 24%
11	V	201	71% 23%
12	I	248	5% 46% 42% 6% 6%
12	N	248	5% 46% 42% 6% 6%
13	G	263	47% 34% 8% 11%
13	L	263	48% 34% 8% 11%
14	O	261	51% 33% 8% 8%
14	Z	261	54% 31% 7% 8%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 48048 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	220	Total	C	N	O	S	0	0
			1656	1044	282	318	12		
1	E	220	Total	C	N	O	S	0	0
			1656	1044	282	318	12		

- Molecule 2 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	199	Total	C	N	O	S	0	0
			1544	976	269	290	9		
2	D	199	Total	C	N	O	S	0	0
			1544	976	269	290	9		

- Molecule 3 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	228	Total	C	N	O	S	0	0
			1781	1138	302	335	6		
3	b	228	Total	C	N	O	S	0	0
			1781	1138	302	335	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	235	Total	C	N	O	S	0	0
			1840	1168	315	346	11		
4	J	235	Total	C	N	O	S	0	0
			1840	1168	315	346	11		

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	236	Total	C	N	O	S	0	0
			1831	1163	304	351	13		
5	K	236	Total	C	N	O	S	0	0
			1831	1163	304	351	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	201	Total	C	N	O	S	0	0
			1512	948	258	294	12		
6	A	201	Total	C	N	O	S	0	0
			1512	948	258	294	12		

- Molecule 7 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	212	Total	C	N	O	S	0	0
			1643	1041	280	312	10		
7	X	212	Total	C	N	O	S	0	0
			1643	1041	280	312	10		

- Molecule 8 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Y	204	Total	C	N	O	S	0	0
			1592	1013	265	295	19		
8	U	204	Total	C	N	O	S	0	0
			1592	1013	265	295	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	214	Total	C	N	O	S	0	0
			1671	1054	289	316	12		
9	W	214	Total	C	N	O	S	0	0
			1671	1054	289	316	12		

- Molecule 10 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	231	Total	C	N	O	S	0	0
			1761	1106	292	352	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	231	Total	C	N	O	S	0	0
			1761	1106	292	352	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	V	196	Total	C	N	O	S	0	0
			1570	1006	267	288	9		
11	T	196	Total	C	N	O	S	0	0
			1570	1006	267	288	9		

- Molecule 12 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	232	Total	C	N	O	S	0	0
			1819	1146	322	346	5		
12	N	232	Total	C	N	O	S	0	0
			1819	1146	322	346	5		

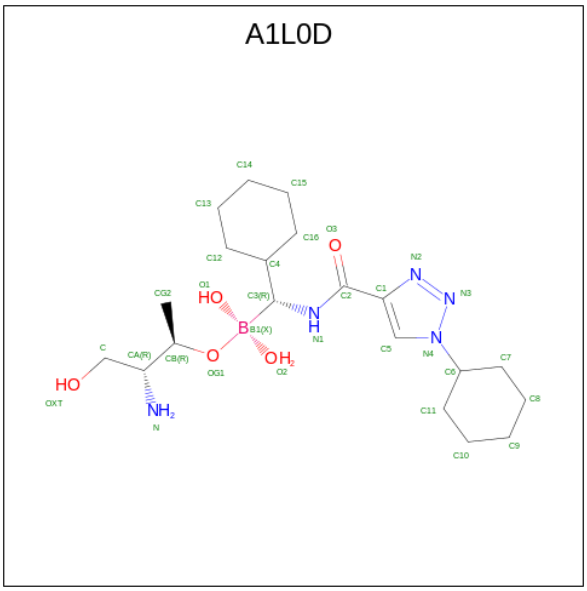
- Molecule 13 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	234	Total	C	N	O	S	0	0
			1836	1150	328	347	11		
13	G	234	Total	C	N	O	S	0	0
			1836	1150	328	347	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	239	Total	C	N	O	S	0	0
			1881	1191	321	359	10		
14	Z	239	Total	C	N	O	S	0	0
			1881	1191	321	359	10		

- Molecule 15 is [(2 {R},3 {R})-3-azanyl-4-oxidanyl-butan-2-yl]oxy-[({R})-cyclohexyl-[(1-cyclohexyl-1,2,3-triazol-4-yl)carbonylamino]methyl]-$l^{3}-oxidanyl-oxidanyl-boron (three-letter code: A1L0D) (formula: $C_{20}H_{38}BN_5O_5$) (labeled as "Ligand of Interest" by depositor).



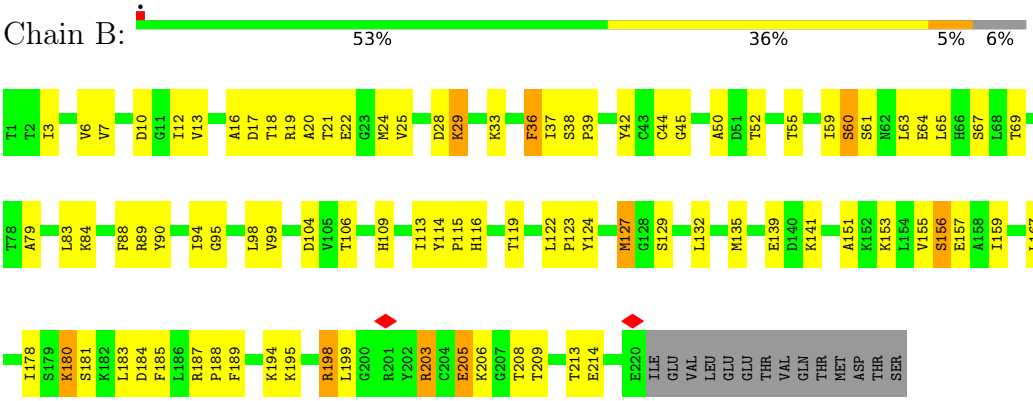
Mol	Chain	Residues	Atoms					AltConf
15	C	1	Total	B	C	N	O	0
			25	1	16	4	4	
15	C	1	Total	B	C	N	O	0
			31	1	20	5	5	
15	F	1	Total	B	C	N	O	0
			31	1	20	5	5	
15	D	1	Total	B	C	N	O	0
			25	1	16	4	4	
15	D	1	Total	B	C	N	O	0
			31	1	20	5	5	
15	A	1	Total	B	C	N	O	0
			31	1	20	5	5	

3 Residue-property plots (i)

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

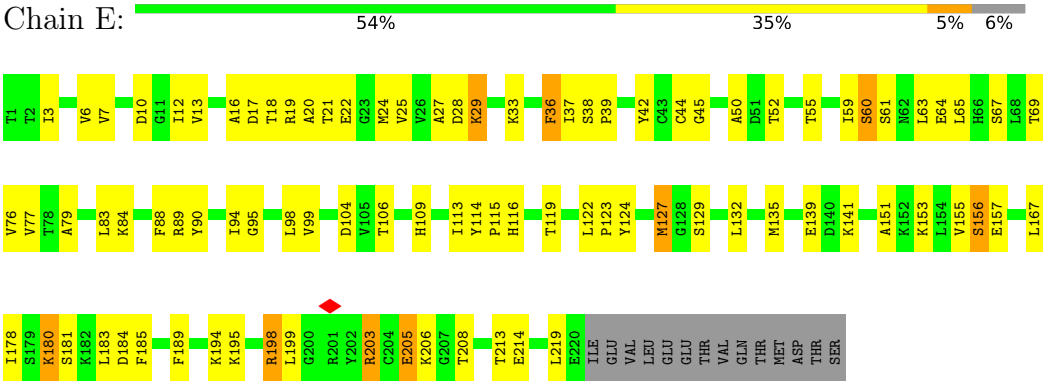
• Molecule 1: Proteasome subunit beta type-7

Chain B:



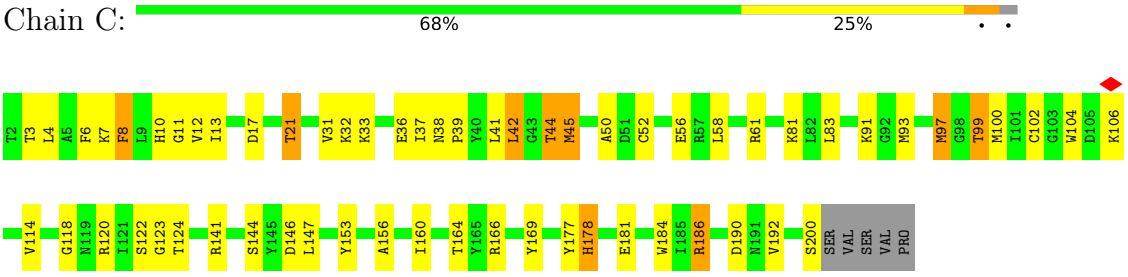
• Molecule 1: Proteasome subunit beta type-7

Chain E:



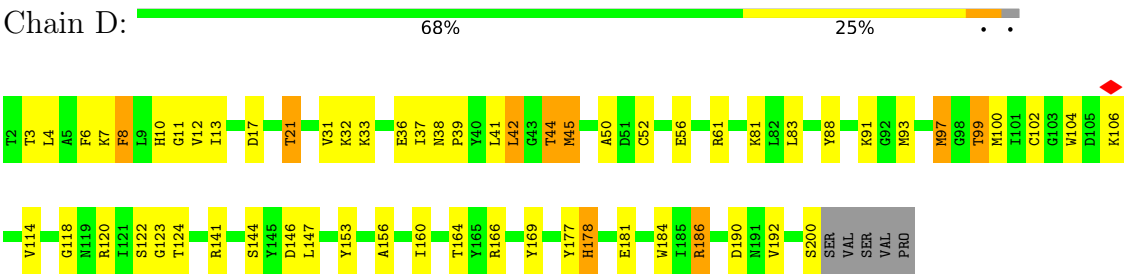
• Molecule 2: Proteasome subunit beta type-5

Chain C:



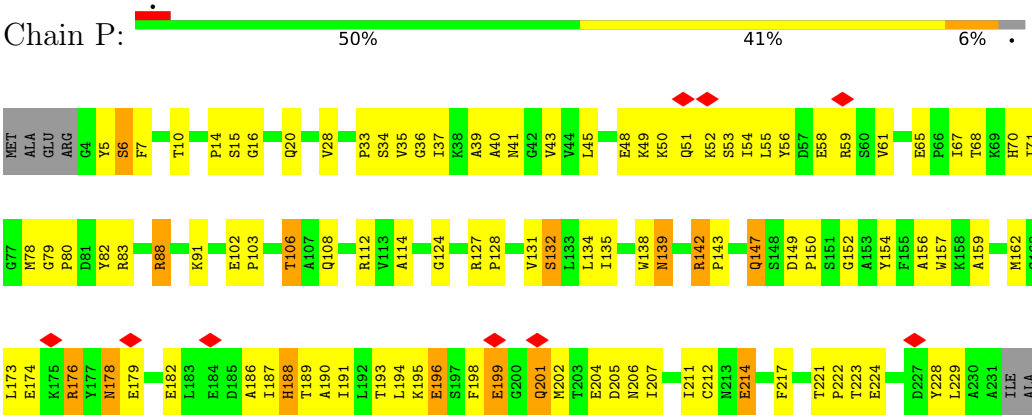
• Molecule 2: Proteasome subunit beta type-5

Chain D:



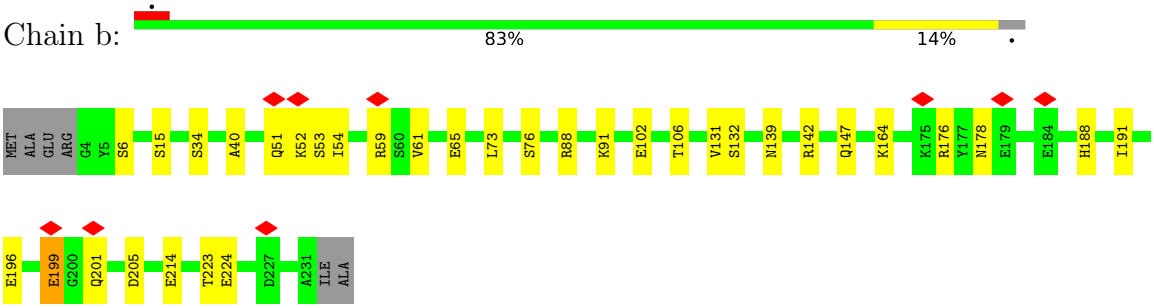
• Molecule 3: Proteasome subunit alpha type-2

Chain P:



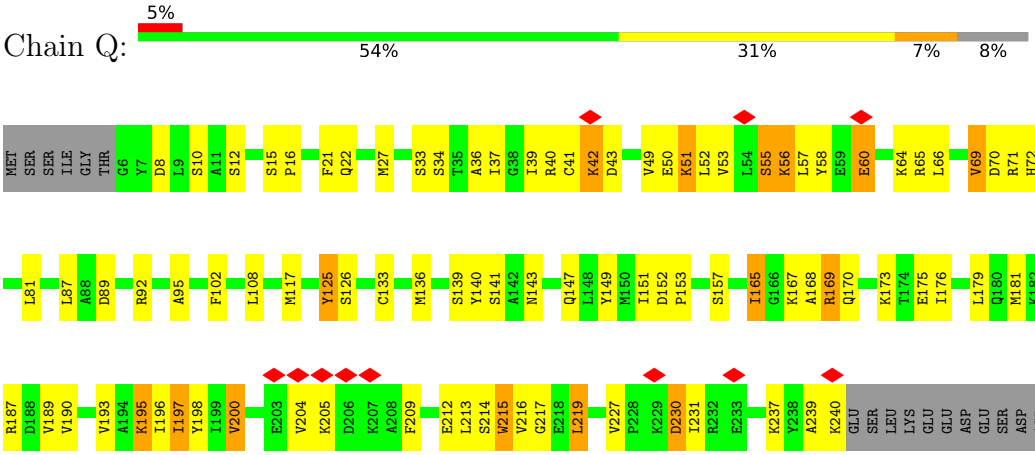
• Molecule 3: Proteasome subunit alpha type-2

Chain b:



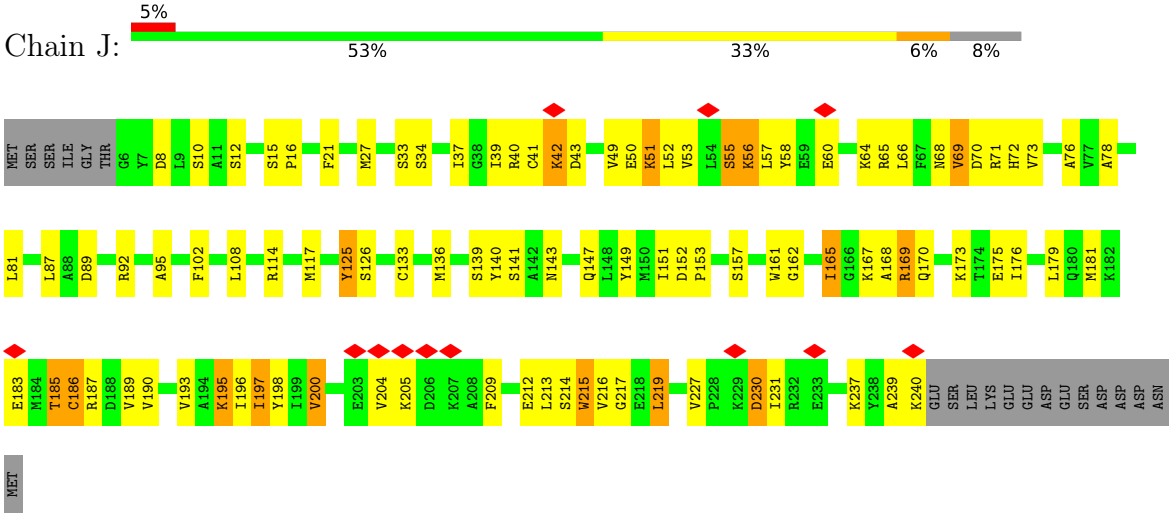
• Molecule 4: Proteasome subunit alpha type-3

Chain Q:



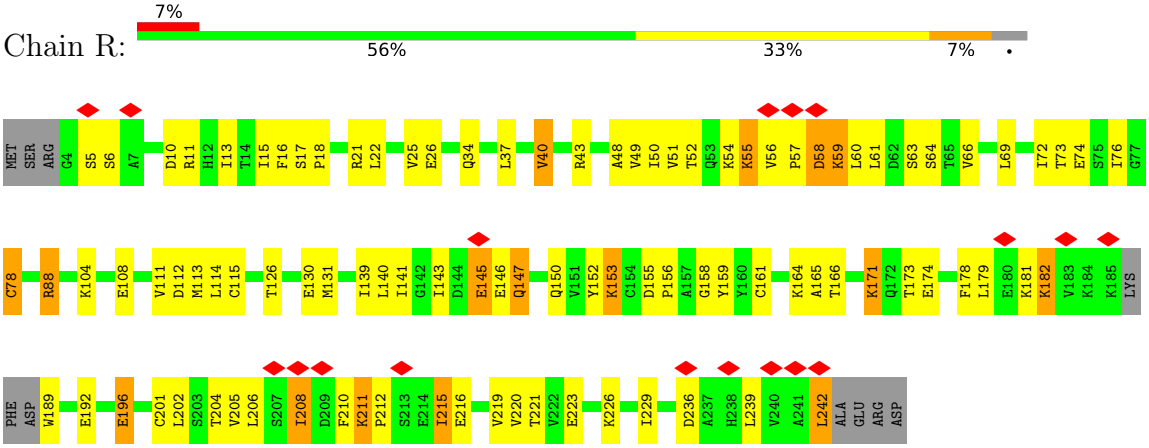
• Molecule 4: Proteasome subunit alpha type-3

Chain J:



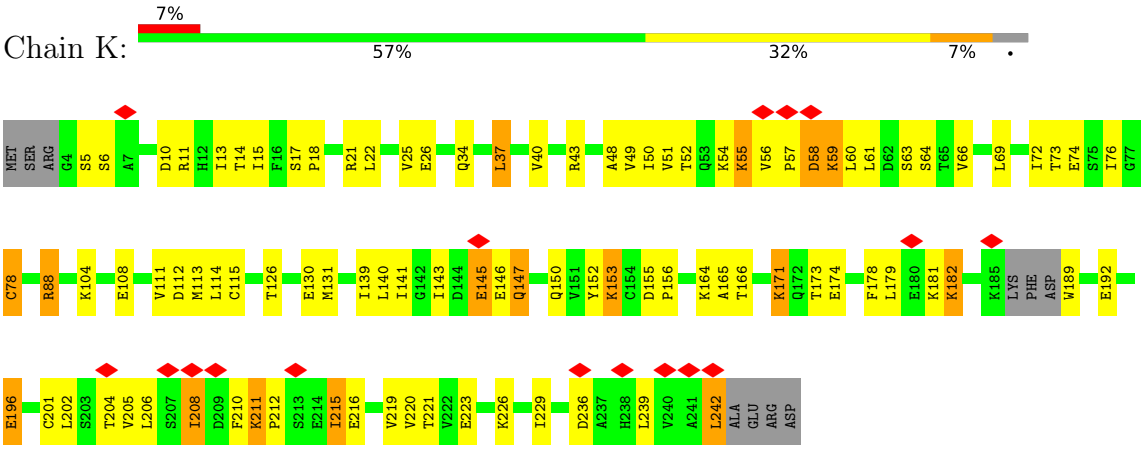
• Molecule 5: Proteasome subunit alpha type-6

Chain R:



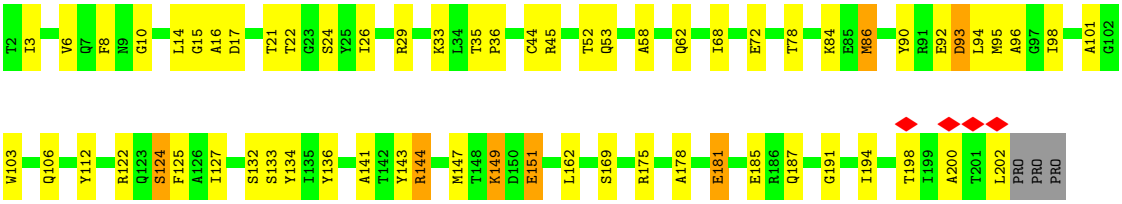
• Molecule 5: Proteasome subunit alpha type-6

Chain K:



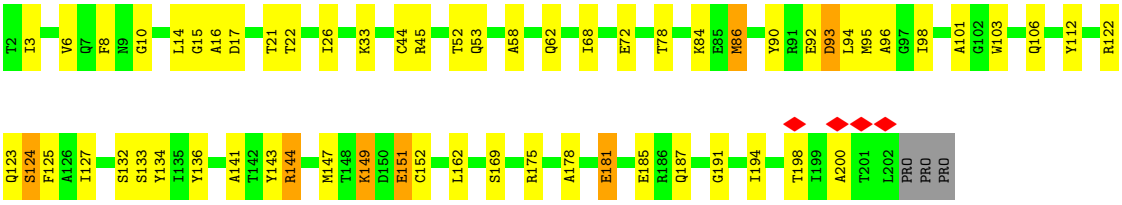
• Molecule 6: Proteasome subunit beta type-6

Chain F:



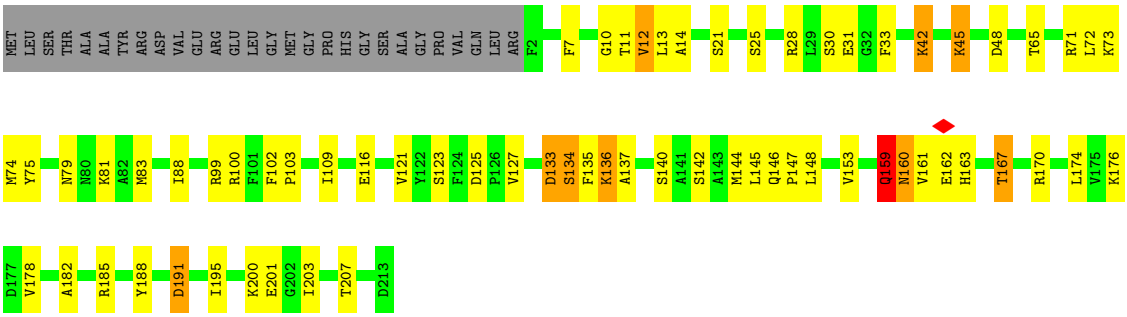
• Molecule 6: Proteasome subunit beta type-6

Chain A:



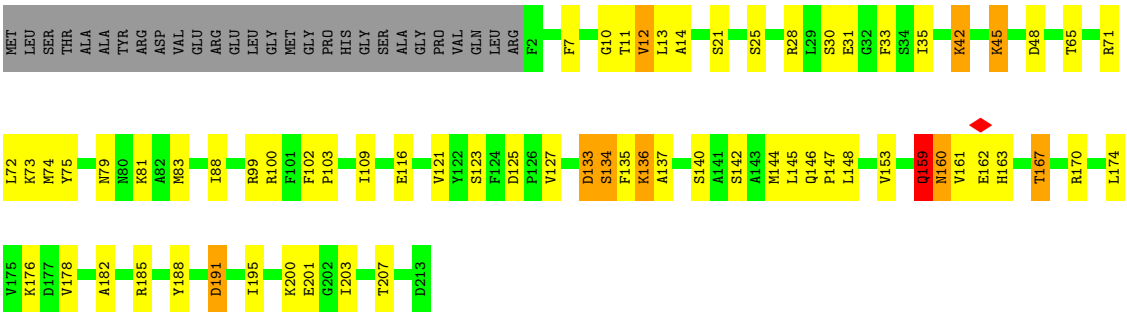
• Molecule 7: Proteasome subunit beta type-1

Chain S:



• Molecule 7: Proteasome subunit beta type-1

Chain X:



• Molecule 8: Proteasome subunit beta type-3

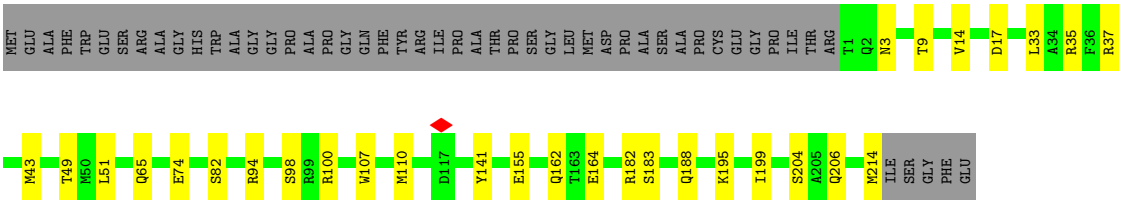
Chain Y:

• Molecule 8: Proteasome subunit beta type-3

Chain U:

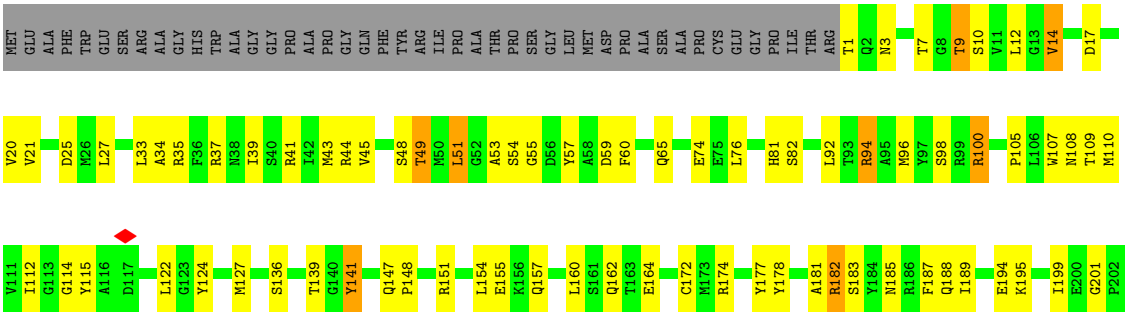
• Molecule 9: Proteasome subunit beta type-4

Chain a:



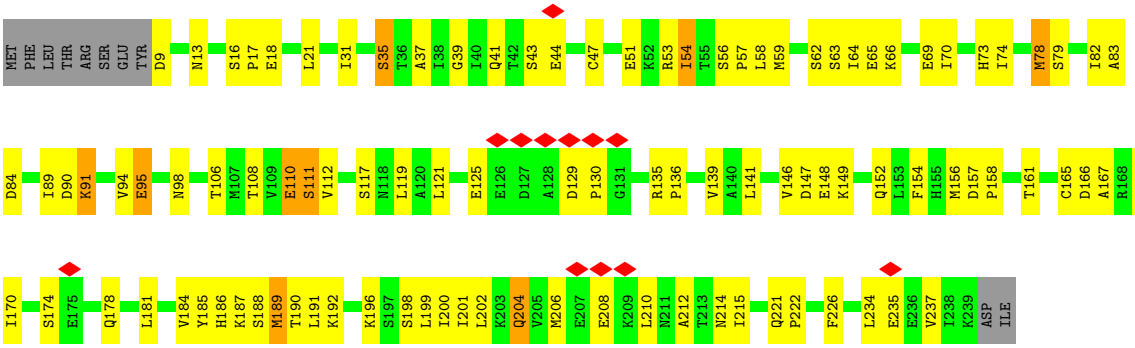
• Molecule 9: Proteasome subunit beta type-4

Chain W:



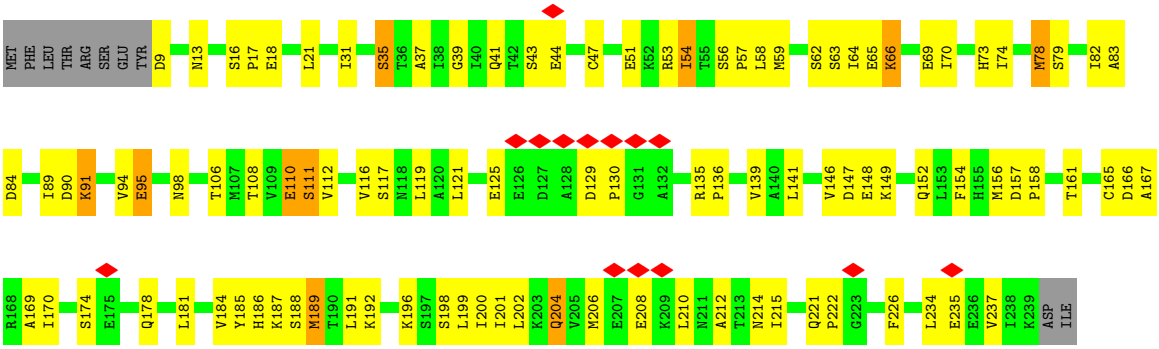
• Molecule 10: Proteasome subunit alpha type-5

Chain H:



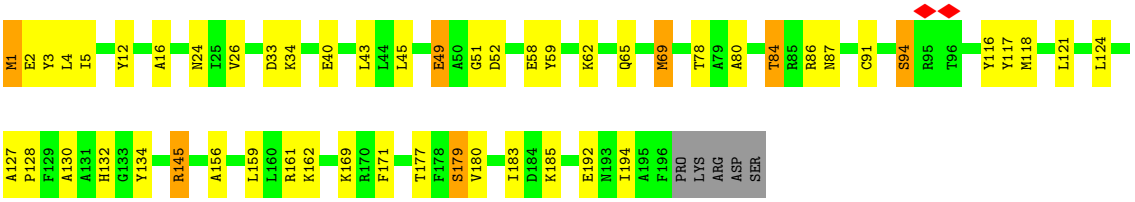
• Molecule 10: Proteasome subunit alpha type-5

Chain M:



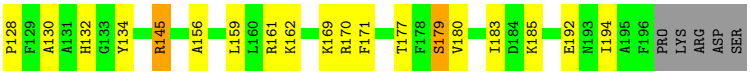
• Molecule 11: Proteasome subunit beta type-2

Chain V:

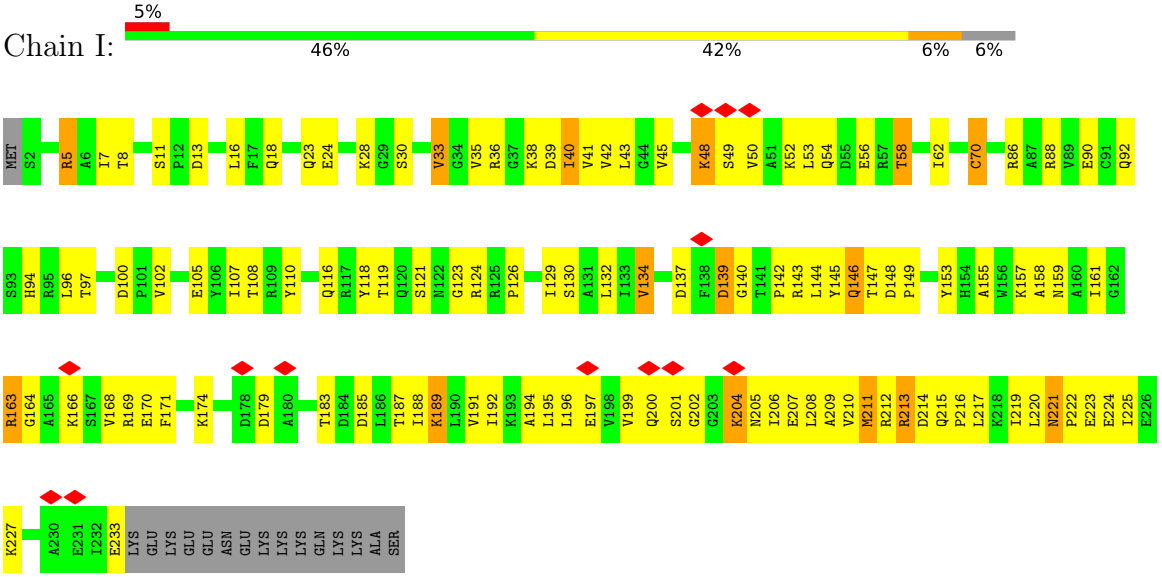


• Molecule 11: Proteasome subunit beta type-2

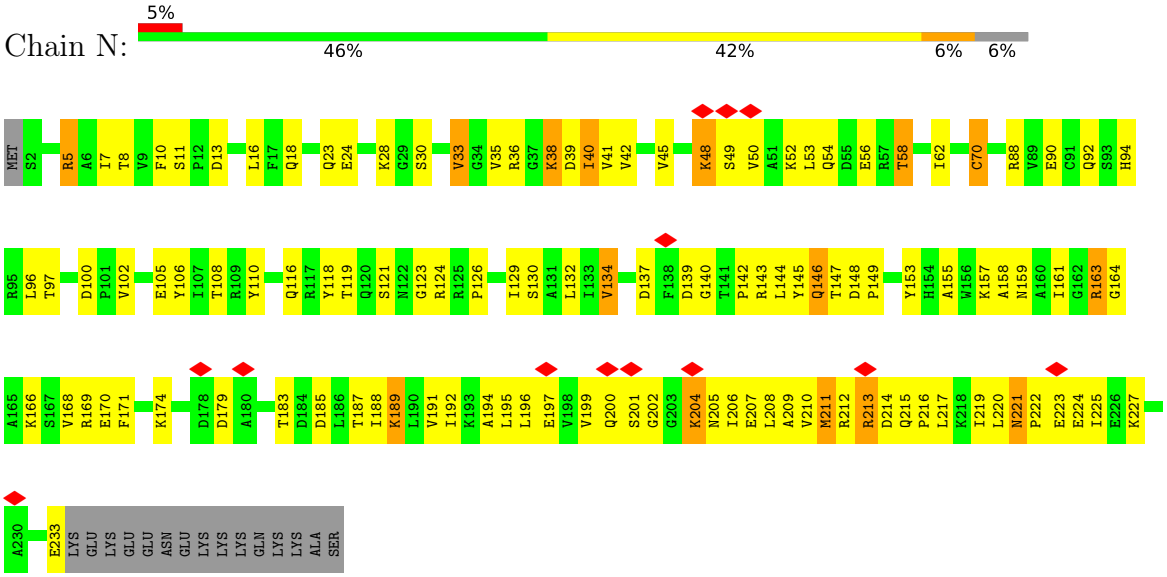
Chain T:



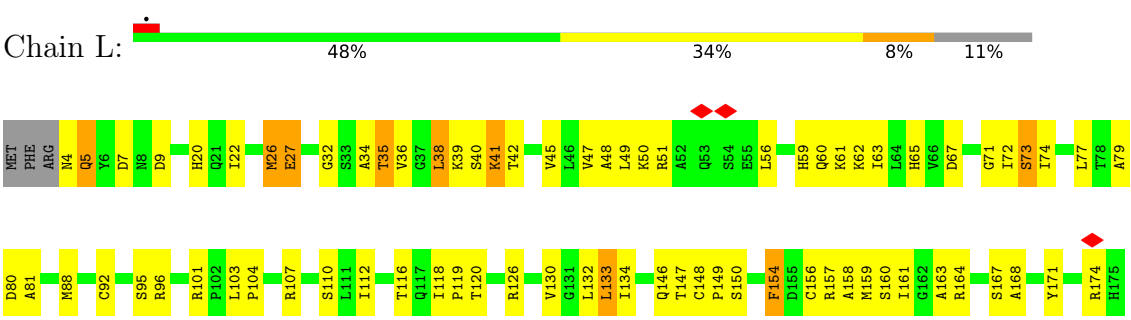
• Molecule 12: Proteasome subunit alpha type-7

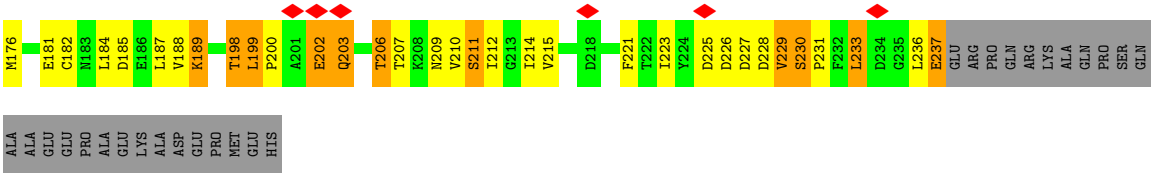


• Molecule 12: Proteasome subunit alpha type-7



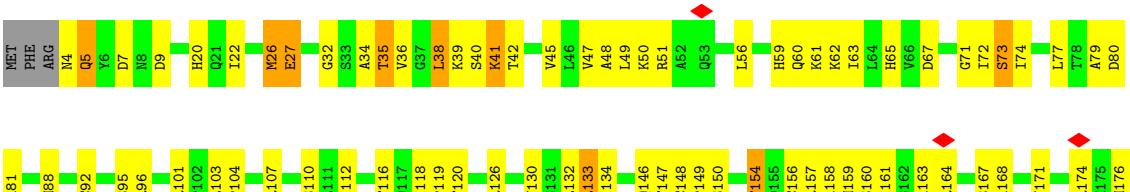
• Molecule 13: Proteasome subunit alpha type-1

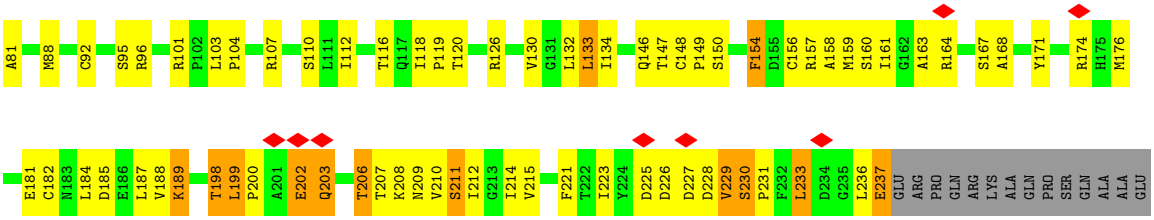




• Molecule 13: Proteasome subunit alpha type-1

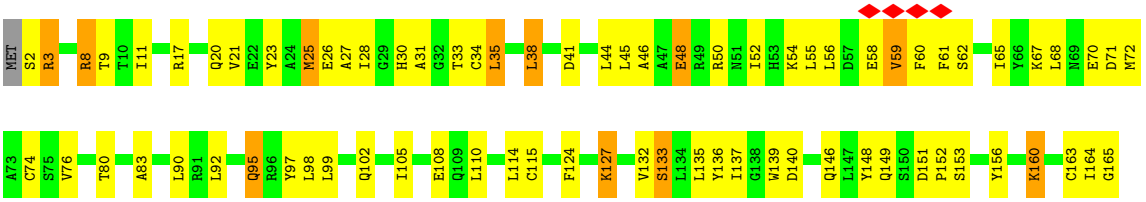
Chain G:

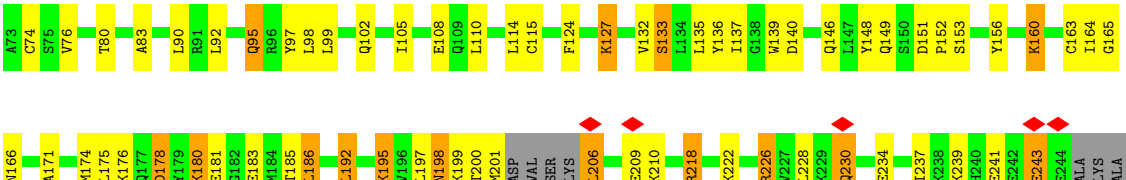


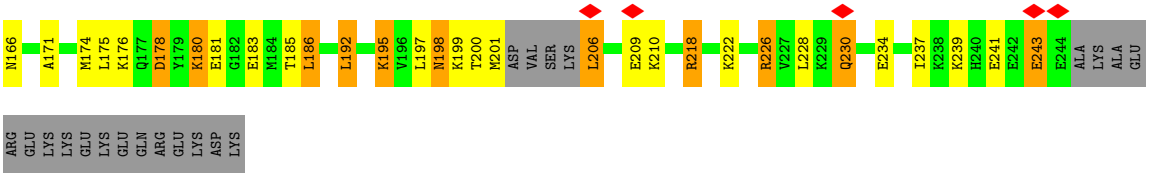


• Molecule 14: Proteasome subunit alpha type-4

Chain O:

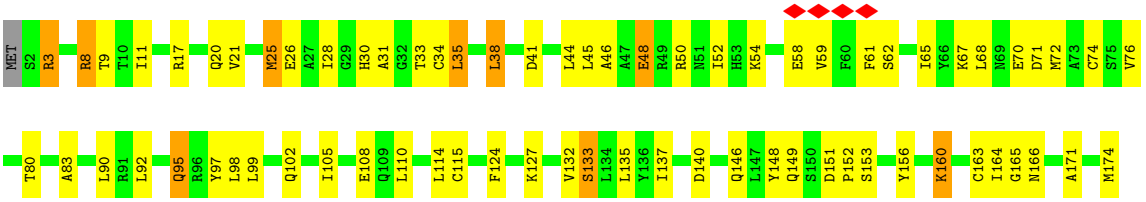


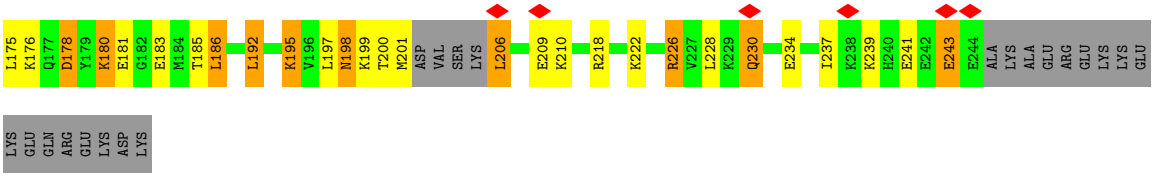




• Molecule 14: Proteasome subunit alpha type-4

Chain Z:




L175 K176 Q177 D178 Y179 K180 E181 G182 E183 M184 T185 L186 L192 K195 V196 L197 N198 K199 T200 M201 ASP VAL SER LYS L206 E209 K210 R218 K222 R226 V227 L228 K229 Q230 E234 I237 K238 K239 H240 E241 E242 E243 E244 ALA LYS ALA GLU ARG GLU LYS LYS GLU
LYS GLU GLN ARG GLU LYS ASP LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	118136	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	48.2	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.196	Depositor
Minimum map value	-0.107	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0282	Depositor
Map size (Å)	292.16095, 292.16095, 292.16095	wwPDB
Map dimensions	254, 254, 254	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15024, 1.15024, 1.15024	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1L0D

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	B	0.25	0/1683	0.45	0/2276
1	E	0.25	0/1683	0.45	0/2276
2	C	0.26	0/1575	0.41	0/2127
2	D	0.26	0/1575	0.41	0/2127
3	P	0.25	0/1820	0.43	0/2466
3	b	0.25	0/1820	0.43	0/2466
4	J	0.24	0/1875	0.42	0/2524
4	Q	0.24	0/1875	0.42	0/2524
5	K	0.23	0/1863	0.43	0/2518
5	R	0.23	0/1863	0.43	0/2518
6	A	0.54	0/1539	0.72	0/2084
6	F	0.54	0/1539	0.71	0/2084
7	S	0.25	0/1674	0.44	0/2257
7	X	0.25	0/1674	0.44	0/2257
8	U	0.26	0/1621	0.45	0/2185
8	Y	0.26	0/1621	0.45	0/2185
9	W	0.26	0/1704	0.46	0/2306
9	a	0.26	0/1704	0.46	0/2306
10	H	0.23	0/1788	0.41	0/2415
10	M	0.23	0/1788	0.41	0/2415
11	T	0.26	0/1602	0.45	0/2167
11	V	0.26	0/1602	0.45	0/2167
12	I	0.23	0/1846	0.42	0/2495
12	N	0.23	0/1846	0.42	0/2495
13	G	0.23	0/1870	0.43	0/2528
13	L	0.23	0/1870	0.43	0/2528
14	O	0.27	0/1910	0.48	0/2573
14	Z	0.27	0/1910	0.48	0/2573
All	All	0.27	0/48740	0.46	0/65842

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	B	1656	0	1685	67	0
1	E	1656	0	1685	66	0
2	C	1544	0	1511	42	0
2	D	1544	0	1511	41	0
3	P	1781	0	1771	115	0
3	b	1781	0	1771	0	0
4	J	1840	0	1827	93	0
4	Q	1840	0	1827	92	0
5	K	1831	0	1841	102	0
5	R	1831	0	1841	104	0
6	A	1512	0	1478	51	0
6	F	1512	0	1478	53	0
7	S	1643	0	1638	41	0
7	X	1643	0	1638	42	0
8	U	1592	0	1612	53	0
8	Y	1592	0	1612	53	0
9	W	1671	0	1648	55	0
9	a	1671	0	1648	0	0
10	H	1761	0	1749	96	0
10	M	1761	0	1749	99	0
11	T	1570	0	1573	35	0
11	V	1570	0	1573	34	0
12	I	1819	0	1845	89	0
12	N	1819	0	1845	91	0
13	G	1836	0	1822	92	0
13	L	1836	0	1822	89	0
14	O	1881	0	1896	109	0
14	Z	1881	0	1896	94	0
15	A	31	0	0	1	0
15	C	56	0	0	1	0
15	D	56	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	F	31	0	0	1	0
All	All	48048	0	47792	1714	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 20.

All (1714) 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)
12:I:41:VAL:HG11	12:I:134:VAL:CG1	1.57	1.32
12:N:41:VAL:HG11	12:N:134:VAL:CG1	1.57	1.30
14:Z:174:MET:HE1	14:Z:199:LYS:CB	1.64	1.26
14:O:174:MET:HE1	14:O:199:LYS:CB	1.66	1.25
10:H:31:ILE:HD11	10:H:158:PRO:HG3	1.24	1.17
12:I:41:VAL:HG11	12:I:134:VAL:HG13	1.19	1.15
10:M:31:ILE:HD11	10:M:158:PRO:CG	1.76	1.15
10:H:31:ILE:HD11	10:H:158:PRO:CG	1.76	1.15
5:K:155:ASP:HB2	5:K:156:PRO:HD2	1.18	1.15
12:N:41:VAL:HG11	12:N:134:VAL:HG13	1.19	1.11
10:M:31:ILE:HD11	10:M:158:PRO:HG3	1.25	1.11
6:A:58:ALA:HB3	6:A:86:MET:HE1	1.21	1.10
12:I:5:ARG:NH1	14:Z:8:ARG:HD2	1.65	1.10
12:N:41:VAL:CG1	12:N:134:VAL:HG11	1.83	1.09
5:R:155:ASP:HB2	5:R:156:PRO:HD2	1.18	1.09
6:F:58:ALA:HB3	6:F:86:MET:HE1	1.34	1.08
12:I:41:VAL:CG1	12:I:134:VAL:HG11	1.83	1.08
14:Z:72:MET:HE2	14:Z:110:LEU:HD23	1.36	1.08
14:O:8:ARG:HD2	12:N:5:ARG:NH1	1.69	1.07
4:Q:56:LYS:HA	4:Q:56:LYS:HE3	1.37	1.07
14:O:174:MET:HE1	14:O:199:LYS:HB2	1.10	1.07
14:Z:174:MET:CE	14:Z:199:LYS:CB	2.33	1.07
14:O:174:MET:CE	14:O:199:LYS:CB	2.33	1.06
14:O:72:MET:HE2	14:O:110:LEU:HD23	1.30	1.06
12:N:94:HIS:CG	12:N:102:VAL:HG12	1.93	1.04
12:N:221:ASN:HB2	12:N:222:PRO:HD2	1.39	1.04
14:Z:174:MET:HE1	14:Z:199:LYS:HB2	1.09	1.04
10:H:18:GLU:O	13:G:27:GLU:HB3	1.57	1.04
12:I:94:HIS:CG	12:I:102:VAL:HG12	1.93	1.03
13:L:27:GLU:HB3	10:M:18:GLU:O	1.57	1.03
4:J:49:VAL:HG11	4:J:65:ARG:HE	1.23	1.03
4:J:56:LYS:HA	4:J:56:LYS:HE3	1.37	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:221:ASN:HB2	12:I:222:PRO:HD2	1.39	1.02
12:N:41:VAL:CG1	12:N:134:VAL:CG1	2.37	1.02
5:R:52:THR:HG23	5:R:216:GLU:HG3	1.42	1.01
5:K:52:THR:HG23	5:K:216:GLU:HG3	1.42	1.01
3:P:48:GLU:HG3	3:P:198:PHE:CE2	1.96	1.01
10:H:31:ILE:CD1	10:H:158:PRO:CG	2.39	1.01
10:M:196:LYS:O	10:M:200:ILE:HD12	1.60	1.00
12:I:41:VAL:CG1	12:I:134:VAL:CG1	2.37	1.00
10:H:196:LYS:O	10:H:200:ILE:HD12	1.60	1.00
12:I:221:ASN:HB2	12:I:222:PRO:CD	1.92	0.99
12:N:221:ASN:HB2	12:N:222:PRO:CD	1.92	0.99
6:F:58:ALA:HB3	6:F:86:MET:CE	1.92	0.99
10:M:31:ILE:CD1	10:M:158:PRO:CG	2.39	0.99
6:A:58:ALA:HB3	6:A:86:MET:CE	1.92	0.99
14:O:72:MET:CE	14:O:110:LEU:HD23	1.93	0.98
4:Q:49:VAL:HG11	4:Q:65:ARG:HE	1.23	0.98
14:Z:72:MET:CE	14:Z:110:LEU:HD23	1.93	0.97
12:I:58:THR:HG22	14:Z:108:GLU:OE2	1.64	0.97
10:H:129:ASP:HB2	10:H:130:PRO:CD	1.94	0.97
12:N:41:VAL:HG11	12:N:134:VAL:HG11	1.40	0.96
10:M:129:ASP:HB2	10:M:130:PRO:CD	1.94	0.95
5:K:196:GLU:HG2	5:K:242:LEU:HD23	1.49	0.94
1:B:208:THR:HG22	8:Y:164:GLU:OE1	1.67	0.94
14:Z:230:GLN:HE21	14:Z:230:GLN:HA	1.32	0.94
14:O:108:GLU:OE2	12:N:58:THR:HG22	1.68	0.94
14:O:230:GLN:HA	14:O:230:GLN:HE21	1.32	0.93
1:E:208:THR:HG22	8:U:164:GLU:OE1	1.68	0.93
10:M:51:GLU:HB3	10:M:206:MET:HE2	1.51	0.92
5:K:155:ASP:HB2	5:K:156:PRO:CD	1.99	0.92
5:R:196:GLU:HG2	5:R:242:LEU:HD23	1.49	0.92
10:H:129:ASP:HB2	10:H:130:PRO:HD2	1.51	0.92
10:M:129:ASP:HB2	10:M:130:PRO:HD2	1.51	0.91
7:S:145:LEU:HD21	7:S:182:ALA:HB2	1.53	0.91
12:I:41:VAL:HG11	12:I:134:VAL:HG11	1.40	0.91
5:R:155:ASP:HB2	5:R:156:PRO:CD	1.99	0.91
5:K:52:THR:CG2	5:K:216:GLU:HG3	2.01	0.91
12:I:48:LYS:HD3	12:I:163:ARG:CZ	2.01	0.91
7:X:145:LEU:HD21	7:X:182:ALA:HB2	1.53	0.91
12:N:48:LYS:HD3	12:N:163:ARG:CZ	2.01	0.90
10:M:166:ASP:HB3	10:M:185:TYR:OH	1.70	0.90
5:R:52:THR:CG2	5:R:216:GLU:HG3	2.01	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:36:GLU:HG2	2:D:184:TRP:CZ2	2.07	0.90
10:H:166:ASP:HB3	10:H:185:TYR:OH	1.70	0.89
13:L:4:ASN:HB3	13:L:5:GLN:HE21	1.37	0.89
2:C:36:GLU:HG2	2:C:184:TRP:CZ2	2.07	0.89
1:B:42:TYR:CE1	1:B:183:LEU:HD11	2.08	0.89
13:G:4:ASN:HB3	13:G:5:GLN:HE21	1.37	0.89
4:J:136:MET:HE2	4:J:165:ILE:HG12	1.55	0.89
12:I:36:ARG:HD2	12:I:142:PRO:O	1.73	0.89
1:E:42:TYR:CE1	1:E:183:LEU:HD11	2.08	0.88
3:P:204:GLU:OE2	3:P:222:PRO:HB3	1.74	0.88
10:H:212:ALA:HB2	10:H:235:GLU:HG2	1.56	0.87
14:O:180:LYS:HB3	14:O:183:GLU:HG3	1.56	0.87
14:Z:180:LYS:HB3	14:Z:183:GLU:HG3	1.56	0.87
10:M:212:ALA:HB2	10:M:235:GLU:HG2	1.56	0.87
12:N:36:ARG:HD2	12:N:142:PRO:O	1.73	0.87
3:P:7:PHE:O	3:P:124:GLY:HA2	1.74	0.87
4:J:56:LYS:HG3	13:G:176:MET:HE1	1.56	0.86
13:G:148:CYS:HB2	13:G:149:PRO:HD2	1.55	0.86
13:L:148:CYS:HB2	13:L:149:PRO:HD2	1.55	0.86
5:K:196:GLU:HG3	5:K:242:LEU:HD21	1.57	0.86
11:T:80:ALA:O	11:T:84:THR:HG22	1.77	0.85
13:L:148:CYS:HB2	13:L:149:PRO:CD	2.05	0.85
13:G:148:CYS:HB2	13:G:149:PRO:CD	2.05	0.85
4:J:72:HIS:O	4:J:139:SER:HB2	1.77	0.84
5:R:196:GLU:HG3	5:R:242:LEU:HD21	1.57	0.84
11:V:1:MET:HG2	11:V:134:TYR:H	1.43	0.84
4:Q:72:HIS:O	4:Q:139:SER:HB2	1.77	0.84
11:V:80:ALA:O	11:V:84:THR:HG22	1.77	0.83
6:A:52:THR:HG22	6:A:96:ALA:HB1	1.59	0.83
4:J:27:MET:HG2	4:J:153:PRO:HG2	1.60	0.83
11:T:80:ALA:O	11:T:84:THR:CG2	2.27	0.83
10:M:110:GLU:HG3	10:M:154:PHE:CZ	2.13	0.83
1:B:206:LYS:HE3	8:Y:160:GLU:OE1	1.79	0.83
3:P:156:ALA:HB2	14:O:59:VAL:HG21	1.61	0.83
3:P:35:VAL:HG21	3:P:193:THR:HG23	1.61	0.82
10:H:110:GLU:HG3	10:H:154:PHE:CZ	2.13	0.82
6:F:52:THR:HG22	6:F:96:ALA:HB1	1.59	0.82
11:V:80:ALA:O	11:V:84:THR:CG2	2.27	0.82
4:J:230:ASP:OD1	4:J:230:ASP:N	2.12	0.82
1:B:203:ARG:HD2	8:Y:161:HIS:NE2	1.94	0.81
11:T:1:MET:HG2	11:T:134:TYR:H	1.43	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:31:ILE:CD1	10:M:158:PRO:HG2	2.10	0.81
4:Q:230:ASP:OD1	4:Q:230:ASP:N	2.12	0.81
3:P:149:ASP:HB2	3:P:150:PRO:HD2	1.62	0.81
13:G:49:LEU:CD2	13:G:199:LEU:HD21	2.11	0.81
4:Q:27:MET:HG2	4:Q:153:PRO:HG2	1.60	0.81
14:Z:174:MET:CE	14:Z:199:LYS:HB2	2.01	0.81
1:E:206:LYS:HE3	8:U:160:GLU:OE1	1.80	0.81
10:H:31:ILE:CD1	10:H:158:PRO:HG2	2.10	0.80
1:E:59:ILE:HG12	1:E:83:LEU:HG	1.64	0.80
13:L:49:LEU:CD2	13:L:199:LEU:HD21	2.11	0.80
1:E:203:ARG:HD2	8:U:161:HIS:NE2	1.96	0.80
3:P:108:GLN:NE2	8:U:77:GLU:HB3	1.95	0.80
12:I:168:VAL:HG13	12:I:194:ALA:HB1	1.63	0.79
14:Z:174:MET:CE	14:Z:199:LYS:HB3	2.11	0.79
1:B:59:ILE:HG12	1:B:83:LEU:HG	1.64	0.79
13:G:49:LEU:HD21	13:G:199:LEU:HD21	1.64	0.79
4:Q:56:LYS:HG3	13:L:176:MET:HE1	1.64	0.79
12:N:168:VAL:HG13	12:N:194:ALA:HB1	1.63	0.79
13:L:49:LEU:HD21	13:L:199:LEU:HD21	1.64	0.79
7:X:123:SER:HB3	7:X:136:LYS:HG2	1.65	0.79
3:P:37:ILE:HD12	3:P:190:ALA:HB2	1.63	0.78
3:P:149:ASP:HB2	3:P:150:PRO:CD	2.13	0.78
4:J:152:ASP:HB2	4:J:153:PRO:HD2	1.65	0.78
7:X:45:LYS:HD2	7:X:203:ILE:HD12	1.65	0.78
5:R:22:LEU:HD13	5:R:126:THR:CG2	2.13	0.78
7:S:123:SER:HB3	7:S:136:LYS:HG2	1.66	0.78
10:M:35:SER:HB2	10:M:51:GLU:HG3	1.66	0.78
2:C:8:PHE:HD1	2:C:8:PHE:H	1.32	0.78
7:S:45:LYS:HD2	7:S:203:ILE:HD12	1.65	0.78
13:G:35:THR:HG21	13:G:73:SER:HB2	1.66	0.78
3:P:198:PHE:HE1	3:P:206:ASN:ND2	1.81	0.78
5:K:22:LEU:HD13	5:K:126:THR:CG2	2.13	0.78
3:P:37:ILE:HD13	3:P:189:THR:HG23	1.66	0.78
5:K:43:ARG:HH21	5:K:164:LYS:HG2	1.49	0.78
5:R:43:ARG:HH21	5:R:164:LYS:HG2	1.49	0.77
14:O:174:MET:CE	14:O:199:LYS:HB3	2.11	0.77
3:P:198:PHE:CE2	3:P:207:ILE:CG2	2.68	0.77
10:H:35:SER:HB2	10:H:51:GLU:HG3	1.66	0.77
6:F:58:ALA:O	6:F:62:GLN:HG3	1.84	0.77
13:L:35:THR:HG21	13:L:73:SER:HB2	1.66	0.77
6:A:58:ALA:O	6:A:62:GLN:HG3	1.85	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:157:ASP:HB2	10:M:158:PRO:CD	2.15	0.77
9:W:115:TYR:HE2	9:W:194:GLU:HG2	1.50	0.77
5:K:196:GLU:CG	5:K:242:LEU:CD2	2.63	0.77
5:R:196:GLU:CG	5:R:242:LEU:CD2	2.63	0.77
2:C:36:GLU:HG2	2:C:184:TRP:CH2	2.20	0.76
10:M:51:GLU:HB3	10:M:206:MET:CE	2.15	0.76
10:M:167:ALA:HB1	10:M:181:LEU:HD22	1.67	0.76
10:H:51:GLU:HB3	10:H:206:MET:CE	2.15	0.76
5:K:59:LYS:O	5:K:59:LYS:HE3	1.85	0.76
14:Z:52:ILE:HD12	14:Z:52:ILE:O	1.86	0.76
2:D:8:PHE:HD1	2:D:8:PHE:H	1.32	0.76
5:R:76:ILE:HD13	5:R:111:VAL:HG22	1.68	0.76
12:N:147:THR:HG22	12:N:153:TYR:HB3	1.67	0.76
10:H:167:ALA:HB1	10:H:181:LEU:HD22	1.67	0.76
2:D:36:GLU:HG2	2:D:184:TRP:CH2	2.20	0.76
1:B:198:ARG:CB	1:B:198:ARG:HH11	1.99	0.76
4:Q:152:ASP:HB2	4:Q:153:PRO:HD2	1.65	0.76
9:W:115:TYR:CE2	9:W:194:GLU:HG2	2.20	0.76
4:Q:136:MET:HE2	4:Q:165:ILE:HG12	1.66	0.76
4:J:136:MET:HE2	4:J:165:ILE:CG1	2.15	0.76
10:H:31:ILE:HD12	10:H:158:PRO:HG2	1.68	0.76
4:Q:56:LYS:HA	4:Q:56:LYS:CE	2.16	0.75
10:M:31:ILE:HD12	10:M:158:PRO:HG2	1.68	0.75
4:J:56:LYS:HA	4:J:56:LYS:CE	2.16	0.75
14:O:52:ILE:O	14:O:52:ILE:HD12	1.86	0.75
5:R:141:ILE:HD12	5:R:220:VAL:HG22	1.68	0.75
10:H:51:GLU:HB3	10:H:206:MET:HE2	1.68	0.75
12:I:147:THR:HG22	12:I:153:TYR:HB3	1.67	0.75
13:L:60:GLN:NE2	10:M:161:THR:HG23	2.01	0.75
8:Y:100:GLY:H	8:Y:101:PRO:HD3	1.50	0.75
4:Q:37:ILE:CD1	4:Q:193:VAL:HG22	2.17	0.75
10:H:157:ASP:HB2	10:H:158:PRO:CD	2.15	0.75
10:M:157:ASP:HB2	10:M:158:PRO:HD2	1.69	0.75
1:E:122:LEU:HB3	1:E:123:PRO:HD2	1.68	0.75
14:O:174:MET:CE	14:O:199:LYS:HB2	2.01	0.75
4:J:37:ILE:CD1	4:J:193:VAL:HG22	2.17	0.75
1:E:198:ARG:CB	1:E:198:ARG:HH11	1.99	0.75
5:R:59:LYS:HE3	5:R:59:LYS:O	1.85	0.74
6:F:124:SER:OG	6:A:200:ALA:HB1	1.88	0.74
14:O:46:ALA:HB1	14:O:197:LEU:HD11	1.69	0.74
8:U:100:GLY:H	8:U:101:PRO:HD3	1.50	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:40:SER:HB3	13:G:187:LEU:HD13	1.68	0.74
1:B:37:ILE:HA	1:B:60:SER:HB2	1.69	0.74
1:B:122:LEU:HB3	1:B:123:PRO:HD2	1.68	0.74
14:Z:46:ALA:HB1	14:Z:197:LEU:HD11	1.69	0.74
4:Q:108:LEU:HD13	4:Q:139:SER:HB3	1.68	0.74
6:F:200:ALA:HB1	6:A:124:SER:OG	1.86	0.74
1:E:20:ALA:HB3	1:E:28:ASP:HB3	1.70	0.74
4:J:37:ILE:HD11	4:J:193:VAL:HG22	1.69	0.74
5:K:76:ILE:HD13	5:K:111:VAL:HG22	1.68	0.74
5:K:52:THR:HG23	5:K:216:GLU:CG	2.18	0.74
14:Z:21:VAL:HG11	14:Z:153:SER:HB3	1.69	0.73
1:E:37:ILE:HA	1:E:60:SER:HB2	1.69	0.73
5:K:141:ILE:HD12	5:K:220:VAL:HG22	1.68	0.73
13:L:168:ALA:HB2	13:L:198:THR:HG22	1.71	0.73
14:Z:151:ASP:HB2	14:Z:152:PRO:HD2	1.70	0.73
4:Q:37:ILE:HD11	4:Q:193:VAL:HG22	1.69	0.73
10:H:157:ASP:HB2	10:H:158:PRO:HD2	1.69	0.73
8:U:26:ARG:HB2	8:U:182:MET:HB2	1.70	0.73
12:N:171:PHE:CB	12:N:197:GLU:OE2	2.37	0.73
1:B:20:ALA:HB3	1:B:28:ASP:HB3	1.70	0.73
5:R:155:ASP:CB	5:R:156:PRO:HD2	2.09	0.73
12:I:171:PHE:CB	12:I:197:GLU:OE2	2.37	0.73
13:L:40:SER:HB3	13:L:187:LEU:HD13	1.68	0.73
12:I:5:ARG:HH12	14:Z:8:ARG:HH11	1.37	0.73
3:P:74:VAL:HG12	3:P:134:LEU:HB2	1.71	0.73
14:O:151:ASP:HB2	14:O:152:PRO:HD2	1.70	0.73
13:L:60:GLN:HE22	10:M:161:THR:HG23	1.54	0.72
4:J:108:LEU:HD13	4:J:139:SER:HB3	1.68	0.72
14:Z:174:MET:CE	14:Z:199:LYS:CG	2.68	0.72
5:K:196:GLU:HG2	5:K:242:LEU:CD2	2.20	0.72
14:O:174:MET:CE	14:O:199:LYS:CG	2.67	0.72
6:F:58:ALA:CB	6:F:86:MET:CE	2.68	0.72
5:K:78:CYS:HB3	5:K:140:LEU:HD23	1.71	0.72
14:O:174:MET:HE2	14:O:199:LYS:CG	2.19	0.72
13:G:168:ALA:HB2	13:G:198:THR:HG22	1.71	0.72
5:R:52:THR:HG23	5:R:216:GLU:CG	2.18	0.72
10:H:110:GLU:HG3	10:H:154:PHE:CE2	2.25	0.72
14:O:21:VAL:HG11	14:O:153:SER:HB3	1.69	0.72
10:H:18:GLU:O	13:G:27:GLU:CB	2.38	0.72
5:R:78:CYS:HB3	5:R:140:LEU:HD23	1.71	0.71
3:P:88:ARG:NH1	3:P:88:ARG:HG3	2.04	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:145:ARG:HH11	11:V:145:ARG:HG3	1.56	0.71
10:M:110:GLU:HG3	10:M:154:PHE:CE2	2.25	0.71
3:P:88:ARG:HG3	3:P:88:ARG:HH11	1.55	0.71
8:Y:26:ARG:HB2	8:Y:182:MET:HB2	1.70	0.71
11:T:145:ARG:HG3	11:T:145:ARG:HH11	1.56	0.71
13:L:79:ALA:HB3	10:M:121:LEU:HD12	1.71	0.71
14:Z:151:ASP:HB2	14:Z:152:PRO:CD	2.21	0.71
4:Q:136:MET:CE	4:Q:165:ILE:CG1	2.69	0.71
5:R:196:GLU:HG3	5:R:242:LEU:CD2	2.21	0.71
7:S:45:LYS:HD2	7:S:203:ILE:CD1	2.21	0.71
4:Q:195:LYS:HA	4:Q:239:ALA:HB1	1.73	0.70
5:R:196:GLU:CG	5:R:242:LEU:HD23	2.20	0.70
10:M:146:VAL:HG11	10:M:222:PRO:HA	1.73	0.70
4:J:136:MET:CE	4:J:165:ILE:CG1	2.69	0.70
14:O:151:ASP:HB2	14:O:152:PRO:CD	2.21	0.70
7:X:45:LYS:HD2	7:X:203:ILE:CD1	2.21	0.70
10:H:146:VAL:HG11	10:H:222:PRO:HA	1.73	0.70
5:K:196:GLU:CG	5:K:242:LEU:HD23	2.20	0.70
3:P:156:ALA:CB	14:O:59:VAL:HG21	2.20	0.70
5:K:196:GLU:HG3	5:K:242:LEU:CD2	2.21	0.70
4:J:195:LYS:HA	4:J:239:ALA:HB1	1.73	0.70
12:I:221:ASN:CB	12:I:222:PRO:CD	2.68	0.70
5:K:88:ARG:HH11	5:K:88:ARG:HG3	1.57	0.70
9:W:157:GLN:HE21	9:W:160:LEU:HD23	1.55	0.70
1:B:24:MET:HE1	7:S:33:PHE:CZ	2.26	0.70
4:Q:57:LEU:HB3	13:L:158:ALA:O	1.92	0.70
14:O:174:MET:HE2	14:O:199:LYS:HD2	1.73	0.70
2:D:3:THR:HB	2:D:44:THR:HG21	1.74	0.69
4:J:136:MET:CE	4:J:165:ILE:HG13	2.22	0.69
10:H:161:THR:HG23	13:G:60:GLN:NE2	2.06	0.69
4:J:152:ASP:HB2	4:J:153:PRO:CD	2.22	0.69
5:K:88:ARG:HG3	5:K:88:ARG:NH1	2.07	0.69
9:W:14:VAL:HG12	9:W:21:VAL:HG12	1.74	0.69
13:G:71:GLY:HA3	13:G:221:PHE:CZ	2.27	0.69
5:R:196:GLU:HG2	5:R:242:LEU:CD2	2.20	0.69
2:C:3:THR:HB	2:C:44:THR:HG21	1.74	0.69
5:R:88:ARG:HH11	5:R:88:ARG:HG3	1.57	0.69
6:A:58:ALA:CB	6:A:86:MET:CE	2.68	0.69
12:N:208:LEU:HD11	12:N:220:LEU:HD12	1.75	0.69
5:R:88:ARG:HG3	5:R:88:ARG:NH1	2.06	0.69
7:X:148:LEU:HD12	7:X:178:VAL:HG12	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:59:LYS:CE	5:R:59:LYS:HA	2.23	0.69
6:F:144:ARG:HH11	6:F:144:ARG:HG3	1.57	0.69
12:I:208:LEU:HD11	12:I:220:LEU:HD12	1.75	0.69
14:Z:174:MET:HE2	14:Z:199:LYS:HD2	1.73	0.69
6:A:144:ARG:HG3	6:A:144:ARG:HH11	1.57	0.69
9:W:92:LEU:HD12	9:W:112:ILE:HD11	1.74	0.69
4:Q:152:ASP:HB2	4:Q:153:PRO:CD	2.22	0.69
12:I:45:VAL:HG23	12:I:62:ILE:HD11	1.75	0.69
14:O:8:ARG:HH11	12:N:5:ARG:HH12	1.40	0.69
3:P:58:GLU:CD	3:P:58:GLU:H	1.95	0.69
4:Q:136:MET:CE	4:Q:165:ILE:HG13	2.22	0.69
7:S:148:LEU:HD12	7:S:178:VAL:HG12	1.75	0.69
14:Z:35:LEU:C	14:Z:35:LEU:HD12	2.13	0.69
14:Z:198:ASN:OD1	14:Z:206:LEU:HD23	1.93	0.69
3:P:198:PHE:HE2	3:P:207:ILE:CG2	2.05	0.68
10:M:91:LYS:HD2	10:M:119:LEU:HD11	1.75	0.68
1:B:151:ALA:O	1:B:155:VAL:HG23	1.94	0.68
7:S:28:ARG:HB2	7:S:191:ASP:OD2	1.94	0.68
14:Z:174:MET:HE2	14:Z:199:LYS:CG	2.22	0.68
12:N:45:VAL:HG23	12:N:62:ILE:HD11	1.75	0.68
3:P:68:THR:HG22	3:P:71:ILE:HB	1.74	0.68
10:H:91:LYS:HD2	10:H:119:LEU:HD11	1.76	0.68
12:N:164:GLY:O	12:N:168:VAL:HG23	1.93	0.68
3:P:74:VAL:CG1	3:P:134:LEU:HB2	2.24	0.68
6:F:17:ASP:OD2	6:F:33:LYS:NZ	2.26	0.68
5:K:43:ARG:NH2	5:K:164:LYS:HG2	2.08	0.68
14:O:35:LEU:C	14:O:35:LEU:HD12	2.13	0.68
4:J:151:ILE:N	4:J:151:ILE:HD12	2.09	0.68
5:K:11:ARG:HG3	5:K:11:ARG:HH11	1.58	0.68
10:M:129:ASP:CB	10:M:130:PRO:CD	2.68	0.68
14:Z:230:GLN:HA	14:Z:230:GLN:NE2	2.07	0.68
2:D:144:SER:HB3	2:D:147:LEU:HD13	1.76	0.68
12:I:164:GLY:O	12:I:168:VAL:HG23	1.93	0.68
12:I:219:ILE:HD12	12:I:219:ILE:N	2.08	0.68
13:L:71:GLY:HA3	13:L:221:PHE:CZ	2.27	0.68
4:Q:186:CYS:O	4:Q:190:VAL:HG23	1.94	0.68
4:J:49:VAL:CG1	4:J:65:ARG:HE	2.04	0.68
4:J:57:LEU:HB3	13:G:158:ALA:O	1.94	0.68
4:J:151:ILE:HG13	4:J:157:SER:HB3	1.75	0.68
13:L:27:GLU:CB	10:M:18:GLU:O	2.38	0.68
10:H:121:LEU:HD12	13:G:79:ALA:HB3	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:17:ASP:OD2	6:A:33:LYS:NZ	2.26	0.68
2:C:144:SER:HB3	2:C:147:LEU:HD13	1.75	0.67
3:P:10:THR:HG23	3:P:20:GLN:HB2	1.76	0.67
1:E:63:LEU:HD11	1:E:79:ALA:HB2	1.76	0.67
1:B:63:LEU:HD11	1:B:79:ALA:HB2	1.76	0.67
4:Q:151:ILE:HD12	4:Q:151:ILE:N	2.09	0.67
7:X:28:ARG:HB2	7:X:191:ASP:OD2	1.94	0.67
14:O:198:ASN:OD1	14:O:206:LEU:HD23	1.94	0.67
12:N:219:ILE:HD12	12:N:219:ILE:N	2.09	0.67
3:P:112:ARG:HH11	3:P:112:ARG:HG3	1.58	0.67
7:S:148:LEU:HD12	7:S:178:VAL:CG1	2.24	0.67
5:R:43:ARG:NH2	5:R:164:LYS:HG2	2.08	0.67
4:J:185:THR:O	4:J:189:VAL:HG23	1.95	0.67
1:E:24:MET:HE2	7:X:33:PHE:CZ	2.29	0.67
5:K:171:LYS:HG3	5:K:206:LEU:CD2	2.25	0.67
11:T:169:LYS:HG2	11:T:169:LYS:O	1.94	0.67
3:P:55:LEU:HD22	5:R:165:ALA:HB3	1.76	0.67
3:P:106:THR:OG1	3:P:139:ASN:ND2	2.27	0.67
3:P:198:PHE:CE1	3:P:206:ASN:ND2	2.62	0.67
4:Q:151:ILE:HG13	4:Q:157:SER:HB3	1.75	0.67
5:R:11:ARG:HH11	5:R:11:ARG:HG3	1.59	0.67
1:E:151:ALA:O	1:E:155:VAL:HG23	1.94	0.67
7:X:148:LEU:HD12	7:X:178:VAL:CG1	2.24	0.67
10:H:161:THR:HG23	13:G:60:GLN:HE22	1.58	0.67
6:A:52:THR:HG22	6:A:96:ALA:CB	2.25	0.67
4:J:186:CYS:O	4:J:190:VAL:HG23	1.94	0.66
1:B:13:VAL:HG12	1:B:155:VAL:HG21	1.77	0.66
5:K:178:PHE:CE1	5:K:201:CYS:HB2	2.30	0.66
3:P:74:VAL:HG12	3:P:134:LEU:CB	2.26	0.66
5:R:178:PHE:CE1	5:R:201:CYS:HB2	2.30	0.66
3:P:48:GLU:HG3	3:P:198:PHE:CD2	2.30	0.66
1:E:13:VAL:HG12	1:E:155:VAL:HG21	1.78	0.66
14:O:226:ARG:O	14:O:226:ARG:HD3	1.95	0.66
13:G:212:ILE:HD12	13:G:229:VAL:HG22	1.77	0.66
9:W:211:ILE:HA	9:W:214:MET:HE3	1.76	0.66
4:Q:56:LYS:HG3	13:L:176:MET:CE	2.26	0.66
13:G:189:LYS:HG3	13:G:236:LEU:CD1	2.26	0.66
11:V:169:LYS:HG2	11:V:169:LYS:O	1.94	0.66
13:L:189:LYS:HG3	13:L:236:LEU:CD1	2.26	0.66
4:Q:136:MET:HE2	4:Q:165:ILE:CG1	2.25	0.66
4:Q:185:THR:O	4:Q:189:VAL:HG23	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:230:GLN:HA	14:O:230:GLN:NE2	2.07	0.66
14:Z:226:ARG:O	14:Z:226:ARG:HD3	1.95	0.66
2:D:4:LEU:C	2:D:4:LEU:HD12	2.16	0.66
10:H:58:LEU:HD13	12:I:158:ALA:O	1.96	0.66
5:K:59:LYS:HA	5:K:59:LYS:CE	2.23	0.66
14:O:174:MET:HE2	14:O:199:LYS:CB	2.24	0.66
2:C:4:LEU:C	2:C:4:LEU:HD12	2.16	0.66
4:Q:50:GLU:O	4:Q:50:GLU:HG3	1.96	0.66
10:H:166:ASP:HB3	10:H:185:TYR:CZ	2.30	0.66
14:O:174:MET:HE1	14:O:199:LYS:HB3	1.69	0.66
13:L:118:ILE:HB	13:L:119:PRO:HD3	1.78	0.65
4:J:50:GLU:HG3	4:J:50:GLU:O	1.97	0.65
4:Q:56:LYS:CG	13:L:176:MET:CE	2.74	0.65
13:G:168:ALA:HB2	13:G:198:THR:CG2	2.27	0.65
3:P:156:ALA:CB	14:O:59:VAL:CG2	2.74	0.65
10:M:166:ASP:HB3	10:M:185:TYR:CZ	2.30	0.65
5:R:171:LYS:HG3	5:R:206:LEU:CD2	2.25	0.65
4:J:27:MET:HG2	4:J:153:PRO:CG	2.26	0.65
1:E:24:MET:CE	7:X:33:PHE:CZ	2.80	0.65
4:Q:49:VAL:CG1	4:Q:65:ARG:HE	2.04	0.65
6:F:52:THR:HG22	6:F:96:ALA:CB	2.25	0.65
13:L:212:ILE:HD12	13:L:229:VAL:HG22	1.77	0.65
8:U:11:MET:HG3	8:U:137:VAL:HG12	1.79	0.65
3:P:188:HIS:CE1	3:P:228:TYR:HD1	2.14	0.65
4:Q:56:LYS:CG	13:L:176:MET:HE2	2.27	0.65
1:B:24:MET:CE	7:S:33:PHE:CZ	2.79	0.64
5:R:171:LYS:HG3	5:R:206:LEU:HD21	1.79	0.64
13:L:168:ALA:HB2	13:L:198:THR:CG2	2.27	0.64
14:O:176:LYS:CG	12:N:53:LEU:HD11	2.28	0.64
5:R:48:ALA:HB3	5:R:220:VAL:CG2	2.27	0.64
12:N:209:ALA:HB1	12:N:217:LEU:HD11	1.80	0.64
13:G:118:ILE:HB	13:G:119:PRO:HD3	1.78	0.64
13:G:189:LYS:CG	13:G:236:LEU:CD1	2.75	0.64
12:I:196:LEU:HD23	12:I:202:GLY:HA3	1.80	0.64
4:Q:27:MET:HG2	4:Q:153:PRO:CG	2.26	0.64
8:Y:11:MET:HG3	8:Y:137:VAL:HG12	1.79	0.64
5:K:59:LYS:HE3	5:K:59:LYS:CA	2.28	0.64
13:L:189:LYS:HG2	13:L:236:LEU:HD12	1.79	0.64
14:O:90:LEU:HG	14:O:114:LEU:HD13	1.80	0.64
3:P:6:SER:O	14:O:127:LYS:HE3	1.97	0.64
11:V:43:LEU:HB2	11:V:183:ILE:HD11	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:43:LEU:HB2	11:T:183:ILE:HD11	1.80	0.64
13:L:189:LYS:CG	13:L:236:LEU:CD1	2.75	0.64
13:G:189:LYS:HG2	13:G:236:LEU:HD12	1.79	0.64
9:W:178:TYR:CE1	9:W:207:THR:HG22	2.33	0.64
7:S:146:GLN:HB3	7:S:147:PRO:HD3	1.80	0.64
5:R:59:LYS:HE3	5:R:59:LYS:CA	2.28	0.63
1:E:13:VAL:CG1	1:E:155:VAL:HG21	2.27	0.63
5:K:48:ALA:HB3	5:K:220:VAL:CG2	2.27	0.63
4:J:56:LYS:CG	13:G:176:MET:CE	2.76	0.63
12:I:209:ALA:HB1	12:I:217:LEU:HD11	1.80	0.63
12:N:196:LEU:HD23	12:N:202:GLY:HA3	1.80	0.63
1:B:139:GLU:OE2	1:B:139:GLU:HA	1.99	0.63
10:H:129:ASP:CB	10:H:130:PRO:CD	2.68	0.63
12:I:140:GLY:HA3	12:I:213:ARG:CZ	2.28	0.63
7:X:146:GLN:HB3	7:X:147:PRO:HD3	1.81	0.63
5:K:171:LYS:HG3	5:K:206:LEU:HD21	1.79	0.63
4:J:12:SER:HB3	4:J:125:TYR:HA	1.80	0.63
13:L:104:PRO:HB2	13:L:107:ARG:HG3	1.80	0.63
12:N:221:ASN:CB	12:N:222:PRO:CD	2.68	0.63
10:H:208:GLU:HB3	10:H:214:ASN:HD21	1.64	0.63
1:B:13:VAL:CG1	1:B:155:VAL:HG21	2.27	0.63
6:F:58:ALA:CB	6:F:86:MET:HE3	2.28	0.63
1:E:42:TYR:CD1	1:E:183:LEU:HD11	2.34	0.63
13:L:176:MET:HG3	13:L:176:MET:O	1.98	0.63
10:M:208:GLU:HB3	10:M:214:ASN:HD21	1.64	0.63
4:Q:87:LEU:HD12	4:Q:133:CYS:SG	2.39	0.63
10:H:191:LEU:HD22	10:H:221:GLN:HG2	1.81	0.63
13:G:104:PRO:HB2	13:G:107:ARG:HG3	1.80	0.63
10:M:191:LEU:HD22	10:M:221:GLN:HG2	1.81	0.63
3:P:48:GLU:CG	3:P:198:PHE:CE2	2.78	0.62
3:P:83:ARG:NH1	5:R:158:GLY:O	2.28	0.62
4:J:49:VAL:HG11	4:J:65:ARG:NE	2.06	0.62
14:Z:41:ASP:OD1	14:Z:41:ASP:N	2.32	0.62
1:B:42:TYR:CD1	1:B:183:LEU:HD11	2.34	0.62
4:J:87:LEU:HD12	4:J:133:CYS:SG	2.39	0.62
14:Z:90:LEU:HG	14:Z:114:LEU:HD13	1.80	0.62
4:J:10:SER:OG	4:J:126:SER:HB3	1.99	0.62
14:O:9:THR:HB	14:O:20:GLN:HG3	1.82	0.62
4:J:52:LEU:HD23	4:J:209:PHE:HB3	1.81	0.62
12:I:94:HIS:ND1	12:I:102:VAL:HG12	2.13	0.62
12:N:140:GLY:HA3	12:N:213:ARG:CZ	2.28	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:65:ARG:HG2	8:U:65:ARG:HH21	1.64	0.62
4:Q:52:LEU:HD23	4:Q:209:PHE:HB3	1.81	0.62
4:Q:12:SER:HB3	4:Q:125:TYR:HA	1.80	0.62
14:O:174:MET:HE2	14:O:199:LYS:CD	2.30	0.62
13:L:4:ASN:HB3	13:L:5:GLN:NE2	2.11	0.62
10:M:31:ILE:CD1	10:M:158:PRO:CD	2.78	0.62
12:N:94:HIS:ND1	12:N:102:VAL:HG12	2.13	0.62
2:D:45:MET:HB3	2:D:52:CYS:HB3	1.82	0.62
1:E:139:GLU:OE2	1:E:139:GLU:HA	1.99	0.62
10:H:191:LEU:CD2	10:H:221:GLN:HG2	2.30	0.62
4:Q:10:SER:OG	4:Q:126:SER:HB3	1.99	0.62
4:Q:179:LEU:HD11	4:Q:196:ILE:HD11	1.81	0.62
5:K:211:LYS:HB3	5:K:212:PRO:HD2	1.82	0.62
13:G:176:MET:O	13:G:176:MET:HG3	1.98	0.62
14:Z:9:THR:HB	14:Z:20:GLN:HG3	1.82	0.62
14:O:35:LEU:HG	14:O:46:ALA:HB3	1.82	0.61
3:P:28:VAL:HG11	3:P:132:SER:HB2	1.81	0.61
3:P:188:HIS:HE1	3:P:228:TYR:CD1	2.19	0.61
4:J:56:LYS:HG3	13:G:176:MET:CE	2.27	0.61
10:H:178:GLN:OE1	10:H:178:GLN:HA	2.00	0.61
14:O:41:ASP:OD1	14:O:41:ASP:N	2.32	0.61
13:G:4:ASN:HB3	13:G:5:GLN:NE2	2.11	0.61
13:G:74:ILE:HG21	13:G:81:ALA:HB1	1.82	0.61
4:J:179:LEU:HD11	4:J:196:ILE:HD11	1.81	0.61
13:G:45:VAL:HG12	13:G:214:ILE:HG23	1.83	0.61
10:M:191:LEU:CD2	10:M:221:GLN:HG2	2.30	0.61
3:P:188:HIS:HE1	3:P:228:TYR:HD1	1.48	0.61
13:L:45:VAL:HG12	13:L:214:ILE:HG23	1.83	0.61
1:B:44:CYS:HB2	1:B:99:VAL:HB	1.82	0.61
10:H:31:ILE:CD1	10:H:158:PRO:CD	2.78	0.61
5:K:88:ARG:HH11	5:K:88:ARG:CG	2.13	0.61
10:M:178:GLN:HA	10:M:178:GLN:OE1	2.00	0.61
1:B:198:ARG:HH11	1:B:198:ARG:CG	2.13	0.61
12:I:50:VAL:HG13	12:I:50:VAL:O	2.00	0.61
3:P:39:ALA:CB	3:P:186:ALA:HB2	2.30	0.61
4:J:108:LEU:HD22	4:J:147:GLN:HB2	1.83	0.61
14:O:137:ILE:HG13	14:O:137:ILE:O	2.00	0.61
10:M:108:THR:O	10:M:112:VAL:HG23	2.01	0.61
14:Z:230:GLN:HE21	14:Z:230:GLN:CA	2.08	0.61
2:C:45:MET:HB3	2:C:52:CYS:HB3	1.82	0.61
10:M:58:LEU:HD13	12:N:158:ALA:O	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Z:35:LEU:HG	14:Z:46:ALA:HB3	1.82	0.61
4:Q:108:LEU:HD22	4:Q:147:GLN:HB2	1.83	0.61
13:L:47:VAL:HG23	13:L:47:VAL:O	2.01	0.61
9:W:44:ARG:HG2	9:W:44:ARG:HH11	1.64	0.61
5:R:50:ILE:HD11	5:R:141:ILE:HG23	1.83	0.60
9:W:7:THR:HA	9:W:55:GLY:O	2.01	0.60
3:P:7:PHE:O	3:P:124:GLY:CA	2.47	0.60
3:P:128:PRO:O	5:R:16:PHE:HE2	1.83	0.60
12:N:50:VAL:HG13	12:N:50:VAL:O	2.00	0.60
9:W:94:ARG:HH21	9:W:94:ARG:HG3	1.65	0.60
8:Y:65:ARG:HH21	8:Y:65:ARG:HG2	1.64	0.60
1:E:198:ARG:HH11	1:E:198:ARG:HB2	1.67	0.60
14:O:95:GLN:HE22	14:O:98:LEU:HD23	1.66	0.60
2:C:38:ASN:HB2	2:C:39:PRO:CD	2.31	0.60
5:R:212:PRO:HG3	5:R:236:ASP:OD1	2.02	0.60
10:H:44:GLU:OE1	10:H:191:LEU:N	2.31	0.60
14:Z:137:ILE:O	14:Z:137:ILE:HG13	2.00	0.60
1:B:198:ARG:HH11	1:B:198:ARG:HB2	1.66	0.60
5:R:211:LYS:HB3	5:R:212:PRO:HD2	1.82	0.60
8:Y:12:ALA:HB3	8:Y:136:VAL:HG23	1.84	0.60
13:L:74:ILE:HG21	13:L:81:ALA:HB1	1.82	0.60
14:Z:95:GLN:HE22	14:Z:98:LEU:HD23	1.66	0.60
3:P:72:GLY:HA3	3:P:217:PHE:CE1	2.36	0.60
5:R:88:ARG:HH11	5:R:88:ARG:CG	2.13	0.60
1:E:198:ARG:HH11	1:E:198:ARG:CG	2.13	0.60
12:N:223:GLU:N	12:N:223:GLU:OE1	2.34	0.60
9:W:45:VAL:HB	9:W:49:THR:HB	1.83	0.60
2:D:38:ASN:HB2	2:D:39:PRO:CD	2.31	0.60
13:G:47:VAL:HG23	13:G:47:VAL:O	2.01	0.60
10:M:44:GLU:O	10:M:222:PRO:HD3	2.02	0.60
3:P:49:LYS:HG2	3:P:49:LYS:O	2.01	0.60
4:Q:49:VAL:HG11	4:Q:65:ARG:NE	2.06	0.60
10:H:56:SER:OG	10:H:57:PRO:HD2	2.02	0.60
5:K:50:ILE:HD11	5:K:141:ILE:HG23	1.83	0.60
5:K:212:PRO:HG3	5:K:236:ASP:OD1	2.02	0.60
12:I:223:GLU:OE1	12:I:223:GLU:N	2.34	0.60
13:G:72:ILE:HG22	13:G:134:ILE:HG13	1.83	0.60
4:J:78:ALA:HB2	4:J:165:ILE:HD12	1.84	0.60
1:E:44:CYS:HB2	1:E:99:VAL:HB	1.82	0.60
10:H:44:GLU:O	10:H:222:PRO:HD3	2.02	0.59
13:G:22:ILE:HD11	13:G:120:THR:HB	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:155:ASP:CB	5:K:156:PRO:HD2	2.09	0.59
12:I:5:ARG:HH11	14:Z:8:ARG:HD2	1.63	0.59
2:D:81:LYS:HG2	12:N:97:THR:O	2.02	0.59
12:I:5:ARG:HH12	14:Z:8:ARG:HD2	1.63	0.59
13:G:237:GLU:N	13:G:237:GLU:OE2	2.35	0.59
10:M:56:SER:OG	10:M:57:PRO:HD2	2.02	0.59
10:H:108:THR:O	10:H:112:VAL:HG23	2.01	0.59
3:P:88:ARG:HH11	3:P:88:ARG:CG	2.14	0.59
4:Q:41:CYS:HB3	4:Q:189:VAL:HG21	1.84	0.59
7:S:127:VAL:HG23	2:D:50:ALA:HB2	1.84	0.59
8:U:12:ALA:HB3	8:U:136:VAL:HG23	1.83	0.59
5:K:54:LYS:O	5:K:54:LYS:HG2	2.02	0.59
13:L:22:ILE:HD11	13:L:120:THR:HB	1.84	0.59
13:L:72:ILE:HG22	13:L:134:ILE:HG13	1.83	0.59
1:B:94:ILE:HG22	1:B:94:ILE:O	2.01	0.59
3:P:198:PHE:CE2	3:P:207:ILE:HG23	2.36	0.59
4:Q:78:ALA:HB2	4:Q:165:ILE:HD12	1.84	0.59
8:Y:130:MET:O	8:Y:130:MET:HG2	2.03	0.59
13:L:32:GLY:O	13:L:163:ALA:N	2.29	0.59
8:U:130:MET:HG2	8:U:130:MET:O	2.03	0.59
1:E:94:ILE:O	1:E:94:ILE:HG22	2.01	0.58
14:O:140:ASP:CG	14:O:146:GLN:HE22	2.06	0.58
14:Z:140:ASP:CG	14:Z:146:GLN:HE22	2.06	0.58
9:W:177:TYR:CE1	9:W:185:ASN:HB2	2.38	0.58
12:I:53:LEU:HD11	14:Z:176:LYS:CG	2.33	0.58
12:N:171:PHE:HB2	12:N:197:GLU:OE2	2.03	0.58
5:R:54:LYS:HG2	5:R:54:LYS:O	2.03	0.58
7:S:123:SER:CB	7:S:136:LYS:HG2	2.33	0.58
4:J:37:ILE:HD11	4:J:193:VAL:CG2	2.34	0.58
14:Z:206:LEU:O	14:Z:206:LEU:HG	2.03	0.58
11:V:145:ARG:HG3	11:V:145:ARG:NH1	2.19	0.58
14:Z:174:MET:HE2	14:Z:199:LYS:CD	2.32	0.58
2:C:104:TRP:CE2	2:C:181:GLU:HG2	2.39	0.58
4:Q:56:LYS:HG2	13:L:176:MET:HE2	1.85	0.58
5:K:11:ARG:HG3	5:K:11:ARG:NH1	2.19	0.58
5:R:212:PRO:HG3	5:R:236:ASP:CG	2.23	0.58
7:X:71:ARG:HA	7:X:74:MET:HE3	1.85	0.58
5:K:206:LEU:HD12	5:K:210:PHE:HZ	1.68	0.58
5:K:212:PRO:HG3	5:K:236:ASP:CG	2.23	0.58
4:Q:64:LYS:HB2	4:Q:212:GLU:OE1	2.04	0.58
7:S:167:THR:HG23	7:S:170:ARG:HB3	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:192:VAL:HG11	8:Y:204:ASP:HB3	1.86	0.58
12:I:199:VAL:HG11	12:I:206:ILE:HD11	1.85	0.58
4:Q:136:MET:CE	4:Q:165:ILE:HG12	2.33	0.58
13:L:41:LYS:HG2	13:L:41:LYS:O	2.04	0.58
10:M:157:ASP:CB	10:M:158:PRO:CD	2.81	0.57
12:N:199:VAL:HG11	12:N:206:ILE:HD11	1.85	0.57
2:D:104:TRP:CE2	2:D:181:GLU:HG2	2.39	0.57
4:J:41:CYS:HB3	4:J:189:VAL:HG21	1.85	0.57
7:S:71:ARG:HA	7:S:74:MET:HE3	1.85	0.57
4:J:64:LYS:HB2	4:J:212:GLU:OE1	2.04	0.57
5:K:72:ILE:HG21	5:K:114:LEU:HD21	1.86	0.57
5:K:192:GLU:H	5:K:192:GLU:CD	2.08	0.57
12:I:171:PHE:HB2	12:I:197:GLU:OE2	2.03	0.57
14:Z:174:MET:HE2	14:Z:199:LYS:CB	2.27	0.57
5:R:17:SER:HB2	5:R:18:PRO:CD	2.35	0.57
11:T:145:ARG:HG3	11:T:145:ARG:NH1	2.19	0.57
4:Q:37:ILE:HD11	4:Q:193:VAL:CG2	2.34	0.57
1:E:106:THR:HB	1:E:109:HIS:HE2	1.70	0.57
12:I:94:HIS:HB3	12:I:102:VAL:CG1	2.34	0.57
10:M:212:ALA:CB	10:M:235:GLU:HG2	2.31	0.57
12:N:94:HIS:HB3	12:N:102:VAL:CG1	2.34	0.57
8:U:65:ARG:HG2	8:U:65:ARG:NH2	2.18	0.57
1:B:76:VAL:HG23	1:B:104:ASP:OD2	2.05	0.57
2:C:50:ALA:HB2	7:X:127:VAL:HG23	1.85	0.57
2:C:192:VAL:HG11	8:U:204:ASP:HB3	1.86	0.57
5:R:206:LEU:HD12	5:R:210:PHE:HZ	1.68	0.57
13:L:49:LEU:HD22	13:L:199:LEU:HD21	1.86	0.57
14:O:48:GLU:O	14:O:48:GLU:HG2	2.03	0.57
10:H:212:ALA:CB	10:H:235:GLU:HG2	2.31	0.57
14:O:186:LEU:HD12	14:O:186:LEU:O	2.05	0.57
3:P:179:GLU:HA	3:P:179:GLU:OE2	2.04	0.57
10:H:83:ALA:HB1	12:I:116:GLN:HG3	1.87	0.57
5:K:17:SER:HB2	5:K:18:PRO:CD	2.35	0.57
13:L:71:GLY:HA3	13:L:221:PHE:CE1	2.40	0.57
14:Z:174:MET:HE1	14:Z:199:LYS:HB3	1.68	0.57
1:B:106:THR:HB	1:B:109:HIS:HE2	1.70	0.57
2:C:8:PHE:CD1	2:C:8:PHE:N	2.73	0.57
5:R:192:GLU:CD	5:R:192:GLU:H	2.08	0.57
13:L:50:LYS:HB3	13:L:59:HIS:HB3	1.86	0.57
13:L:65:HIS:CE1	13:L:223:ILE:HG13	2.39	0.57
14:O:206:LEU:HG	14:O:206:LEU:O	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Z:48:GLU:O	14:Z:48:GLU:HG2	2.04	0.57
9:W:201:GLY:HA2	9:W:203:LEU:HG	1.86	0.57
5:R:72:ILE:HG21	5:R:114:LEU:HD21	1.86	0.57
5:K:17:SER:HB2	5:K:18:PRO:HD2	1.87	0.57
5:K:145:GLU:N	5:K:145:GLU:OE1	2.38	0.57
13:L:154:PHE:N	13:L:154:PHE:CD1	2.73	0.56
14:O:72:MET:HE2	14:O:110:LEU:CD2	2.21	0.56
10:M:44:GLU:OE1	10:M:191:LEU:N	2.31	0.56
14:Z:186:LEU:HD12	14:Z:186:LEU:O	2.05	0.56
12:N:148:ASP:HB2	12:N:149:PRO:HD2	1.87	0.56
7:X:167:THR:HG23	7:X:170:ARG:HB3	1.86	0.56
13:L:237:GLU:N	13:L:237:GLU:OE2	2.35	0.56
10:M:79:SER:O	10:M:139:VAL:HG23	2.05	0.56
8:U:170:MET:HE2	8:U:184:VAL:HG13	1.87	0.56
1:B:50:ALA:CB	8:Y:126:ILE:HG13	2.36	0.56
4:Q:39:ILE:HD12	4:Q:193:VAL:HG23	1.87	0.56
5:R:17:SER:HB2	5:R:18:PRO:HD2	1.87	0.56
8:Y:163:PHE:CE1	8:Y:197:ARG:HD3	2.41	0.56
8:Y:192:ASP:OD1	8:Y:192:ASP:N	2.39	0.56
13:L:148:CYS:CB	13:L:149:PRO:CD	2.77	0.56
13:G:65:HIS:CE1	13:G:223:ILE:HG13	2.39	0.56
13:G:154:PHE:N	13:G:154:PHE:CD1	2.73	0.56
8:U:163:PHE:CE1	8:U:197:ARG:HD3	2.41	0.56
9:W:25:ASP:HA	9:W:187:PHE:HA	1.86	0.56
1:B:17:ASP:O	1:B:33:LYS:HD2	2.05	0.56
3:P:134:LEU:HG	3:P:162:MET:HE3	1.88	0.56
11:V:69:MET:HG3	12:I:88:ARG:HG2	1.87	0.56
13:L:126:ARG:HD3	10:M:13:ASN:HB3	1.88	0.56
6:A:8:PHE:CZ	6:A:149:LYS:HG2	2.41	0.56
2:C:81:LYS:HG2	12:I:97:THR:O	2.05	0.56
5:R:11:ARG:HG3	5:R:11:ARG:NH1	2.19	0.56
5:R:143:ILE:HG13	5:R:221:THR:O	2.06	0.56
4:J:78:ALA:CB	4:J:165:ILE:HD12	2.36	0.56
10:H:79:SER:O	10:H:139:VAL:HG23	2.05	0.56
13:G:50:LYS:HB3	13:G:59:HIS:HB3	1.86	0.56
13:G:200:PRO:HG2	13:G:203:GLN:HG3	1.88	0.56
6:F:8:PHE:CZ	6:F:149:LYS:HG2	2.41	0.56
4:J:51:LYS:HG3	4:J:212:GLU:OE2	2.06	0.56
4:J:108:LEU:HD23	4:J:149:TYR:CD1	2.41	0.56
1:E:17:ASP:O	1:E:33:LYS:HD2	2.05	0.56
1:E:76:VAL:HG23	1:E:104:ASP:OD2	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:41:LYS:HG2	13:G:41:LYS:O	2.04	0.56
5:R:69:LEU:CD1	5:R:229:ILE:HD12	2.36	0.56
4:J:40:ARG:HG2	4:J:40:ARG:O	2.06	0.56
10:H:51:GLU:HB3	10:H:206:MET:HE1	1.87	0.56
11:T:49:GLU:HB3	11:T:52:ASP:HB2	1.87	0.56
5:R:145:GLU:OE1	5:R:145:GLU:N	2.38	0.56
11:V:49:GLU:HB3	11:V:52:ASP:HB2	1.87	0.56
12:I:132:LEU:HG	12:I:161:ILE:HD13	1.87	0.56
13:L:189:LYS:HG2	13:L:236:LEU:CD1	2.36	0.56
14:O:8:ARG:HD2	12:N:5:ARG:HH12	1.65	0.56
13:G:71:GLY:HA3	13:G:221:PHE:CE1	2.40	0.56
3:P:176:ARG:HH11	3:P:176:ARG:HG3	1.71	0.56
4:Q:78:ALA:CB	4:Q:165:ILE:HD12	2.36	0.56
4:J:68:ASN:HB3	9:W:76:LEU:HD22	1.86	0.56
8:Y:65:ARG:HG2	8:Y:65:ARG:NH2	2.18	0.56
7:X:45:LYS:CD	7:X:203:ILE:HD12	2.35	0.56
7:S:14:ALA:HB2	7:S:109:ILE:HG21	1.88	0.56
7:S:45:LYS:CD	7:S:203:ILE:HD12	2.35	0.56
11:V:118:MET:HE2	11:V:124:LEU:HD13	1.88	0.56
9:W:177:TYR:CZ	9:W:185:ASN:HB2	2.41	0.55
4:Q:108:LEU:HD23	4:Q:149:TYR:CD1	2.41	0.55
6:F:92:GLU:OE1	6:F:92:GLU:HA	2.07	0.55
12:I:134:VAL:HG23	12:I:144:LEU:HD13	1.88	0.55
9:W:109:THR:HG22	9:W:139:THR:HG21	1.89	0.55
7:X:123:SER:CB	7:X:136:LYS:HG2	2.33	0.55
10:H:129:ASP:HB2	10:H:130:PRO:HD3	1.85	0.55
5:K:143:ILE:HG13	5:K:221:THR:O	2.06	0.55
11:V:12:TYR:OH	11:V:156:ALA:HB2	2.06	0.55
11:T:69:MET:HG3	12:N:88:ARG:HG2	1.88	0.55
11:T:118:MET:HE2	11:T:124:LEU:HD13	1.88	0.55
12:N:132:LEU:HG	12:N:161:ILE:HD13	1.87	0.55
9:W:12:LEU:HD11	9:W:172:CYS:HB3	1.87	0.55
5:K:56:VAL:O	5:K:56:VAL:HG12	2.07	0.55
5:K:69:LEU:CD1	5:K:229:ILE:HD12	2.36	0.55
13:L:40:SER:HB3	13:L:187:LEU:CD1	2.36	0.55
10:M:135:ARG:HB2	10:M:136:PRO:HD2	1.88	0.55
14:Z:175:LEU:HD23	14:Z:192:LEU:CD1	2.36	0.55
7:S:127:VAL:HG23	2:D:50:ALA:CB	2.37	0.55
14:O:175:LEU:HD23	14:O:192:LEU:CD1	2.36	0.55
14:O:176:LYS:HG3	12:N:53:LEU:HD11	1.87	0.55
12:N:134:VAL:HG23	12:N:144:LEU:HD13	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:39:ILE:HD12	4:J:193:VAL:HG23	1.87	0.55
13:L:200:PRO:HG2	13:L:203:GLN:HG3	1.88	0.55
4:Q:51:LYS:HG3	4:Q:212:GLU:OE2	2.06	0.55
5:R:56:VAL:O	5:R:56:VAL:HG12	2.07	0.55
12:I:23:GLN:HG3	12:I:149:PRO:HG2	1.88	0.55
13:G:189:LYS:CG	13:G:236:LEU:HD12	2.37	0.55
8:U:192:ASP:N	8:U:192:ASP:OD1	2.39	0.55
3:P:198:PHE:HE2	3:P:207:ILE:HG22	1.72	0.55
4:Q:136:MET:HE3	4:Q:165:ILE:CG1	2.37	0.55
5:R:50:ILE:HG13	5:R:141:ILE:HG21	1.89	0.55
1:E:50:ALA:CB	8:U:126:ILE:HG13	2.37	0.55
12:I:148:ASP:HB2	12:I:149:PRO:HD2	1.87	0.55
5:R:112:ASP:HB3	5:R:152:TYR:CZ	2.42	0.55
4:J:37:ILE:C	4:J:37:ILE:HD12	2.28	0.55
11:T:12:TYR:OH	11:T:156:ALA:HB2	2.06	0.55
13:L:189:LYS:CG	13:L:236:LEU:HD12	2.37	0.55
3:P:147:GLN:CG	3:P:162:MET:CE	2.84	0.54
2:D:61:ARG:NH2	10:M:98:ASN:OD1	2.38	0.54
1:E:199:LEU:CD1	7:X:176:LYS:HD2	2.38	0.54
9:W:51:LEU:HD23	9:W:51:LEU:C	2.27	0.54
3:P:221:THR:HB	3:P:222:PRO:HD2	1.88	0.54
4:Q:40:ARG:O	4:Q:40:ARG:HG2	2.06	0.54
4:Q:42:LYS:HG3	4:Q:42:LYS:O	2.07	0.54
5:R:22:LEU:CD1	5:R:126:THR:CG2	2.85	0.54
10:H:135:ARG:HB2	10:H:136:PRO:HD2	1.88	0.54
10:H:157:ASP:CB	10:H:158:PRO:CD	2.81	0.54
5:K:112:ASP:HB3	5:K:152:TYR:CZ	2.42	0.54
11:T:4:LEU:HD22	11:T:45:LEU:HB3	1.89	0.54
9:W:96:MET:HE3	9:W:127:MET:HA	1.89	0.54
7:X:14:ALA:HB2	7:X:109:ILE:HG21	1.88	0.54
10:H:37:ALA:HB3	10:H:170:ILE:HG12	1.88	0.54
11:V:4:LEU:HD22	11:V:45:LEU:HB3	1.89	0.54
14:O:3:ARG:HG3	14:O:3:ARG:O	2.06	0.54
12:N:8:THR:HG22	12:N:16:LEU:HD22	1.89	0.54
3:P:78:MET:CE	5:R:16:PHE:HE1	2.21	0.54
13:G:49:LEU:HD22	13:G:199:LEU:HD21	1.86	0.54
6:A:92:GLU:OE1	6:A:92:GLU:HA	2.07	0.54
8:U:12:ALA:HB3	8:U:136:VAL:CG2	2.38	0.54
2:C:50:ALA:CB	7:X:127:VAL:HG23	2.38	0.54
4:J:42:LYS:HG3	4:J:42:LYS:O	2.07	0.54
10:H:91:LYS:NZ	10:H:95:GLU:HG2	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Z:3:ARG:HG3	14:Z:3:ARG:O	2.06	0.54
6:A:178:ALA:HB3	6:A:185:GLU:HB2	1.90	0.54
8:U:137:VAL:HG11	8:U:145:MET:HB3	1.90	0.54
1:E:18:THR:OG1	1:E:171:SER:HB3	2.08	0.54
12:I:146:GLN:OE1	12:I:159:ASN:ND2	2.41	0.54
13:G:148:CYS:CB	13:G:149:PRO:CD	2.77	0.54
1:E:29:LYS:HE2	7:X:185:ARG:NH2	2.23	0.54
13:L:27:GLU:OE1	13:L:27:GLU:HA	2.07	0.54
14:Z:175:LEU:HD23	14:Z:192:LEU:HD11	1.90	0.54
11:T:62:LYS:HG3	12:N:92:GLN:HB3	1.89	0.53
12:N:23:GLN:HG3	12:N:149:PRO:HG2	1.88	0.53
9:W:1:THR:N	9:W:105:PRO:O	2.41	0.53
1:B:18:THR:OG1	1:B:171:SER:HB3	2.08	0.53
8:Y:12:ALA:HB3	8:Y:136:VAL:CG2	2.38	0.53
8:Y:137:VAL:HG11	8:Y:145:MET:HB3	1.90	0.53
11:V:59:TYR:HE2	11:V:87:ASN:OD1	1.92	0.53
3:P:37:ILE:CD1	3:P:189:THR:HG23	2.37	0.53
5:K:50:ILE:HG13	5:K:141:ILE:HG21	1.89	0.53
13:L:56:LEU:HD13	10:M:167:ALA:HB3	1.90	0.53
14:O:148:TYR:HE1	12:N:58:THR:HG21	1.74	0.53
13:G:27:GLU:OE1	13:G:27:GLU:HA	2.07	0.53
13:G:40:SER:HB3	13:G:187:LEU:CD1	2.36	0.53
10:M:91:LYS:NZ	10:M:95:GLU:HG2	2.23	0.53
5:R:210:PHE:O	5:R:239:LEU:CD1	2.57	0.53
6:F:178:ALA:HB3	6:F:185:GLU:HB2	1.90	0.53
1:E:183:LEU:HD23	1:E:183:LEU:O	2.09	0.53
14:O:174:MET:CE	14:O:199:LYS:HG3	2.38	0.53
13:G:32:GLY:O	13:G:163:ALA:N	2.29	0.53
12:N:40:ILE:HG13	12:N:212:ARG:HG2	1.89	0.53
3:P:156:ALA:HB2	14:O:59:VAL:CG2	2.35	0.53
4:Q:37:ILE:C	4:Q:37:ILE:HD12	2.28	0.53
5:R:210:PHE:O	5:R:239:LEU:HD13	2.09	0.53
5:K:59:LYS:HE3	5:K:59:LYS:HA	1.90	0.53
5:K:59:LYS:CE	5:K:59:LYS:CA	2.86	0.53
10:M:37:ALA:HB3	10:M:170:ILE:HG12	1.88	0.53
10:M:206:MET:HE1	10:M:215:ILE:HG22	1.90	0.53
14:O:176:LYS:HG2	12:N:53:LEU:CD1	2.38	0.53
1:B:199:LEU:CD1	7:S:176:LYS:HD2	2.39	0.53
3:P:33:PRO:HA	3:P:162:MET:O	2.09	0.53
5:R:22:LEU:HD13	5:R:126:THR:HG23	1.89	0.53
10:H:13:ASN:HB3	13:G:126:ARG:HD3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:145:ARG:HG3	11:T:145:ARG:O	2.09	0.53
12:I:41:VAL:HG12	12:I:134:VAL:HG11	1.86	0.53
14:O:175:LEU:HD23	14:O:192:LEU:HD11	1.90	0.53
14:O:176:LYS:CG	12:N:53:LEU:CD1	2.87	0.53
12:N:7:ILE:HG22	12:N:18:GLN:HG3	1.90	0.53
9:W:94:ARG:HG3	9:W:94:ARG:NH2	2.24	0.53
1:B:183:LEU:HD23	1:B:183:LEU:O	2.09	0.53
7:S:72:LEU:HD21	7:S:88:ILE:HG12	1.91	0.53
7:X:72:LEU:HD21	7:X:88:ILE:HG12	1.91	0.53
5:K:22:LEU:HD13	5:K:126:THR:HG23	1.89	0.53
12:I:7:ILE:HG22	12:I:18:GLN:HG3	1.90	0.53
12:I:8:THR:HG22	12:I:16:LEU:HD22	1.89	0.53
5:R:58:ASP:OD1	5:R:58:ASP:N	2.41	0.53
4:J:176:ILE:HG22	5:K:60:LEU:HD21	1.89	0.53
7:X:102:PHE:N	7:X:103:PRO:CD	2.72	0.53
8:U:13:MET:HB3	8:U:162:LEU:HD11	1.90	0.53
7:S:102:PHE:N	7:S:103:PRO:CD	2.72	0.52
12:N:148:ASP:HB2	12:N:149:PRO:CD	2.39	0.52
2:C:10:HIS:O	2:C:178:HIS:HE1	1.92	0.52
5:K:22:LEU:CD1	5:K:126:THR:CG2	2.85	0.52
5:K:58:ASP:OD1	5:K:58:ASP:N	2.41	0.52
5:K:210:PHE:O	5:K:239:LEU:CD1	2.57	0.52
12:I:40:ILE:HG13	12:I:212:ARG:HG2	1.89	0.52
8:U:168:GLN:O	8:U:172:ASN:ND2	2.38	0.52
2:C:11:GLY:HA2	2:C:104:TRP:CZ3	2.44	0.52
2:D:10:HIS:O	2:D:178:HIS:HE1	1.92	0.52
11:T:59:TYR:HE2	11:T:87:ASN:OD1	1.92	0.52
13:L:209:ASN:OD1	13:L:210:VAL:HG23	2.09	0.52
8:Y:13:MET:HB3	8:Y:162:LEU:HD11	1.91	0.52
14:Z:174:MET:CE	14:Z:199:LYS:HG3	2.38	0.52
2:C:177:TYR:CE2	2:C:186:ARG:HG2	2.45	0.52
2:D:11:GLY:HA2	2:D:104:TRP:CZ3	2.45	0.52
1:B:29:LYS:HE2	7:S:185:ARG:NH2	2.24	0.52
8:Y:170:MET:HE2	8:Y:184:VAL:HG13	1.91	0.52
10:H:51:GLU:CB	10:H:206:MET:HE1	2.40	0.52
14:O:226:ARG:HD3	14:O:226:ARG:C	2.30	0.52
12:N:146:GLN:OE1	12:N:159:ASN:ND2	2.41	0.52
3:P:37:ILE:HD12	3:P:190:ALA:CB	2.38	0.52
5:K:210:PHE:O	5:K:239:LEU:HD13	2.09	0.52
13:G:34:ALA:HA	13:G:161:ILE:O	2.10	0.52
12:N:208:LEU:HD11	12:N:220:LEU:CD1	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:93:ASP:OD1	6:F:93:ASP:N	2.42	0.52
2:D:177:TYR:CE2	2:D:186:ARG:HG2	2.45	0.52
13:G:209:ASN:OD1	13:G:210:VAL:HG23	2.09	0.52
14:Z:226:ARG:HD3	14:Z:226:ARG:C	2.30	0.52
11:V:145:ARG:HG3	11:V:145:ARG:O	2.09	0.52
6:F:17:ASP:O	6:F:33:LYS:HD2	2.11	0.51
1:B:69:THR:HG22	5:K:113:MET:CE	2.40	0.51
1:B:72:ARG:NH2	5:K:112:ASP:OD1	2.42	0.51
3:P:48:GLU:HA	3:P:207:ILE:HG22	1.92	0.51
3:P:112:ARG:HG3	3:P:112:ARG:NH1	2.23	0.51
5:R:112:ASP:OD1	1:E:72:ARG:NH2	2.44	0.51
11:V:62:LYS:HG3	12:I:92:GLN:HB3	1.92	0.51
6:A:17:ASP:O	6:A:33:LYS:HD2	2.11	0.51
1:B:180:LYS:O	1:B:180:LYS:HG2	2.10	0.51
2:C:38:ASN:CB	2:C:39:PRO:CD	2.88	0.51
3:P:75:TYR:HB3	3:P:82:TYR:CD1	2.45	0.51
2:D:3:THR:HG21	2:D:44:THR:HG22	1.92	0.51
5:K:22:LEU:HD13	5:K:126:THR:HG22	1.92	0.51
10:M:74:ILE:HD13	10:M:112:VAL:HG21	1.93	0.51
5:R:22:LEU:HD13	5:R:126:THR:HG22	1.92	0.51
10:H:186:HIS:CE1	10:H:189:MET:HG3	2.46	0.51
13:L:34:ALA:HA	13:L:161:ILE:O	2.10	0.51
13:G:5:GLN:HE21	13:G:5:GLN:H	1.59	0.51
8:Y:21:ILE:HG22	8:Y:187:HIS:HB2	1.93	0.51
8:Y:68:PHE:CE2	14:Z:95:GLN:HB3	2.45	0.51
7:X:7:PHE:HE2	7:X:188:TYR:CE2	2.29	0.51
12:I:148:ASP:HB2	12:I:149:PRO:CD	2.39	0.51
10:M:186:HIS:CE1	10:M:189:MET:HG3	2.45	0.51
6:A:93:ASP:N	6:A:93:ASP:OD1	2.42	0.51
9:W:12:LEU:CD1	9:W:172:CYS:HB3	2.40	0.51
9:W:27:LEU:HD11	9:W:34:ALA:HB1	1.92	0.51
13:L:5:GLN:HE21	13:L:5:GLN:H	1.59	0.51
12:N:70:CYS:HB3	12:N:211:MET:CE	2.41	0.51
7:S:7:PHE:HE2	7:S:188:TYR:CE2	2.29	0.51
2:D:38:ASN:CB	2:D:39:PRO:CD	2.87	0.51
10:H:74:ILE:HD13	10:H:112:VAL:HG21	1.93	0.51
2:C:3:THR:HG21	2:C:44:THR:HG22	1.92	0.51
8:Y:168:GLN:O	8:Y:172:ASN:ND2	2.38	0.51
10:H:200:ILE:O	10:H:204:GLN:HG3	2.10	0.51
14:O:135:LEU:CD2	14:O:149:GLN:HG3	2.41	0.51
10:M:200:ILE:O	10:M:204:GLN:HG3	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:9:THR:O	9:W:54:SER:HB2	2.11	0.51
9:W:10:SER:HB3	9:W:139:THR:O	2.11	0.51
7:S:75:TYR:CD1	7:S:83:MET:HG3	2.46	0.51
14:O:192:LEU:O	14:O:192:LEU:HD22	2.11	0.51
10:M:63:SER:HB3	12:N:155:ALA:HB3	1.92	0.51
10:M:210:LEU:O	10:M:210:LEU:HD23	2.11	0.51
8:U:21:ILE:HG22	8:U:187:HIS:HB2	1.93	0.51
10:H:63:SER:HB3	12:I:155:ALA:HB3	1.93	0.51
10:H:147:ASP:N	10:H:147:ASP:OD1	2.44	0.51
13:L:79:ALA:HB3	10:M:121:LEU:CD1	2.39	0.51
8:U:26:ARG:HG3	8:U:182:MET:HG3	1.92	0.51
4:Q:66:LEU:HD23	4:Q:76:ALA:HA	1.93	0.50
14:O:230:GLN:HE21	14:O:230:GLN:CA	2.08	0.50
14:Z:45:LEU:HG	14:Z:137:ILE:HG21	1.94	0.50
14:Z:192:LEU:O	14:Z:192:LEU:HD22	2.11	0.50
6:A:3:ILE:HG21	6:A:44:CYS:HB3	1.93	0.50
3:P:147:GLN:HG2	3:P:162:MET:CE	2.42	0.50
5:R:25:VAL:HG21	5:R:126:THR:HG23	1.93	0.50
4:J:56:LYS:CG	13:G:176:MET:HE2	2.40	0.50
8:Y:26:ARG:HG3	8:Y:182:MET:HG3	1.92	0.50
8:Y:27:PHE:HB2	8:Y:38:PHE:HB2	1.94	0.50
13:G:189:LYS:HG2	13:G:236:LEU:CD1	2.36	0.50
6:A:14:LEU:HD21	6:A:101:ALA:HB3	1.93	0.50
6:F:3:ILE:HG21	6:F:44:CYS:HB3	1.93	0.50
5:K:25:VAL:HG21	5:K:126:THR:HG23	1.93	0.50
11:T:16:ALA:HA	11:T:179:SER:O	2.12	0.50
12:I:58:THR:HG21	14:Z:148:TYR:HE1	1.76	0.50
12:I:94:HIS:CB	12:I:102:VAL:HG12	2.40	0.50
5:R:113:MET:CE	1:E:69:THR:HG22	2.42	0.50
5:R:182:LYS:HB3	5:R:189:TRP:HH2	1.77	0.50
7:X:35:ILE:O	9:W:151:ARG:NH2	2.22	0.50
7:X:75:TYR:CD1	7:X:83:MET:HG3	2.46	0.50
10:H:210:LEU:O	10:H:210:LEU:HD23	2.11	0.50
12:I:70:CYS:HB3	12:I:211:MET:CE	2.41	0.50
12:I:208:LEU:HD11	12:I:220:LEU:CD1	2.39	0.50
13:G:67:ASP:OD2	13:G:92:CYS:HB3	2.12	0.50
7:X:161:VAL:HG12	7:X:163:HIS:CD2	2.46	0.50
5:K:182:LYS:HB3	5:K:189:TRP:HH2	1.77	0.50
10:M:129:ASP:HB2	10:M:130:PRO:HD3	1.85	0.50
10:M:147:ASP:N	10:M:147:ASP:OD1	2.44	0.50
1:E:198:ARG:CG	1:E:198:ARG:NH1	2.73	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ILE:HG13	1:B:119:THR:HG22	1.94	0.50
13:G:5:GLN:NE2	13:G:5:GLN:H	2.10	0.50
14:Z:175:LEU:CD2	14:Z:192:LEU:HD13	2.42	0.50
6:A:58:ALA:CB	6:A:86:MET:HE3	2.42	0.50
5:R:178:PHE:CZ	5:R:182:LYS:HD3	2.47	0.50
4:J:56:LYS:HG2	13:G:176:MET:HE2	1.93	0.50
12:I:108:THR:HG21	12:I:145:TYR:HB3	1.94	0.50
6:A:144:ARG:HH11	6:A:144:ARG:CG	2.24	0.50
8:U:47:ARG:HD3	8:U:111:LEU:HD12	1.93	0.50
1:E:45:GLY:HA3	1:E:52:THR:HG21	1.94	0.50
10:H:31:ILE:HG22	10:H:31:ILE:O	2.11	0.50
11:T:58:GLU:HB3	12:N:96:LEU:HD11	1.93	0.50
13:L:50:LYS:CB	13:L:59:HIS:HB3	2.42	0.50
14:O:95:GLN:HB3	8:U:68:PHE:CE2	2.47	0.50
8:U:27:PHE:HB2	8:U:38:PHE:HB2	1.94	0.50
4:Q:52:LEU:HD23	4:Q:209:PHE:CB	2.42	0.49
4:Q:56:LYS:CE	4:Q:56:LYS:CA	2.86	0.49
1:E:3:ILE:HD11	1:E:127:MET:HB3	1.95	0.49
14:O:175:LEU:CD2	14:O:192:LEU:HD13	2.42	0.49
12:N:108:THR:HG21	12:N:145:TYR:HB3	1.94	0.49
8:Y:47:ARG:HD3	8:Y:111:LEU:HD12	1.93	0.49
5:K:178:PHE:CZ	5:K:182:LYS:HD3	2.47	0.49
12:N:206:ILE:HG22	12:N:206:ILE:O	2.11	0.49
5:R:59:LYS:HE3	5:R:59:LYS:C	2.33	0.49
7:S:161:VAL:HG12	7:S:163:HIS:CD2	2.46	0.49
12:I:53:LEU:CD1	14:Z:176:LYS:HG2	2.42	0.49
12:I:171:PHE:HB3	12:I:197:GLU:OE2	2.11	0.49
13:G:50:LYS:CB	13:G:59:HIS:HB3	2.42	0.49
14:Z:135:LEU:CD2	14:Z:149:GLN:HG3	2.41	0.49
1:B:42:TYR:HE1	1:B:183:LEU:HD11	1.73	0.49
2:C:153:TYR:OH	2:C:178:HIS:HD2	1.95	0.49
4:Q:33:SER:OG	4:Q:65:ARG:NH1	2.45	0.49
4:Q:69:VAL:HG23	4:Q:73:VAL:HB	1.95	0.49
4:J:66:LEU:HD23	4:J:76:ALA:HA	1.93	0.49
1:E:113:ILE:HG13	1:E:119:THR:HG22	1.94	0.49
1:E:180:LYS:O	1:E:180:LYS:HG2	2.10	0.49
13:L:5:GLN:NE2	13:L:5:GLN:H	2.10	0.49
14:O:45:LEU:HG	14:O:137:ILE:HG21	1.94	0.49
10:M:83:ALA:HB1	12:N:116:GLN:HG3	1.94	0.49
1:B:3:ILE:HD11	1:B:127:MET:HB3	1.95	0.49
3:P:176:ARG:HH11	3:P:176:ARG:CG	2.25	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:37:ILE:HD11	4:Q:193:VAL:HG13	1.95	0.49
4:J:52:LEU:HD23	4:J:209:PHE:CB	2.42	0.49
11:T:80:ALA:O	11:T:84:THR:HG23	2.12	0.49
12:N:94:HIS:CG	12:N:102:VAL:CG1	2.82	0.49
9:W:174:ARG:HD3	9:W:206:GLN:O	2.12	0.49
1:B:36:PHE:CD1	1:B:36:PHE:C	2.85	0.49
2:C:97:MET:O	2:C:97:MET:HG3	2.13	0.49
6:F:14:LEU:HD21	6:F:101:ALA:HB3	1.93	0.49
2:D:97:MET:HG3	2:D:97:MET:O	2.12	0.49
1:E:36:PHE:CD1	1:E:36:PHE:C	2.85	0.49
10:H:110:GLU:CG	10:H:154:PHE:CE2	2.95	0.49
12:I:206:ILE:O	12:I:206:ILE:HG22	2.11	0.49
12:N:94:HIS:CB	12:N:102:VAL:HG12	2.40	0.49
9:W:109:THR:HG22	9:W:139:THR:CG2	2.42	0.49
10:H:31:ILE:CD1	10:H:158:PRO:HD3	2.43	0.49
10:H:110:GLU:CG	10:H:154:PHE:CZ	2.93	0.49
13:L:36:VAL:HB	13:L:47:VAL:CG2	2.43	0.49
13:G:36:VAL:HB	13:G:47:VAL:CG2	2.43	0.49
14:Z:76:VAL:HG11	14:Z:83:ALA:HB1	1.95	0.49
12:N:42:VAL:HB	12:N:191:VAL:HG21	1.94	0.49
1:B:24:MET:HE2	7:S:33:PHE:CZ	2.48	0.49
4:Q:117:MET:HA	4:Q:117:MET:CE	2.43	0.49
4:J:69:VAL:HG23	4:J:73:VAL:HB	1.95	0.49
1:E:24:MET:HE1	7:X:33:PHE:CZ	2.46	0.49
10:H:21:LEU:HD21	13:G:126:ARG:HD2	1.93	0.49
10:H:59:MET:SD	10:H:64:ILE:HD11	2.53	0.49
13:G:171:TYR:CD1	13:G:171:TYR:C	2.86	0.49
10:M:110:GLU:CG	10:M:154:PHE:CE2	2.96	0.49
13:L:67:ASP:OD2	13:L:92:CYS:HB3	2.12	0.49
13:L:171:TYR:CD1	13:L:171:TYR:C	2.86	0.49
6:A:52:THR:HG22	6:A:98:ILE:HD11	1.94	0.49
1:B:198:ARG:CG	1:B:198:ARG:NH1	2.73	0.49
2:D:153:TYR:OH	2:D:178:HIS:HD2	1.95	0.49
10:H:121:LEU:CD1	13:G:79:ALA:HB3	2.42	0.49
5:K:59:LYS:HE3	5:K:59:LYS:C	2.33	0.49
5:K:178:PHE:CD1	5:K:178:PHE:C	2.86	0.49
13:G:49:LEU:HG	13:G:49:LEU:O	2.12	0.49
10:M:31:ILE:O	10:M:31:ILE:HG22	2.11	0.49
9:W:51:LEU:HD23	9:W:51:LEU:O	2.12	0.49
10:H:82:ILE:HD13	10:H:82:ILE:N	2.28	0.48
12:I:42:VAL:HB	12:I:191:VAL:HG21	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:34:CYS:HB2	14:O:164:ILE:HG13	1.95	0.48
14:Z:30:HIS:O	14:Z:50:ARG:NH2	2.28	0.48
12:N:195:LEU:HD13	12:N:206:ILE:HG23	1.95	0.48
1:B:45:GLY:HA3	1:B:52:THR:HG21	1.94	0.48
4:Q:69:VAL:HA	4:Q:92:ARG:HG3	1.95	0.48
5:R:178:PHE:CD1	5:R:178:PHE:C	2.86	0.48
12:I:33:VAL:CG2	12:I:191:VAL:HG13	2.43	0.48
13:L:26:MET:CE	13:L:150:SER:HB3	2.43	0.48
13:L:49:LEU:HG	13:L:49:LEU:O	2.12	0.48
14:O:28:ILE:O	14:O:165:GLY:HA2	2.13	0.48
3:P:187:ILE:HD11	3:P:211:ILE:HG21	1.95	0.48
6:F:52:THR:HG22	6:F:98:ILE:HD11	1.94	0.48
7:S:75:TYR:CD1	7:S:75:TYR:C	2.86	0.48
11:V:16:ALA:HA	11:V:179:SER:O	2.12	0.48
12:N:33:VAL:CG2	12:N:191:VAL:HG13	2.43	0.48
3:P:50:LYS:HE3	3:P:50:LYS:HB3	1.45	0.48
5:R:165:ALA:HB1	5:R:179:LEU:HD22	1.94	0.48
7:S:10:GLY:HA3	7:S:42:LYS:HE3	1.95	0.48
4:J:55:SER:HB2	4:J:58:TYR:CE2	2.48	0.48
7:X:75:TYR:CD1	7:X:75:TYR:C	2.86	0.48
5:K:104:LYS:HE3	5:K:104:LYS:HB3	1.49	0.48
11:V:4:LEU:HB2	11:V:132:HIS:HB2	1.95	0.48
12:I:195:LEU:HD13	12:I:206:ILE:HG23	1.95	0.48
12:N:171:PHE:HB3	12:N:197:GLU:OE2	2.11	0.48
4:Q:108:LEU:HD13	4:Q:139:SER:CB	2.41	0.48
2:D:166:ARG:NH1	8:Y:33:MET:O	2.46	0.48
4:J:37:ILE:HD11	4:J:193:VAL:HG13	1.95	0.48
5:K:165:ALA:HB1	5:K:179:LEU:HD22	1.94	0.48
14:O:25:MET:HA	14:O:28:ILE:HD12	1.95	0.48
6:A:22:THR:O	6:A:22:THR:OG1	2.31	0.48
2:C:141:ARG:HD2	11:T:162:LYS:HB3	1.95	0.48
4:J:56:LYS:CE	4:J:56:LYS:CA	2.86	0.48
14:O:135:LEU:HD21	14:O:149:GLN:HG3	1.95	0.48
1:B:205:GLU:H	1:B:205:GLU:HG2	1.50	0.48
2:C:166:ARG:NH1	8:U:33:MET:O	2.46	0.48
3:P:198:PHE:CZ	3:P:207:ILE:HG23	2.49	0.48
4:Q:136:MET:HE3	4:Q:165:ILE:HG13	1.91	0.48
4:Q:176:ILE:HG22	5:R:60:LEU:HD21	1.95	0.48
4:J:69:VAL:HA	4:J:92:ARG:HG3	1.95	0.48
1:E:219:LEU:N	8:U:192:ASP:O	2.44	0.48
10:H:73:HIS:CE1	10:H:106:THR:HB	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:52:THR:HG22	5:K:216:GLU:HG3	1.93	0.48
5:K:78:CYS:CB	5:K:140:LEU:HD23	2.42	0.48
11:T:49:GLU:OE2	11:T:49:GLU:HA	2.14	0.48
14:O:76:VAL:HG11	14:O:83:ALA:HB1	1.95	0.48
10:M:59:MET:SD	10:M:64:ILE:HD11	2.53	0.48
10:M:73:HIS:CE1	10:M:106:THR:HB	2.49	0.48
14:Z:28:ILE:O	14:Z:165:GLY:HA2	2.13	0.48
6:A:90:TYR:HB2	6:A:94:LEU:CD1	2.44	0.48
3:P:39:ALA:HB2	3:P:186:ALA:HB2	1.96	0.48
4:Q:51:LYS:HB3	4:Q:51:LYS:HE2	1.37	0.48
5:R:52:THR:HG22	5:R:216:GLU:HG3	1.93	0.48
4:J:37:ILE:HD13	4:J:193:VAL:HG22	1.94	0.48
13:L:116:THR:HG22	13:L:116:THR:O	2.14	0.48
14:O:30:HIS:O	14:O:50:ARG:NH2	2.28	0.48
13:G:132:LEU:HB2	13:G:147:THR:OG1	2.14	0.48
14:Z:135:LEU:HD21	14:Z:149:GLN:HG3	1.95	0.48
3:P:79:GLY:N	3:P:80:PRO:CD	2.77	0.48
6:F:3:ILE:CG2	6:F:44:CYS:HB3	2.44	0.48
6:F:90:TYR:HB2	6:F:94:LEU:CD1	2.44	0.48
6:F:144:ARG:HH11	6:F:144:ARG:CG	2.24	0.48
7:X:10:GLY:HA3	7:X:42:LYS:HE3	1.95	0.48
3:P:135:ILE:H	3:P:135:ILE:HD12	1.78	0.47
7:S:134:SER:HB2	7:S:135:PHE:CD1	2.49	0.47
4:J:117:MET:HA	4:J:117:MET:CE	2.43	0.47
6:F:45:ARG:NH2	6:F:53:GLN:HG3	2.29	0.47
1:E:7:VAL:HG22	1:E:12:ILE:CD1	2.44	0.47
1:E:203:ARG:HD2	8:U:161:HIS:CD2	2.50	0.47
11:T:4:LEU:HB2	11:T:132:HIS:HB2	1.95	0.47
12:I:209:ALA:CB	12:I:217:LEU:HD11	2.44	0.47
14:O:171:ALA:HB2	14:O:200:THR:HG21	1.96	0.47
14:Z:34:CYS:HB2	14:Z:164:ILE:HG13	1.95	0.47
9:W:189:ILE:HG22	9:W:189:ILE:O	2.14	0.47
3:P:202:MET:HG3	3:P:207:ILE:HG12	1.95	0.47
7:X:134:SER:HB2	7:X:135:PHE:CD1	2.48	0.47
13:L:77:LEU:HB2	13:L:80:ASP:HB2	1.96	0.47
13:G:26:MET:CE	13:G:150:SER:HB3	2.43	0.47
6:A:3:ILE:CG2	6:A:44:CYS:HB3	2.44	0.47
12:N:204:LYS:HE2	12:N:204:LYS:HB3	1.51	0.47
9:W:12:LEU:CD1	9:W:172:CYS:CB	2.93	0.47
3:P:147:GLN:HG3	3:P:162:MET:CE	2.45	0.47
14:O:124:PHE:HB2	12:N:123:GLY:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:16:SER:HB2	10:M:17:PRO:HD2	1.95	0.47
6:A:17:ASP:CG	6:A:33:LYS:NZ	2.68	0.47
6:F:162:LEU:HD11	6:A:141:ALA:HB2	1.97	0.47
12:I:53:LEU:HD11	14:Z:176:LYS:HG3	1.96	0.47
4:Q:197:ILE:HD12	4:Q:197:ILE:HA	1.68	0.47
5:R:69:LEU:HD12	5:R:229:ILE:HD12	1.96	0.47
10:H:16:SER:HB2	10:H:17:PRO:HD2	1.95	0.47
13:L:41:LYS:HG2	13:L:42:THR:HG23	1.96	0.47
10:M:82:ILE:HD13	10:M:82:ILE:N	2.28	0.47
14:Z:25:MET:HA	14:Z:28:ILE:HD12	1.95	0.47
6:A:112:TYR:CE1	6:A:122:ARG:HG3	2.49	0.47
9:W:9:THR:O	9:W:41:ARG:NH2	2.47	0.47
2:C:8:PHE:CE1	2:C:13:ILE:HG12	2.50	0.47
2:C:61:ARG:NH2	10:H:98:ASN:OD1	2.41	0.47
2:C:160:ILE:O	2:C:164:THR:HG23	2.14	0.47
3:P:43:VAL:O	3:P:212:CYS:N	2.44	0.47
3:P:68:THR:HG23	3:P:70:HIS:H	1.79	0.47
3:P:147:GLN:HE21	3:P:157:TRP:HE1	1.61	0.47
3:P:154:TYR:HE1	14:O:60:PHE:CZ	2.33	0.47
3:P:171:THR:O	3:P:174:GLU:HG2	2.13	0.47
3:P:202:MET:HG2	3:P:229:LEU:HD11	1.96	0.47
4:Q:151:ILE:HG13	4:Q:157:SER:CB	2.43	0.47
5:R:139:ILE:HG12	5:R:153:LYS:CG	2.45	0.47
6:F:112:TYR:CE1	6:F:122:ARG:HG3	2.49	0.47
5:K:69:LEU:HD12	5:K:229:ILE:HD12	1.96	0.47
5:K:139:ILE:HG12	5:K:153:LYS:CG	2.45	0.47
13:L:88:MET:HE3	13:L:112:ILE:HD11	1.97	0.47
13:L:212:ILE:CD1	13:L:229:VAL:HG22	2.44	0.47
14:O:176:LYS:HG2	12:N:53:LEU:HD11	1.97	0.47
13:G:77:LEU:HB2	13:G:80:ASP:HB2	1.96	0.47
10:M:31:ILE:CD1	10:M:158:PRO:HD3	2.43	0.47
14:Z:33:THR:OG1	14:Z:166:ASN:O	2.30	0.47
2:C:83:LEU:HD21	2:C:99:THR:HG21	1.96	0.47
4:Q:55:SER:HB2	4:Q:58:TYR:CE2	2.49	0.47
6:F:17:ASP:CG	6:F:33:LYS:NZ	2.68	0.47
8:Y:163:PHE:CE1	8:Y:197:ARG:CD	2.97	0.47
10:H:117:SER:OG	10:H:156:MET:HG3	2.15	0.47
10:H:215:ILE:HD11	10:H:234:LEU:HD13	1.97	0.47
3:P:67:ILE:HG13	3:P:73:LEU:HD13	1.97	0.47
3:P:72:GLY:HA3	3:P:217:PHE:CD1	2.50	0.47
3:P:127:ARG:HH21	5:R:126:THR:HG22	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:141:ALA:HB2	6:A:162:LEU:HD11	1.97	0.47
2:D:8:PHE:CD1	2:D:8:PHE:N	2.73	0.47
11:V:49:GLU:OE2	11:V:49:GLU:HA	2.14	0.47
14:O:38:LEU:HB3	14:O:160:LYS:O	2.15	0.47
13:G:41:LYS:HG2	13:G:42:THR:HG23	1.96	0.47
10:M:215:ILE:HD11	10:M:234:LEU:HD13	1.97	0.47
14:Z:171:ALA:HB2	14:Z:200:THR:HG21	1.96	0.47
6:A:45:ARG:NH2	6:A:53:GLN:HG3	2.30	0.47
8:U:163:PHE:CE1	8:U:197:ARG:CD	2.97	0.47
3:P:56:TYR:HD2	5:R:161:CYS:SG	2.38	0.47
6:F:52:THR:CG2	6:F:96:ALA:CB	2.92	0.47
4:J:151:ILE:HG13	4:J:157:SER:CB	2.43	0.47
1:E:38:SER:HB2	1:E:39:PRO:HD2	1.97	0.47
10:H:90:ASP:O	10:H:94:VAL:HG23	2.14	0.47
5:K:208:ILE:O	5:K:208:ILE:HG23	2.15	0.47
11:T:2:GLU:HG2	11:T:34:LYS:CE	2.45	0.47
11:T:180:VAL:HG21	11:T:194:ILE:HD12	1.97	0.47
12:I:53:LEU:CD1	14:Z:176:LYS:CG	2.93	0.47
14:Z:38:LEU:HB3	14:Z:160:LYS:O	2.15	0.47
1:B:7:VAL:HG22	1:B:12:ILE:CD1	2.44	0.46
2:D:38:ASN:HB2	2:D:39:PRO:HD2	1.97	0.46
2:D:160:ILE:O	2:D:164:THR:HG23	2.14	0.46
4:J:169:ARG:HG2	4:J:169:ARG:HH11	1.81	0.46
5:K:69:LEU:HD13	5:K:229:ILE:CD1	2.45	0.46
5:K:171:LYS:HG3	5:K:206:LEU:HD23	1.96	0.46
11:V:2:GLU:HG2	11:V:34:LYS:CE	2.45	0.46
10:M:90:ASP:O	10:M:94:VAL:HG23	2.15	0.46
10:M:201:ILE:HA	10:M:204:GLN:CD	2.36	0.46
12:N:41:VAL:HG12	12:N:134:VAL:HG11	1.86	0.46
8:U:154:GLU:O	8:U:157:MET:HG3	2.16	0.46
6:F:98:ILE:HD13	6:F:98:ILE:N	2.30	0.46
2:D:8:PHE:CE1	2:D:13:ILE:HG12	2.50	0.46
13:L:132:LEU:HB2	13:L:147:THR:OG1	2.14	0.46
2:C:7:LYS:HE2	2:C:123:GLY:O	2.15	0.46
5:R:69:LEU:HD13	5:R:229:ILE:CD1	2.45	0.46
6:F:22:THR:O	6:F:22:THR:OG1	2.31	0.46
7:S:159:GLN:HB3	7:S:160:ASN:H	1.58	0.46
4:J:66:LEU:HD13	4:J:214:SER:HB2	1.97	0.46
7:X:72:LEU:HD23	7:X:83:MET:SD	2.56	0.46
12:I:137:ASP:OD2	12:I:143:ARG:NE	2.45	0.46
12:I:192:ILE:HD11	12:I:208:LEU:HD21	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:33:THR:OG1	14:O:166:ASN:O	2.30	0.46
13:G:116:THR:O	13:G:116:THR:HG22	2.14	0.46
12:N:209:ALA:CB	12:N:217:LEU:HD11	2.44	0.46
9:W:27:LEU:CD1	9:W:34:ALA:HB1	2.46	0.46
3:P:201:GLN:NE2	3:P:201:GLN:H	2.14	0.46
6:F:21:THR:HG22	6:F:26:ILE:HA	1.98	0.46
10:H:167:ALA:HB3	13:G:56:LEU:HD13	1.97	0.46
10:M:117:SER:OG	10:M:156:MET:HG3	2.15	0.46
14:Z:28:ILE:HG21	14:Z:133:SER:HB2	1.97	0.46
9:W:9:THR:CG2	9:W:182:ARG:HB3	2.46	0.46
9:W:136:SER:HB3	9:W:154:LEU:HD11	1.96	0.46
1:B:38:SER:HB2	1:B:39:PRO:CD	2.46	0.46
2:C:21:THR:HG21	2:C:169:TYR:CD1	2.51	0.46
3:P:142:ARG:HG2	3:P:143:PRO:HD2	1.97	0.46
2:D:7:LYS:HE2	2:D:123:GLY:O	2.15	0.46
8:Y:154:GLU:O	8:Y:157:MET:HG3	2.15	0.46
10:H:91:LYS:HZ3	10:H:95:GLU:HG2	1.80	0.46
10:M:39:GLY:O	10:M:167:ALA:HA	2.15	0.46
12:N:192:ILE:HD11	12:N:208:LEU:HD21	1.98	0.46
1:B:203:ARG:HD2	8:Y:161:HIS:CD2	2.48	0.46
2:C:38:ASN:HB2	2:C:39:PRO:HD2	1.97	0.46
3:P:70:HIS:CE1	3:P:103:PRO:HB3	2.50	0.46
4:Q:169:ARG:HH11	4:Q:169:ARG:HG2	1.81	0.46
11:V:180:VAL:HG21	11:V:194:ILE:HD12	1.97	0.46
12:I:94:HIS:CG	12:I:102:VAL:CG1	2.82	0.46
12:I:94:HIS:CB	12:I:102:VAL:CG1	2.93	0.46
12:I:139:ASP:OD1	12:I:139:ASP:N	2.35	0.46
14:O:11:ILE:HG22	12:N:7:ILE:HG23	1.97	0.46
14:O:28:ILE:HG21	14:O:133:SER:HB2	1.97	0.46
13:G:188:VAL:O	13:G:188:VAL:HG12	2.16	0.46
13:G:202:GLU:H	13:G:202:GLU:HG3	1.41	0.46
6:A:98:ILE:HD13	6:A:98:ILE:N	2.30	0.46
12:N:94:HIS:CB	12:N:102:VAL:CG1	2.93	0.46
9:W:147:GLN:HB3	9:W:148:PRO:HD3	1.97	0.46
5:R:104:LYS:HE3	5:R:104:LYS:HB3	1.49	0.46
6:F:21:THR:HG21	9:W:181:ALA:HB2	1.98	0.46
2:D:83:LEU:HD21	2:D:99:THR:HG21	1.96	0.46
7:X:136:LYS:HD2	7:X:137:ALA:H	1.81	0.46
11:T:127:ALA:HB1	11:T:128:PRO:HD2	1.98	0.46
13:L:188:VAL:O	13:L:188:VAL:HG12	2.16	0.46
14:O:95:GLN:NE2	14:O:98:LEU:HD23	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:48:LYS:HD3	12:N:163:ARG:NH2	2.30	0.46
3:P:172:PHE:CD2	3:P:196:GLU:OE1	2.69	0.46
3:P:195:LYS:HG3	3:P:202:MET:HE3	1.98	0.46
4:Q:108:LEU:HD23	4:Q:149:TYR:HD1	1.81	0.46
5:R:208:ILE:O	5:R:208:ILE:HG23	2.15	0.46
4:J:108:LEU:HD13	4:J:139:SER:CB	2.41	0.46
4:J:162:GLY:HA3	5:K:60:LEU:HD22	1.98	0.46
11:V:127:ALA:HB1	11:V:128:PRO:HD2	1.98	0.46
12:N:38:LYS:HD2	12:N:38:LYS:HA	1.60	0.46
1:B:114:TYR:HB3	1:B:115:PRO:HD2	1.97	0.46
3:P:221:THR:HB	3:P:222:PRO:CD	2.46	0.46
6:F:8:PHE:CZ	6:F:149:LYS:CG	2.99	0.46
10:H:201:ILE:HA	10:H:204:GLN:CD	2.36	0.46
11:V:4:LEU:HD22	11:V:45:LEU:HD23	1.98	0.46
11:V:58:GLU:HB3	12:I:96:LEU:HD11	1.97	0.46
14:O:174:MET:SD	14:O:195:LYS:HD3	2.56	0.46
10:M:91:LYS:HZ2	10:M:95:GLU:HG2	1.81	0.46
14:Z:72:MET:HE1	14:Z:110:LEU:HD23	1.92	0.46
12:N:90:GLU:HG2	12:N:110:TYR:CD2	2.51	0.46
2:C:37:ILE:HG21	2:C:41:LEU:HD23	1.98	0.46
4:J:136:MET:HE3	4:J:165:ILE:HG13	1.96	0.46
12:I:219:ILE:N	12:I:219:ILE:CD1	2.79	0.46
14:O:115:CYS:SG	14:O:156:TYR:HB3	2.56	0.46
12:N:35:VAL:HG23	12:N:191:VAL:HG22	1.97	0.46
8:U:25:ARG:HG3	8:U:183:GLY:C	2.36	0.46
3:P:56:TYR:HE2	5:R:159:TYR:HH	1.64	0.45
3:P:187:ILE:O	3:P:187:ILE:HG22	2.15	0.45
7:S:72:LEU:HD23	7:S:83:MET:SD	2.56	0.45
1:E:114:TYR:HB3	1:E:115:PRO:HD2	1.97	0.45
1:E:122:LEU:HB3	1:E:123:PRO:CD	2.44	0.45
10:H:135:ARG:HD3	12:I:8:THR:O	2.16	0.45
12:I:90:GLU:HG2	12:I:110:TYR:CD2	2.51	0.45
12:I:123:GLY:O	14:Z:124:PHE:HB2	2.15	0.45
14:O:97:TYR:CD2	14:O:105:ILE:HG13	2.51	0.45
13:G:81:ALA:HB2	13:G:130:VAL:HG21	1.98	0.45
14:Z:115:CYS:SG	14:Z:156:TYR:HB3	2.56	0.45
6:A:8:PHE:CZ	6:A:149:LYS:CG	2.99	0.45
6:A:21:THR:HG22	6:A:26:ILE:HA	1.97	0.45
8:U:106:PRO:HG2	8:U:123:LEU:HD13	1.98	0.45
7:S:136:LYS:HD2	7:S:137:ALA:H	1.81	0.45
10:H:69:GLU:HB2	10:H:226:PHE:CD2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:126:ARG:HD2	10:M:21:LEU:HD21	1.97	0.45
14:O:8:ARG:HD2	12:N:5:ARG:HH11	1.68	0.45
14:O:243:GLU:HA	14:O:243:GLU:OE2	2.16	0.45
14:Z:243:GLU:HA	14:Z:243:GLU:OE2	2.16	0.45
6:A:52:THR:CG2	6:A:96:ALA:CB	2.92	0.45
15:A:301:A1L0D:CB	15:A:301:A1L0D:O2	2.64	0.45
1:B:156:SER:HG	1:B:189:PHE:HE2	1.62	0.45
3:P:201:GLN:H	3:P:201:GLN:HE21	1.63	0.45
5:R:48:ALA:HB3	5:R:220:VAL:HG22	1.98	0.45
2:D:118:GLY:HA3	11:T:51:GLY:HA3	1.99	0.45
2:D:153:TYR:OH	2:D:178:HIS:CD2	2.70	0.45
7:X:136:LYS:HD3	7:X:136:LYS:HA	1.76	0.45
10:H:39:GLY:O	10:H:167:ALA:HA	2.15	0.45
12:I:35:VAL:HG23	12:I:191:VAL:HG22	1.97	0.45
12:I:200:GLN:NE2	12:I:201:SER:HB2	2.32	0.45
10:M:91:LYS:CD	10:M:119:LEU:HD11	2.45	0.45
2:C:6:PHE:HA	2:C:124:THR:O	2.17	0.45
15:F:301:A1L0D:CB	15:F:301:A1L0D:O2	2.65	0.45
2:D:21:THR:HG21	2:D:169:TYR:CD1	2.51	0.45
7:X:14:ALA:HB2	7:X:109:ILE:CG2	2.47	0.45
11:T:121:LEU:O	8:U:57:THR:CB	2.64	0.45
14:Z:174:MET:SD	14:Z:195:LYS:HD3	2.56	0.45
1:B:203:ARG:HD2	8:Y:161:HIS:CE1	2.52	0.45
4:Q:60:GLU:H	4:Q:60:GLU:HG2	1.59	0.45
6:F:15:GLY:HA2	6:F:175:ARG:O	2.17	0.45
2:D:37:ILE:HG21	2:D:41:LEU:HD23	1.98	0.45
4:J:56:LYS:CG	13:G:176:MET:HE1	2.31	0.45
8:Y:25:ARG:HG3	8:Y:183:GLY:C	2.36	0.45
5:K:239:LEU:HA	5:K:242:LEU:HD11	1.99	0.45
12:I:204:LYS:HE2	12:I:204:LYS:HB3	1.51	0.45
14:Z:175:LEU:CD2	14:Z:192:LEU:CD1	2.94	0.45
1:B:38:SER:HB2	1:B:39:PRO:HD2	1.97	0.45
1:B:171:SER:HB3	1:B:172:ASN:H	1.55	0.45
1:E:38:SER:HB2	1:E:39:PRO:CD	2.46	0.45
12:I:7:ILE:HG23	14:Z:11:ILE:HG22	1.98	0.45
13:L:7:ASP:HA	13:L:20:HIS:HB2	1.98	0.45
14:O:44:LEU:C	14:O:44:LEU:HD12	2.37	0.45
14:Z:31:ALA:O	14:Z:166:ASN:CB	2.65	0.45
14:Z:44:LEU:C	14:Z:44:LEU:HD12	2.37	0.45
14:Z:97:TYR:CD2	14:Z:105:ILE:HG13	2.51	0.45
8:U:142:SER:HA	8:U:145:MET:HE3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:THR:O	8:Y:197:ARG:HB3	2.17	0.45
2:C:153:TYR:OH	2:C:178:HIS:CD2	2.70	0.45
4:Q:66:LEU:HD13	4:Q:214:SER:HB2	1.97	0.45
2:D:17:ASP:OD2	2:D:33:LYS:NZ	2.50	0.45
1:E:195:LYS:NZ	8:U:150:GLU:OE1	2.43	0.45
14:O:31:ALA:O	14:O:166:ASN:CB	2.65	0.45
10:M:69:GLU:HB2	10:M:226:PHE:CD2	2.51	0.45
2:C:17:ASP:OD2	2:C:33:LYS:NZ	2.50	0.45
10:H:16:SER:HB2	10:H:17:PRO:CD	2.47	0.45
10:H:91:LYS:CA	10:H:91:LYS:HE2	2.47	0.45
13:L:35:THR:O	13:L:160:SER:HA	2.16	0.45
13:G:35:THR:O	13:G:160:SER:HA	2.16	0.45
12:N:119:THR:HG22	12:N:126:PRO:HB3	1.99	0.45
12:N:200:GLN:NE2	12:N:201:SER:HB2	2.32	0.45
4:Q:179:LEU:CD1	4:Q:196:ILE:HD11	2.46	0.45
10:M:16:SER:HB2	10:M:17:PRO:CD	2.47	0.45
14:Z:156:TYR:CD1	14:Z:156:TYR:C	2.90	0.45
3:P:45:LEU:HD13	3:P:74:VAL:HB	1.99	0.45
3:P:198:PHE:O	3:P:198:PHE:CD1	2.70	0.45
4:J:161:TRP:N	5:K:60:LEU:O	2.49	0.45
8:Y:158:ASP:HB2	8:Y:159:PRO:HD2	1.99	0.45
10:H:169:ALA:O	10:H:174:SER:HB2	2.16	0.45
12:I:48:LYS:HD3	12:I:163:ARG:NH2	2.29	0.45
13:L:63:ILE:HD12	13:L:211:SER:HB3	1.98	0.45
14:O:156:TYR:CD1	14:O:156:TYR:C	2.90	0.45
13:G:63:ILE:HD12	13:G:211:SER:HB3	1.98	0.45
4:Q:102:PHE:HB3	6:F:78:THR:HG23	1.99	0.44
5:R:78:CYS:CB	5:R:140:LEU:HD23	2.42	0.44
5:R:139:ILE:HG12	5:R:153:LYS:HG3	1.99	0.44
5:R:171:LYS:HB3	5:R:205:VAL:HG11	1.98	0.44
6:F:144:ARG:HG3	6:F:144:ARG:NH1	2.30	0.44
4:J:197:ILE:HD12	4:J:197:ILE:HA	1.68	0.44
5:K:171:LYS:HB3	5:K:205:VAL:HG11	1.98	0.44
11:T:4:LEU:HD22	11:T:45:LEU:HD23	1.98	0.44
14:O:28:ILE:HD11	14:O:152:PRO:HG3	1.99	0.44
14:O:151:ASP:CB	14:O:152:PRO:CD	2.89	0.44
10:M:169:ALA:O	10:M:174:SER:HB2	2.16	0.44
8:U:97:LYS:HB2	8:U:101:PRO:HA	2.00	0.44
6:F:134:TYR:HA	6:A:133:SER:O	2.17	0.44
8:Y:97:LYS:HB2	8:Y:101:PRO:HA	1.99	0.44
5:K:59:LYS:HA	5:K:59:LYS:HD2	1.71	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:176:LYS:HG3	12:N:53:LEU:CD1	2.47	0.44
12:N:137:ASP:OD2	12:N:143:ARG:NE	2.45	0.44
9:W:44:ARG:HG2	9:W:44:ARG:NH1	2.32	0.44
2:C:42:LEU:HD13	2:C:184:TRP:CD1	2.52	0.44
3:P:78:MET:HE3	5:R:16:PHE:HE1	1.82	0.44
3:P:156:ALA:CB	14:O:59:VAL:HG22	2.45	0.44
7:S:121:VAL:HG12	7:S:133:ASP:OD1	2.17	0.44
7:X:121:VAL:HG12	7:X:133:ASP:OD1	2.17	0.44
13:G:7:ASP:HA	13:G:20:HIS:HB2	1.98	0.44
8:U:67:LYS:HD3	8:U:67:LYS:HA	1.82	0.44
2:C:58:LEU:HD12	2:C:58:LEU:HA	1.82	0.44
3:P:67:ILE:CG1	3:P:73:LEU:HD13	2.48	0.44
3:P:108:GLN:CD	8:U:77:GLU:HB3	2.38	0.44
4:Q:51:LYS:O	4:Q:209:PHE:HB2	2.18	0.44
4:Q:215:TRP:CZ2	4:Q:219:LEU:HD11	2.53	0.44
5:R:147:GLN:HG2	5:R:150:GLN:HE22	1.83	0.44
5:R:239:LEU:HA	5:R:242:LEU:HD11	1.99	0.44
7:S:135:PHE:CD1	7:S:153:VAL:HG11	2.53	0.44
2:D:42:LEU:HD13	2:D:184:TRP:CD1	2.52	0.44
4:J:176:ILE:HG22	5:K:60:LEU:CD2	2.48	0.44
4:J:179:LEU:CD1	4:J:196:ILE:HD11	2.46	0.44
1:E:88:PHE:HA	1:E:116:HIS:O	2.17	0.44
13:L:215:VAL:O	13:L:215:VAL:HG13	2.18	0.44
10:M:136:PRO:O	12:N:10:PHE:HE2	1.99	0.44
1:B:88:PHE:HA	1:B:116:HIS:O	2.17	0.44
2:C:118:GLY:HA3	11:V:51:GLY:HA3	1.99	0.44
3:P:139:ASN:ND2	3:P:139:ASN:N	2.65	0.44
4:J:70:ASP:OD2	4:J:95:ALA:HB1	2.18	0.44
1:E:25:VAL:HG13	7:X:144:MET:HE1	2.00	0.44
10:H:91:LYS:CD	10:H:119:LEU:HD11	2.45	0.44
5:K:48:ALA:HB3	5:K:220:VAL:HG22	1.99	0.44
11:V:26:VAL:HA	11:T:170:ARG:O	2.16	0.44
11:V:78:THR:HG23	11:V:116:TYR:OH	2.18	0.44
11:T:78:THR:HG23	11:T:116:TYR:OH	2.17	0.44
13:L:81:ALA:HB2	13:L:130:VAL:HG21	1.98	0.44
13:L:189:LYS:CG	13:L:236:LEU:HD11	2.48	0.44
14:O:95:GLN:NE2	8:U:71:ASN:HD22	2.15	0.44
9:W:14:VAL:HG12	9:W:21:VAL:CG1	2.45	0.44
3:P:186:ALA:HA	3:P:189:THR:HG22	2.00	0.44
7:S:79:ASN:ND2	10:M:111:SER:OG	2.50	0.44
15:D:301:A1L0D:C4	15:D:301:A1L0D:O2	2.66	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:175:LEU:CD2	14:O:192:LEU:CD1	2.95	0.44
13:G:189:LYS:CG	13:G:236:LEU:HD11	2.48	0.44
8:U:13:MET:HB2	8:U:166:ILE:HD12	2.00	0.44
8:U:158:ASP:HB2	8:U:159:PRO:HD2	1.99	0.44
1:B:90:TYR:CD2	1:B:94:ILE:HD12	2.53	0.44
1:B:187:ARG:HA	1:B:188:PRO:HA	1.76	0.44
6:F:133:SER:O	6:A:134:TYR:HA	2.17	0.44
7:S:14:ALA:HB2	7:S:109:ILE:CG2	2.47	0.44
2:D:6:PHE:HA	2:D:124:THR:O	2.17	0.44
2:D:141:ARG:HD2	11:V:162:LYS:HB3	1.99	0.44
4:J:51:LYS:O	4:J:209:PHE:HB2	2.18	0.44
8:Y:21:ILE:CG2	8:Y:187:HIS:HB2	2.48	0.44
10:M:110:GLU:CG	10:M:154:PHE:CZ	2.93	0.44
10:M:135:ARG:HD3	12:N:8:THR:O	2.18	0.44
5:R:17:SER:CB	5:R:18:PRO:CD	2.96	0.44
5:R:113:MET:HE3	1:E:69:THR:HG22	2.00	0.44
4:J:52:LEU:CD2	4:J:209:PHE:HB3	2.47	0.44
14:O:198:ASN:HB2	14:O:206:LEU:CD2	2.48	0.44
13:G:73:SER:OG	13:G:133:LEU:HB2	2.18	0.44
13:G:229:VAL:HG12	13:G:233:LEU:HD12	2.00	0.44
14:Z:72:MET:HE2	14:Z:110:LEU:CD2	2.26	0.44
4:J:108:LEU:HD23	4:J:149:TYR:HD1	1.81	0.44
5:K:17:SER:CB	5:K:18:PRO:CD	2.96	0.44
13:L:229:VAL:HG12	13:L:233:LEU:HD12	2.00	0.44
14:Z:206:LEU:HA	14:Z:210:LYS:NZ	2.32	0.44
12:N:188:ILE:O	12:N:192:ILE:HD12	2.18	0.44
1:B:42:TYR:CE1	1:B:183:LEU:CD1	2.92	0.43
5:R:10:ASP:HA	5:R:15:ILE:HG13	2.00	0.43
6:F:149:LYS:HE3	6:F:149:LYS:HB3	1.83	0.43
4:J:136:MET:HE3	4:J:165:ILE:CG1	2.48	0.43
8:Y:42:PHE:HA	8:Y:43:PRO:HD3	1.84	0.43
8:Y:57:THR:CB	11:V:121:LEU:O	2.66	0.43
8:Y:106:PRO:HG2	8:Y:123:LEU:HD13	1.98	0.43
5:K:139:ILE:HG12	5:K:153:LYS:HG3	1.99	0.43
12:I:119:THR:HG22	12:I:126:PRO:HB3	1.99	0.43
12:I:225:ILE:O	12:I:225:ILE:HG22	2.18	0.43
10:M:91:LYS:CA	10:M:91:LYS:HE2	2.47	0.43
14:Z:52:ILE:H	14:Z:52:ILE:HG13	1.65	0.43
6:A:15:GLY:HA2	6:A:175:ARG:O	2.17	0.43
12:N:188:ILE:HD11	12:N:210:VAL:HG11	2.00	0.43
3:P:201:GLN:NE2	3:P:201:GLN:N	2.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:15:SER:HB2	4:Q:16:PRO:HD2	2.00	0.43
1:E:42:TYR:CE1	1:E:183:LEU:CD1	2.92	0.43
1:E:90:TYR:CD2	1:E:94:ILE:HD12	2.53	0.43
1:E:171:SER:HB3	1:E:172:ASN:H	1.55	0.43
1:E:213:THR:O	8:U:197:ARG:HB3	2.18	0.43
10:M:135:ARG:HH21	10:M:135:ARG:HG3	1.83	0.43
1:B:209:THR:HG21	8:Y:167:SER:HB3	2.00	0.43
4:Q:37:ILE:HD13	4:Q:193:VAL:HG22	1.94	0.43
4:Q:117:MET:HA	4:Q:117:MET:HE2	1.99	0.43
6:A:17:ASP:CG	6:A:33:LYS:HZ3	2.21	0.43
6:A:127:ILE:HD12	6:A:132:SER:HB2	2.01	0.43
15:C:301:A1L0D:C4	15:C:301:A1L0D:O2	2.66	0.43
6:F:144:ARG:CG	6:F:144:ARG:NH1	2.81	0.43
4:J:51:LYS:HB3	4:J:51:LYS:HE2	1.37	0.43
4:J:162:GLY:O	5:K:60:LEU:HB3	2.18	0.43
4:J:215:TRP:CZ2	4:J:219:LEU:HD11	2.53	0.43
7:X:159:GLN:HB3	7:X:160:ASN:H	1.58	0.43
5:K:21:ARG:NH2	5:K:26:GLU:OE1	2.50	0.43
13:L:73:SER:OG	13:L:133:LEU:HB2	2.18	0.43
9:W:39:ILE:HD12	9:W:57:TYR:CE1	2.53	0.43
4:Q:8:ASP:O	4:Q:22:GLN:NE2	2.37	0.43
4:Q:52:LEU:CD2	4:Q:209:PHE:HB3	2.47	0.43
4:Q:70:ASP:OD2	4:Q:95:ALA:HB1	2.18	0.43
4:J:102:PHE:HB3	6:A:78:THR:HG23	2.00	0.43
4:J:114:ARG:HA	4:J:114:ARG:HD2	1.85	0.43
10:H:95:GLU:OE2	10:H:95:GLU:HA	2.19	0.43
5:K:182:LYS:HB3	5:K:189:TRP:CH2	2.54	0.43
11:V:80:ALA:O	11:V:84:THR:HG23	2.12	0.43
14:O:31:ALA:O	14:O:166:ASN:HB2	2.18	0.43
10:M:78:MET:HB3	10:M:141:LEU:HD23	2.01	0.43
10:M:202:LEU:HD23	10:M:215:ILE:HG21	2.00	0.43
14:Z:28:ILE:HD11	14:Z:152:PRO:HG3	1.99	0.43
14:Z:35:LEU:C	14:Z:35:LEU:CD1	2.86	0.43
8:U:70:LEU:O	8:U:74:GLU:HG3	2.19	0.43
9:W:59:ASP:HB3	9:W:108:ASN:OD1	2.19	0.43
1:B:25:VAL:HG13	7:S:144:MET:HE1	2.01	0.43
4:Q:27:MET:CE	4:Q:153:PRO:HD2	2.49	0.43
4:Q:151:ILE:N	4:Q:151:ILE:CD1	2.79	0.43
10:H:35:SER:CB	10:H:51:GLU:HG3	2.44	0.43
14:O:206:LEU:HA	14:O:210:LYS:NZ	2.32	0.43
13:G:103:LEU:HD12	13:G:104:PRO:HD2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:107:ARG:NH2	9:W:81:HIS:O	2.51	0.43
6:A:103:TRP:CZ2	6:A:181:GLU:HB2	2.54	0.43
12:N:225:ILE:O	12:N:225:ILE:HG22	2.18	0.43
9:W:147:GLN:OE1	9:W:147:GLN:HA	2.19	0.43
1:B:3:ILE:HG22	1:B:16:ALA:HB2	2.00	0.43
5:R:113:MET:HE1	1:E:70:THR:HG22	2.00	0.43
5:R:139:ILE:HD13	5:R:166:THR:HG23	2.01	0.43
8:Y:70:LEU:O	8:Y:74:GLU:HG3	2.19	0.43
10:H:202:LEU:HD23	10:H:215:ILE:HG21	2.00	0.43
11:T:3:TYR:OH	11:T:5:ILE:HD12	2.19	0.43
13:G:230:SER:CB	13:G:231:PRO:HD3	2.49	0.43
10:M:54:ILE:O	10:M:54:ILE:HG22	2.18	0.43
14:Z:198:ASN:HB2	14:Z:206:LEU:CD2	2.48	0.43
8:U:24:ASP:O	8:U:40:LYS:HE3	2.19	0.43
3:P:188:HIS:CE1	3:P:228:TYR:CD1	2.97	0.43
4:J:33:SER:OG	4:J:65:ARG:NH1	2.44	0.43
7:X:135:PHE:CD1	7:X:153:VAL:HG11	2.53	0.43
10:H:199:LEU:HD12	10:H:237:VAL:HG12	2.01	0.43
13:G:215:VAL:O	13:G:215:VAL:HG13	2.18	0.43
14:Z:95:GLN:NE2	14:Z:98:LEU:HD23	2.31	0.43
14:Z:99:LEU:O	14:Z:99:LEU:HG	2.19	0.43
3:P:35:VAL:HG21	3:P:193:THR:CG2	2.40	0.43
6:F:14:LEU:N	6:F:14:LEU:HD12	2.34	0.43
7:S:133:ASP:OD1	7:S:133:ASP:N	2.52	0.43
4:J:15:SER:HB2	4:J:16:PRO:HD2	2.01	0.43
8:Y:100:GLY:H	8:Y:101:PRO:CD	2.27	0.43
1:E:3:ILE:HG22	1:E:16:ALA:HB2	2.00	0.43
10:H:78:MET:HB3	10:H:141:LEU:HD23	2.01	0.43
10:H:135:ARG:HH21	10:H:135:ARG:HG3	1.83	0.43
5:K:178:PHE:CE1	5:K:182:LYS:HD3	2.54	0.43
14:Z:9:THR:CB	14:Z:20:GLN:HG3	2.48	0.43
14:Z:31:ALA:O	14:Z:166:ASN:HB2	2.18	0.43
8:U:21:ILE:CG2	8:U:187:HIS:HB2	2.48	0.43
3:P:16:GLY:O	14:O:27:ALA:HB2	2.18	0.43
5:R:171:LYS:HG3	5:R:206:LEU:HD23	1.97	0.43
8:Y:13:MET:HB2	8:Y:166:ILE:HD12	2.00	0.43
8:Y:24:ASP:O	8:Y:40:LYS:HE3	2.19	0.43
5:K:147:GLN:HG2	5:K:150:GLN:HE22	1.83	0.43
13:L:35:THR:HG23	13:L:48:ALA:CB	2.49	0.43
13:L:49:LEU:HD22	13:L:199:LEU:CD2	2.48	0.43
13:G:35:THR:CG2	13:G:48:ALA:HB2	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:LEU:HD12	7:S:33:PHE:HA	2.01	0.42
1:B:195:LYS:NZ	8:Y:150:GLU:OE1	2.41	0.42
5:R:49:VAL:HG22	5:R:219:VAL:HG12	2.01	0.42
5:R:174:GLU:CD	5:R:174:GLU:N	2.73	0.42
4:J:151:ILE:N	4:J:151:ILE:CD1	2.79	0.42
1:E:167:LEU:HD12	7:X:33:PHE:HA	2.01	0.42
5:K:10:ASP:HA	5:K:15:ILE:HG13	2.00	0.42
11:V:2:GLU:HG2	11:V:34:LYS:HE3	2.00	0.42
12:I:188:ILE:O	12:I:192:ILE:HD12	2.18	0.42
13:L:230:SER:CB	13:L:231:PRO:HD3	2.49	0.42
13:G:35:THR:HG23	13:G:48:ALA:CB	2.49	0.42
10:M:199:LEU:HD12	10:M:237:VAL:HG12	2.01	0.42
14:Z:68:LEU:HD21	14:Z:74:CYS:SG	2.59	0.42
6:A:3:ILE:HG22	6:A:16:ALA:HB2	2.01	0.42
3:P:127:ARG:HD2	5:R:16:PHE:CE2	2.54	0.42
3:P:178:ASN:HD22	3:P:178:ASN:HA	1.56	0.42
4:Q:36:ALA:O	4:Q:136:MET:HE1	2.19	0.42
4:Q:215:TRP:O	4:Q:215:TRP:HD1	2.02	0.42
5:R:178:PHE:CE1	5:R:182:LYS:HD3	2.54	0.42
6:F:29:ARG:CZ	9:W:211:ILE:HD11	2.48	0.42
8:Y:189:ILE:HG23	8:Y:194:ILE:CD1	2.50	0.42
7:X:79:ASN:ND2	10:H:111:SER:OG	2.52	0.42
10:H:54:ILE:O	10:H:54:ILE:HG22	2.18	0.42
14:O:52:ILE:H	14:O:52:ILE:HG13	1.65	0.42
14:Z:174:MET:HE2	14:Z:199:LYS:HB3	1.94	0.42
9:W:53:ALA:HB3	9:W:60:PHE:CD1	2.54	0.42
1:B:6:VAL:HG12	1:B:124:TYR:CB	2.49	0.42
6:F:35:THR:HA	6:F:36:PRO:HD3	1.83	0.42
6:F:103:TRP:CZ2	6:F:181:GLU:HB2	2.54	0.42
14:O:102:GLN:NE2	8:U:64:GLN:HG2	2.33	0.42
13:G:62:LYS:HB3	13:G:62:LYS:HE3	1.77	0.42
10:M:70:ILE:HD11	10:M:89:ILE:HD12	2.02	0.42
6:A:14:LEU:N	6:A:14:LEU:HD12	2.34	0.42
6:F:127:ILE:HD12	6:F:132:SER:HB2	2.01	0.42
4:J:215:TRP:HD1	4:J:215:TRP:O	2.02	0.42
10:H:186:HIS:ND1	10:H:186:HIS:N	2.68	0.42
10:H:215:ILE:CD1	10:H:234:LEU:HD13	2.49	0.42
5:K:10:ASP:N	5:K:10:ASP:OD1	2.50	0.42
12:I:188:ILE:HD11	12:I:210:VAL:HG11	2.00	0.42
13:L:60:GLN:NE2	10:M:161:THR:CG2	2.79	0.42
10:M:95:GLU:HA	10:M:95:GLU:OE2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:148:ASP:CB	12:N:149:PRO:CD	2.97	0.42
8:U:189:ILE:HG23	8:U:194:ILE:CD1	2.50	0.42
9:W:9:THR:O	9:W:54:SER:CB	2.67	0.42
9:W:9:THR:HB	9:W:10:SER:H	1.54	0.42
3:P:156:ALA:O	14:O:56:LEU:HD23	2.19	0.42
8:Y:81:ILE:HD11	8:Y:85:THR:HG22	2.02	0.42
5:K:174:GLU:N	5:K:174:GLU:CD	2.73	0.42
3:P:159:ALA:HB3	14:O:55:LEU:HD13	2.00	0.42
4:Q:140:TYR:CG	4:Q:217:GLY:HA2	2.54	0.42
5:R:21:ARG:NH2	5:R:26:GLU:OE1	2.50	0.42
4:J:140:TYR:CG	4:J:217:GLY:HA2	2.55	0.42
11:T:2:GLU:HG2	11:T:34:LYS:HE3	2.00	0.42
12:I:199:VAL:O	12:I:199:VAL:HG13	2.19	0.42
14:O:176:LYS:HG2	12:N:53:LEU:HD12	2.02	0.42
13:G:88:MET:HE3	13:G:112:ILE:HD11	2.01	0.42
13:G:212:ILE:CD1	13:G:229:VAL:HG22	2.44	0.42
6:A:147:MET:HG2	6:A:151:GLU:HB3	2.01	0.42
1:B:122:LEU:HB3	1:B:123:PRO:CD	2.44	0.42
4:Q:73:VAL:HG13	4:Q:108:LEU:CD1	2.50	0.42
4:Q:139:SER:HA	4:Q:216:VAL:HG11	2.02	0.42
4:J:27:MET:CE	4:J:153:PRO:HD2	2.49	0.42
1:E:6:VAL:HG12	1:E:124:TYR:CB	2.49	0.42
10:H:204:GLN:HG3	10:H:204:GLN:H	1.71	0.42
5:K:37:LEU:HD12	5:K:37:LEU:HA	1.80	0.42
13:L:35:THR:CG2	13:L:48:ALA:HB2	2.49	0.42
13:L:103:LEU:HD12	13:L:104:PRO:HD2	2.01	0.42
10:M:202:LEU:HD23	10:M:206:MET:HE3	2.02	0.42
14:Z:178:ASP:OD2	14:Z:195:LYS:HE3	2.20	0.42
3:P:41:ASN:HD21	3:P:182:GLU:HG3	1.83	0.42
5:R:10:ASP:OD1	5:R:10:ASP:N	2.50	0.42
5:R:13:ILE:HG13	5:R:15:ILE:HG12	2.02	0.42
5:R:192:GLU:CD	5:R:192:GLU:N	2.73	0.42
6:F:10:GLY:O	6:F:103:TRP:CD1	2.73	0.42
6:F:143:TYR:CD1	6:F:143:TYR:C	2.93	0.42
4:J:215:TRP:O	4:J:215:TRP:CD1	2.73	0.42
7:X:133:ASP:OD1	7:X:133:ASP:N	2.52	0.42
11:V:117:TYR:HD2	11:V:130:ALA:HB1	1.85	0.42
14:O:68:LEU:HD21	14:O:74:CYS:SG	2.59	0.42
14:O:178:ASP:OD2	14:O:195:LYS:HE3	2.20	0.42
10:M:35:SER:CB	10:M:51:GLU:HG3	2.44	0.42
6:A:10:GLY:O	6:A:103:TRP:CD1	2.73	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:147:MET:HG2	6:F:151:GLU:HB3	2.01	0.42
4:J:73:VAL:HG13	4:J:108:LEU:CD1	2.50	0.42
1:E:3:ILE:HG22	1:E:16:ALA:CB	2.50	0.42
5:K:139:ILE:HD13	5:K:166:THR:HG23	2.01	0.42
5:K:192:GLU:CD	5:K:192:GLU:N	2.73	0.42
11:V:3:TYR:OH	11:V:5:ILE:HD12	2.19	0.42
12:I:148:ASP:CB	12:I:149:PRO:CD	2.97	0.42
10:M:215:ILE:CD1	10:M:234:LEU:HD13	2.49	0.42
9:W:20:VAL:HG11	9:W:122:LEU:HD13	2.01	0.42
3:P:172:PHE:CD1	3:P:172:PHE:C	2.93	0.42
6:F:24:SER:HB2	9:W:141:TYR:CE1	2.54	0.42
2:D:45:MET:HB3	2:D:52:CYS:CB	2.49	0.42
13:L:62:LYS:HB3	13:L:62:LYS:HE3	1.77	0.42
13:G:206:THR:O	13:G:233:LEU:HD11	2.20	0.42
12:N:199:VAL:O	12:N:199:VAL:HG13	2.19	0.42
9:W:48:SER:O	9:W:114:GLY:HA2	2.19	0.42
9:W:124:TYR:CD1	9:W:124:TYR:C	2.93	0.42
2:D:7:LYS:HB3	2:D:12:VAL:HG22	2.01	0.41
4:J:213:LEU:HB3	4:J:227:VAL:HG21	2.01	0.41
10:H:234:LEU:HD23	10:H:234:LEU:HA	1.85	0.41
5:K:13:ILE:HG13	5:K:15:ILE:HG12	2.02	0.41
13:L:206:THR:O	13:L:233:LEU:HD11	2.20	0.41
13:G:38:LEU:HD11	13:G:187:LEU:HG	2.02	0.41
14:Z:33:THR:HG23	14:Z:163:CYS:SG	2.60	0.41
9:W:100:ARG:O	9:W:100:ARG:HG2	2.20	0.41
3:P:159:ALA:HB1	3:P:173:LEU:HD22	2.00	0.41
5:R:55:LYS:NZ	5:R:55:LYS:HB3	2.35	0.41
5:R:59:LYS:HE3	5:R:59:LYS:HA	1.90	0.41
8:Y:112:ASP:HA	8:Y:113:PRO:HD3	1.86	0.41
8:Y:116:PHE:CE1	8:Y:191:LYS:HE3	2.56	0.41
1:E:106:THR:O	1:E:106:THR:HG22	2.20	0.41
1:E:206:LYS:HB3	1:E:206:LYS:HE2	1.83	0.41
10:H:18:GLU:CD	10:H:18:GLU:N	2.73	0.41
10:H:210:LEU:HD12	10:H:215:ILE:HG21	2.01	0.41
14:O:99:LEU:O	14:O:99:LEU:HG	2.19	0.41
6:A:149:LYS:HB3	6:A:149:LYS:HE3	1.83	0.41
8:U:6:ASN:HA	8:U:28:GLY:O	2.20	0.41
1:B:106:THR:O	1:B:106:THR:HG22	2.20	0.41
2:C:7:LYS:HB3	2:C:12:VAL:HG22	2.01	0.41
3:P:5:TYR:CE1	14:O:2:SER:HB2	2.56	0.41
3:P:114:ALA:HB1	3:P:152:GLY:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:135:ILE:HD12	3:P:135:ILE:N	2.35	0.41
3:P:138:TRP:CD1	3:P:214:GLU:HA	2.55	0.41
4:Q:213:LEU:HB3	4:Q:227:VAL:HG21	2.01	0.41
7:S:100:ARG:HH11	7:S:100:ARG:HG3	1.86	0.41
4:J:41:CYS:HG	4:J:186:CYS:HG	1.68	0.41
8:Y:10:VAL:HG12	8:Y:23:ALA:HB2	2.03	0.41
5:K:49:VAL:HG22	5:K:219:VAL:HG12	2.01	0.41
11:T:117:TYR:HD2	11:T:130:ALA:HB1	1.85	0.41
13:L:38:LEU:HD11	13:L:187:LEU:HG	2.03	0.41
6:A:143:TYR:CD1	6:A:143:TYR:C	2.93	0.41
5:R:182:LYS:HB3	5:R:189:TRP:CH2	2.54	0.41
6:F:6:VAL:HG23	6:F:125:PHE:HB3	2.02	0.41
8:Y:64:GLN:HG2	14:Z:102:GLN:NE2	2.36	0.41
1:E:205:GLU:H	1:E:205:GLU:HG2	1.50	0.41
9:W:147:GLN:N	9:W:148:PRO:CD	2.82	0.41
1:B:3:ILE:HG22	1:B:16:ALA:CB	2.50	0.41
1:B:22:GLU:O	1:B:22:GLU:HG3	2.21	0.41
4:Q:176:ILE:HG22	5:R:60:LEU:CD2	2.51	0.41
4:Q:215:TRP:O	4:Q:215:TRP:CD1	2.73	0.41
1:E:156:SER:HG	1:E:189:PHE:HE2	1.65	0.41
10:H:70:ILE:HD11	10:H:89:ILE:HD12	2.02	0.41
11:V:91:CYS:HA	11:V:94:SER:HB3	2.03	0.41
11:T:159:LEU:O	11:T:159:LEU:HD12	2.21	0.41
12:I:185:ASP:HB3	12:I:189:LYS:NZ	2.35	0.41
10:M:186:HIS:ND1	10:M:186:HIS:N	2.68	0.41
6:A:6:VAL:HG23	6:A:125:PHE:HB3	2.02	0.41
8:U:26:ARG:HB2	8:U:182:MET:CB	2.47	0.41
1:B:69:THR:HG22	5:K:113:MET:HE3	2.01	0.41
1:B:159:ILE:CG2	1:B:173:ILE:HG12	2.51	0.41
3:P:36:GLY:O	3:P:159:ALA:HA	2.20	0.41
4:Q:27:MET:HE3	4:Q:153:PRO:HD2	2.01	0.41
4:J:139:SER:HA	4:J:216:VAL:HG11	2.02	0.41
5:K:55:LYS:NZ	5:K:55:LYS:HB3	2.35	0.41
14:O:33:THR:HG23	14:O:163:CYS:SG	2.60	0.41
12:N:94:HIS:HD2	12:N:106:TYR:CZ	2.39	0.41
8:U:81:ILE:HD11	8:U:85:THR:HG22	2.02	0.41
4:J:117:MET:HA	4:J:117:MET:HE2	2.02	0.41
4:J:168:ALA:HB1	4:J:200:VAL:HG22	2.03	0.41
1:E:22:GLU:HG3	1:E:22:GLU:O	2.21	0.41
1:E:42:TYR:HB2	1:E:178:ILE:HD11	2.03	0.41
5:K:115:CYS:SG	5:K:152:TYR:HB3	2.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:207:THR:HG22	13:L:233:LEU:CD1	2.51	0.41
6:A:6:VAL:CG1	6:A:152:CYS:HB3	2.51	0.41
6:A:144:ARG:CG	6:A:144:ARG:NH1	2.81	0.41
2:C:4:LEU:C	2:C:4:LEU:CD1	2.88	0.41
2:C:13:ILE:HG21	2:C:156:ALA:HB2	2.03	0.41
3:P:14:PRO:HA	14:O:23:TYR:CD1	2.56	0.41
4:Q:56:LYS:HG2	13:L:176:MET:CE	2.47	0.41
5:R:210:PHE:HB3	5:R:215:ILE:HG12	2.03	0.41
5:R:239:LEU:HA	5:R:239:LEU:HD23	1.85	0.41
7:S:136:LYS:HD3	7:S:136:LYS:HA	1.76	0.41
10:M:210:LEU:HD12	10:M:215:ILE:HG21	2.01	0.41
12:N:185:ASP:HB3	12:N:189:LYS:NZ	2.35	0.41
3:P:73:LEU:HD12	3:P:135:ILE:HG23	2.02	0.41
4:Q:8:ASP:HB3	4:Q:21:PHE:CB	2.51	0.41
5:R:51:VAL:HG23	5:R:202:LEU:HD22	2.02	0.41
6:F:202:LEU:HD11	6:A:123:GLN:HA	2.03	0.41
8:Y:100:GLY:N	8:Y:101:PRO:HD3	2.24	0.41
1:E:113:ILE:HD12	1:E:113:ILE:N	2.36	0.41
7:X:12:VAL:HG12	7:X:25:SER:HB3	2.03	0.41
10:H:206:MET:HE3	10:H:215:ILE:CG2	2.50	0.41
5:K:210:PHE:HB3	5:K:215:ILE:HG12	2.03	0.41
14:O:35:LEU:HD12	14:O:35:LEU:O	2.21	0.41
13:G:118:ILE:CB	13:G:119:PRO:HD3	2.49	0.41
13:G:207:THR:HG22	13:G:233:LEU:CD1	2.51	0.41
10:M:191:LEU:CD2	10:M:221:GLN:CG	2.99	0.41
6:A:127:ILE:HD11	6:A:136:TYR:CE1	2.56	0.41
8:U:10:VAL:HG12	8:U:23:ALA:HB2	2.03	0.41
6:F:3:ILE:HG22	6:F:16:ALA:HB2	2.01	0.41
4:J:8:ASP:HB3	4:J:21:PHE:CB	2.51	0.41
8:Y:71:ASN:HD22	14:Z:95:GLN:NE2	2.19	0.41
7:X:100:ARG:HG3	7:X:100:ARG:HH11	1.86	0.41
5:K:25:VAL:CG2	5:K:126:THR:HG23	2.51	0.41
13:G:50:LYS:HE2	13:G:59:HIS:HB2	2.03	0.41
13:G:59:HIS:CD2	13:G:208:LYS:O	2.74	0.41
10:M:31:ILE:HD13	10:M:158:PRO:HD3	2.02	0.41
12:N:118:TYR:CD2	12:N:124:ARG:HD3	2.56	0.41
12:N:209:ALA:HB1	12:N:217:LEU:CD1	2.50	0.41
8:U:65:ARG:HH21	8:U:65:ARG:CG	2.32	0.41
1:B:42:TYR:HB2	1:B:178:ILE:HD11	2.03	0.40
3:P:159:ALA:O	14:O:55:LEU:HD13	2.21	0.40
4:Q:168:ALA:HB1	4:Q:200:VAL:HG22	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:12:VAL:HG12	7:S:25:SER:HB3	2.03	0.40
2:D:13:ILE:HG21	2:D:156:ALA:HB2	2.03	0.40
12:I:40:ILE:HG13	12:I:212:ARG:CG	2.50	0.40
12:I:43:LEU:HD12	12:I:70:CYS:SG	2.62	0.40
12:I:107:ILE:HD12	12:I:107:ILE:HA	1.95	0.40
13:G:49:LEU:HD22	13:G:199:LEU:CD2	2.48	0.40
10:M:35:SER:OG	10:M:66:LYS:CE	2.70	0.40
10:M:89:ILE:HD13	10:M:89:ILE:HA	1.85	0.40
14:Z:35:LEU:HD12	14:Z:35:LEU:O	2.21	0.40
3:P:74:VAL:HG12	3:P:134:LEU:HB3	2.03	0.40
3:P:194:LEU:HD23	3:P:194:LEU:HA	1.85	0.40
5:R:115:CYS:SG	5:R:152:TYR:HB3	2.60	0.40
2:D:88:TYR:CD2	11:T:55:GLN:NE2	2.89	0.40
8:Y:6:ASN:HA	8:Y:28:GLY:O	2.20	0.40
12:I:118:TYR:CD2	12:I:124:ARG:HD3	2.56	0.40
14:O:136:TYR:CD1	14:O:136:TYR:N	2.89	0.40
10:M:18:GLU:N	10:M:18:GLU:CD	2.73	0.40
1:B:69:THR:HG22	5:K:113:MET:HE1	2.01	0.40
2:C:8:PHE:HD1	2:C:8:PHE:N	2.09	0.40
3:P:28:VAL:CG1	3:P:132:SER:HB2	2.47	0.40
5:R:40:VAL:HG22	5:R:202:LEU:HD13	2.02	0.40
6:F:127:ILE:HD11	6:F:136:TYR:CE1	2.56	0.40
8:Y:34:VAL:HG12	8:Y:35:THR:HG23	2.03	0.40
10:H:31:ILE:HD13	10:H:158:PRO:HD3	2.02	0.40
10:H:44:GLU:OE1	10:H:190:THR:HA	2.21	0.40
5:K:51:VAL:HG23	5:K:202:LEU:HD22	2.02	0.40
11:V:159:LEU:HD12	11:V:159:LEU:O	2.21	0.40
1:E:22:GLU:HG2	1:E:27:ALA:HB2	2.04	0.40
5:K:14:THR:HB	5:K:126:THR:O	2.22	0.40
13:L:202:GLU:H	13:L:202:GLU:HG3	1.41	0.40
14:O:139:TRP:CE2	14:O:218:ARG:HD2	2.57	0.40
14:Z:97:TYR:C	14:Z:97:TYR:CD1	2.94	0.40
8:U:44:MET:HE3	8:U:50:ILE:HG21	2.03	0.40
9:W:76:LEU:HD23	9:W:76:LEU:HA	1.92	0.40
2:C:114:VAL:HG22	2:C:120:ARG:HG3	2.03	0.40
2:D:114:VAL:HG22	2:D:120:ARG:HG3	2.03	0.40
5:K:43:ARG:HE	5:K:164:LYS:HA	1.87	0.40
11:T:41:LYS:HB2	11:T:41:LYS:HE3	1.79	0.40
14:O:97:TYR:CD1	14:O:97:TYR:C	2.94	0.40
10:M:51:GLU:CB	10:M:206:MET:CE	2.93	0.40
10:M:116:VAL:O	10:M:116:VAL:HG12	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:144:ARG:HG3	6:A:144:ARG:NH1	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	218/234 (93%)	210 (96%)	7 (3%)	1 (0%)	29	48
1	E	218/234 (93%)	210 (96%)	7 (3%)	1 (0%)	29	48
2	C	197/204 (97%)	189 (96%)	8 (4%)	0	100	100
2	D	197/204 (97%)	189 (96%)	8 (4%)	0	100	100
3	P	226/234 (97%)	210 (93%)	12 (5%)	4 (2%)	8	14
3	b	226/234 (97%)	210 (93%)	12 (5%)	4 (2%)	8	14
4	J	233/255 (91%)	220 (94%)	13 (6%)	0	100	100
4	Q	233/255 (91%)	219 (94%)	14 (6%)	0	100	100
5	K	232/246 (94%)	219 (94%)	12 (5%)	1 (0%)	34	54
5	R	232/246 (94%)	219 (94%)	12 (5%)	1 (0%)	34	54
6	A	199/204 (98%)	189 (95%)	9 (4%)	1 (0%)	29	48
6	F	199/204 (98%)	189 (95%)	9 (4%)	1 (0%)	29	48
7	S	210/240 (88%)	197 (94%)	11 (5%)	2 (1%)	15	28
7	X	210/240 (88%)	197 (94%)	11 (5%)	2 (1%)	15	28
8	U	202/205 (98%)	190 (94%)	11 (5%)	1 (0%)	29	48
8	Y	202/205 (98%)	190 (94%)	11 (5%)	1 (0%)	29	48
9	W	212/264 (80%)	201 (95%)	9 (4%)	2 (1%)	17	31
9	a	212/264 (80%)	201 (95%)	9 (4%)	2 (1%)	17	31
10	H	229/241 (95%)	214 (93%)	15 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	M	229/241 (95%)	214 (93%)	15 (7%)	0	100	100
11	T	194/201 (96%)	189 (97%)	4 (2%)	1 (0%)	29	48
11	V	194/201 (96%)	189 (97%)	4 (2%)	1 (0%)	29	48
12	I	230/248 (93%)	215 (94%)	14 (6%)	1 (0%)	34	54
12	N	230/248 (93%)	215 (94%)	14 (6%)	1 (0%)	34	54
13	G	232/263 (88%)	217 (94%)	14 (6%)	1 (0%)	34	54
13	L	232/263 (88%)	217 (94%)	14 (6%)	1 (0%)	34	54
14	O	235/261 (90%)	228 (97%)	6 (3%)	1 (0%)	34	54
14	Z	235/261 (90%)	228 (97%)	6 (3%)	1 (0%)	34	54
All	All	6098/6600 (92%)	5775 (95%)	291 (5%)	32 (0%)	32	48

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	Y	78	GLY
14	O	59	VAL
14	Z	59	VAL
8	U	78	GLY
1	B	95	GLY
3	P	40	ALA
3	P	199	GLU
5	R	57	PRO
6	F	191	GLY
1	E	95	GLY
9	a	107	TRP
5	K	57	PRO
3	b	40	ALA
3	b	199	GLU
11	V	24	ASN
11	T	24	ASN
6	A	191	GLY
9	W	107	TRP
7	S	191	ASP
7	X	191	ASP
13	L	225	ASP
13	G	225	ASP
3	P	54	ILE
7	S	159	GLN
7	X	159	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	b	54	ILE
12	I	216	PRO
12	N	216	PRO
3	P	53	SER
3	b	53	SER
9	a	17	ASP
9	W	17	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	181/195 (93%)	147 (81%)	34 (19%)	1 2
1	E	181/195 (93%)	147 (81%)	34 (19%)	1 2
2	C	155/160 (97%)	134 (86%)	21 (14%)	4 7
2	D	155/160 (97%)	134 (86%)	21 (14%)	4 7
3	P	187/191 (98%)	156 (83%)	31 (17%)	2 4
3	b	187/191 (98%)	156 (83%)	31 (17%)	2 4
4	J	192/211 (91%)	154 (80%)	38 (20%)	1 2
4	Q	192/211 (91%)	154 (80%)	38 (20%)	1 2
5	K	201/210 (96%)	166 (83%)	35 (17%)	2 3
5	R	201/210 (96%)	166 (83%)	35 (17%)	2 3
6	A	158/161 (98%)	142 (90%)	16 (10%)	7 14
6	F	158/161 (98%)	142 (90%)	16 (10%)	7 14
7	S	177/198 (89%)	148 (84%)	29 (16%)	2 4
7	X	177/198 (89%)	148 (84%)	29 (16%)	2 4
8	U	174/175 (99%)	157 (90%)	17 (10%)	8 15
8	Y	174/175 (99%)	157 (90%)	17 (10%)	8 15
9	W	176/212 (83%)	147 (84%)	29 (16%)	2 4
9	a	176/212 (83%)	148 (84%)	28 (16%)	2 4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	H	193/203 (95%)	165 (86%)	28 (14%)	3 6
10	M	193/203 (95%)	165 (86%)	28 (14%)	3 6
11	T	166/171 (97%)	150 (90%)	16 (10%)	8 16
11	V	166/171 (97%)	150 (90%)	16 (10%)	8 16
12	I	195/211 (92%)	148 (76%)	47 (24%)	0 1
12	N	195/211 (92%)	149 (76%)	46 (24%)	1 1
13	G	200/224 (89%)	158 (79%)	42 (21%)	1 2
13	L	200/224 (89%)	158 (79%)	42 (21%)	1 2
14	O	201/221 (91%)	157 (78%)	44 (22%)	1 1
14	Z	201/221 (91%)	157 (78%)	44 (22%)	1 1
All	All	5112/5486 (93%)	4260 (83%)	852 (17%)	5 4

All (852) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	10	ASP
1	B	19	ARG
1	B	21	THR
1	B	29	LYS
1	B	36	PHE
1	B	55	THR
1	B	60	SER
1	B	61	SER
1	B	64	GLU
1	B	65	LEU
1	B	67	SER
1	B	72	ARG
1	B	77	VAL
1	B	84	LYS
1	B	89	ARG
1	B	98	LEU
1	B	127	MET
1	B	129	SER
1	B	132	LEU
1	B	135	MET
1	B	141	LYS
1	B	153	LYS
1	B	156	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	157	GLU
1	B	171	SER
1	B	180	LYS
1	B	181	SER
1	B	184	ASP
1	B	185	PHE
1	B	194	LYS
1	B	198	ARG
1	B	203	ARG
1	B	205	GLU
1	B	214	GLU
2	C	8	PHE
2	C	21	THR
2	C	31	VAL
2	C	32	LYS
2	C	42	LEU
2	C	44	THR
2	C	45	MET
2	C	56	GLU
2	C	91	LYS
2	C	93	MET
2	C	97	MET
2	C	99	THR
2	C	100	MET
2	C	102	CYS
2	C	106	LYS
2	C	122	SER
2	C	146	ASP
2	C	178	HIS
2	C	186	ARG
2	C	190	ASP
2	C	200	SER
3	P	6	SER
3	P	15	SER
3	P	34	SER
3	P	51	GLN
3	P	52	LYS
3	P	59	ARG
3	P	61	VAL
3	P	65	GLU
3	P	73	LEU
3	P	76	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	P	88	ARG
3	P	91	LYS
3	P	102	GLU
3	P	106	THR
3	P	131	VAL
3	P	132	SER
3	P	139	ASN
3	P	142	ARG
3	P	147	GLN
3	P	164	LYS
3	P	176	ARG
3	P	178	ASN
3	P	188	HIS
3	P	191	ILE
3	P	196	GLU
3	P	199	GLU
3	P	201	GLN
3	P	205	ASP
3	P	214	GLU
3	P	223	THR
3	P	224	GLU
4	Q	34	SER
4	Q	42	LYS
4	Q	43	ASP
4	Q	51	LYS
4	Q	53	VAL
4	Q	55	SER
4	Q	56	LYS
4	Q	60	GLU
4	Q	69	VAL
4	Q	71	ARG
4	Q	81	LEU
4	Q	89	ASP
4	Q	125	TYR
4	Q	141	SER
4	Q	143	ASN
4	Q	165	ILE
4	Q	167	LYS
4	Q	169	ARG
4	Q	170	GLN
4	Q	173	LYS
4	Q	175	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	Q	181	MET
4	Q	183	GLU
4	Q	185	THR
4	Q	186	CYS
4	Q	187	ARG
4	Q	195	LYS
4	Q	197	ILE
4	Q	198	TYR
4	Q	200	VAL
4	Q	204	VAL
4	Q	205	LYS
4	Q	215	TRP
4	Q	219	LEU
4	Q	230	ASP
4	Q	231	ILE
4	Q	237	LYS
4	Q	240	LYS
5	R	5	SER
5	R	6	SER
5	R	34	GLN
5	R	37	LEU
5	R	40	VAL
5	R	55	LYS
5	R	58	ASP
5	R	59	LYS
5	R	61	LEU
5	R	63	SER
5	R	64	SER
5	R	66	VAL
5	R	73	THR
5	R	74	GLU
5	R	78	CYS
5	R	88	ARG
5	R	108	GLU
5	R	130	GLU
5	R	131	MET
5	R	145	GLU
5	R	146	GLU
5	R	147	GLN
5	R	153	LYS
5	R	171	LYS
5	R	173	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	R	181	LYS
5	R	182	LYS
5	R	196	GLU
5	R	204	THR
5	R	208	ILE
5	R	211	LYS
5	R	215	ILE
5	R	223	GLU
5	R	226	LYS
5	R	242	LEU
6	F	68	ILE
6	F	72	GLU
6	F	84	LYS
6	F	86	MET
6	F	93	ASP
6	F	95	MET
6	F	106	GLN
6	F	124	SER
6	F	144	ARG
6	F	149	LYS
6	F	151	GLU
6	F	169	SER
6	F	181	GLU
6	F	187	GLN
6	F	194	ILE
6	F	198	THR
7	S	11	THR
7	S	12	VAL
7	S	13	LEU
7	S	21	SER
7	S	30	SER
7	S	31	GLU
7	S	42	LYS
7	S	45	LYS
7	S	48	ASP
7	S	65	THR
7	S	73	LYS
7	S	81	LYS
7	S	99	ARG
7	S	116	GLU
7	S	125	ASP
7	S	133	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	S	134	SER
7	S	136	LYS
7	S	140	SER
7	S	142	SER
7	S	159	GLN
7	S	160	ASN
7	S	162	GLU
7	S	167	THR
7	S	174	LEU
7	S	195	ILE
7	S	200	LYS
7	S	201	GLU
7	S	207	THR
2	D	8	PHE
2	D	21	THR
2	D	31	VAL
2	D	32	LYS
2	D	42	LEU
2	D	44	THR
2	D	45	MET
2	D	56	GLU
2	D	91	LYS
2	D	93	MET
2	D	97	MET
2	D	99	THR
2	D	100	MET
2	D	102	CYS
2	D	106	LYS
2	D	122	SER
2	D	146	ASP
2	D	178	HIS
2	D	186	ARG
2	D	190	ASP
2	D	200	SER
4	J	34	SER
4	J	42	LYS
4	J	43	ASP
4	J	51	LYS
4	J	53	VAL
4	J	55	SER
4	J	56	LYS
4	J	60	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	J	69	VAL
4	J	71	ARG
4	J	81	LEU
4	J	89	ASP
4	J	125	TYR
4	J	141	SER
4	J	143	ASN
4	J	165	ILE
4	J	167	LYS
4	J	169	ARG
4	J	170	GLN
4	J	173	LYS
4	J	175	GLU
4	J	181	MET
4	J	183	GLU
4	J	185	THR
4	J	186	CYS
4	J	187	ARG
4	J	195	LYS
4	J	197	ILE
4	J	198	TYR
4	J	200	VAL
4	J	204	VAL
4	J	205	LYS
4	J	215	TRP
4	J	219	LEU
4	J	230	ASP
4	J	231	ILE
4	J	237	LYS
4	J	240	LYS
8	Y	2	ILE
8	Y	4	SER
8	Y	14	LYS
8	Y	16	LYS
8	Y	26	ARG
8	Y	70	LEU
8	Y	76	LYS
8	Y	114	LYS
8	Y	125	LEU
8	Y	134	ASP
8	Y	138	SER
8	Y	144	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	Y	180	SER
8	Y	192	ASP
8	Y	193	LYS
8	Y	197	ARG
8	Y	200	LYS
1	E	10	ASP
1	E	19	ARG
1	E	21	THR
1	E	29	LYS
1	E	36	PHE
1	E	55	THR
1	E	60	SER
1	E	61	SER
1	E	64	GLU
1	E	65	LEU
1	E	67	SER
1	E	72	ARG
1	E	77	VAL
1	E	84	LYS
1	E	89	ARG
1	E	98	LEU
1	E	127	MET
1	E	129	SER
1	E	132	LEU
1	E	135	MET
1	E	141	LYS
1	E	153	LYS
1	E	156	SER
1	E	157	GLU
1	E	171	SER
1	E	180	LYS
1	E	181	SER
1	E	184	ASP
1	E	185	PHE
1	E	194	LYS
1	E	198	ARG
1	E	203	ARG
1	E	205	GLU
1	E	214	GLU
7	X	11	THR
7	X	12	VAL
7	X	13	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	X	21	SER
7	X	30	SER
7	X	31	GLU
7	X	42	LYS
7	X	45	LYS
7	X	48	ASP
7	X	65	THR
7	X	73	LYS
7	X	81	LYS
7	X	99	ARG
7	X	116	GLU
7	X	125	ASP
7	X	133	ASP
7	X	134	SER
7	X	136	LYS
7	X	140	SER
7	X	142	SER
7	X	159	GLN
7	X	160	ASN
7	X	162	GLU
7	X	167	THR
7	X	174	LEU
7	X	195	ILE
7	X	200	LYS
7	X	201	GLU
7	X	207	THR
9	a	3	ASN
9	a	9	THR
9	a	14	VAL
9	a	33	LEU
9	a	35	ARG
9	a	37	ARG
9	a	43	MET
9	a	49	THR
9	a	51	LEU
9	a	65	GLN
9	a	74	GLU
9	a	82	SER
9	a	94	ARG
9	a	98	SER
9	a	100	ARG
9	a	110	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	a	141	TYR
9	a	155	GLU
9	a	162	GLN
9	a	164	GLU
9	a	182	ARG
9	a	183	SER
9	a	188	GLN
9	a	195	LYS
9	a	199	ILE
9	a	204	SER
9	a	206	GLN
9	a	214	MET
10	H	9	ASP
10	H	35	SER
10	H	41	GLN
10	H	43	SER
10	H	47	CYS
10	H	53	ARG
10	H	54	ILE
10	H	62	SER
10	H	65	GLU
10	H	66	LYS
10	H	78	MET
10	H	84	ASP
10	H	91	LYS
10	H	95	GLU
10	H	110	GLU
10	H	111	SER
10	H	125	GLU
10	H	148	GLU
10	H	149	LYS
10	H	152	GLN
10	H	165	CYS
10	H	184	VAL
10	H	187	LYS
10	H	188	SER
10	H	189	MET
10	H	192	LYS
10	H	198	SER
10	H	204	GLN
5	K	5	SER
5	K	6	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	K	34	GLN
5	K	37	LEU
5	K	40	VAL
5	K	55	LYS
5	K	58	ASP
5	K	59	LYS
5	K	61	LEU
5	K	63	SER
5	K	64	SER
5	K	66	VAL
5	K	73	THR
5	K	74	GLU
5	K	78	CYS
5	K	88	ARG
5	K	108	GLU
5	K	130	GLU
5	K	131	MET
5	K	145	GLU
5	K	146	GLU
5	K	147	GLN
5	K	153	LYS
5	K	171	LYS
5	K	173	THR
5	K	181	LYS
5	K	182	LYS
5	K	196	GLU
5	K	204	THR
5	K	208	ILE
5	K	211	LYS
5	K	215	ILE
5	K	223	GLU
5	K	226	LYS
5	K	242	LEU
3	b	6	SER
3	b	15	SER
3	b	34	SER
3	b	51	GLN
3	b	52	LYS
3	b	59	ARG
3	b	61	VAL
3	b	65	GLU
3	b	73	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	b	76	SER
3	b	88	ARG
3	b	91	LYS
3	b	102	GLU
3	b	106	THR
3	b	131	VAL
3	b	132	SER
3	b	139	ASN
3	b	142	ARG
3	b	147	GLN
3	b	164	LYS
3	b	176	ARG
3	b	178	ASN
3	b	188	HIS
3	b	191	ILE
3	b	196	GLU
3	b	199	GLU
3	b	201	GLN
3	b	205	ASP
3	b	214	GLU
3	b	223	THR
3	b	224	GLU
11	V	1	MET
11	V	33	ASP
11	V	40	GLU
11	V	49	GLU
11	V	65	GLN
11	V	69	MET
11	V	84	THR
11	V	86	ARG
11	V	94	SER
11	V	145	ARG
11	V	161	ARG
11	V	171	PHE
11	V	177	THR
11	V	179	SER
11	V	185	LYS
11	V	192	GLU
11	T	1	MET
11	T	33	ASP
11	T	40	GLU
11	T	49	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	T	65	GLN
11	T	69	MET
11	T	84	THR
11	T	86	ARG
11	T	94	SER
11	T	145	ARG
11	T	161	ARG
11	T	171	PHE
11	T	177	THR
11	T	179	SER
11	T	185	LYS
11	T	192	GLU
12	I	5	ARG
12	I	11	SER
12	I	13	ASP
12	I	24	GLU
12	I	28	LYS
12	I	30	SER
12	I	33	VAL
12	I	38	LYS
12	I	39	ASP
12	I	40	ILE
12	I	48	LYS
12	I	49	SER
12	I	52	LYS
12	I	54	GLN
12	I	56	GLU
12	I	58	THR
12	I	70	CYS
12	I	86	ARG
12	I	100	ASP
12	I	105	GLU
12	I	121	SER
12	I	129	ILE
12	I	130	SER
12	I	134	VAL
12	I	139	ASP
12	I	146	GLN
12	I	157	LYS
12	I	163	ARG
12	I	166	LYS
12	I	169	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	I	170	GLU
12	I	174	LYS
12	I	179	ASP
12	I	183	THR
12	I	187	THR
12	I	189	LYS
12	I	204	LYS
12	I	205	ASN
12	I	207	GLU
12	I	211	MET
12	I	213	ARG
12	I	214	ASP
12	I	215	GLN
12	I	221	ASN
12	I	224	GLU
12	I	227	LYS
12	I	233	GLU
13	L	5	GLN
13	L	9	ASP
13	L	26	MET
13	L	27	GLU
13	L	35	THR
13	L	38	LEU
13	L	39	LYS
13	L	41	LYS
13	L	51	ARG
13	L	61	LYS
13	L	73	SER
13	L	95	SER
13	L	96	ARG
13	L	101	ARG
13	L	110	SER
13	L	133	LEU
13	L	146	GLN
13	L	154	PHE
13	L	156	CYS
13	L	157	ARG
13	L	159	MET
13	L	164	ARG
13	L	167	SER
13	L	174	ARG
13	L	181	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	L	182	CYS
13	L	184	LEU
13	L	185	ASP
13	L	189	LYS
13	L	198	THR
13	L	199	LEU
13	L	202	GLU
13	L	203	GLN
13	L	206	THR
13	L	211	SER
13	L	226	ASP
13	L	227	ASP
13	L	228	ASP
13	L	229	VAL
13	L	230	SER
13	L	233	LEU
13	L	237	GLU
14	O	3	ARG
14	O	8	ARG
14	O	17	ARG
14	O	25	MET
14	O	26	GLU
14	O	35	LEU
14	O	38	LEU
14	O	48	GLU
14	O	54	LYS
14	O	58	GLU
14	O	61	PHE
14	O	62	SER
14	O	65	ILE
14	O	67	LYS
14	O	70	GLU
14	O	71	ASP
14	O	80	THR
14	O	92	LEU
14	O	95	GLN
14	O	127	LYS
14	O	132	VAL
14	O	133	SER
14	O	160	LYS
14	O	178	ASP
14	O	180	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	O	181	GLU
14	O	185	THR
14	O	186	LEU
14	O	192	LEU
14	O	195	LYS
14	O	198	ASN
14	O	201	MET
14	O	206	LEU
14	O	209	GLU
14	O	218	ARG
14	O	222	LYS
14	O	226	ARG
14	O	228	LEU
14	O	230	GLN
14	O	234	GLU
14	O	237	ILE
14	O	239	LYS
14	O	241	GLU
14	O	243	GLU
13	G	5	GLN
13	G	9	ASP
13	G	26	MET
13	G	27	GLU
13	G	35	THR
13	G	38	LEU
13	G	39	LYS
13	G	41	LYS
13	G	51	ARG
13	G	61	LYS
13	G	73	SER
13	G	95	SER
13	G	96	ARG
13	G	101	ARG
13	G	110	SER
13	G	133	LEU
13	G	146	GLN
13	G	154	PHE
13	G	156	CYS
13	G	157	ARG
13	G	159	MET
13	G	164	ARG
13	G	167	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	G	174	ARG
13	G	181	GLU
13	G	182	CYS
13	G	184	LEU
13	G	185	ASP
13	G	189	LYS
13	G	198	THR
13	G	199	LEU
13	G	202	GLU
13	G	203	GLN
13	G	206	THR
13	G	211	SER
13	G	226	ASP
13	G	227	ASP
13	G	228	ASP
13	G	229	VAL
13	G	230	SER
13	G	233	LEU
13	G	237	GLU
10	M	9	ASP
10	M	35	SER
10	M	41	GLN
10	M	43	SER
10	M	47	CYS
10	M	53	ARG
10	M	54	ILE
10	M	62	SER
10	M	65	GLU
10	M	66	LYS
10	M	78	MET
10	M	84	ASP
10	M	91	LYS
10	M	95	GLU
10	M	110	GLU
10	M	111	SER
10	M	125	GLU
10	M	148	GLU
10	M	149	LYS
10	M	152	GLN
10	M	165	CYS
10	M	184	VAL
10	M	187	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	M	188	SER
10	M	189	MET
10	M	192	LYS
10	M	198	SER
10	M	204	GLN
14	Z	3	ARG
14	Z	8	ARG
14	Z	17	ARG
14	Z	25	MET
14	Z	26	GLU
14	Z	35	LEU
14	Z	38	LEU
14	Z	48	GLU
14	Z	54	LYS
14	Z	58	GLU
14	Z	61	PHE
14	Z	62	SER
14	Z	65	ILE
14	Z	67	LYS
14	Z	70	GLU
14	Z	71	ASP
14	Z	80	THR
14	Z	92	LEU
14	Z	95	GLN
14	Z	127	LYS
14	Z	132	VAL
14	Z	133	SER
14	Z	160	LYS
14	Z	178	ASP
14	Z	180	LYS
14	Z	181	GLU
14	Z	185	THR
14	Z	186	LEU
14	Z	192	LEU
14	Z	195	LYS
14	Z	198	ASN
14	Z	201	MET
14	Z	206	LEU
14	Z	209	GLU
14	Z	218	ARG
14	Z	222	LYS
14	Z	226	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	Z	228	LEU
14	Z	230	GLN
14	Z	234	GLU
14	Z	237	ILE
14	Z	239	LYS
14	Z	241	GLU
14	Z	243	GLU
6	A	68	ILE
6	A	72	GLU
6	A	84	LYS
6	A	86	MET
6	A	93	ASP
6	A	95	MET
6	A	106	GLN
6	A	124	SER
6	A	144	ARG
6	A	149	LYS
6	A	151	GLU
6	A	169	SER
6	A	181	GLU
6	A	187	GLN
6	A	194	ILE
6	A	198	THR
12	N	5	ARG
12	N	11	SER
12	N	13	ASP
12	N	24	GLU
12	N	28	LYS
12	N	30	SER
12	N	33	VAL
12	N	38	LYS
12	N	39	ASP
12	N	40	ILE
12	N	48	LYS
12	N	49	SER
12	N	52	LYS
12	N	54	GLN
12	N	56	GLU
12	N	58	THR
12	N	70	CYS
12	N	100	ASP
12	N	105	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	N	121	SER
12	N	129	ILE
12	N	130	SER
12	N	134	VAL
12	N	139	ASP
12	N	146	GLN
12	N	157	LYS
12	N	163	ARG
12	N	166	LYS
12	N	169	ARG
12	N	170	GLU
12	N	174	LYS
12	N	179	ASP
12	N	183	THR
12	N	187	THR
12	N	189	LYS
12	N	204	LYS
12	N	205	ASN
12	N	207	GLU
12	N	211	MET
12	N	213	ARG
12	N	214	ASP
12	N	215	GLN
12	N	221	ASN
12	N	224	GLU
12	N	227	LYS
12	N	233	GLU
8	U	2	ILE
8	U	4	SER
8	U	14	LYS
8	U	16	LYS
8	U	26	ARG
8	U	70	LEU
8	U	76	LYS
8	U	114	LYS
8	U	125	LEU
8	U	134	ASP
8	U	138	SER
8	U	144	GLN
8	U	180	SER
8	U	192	ASP
8	U	193	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	U	197	ARG
8	U	200	LYS
9	W	3	ASN
9	W	9	THR
9	W	14	VAL
9	W	33	LEU
9	W	35	ARG
9	W	37	ARG
9	W	43	MET
9	W	49	THR
9	W	51	LEU
9	W	65	GLN
9	W	74	GLU
9	W	82	SER
9	W	94	ARG
9	W	98	SER
9	W	100	ARG
9	W	110	MET
9	W	141	TYR
9	W	155	GLU
9	W	162	GLN
9	W	164	GLU
9	W	182	ARG
9	W	183	SER
9	W	188	GLN
9	W	195	LYS
9	W	199	ILE
9	W	203	LEU
9	W	204	SER
9	W	206	GLN
9	W	214	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	66	HIS
2	C	178	HIS
2	C	196	HIS
3	P	108	GLN
3	P	111	GLN
3	P	139	ASN
3	P	147	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	P	168	ASN
3	P	178	ASN
3	P	188	HIS
3	P	201	GLN
4	Q	63	ASN
5	R	34	GLN
5	R	90	GLN
5	R	150	GLN
6	F	40	HIS
6	F	77	HIS
6	F	123	GLN
6	F	180	GLN
7	S	79	ASN
7	S	131	GLN
7	S	159	GLN
7	S	163	HIS
2	D	178	HIS
2	D	196	HIS
4	J	63	ASN
1	E	66	HIS
7	X	58	HIS
7	X	79	ASN
7	X	131	GLN
7	X	159	GLN
7	X	163	HIS
9	a	81	HIS
9	a	157	GLN
9	a	188	GLN
10	H	122	GLN
10	H	152	GLN
10	H	227	HIS
5	K	34	GLN
5	K	90	GLN
5	K	150	GLN
3	b	108	GLN
3	b	111	GLN
3	b	139	ASN
3	b	147	GLN
3	b	168	ASN
3	b	178	ASN
3	b	188	HIS
3	b	201	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	V	55	GLN
11	V	71	ASN
11	V	132	HIS
11	V	190	ASN
11	T	55	GLN
11	T	71	ASN
11	T	132	HIS
11	T	190	ASN
12	I	23	GLN
12	I	92	GLN
12	I	146	GLN
12	I	159	ASN
12	I	200	GLN
12	I	221	ASN
13	L	5	GLN
13	L	60	GLN
13	L	183	ASN
13	L	190	HIS
14	O	40	ASN
14	O	95	GLN
14	O	102	GLN
14	O	146	GLN
14	O	230	GLN
13	G	5	GLN
13	G	60	GLN
13	G	183	ASN
13	G	190	HIS
10	M	122	GLN
10	M	152	GLN
10	M	214	ASN
10	M	227	HIS
14	Z	40	ASN
14	Z	95	GLN
14	Z	102	GLN
14	Z	146	GLN
14	Z	230	GLN
6	A	40	HIS
6	A	77	HIS
6	A	123	GLN
6	A	180	GLN
12	N	23	GLN
12	N	92	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	N	146	GLN
12	N	159	ASN
12	N	200	GLN
12	N	221	ASN
9	W	81	HIS
9	W	157	GLN
9	W	188	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	A1L0D	C	302	2	25,33,33	0.82	1 (4%)	24,46,46	1.42	2 (8%)
15	A1L0D	C	301	-	20,27,33	0.66	1 (5%)	23,38,46	1.50	2 (8%)
15	A1L0D	A	301	6	25,33,33	0.79	1 (4%)	24,46,46	1.32	2 (8%)
15	A1L0D	F	301	6	25,33,33	0.80	1 (4%)	24,46,46	1.32	2 (8%)
15	A1L0D	D	302	2	25,33,33	0.81	1 (4%)	24,46,46	1.40	2 (8%)
15	A1L0D	D	301	-	20,27,33	0.65	1 (5%)	23,38,46	1.50	2 (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
15	A1L0D	C	302	2	-	1/11/49/49	0/3/3/3
15	A1L0D	C	301	-	-	2/5/38/49	0/3/3/3
15	A1L0D	A	301	6	-	0/11/49/49	0/3/3/3
15	A1L0D	F	301	6	-	0/11/49/49	0/3/3/3
15	A1L0D	D	302	2	-	2/11/49/49	0/3/3/3
15	A1L0D	D	301	-	-	2/5/38/49	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	D	302	A1L0D	OXT-C	-2.57	1.31	1.42
15	C	302	A1L0D	OXT-C	-2.57	1.31	1.42
15	A	301	A1L0D	OXT-C	-2.54	1.31	1.42
15	F	301	A1L0D	OXT-C	-2.53	1.31	1.42
15	C	301	A1L0D	N2-N3	-2.05	1.30	1.34
15	D	301	A1L0D	N2-N3	-2.04	1.30	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	D	301	A1L0D	C5-N4-C6	6.08	130.87	125.48
15	C	301	A1L0D	C5-N4-C6	6.08	130.87	125.48
15	C	302	A1L0D	C5-N4-C6	5.84	130.66	125.48
15	D	302	A1L0D	C5-N4-C6	5.77	130.60	125.48
15	F	301	A1L0D	C5-N4-C6	4.89	129.81	125.48
15	A	301	A1L0D	C5-N4-C6	4.83	129.76	125.48
15	F	301	A1L0D	C12-C4-C3	-2.70	109.50	112.16
15	A	301	A1L0D	C12-C4-C3	-2.69	109.51	112.16
15	D	301	A1L0D	C8-C7-C6	-2.58	107.75	111.57
15	C	301	A1L0D	C8-C7-C6	-2.58	107.75	111.57
15	D	302	A1L0D	C16-C4-C3	-2.03	110.16	112.16
15	C	302	A1L0D	C16-C4-C3	-2.03	110.16	112.16

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	C	301	A1L0D	N1-C3-C4-C12
15	C	302	A1L0D	OXT-C-CA-N
15	D	301	A1L0D	N1-C3-C4-C12
15	D	302	A1L0D	OXT-C-CA-N
15	C	301	A1L0D	N1-C3-C4-C16
15	D	301	A1L0D	N1-C3-C4-C16
15	D	302	A1L0D	OXT-C-CA-CB

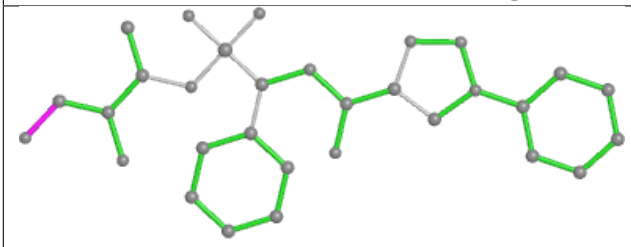
There are no ring outliers.

4 monomers are involved in 4 short contacts:

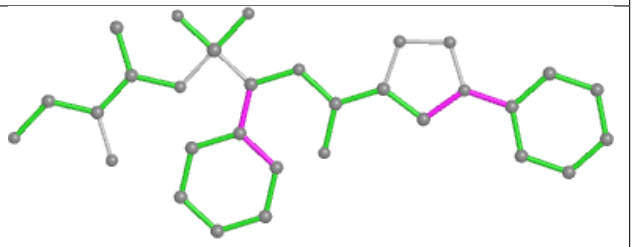
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	301	A1L0D	1	0
15	A	301	A1L0D	1	0
15	F	301	A1L0D	1	0
15	D	301	A1L0D	1	0

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

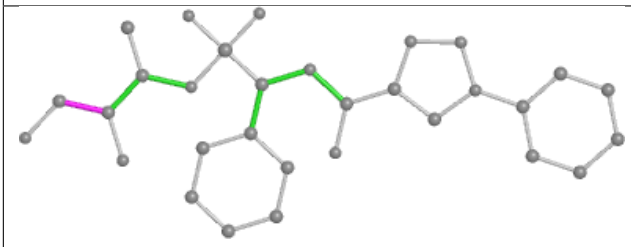
Ligand A1L0D C 302



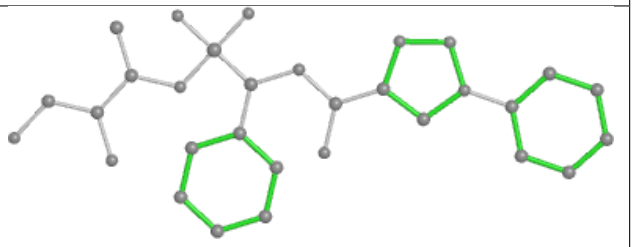
Bond lengths



Bond angles

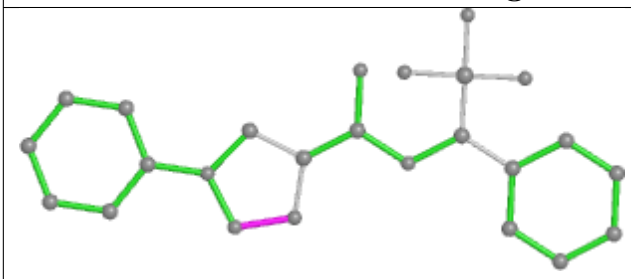


Torsions

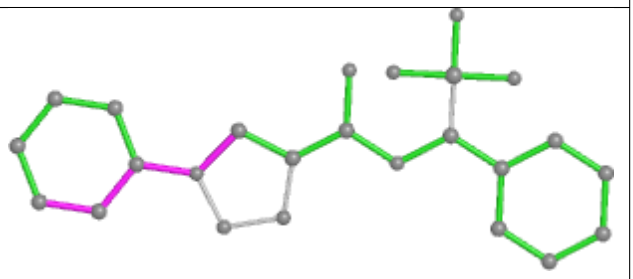


Rings

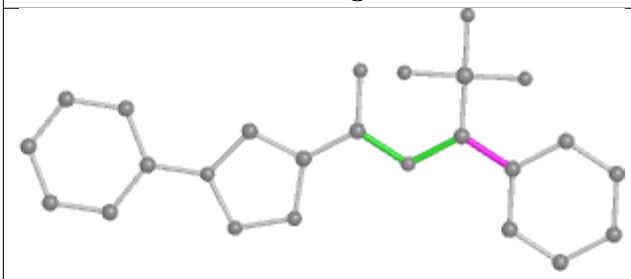
Ligand A1L0D C 301



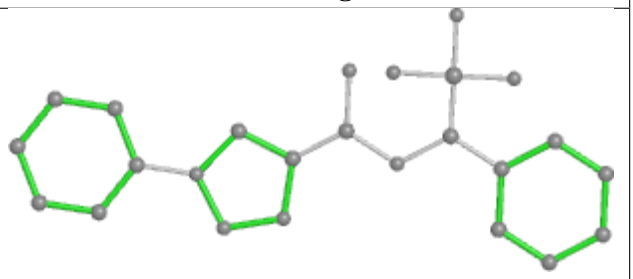
Bond lengths



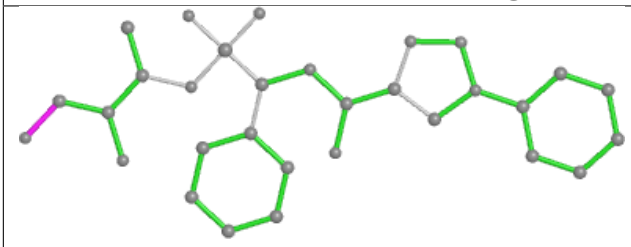
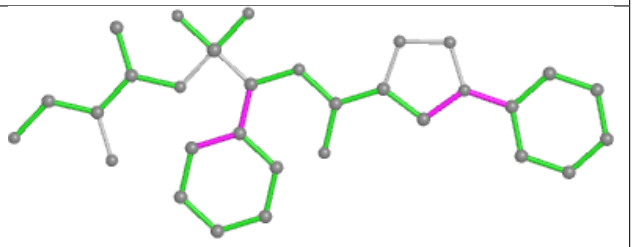
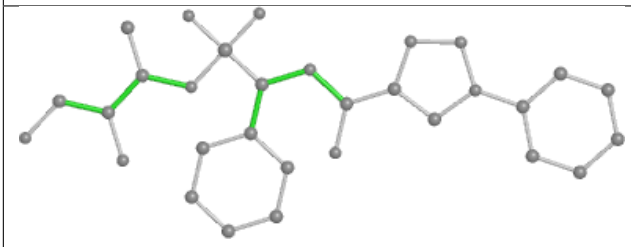
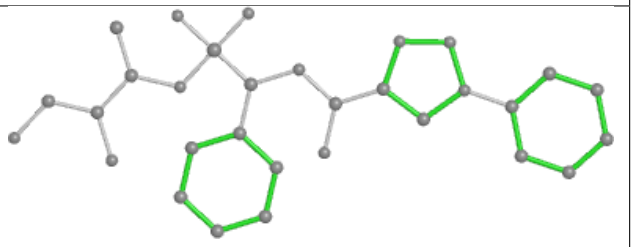
Bond angles

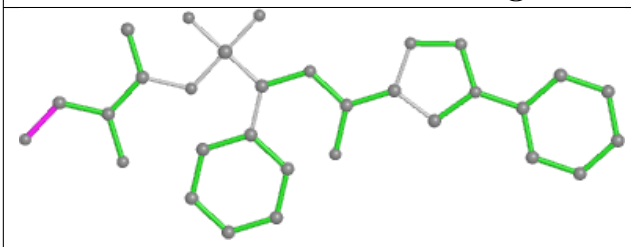
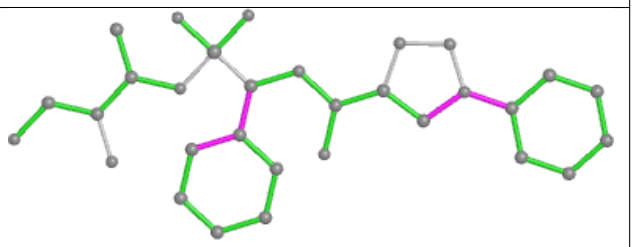
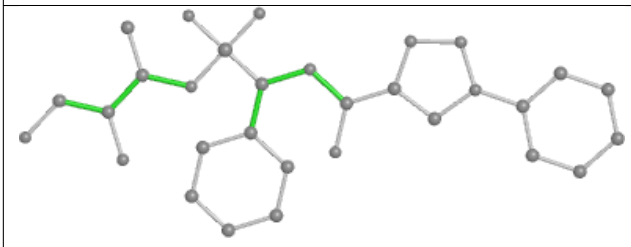
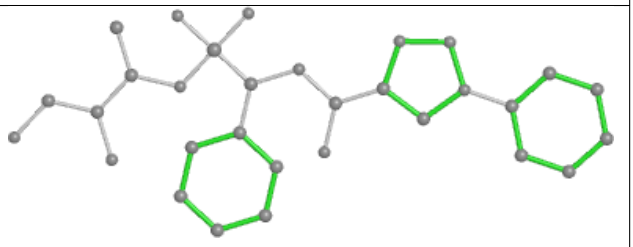


Torsions

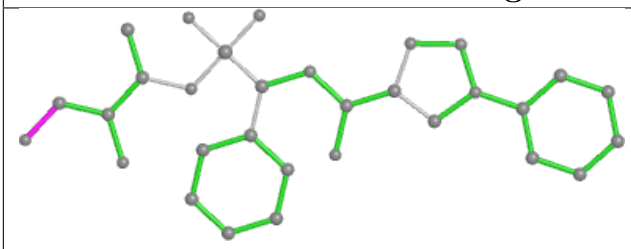


Rings

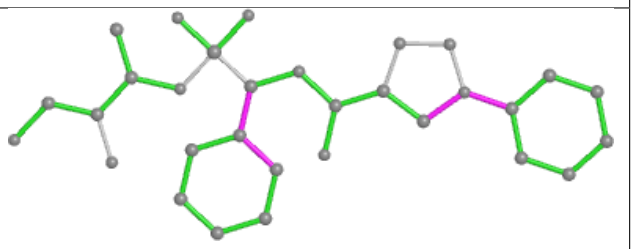
Ligand A1L0D A 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand A1L0D F 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

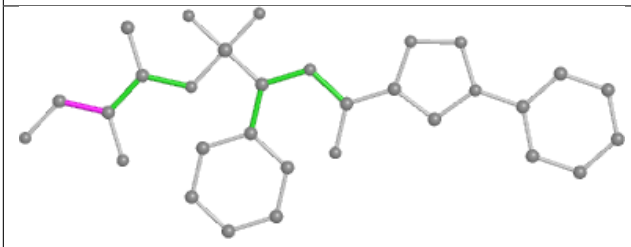
Ligand A1L0D D 302



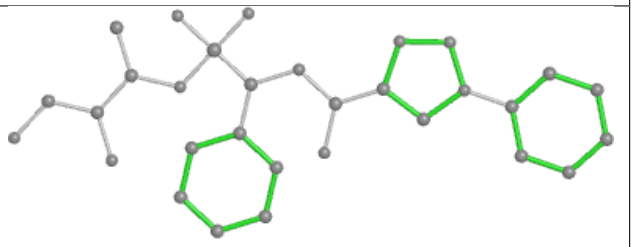
Bond lengths



Bond angles

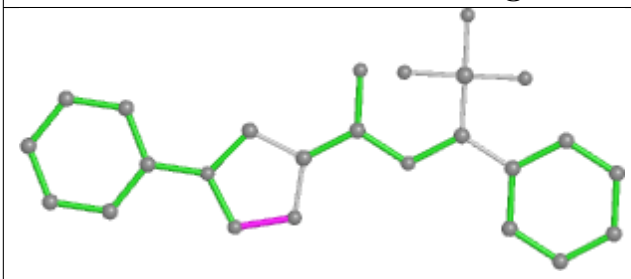


Torsions

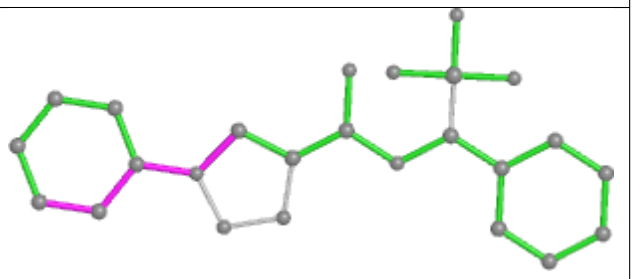


Rings

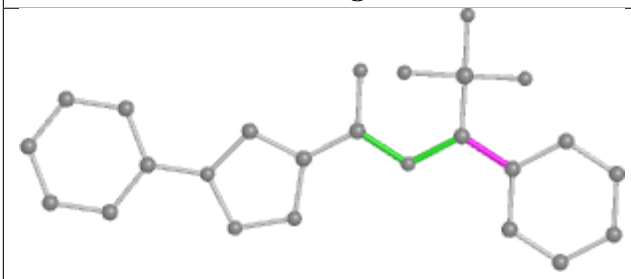
Ligand A1L0D D 301



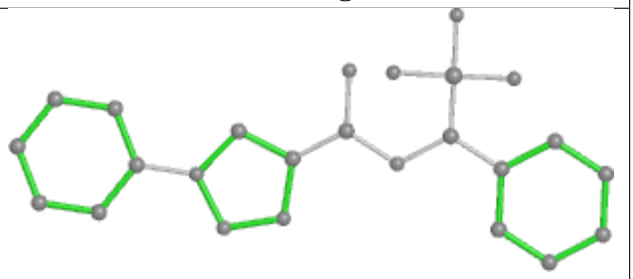
Bond lengths



Bond angles



Torsions



Rings

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.

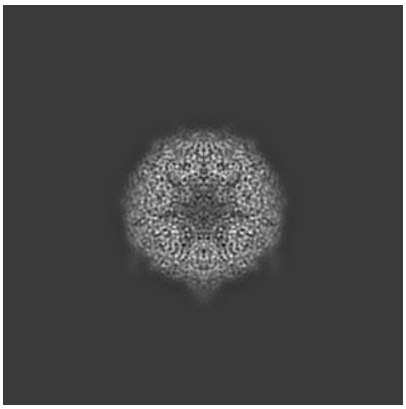
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-39612. These allow visual inspection of the internal detail of the map and identification of artifacts.

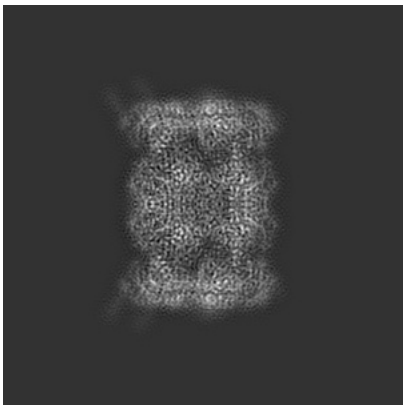
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

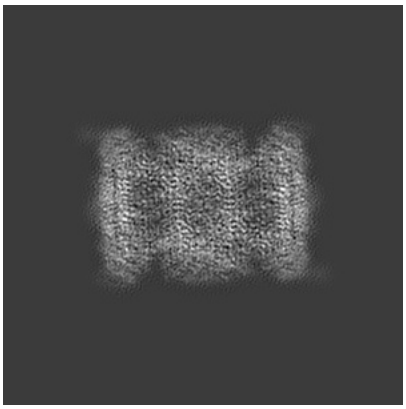
6.1.1 Primary map



X

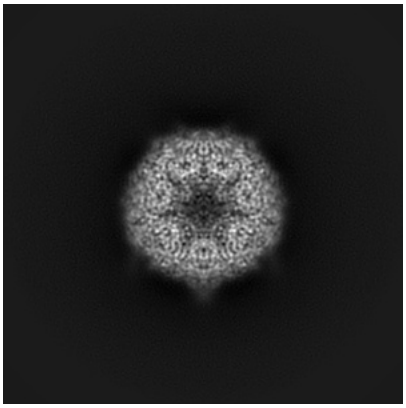


Y

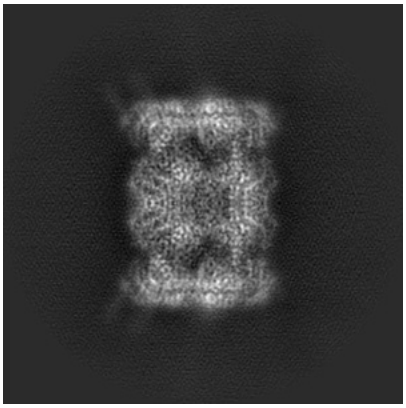


Z

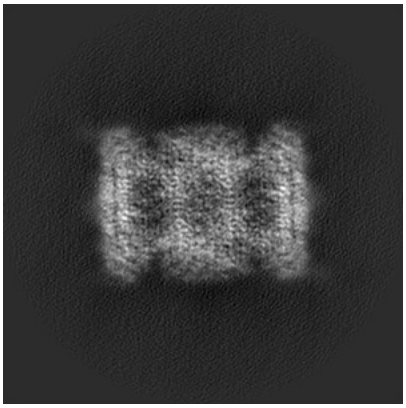
6.1.2 Raw map



X



Y

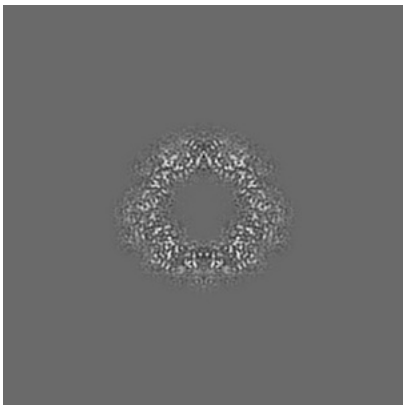


Z

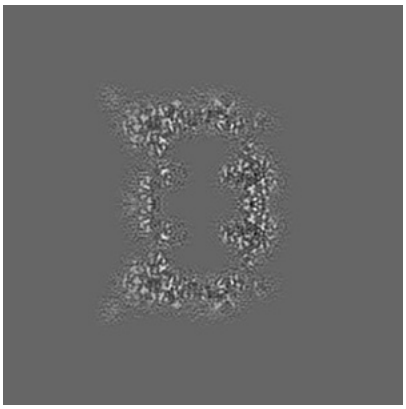
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

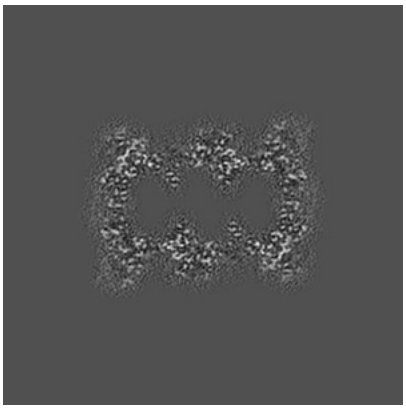
6.2.1 Primary map



X Index: 127

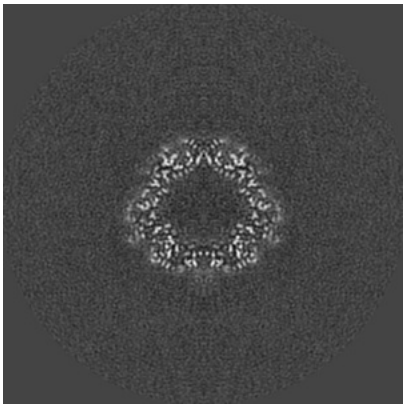


Y Index: 127

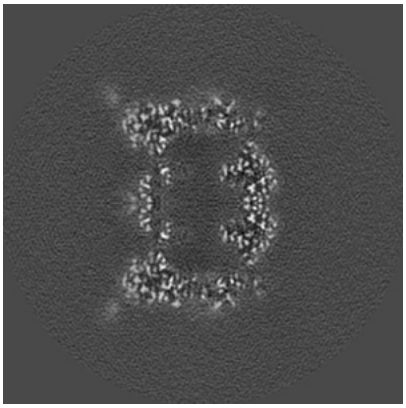


Z Index: 127

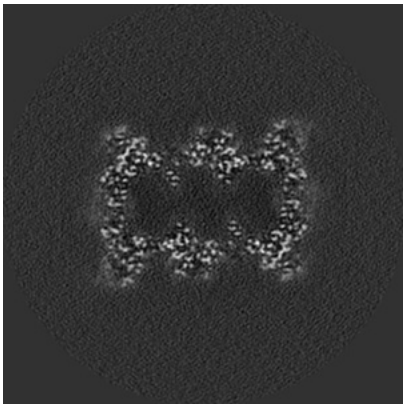
6.2.2 Raw map



X Index: 127



Y Index: 127

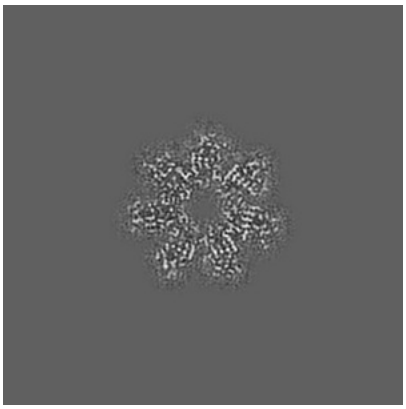


Z Index: 127

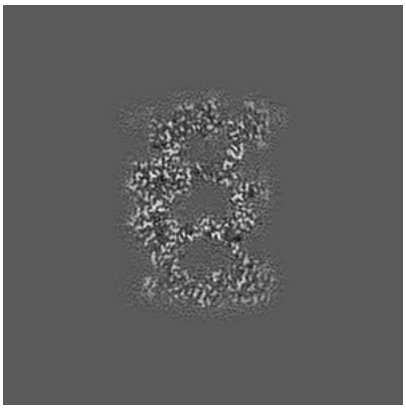
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

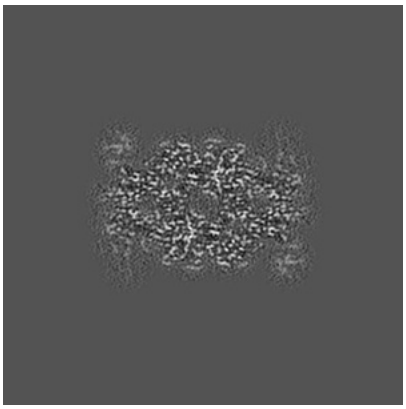
6.3.1 Primary map



X Index: 110

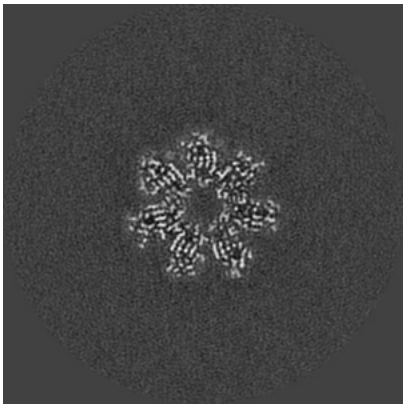


Y Index: 110

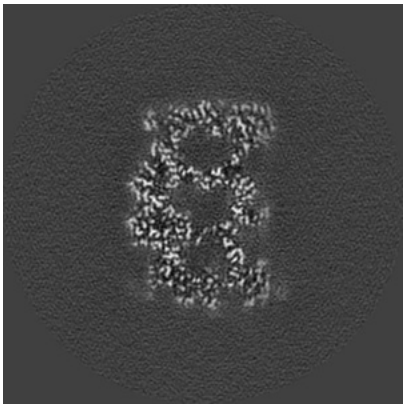


Z Index: 148

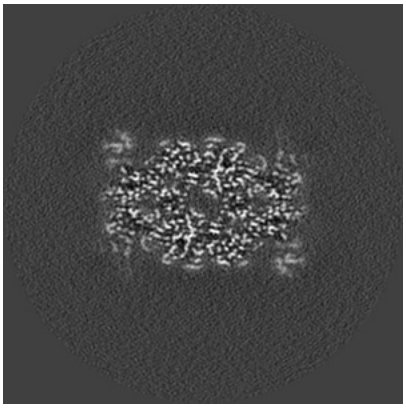
6.3.2 Raw map



X Index: 144



Y Index: 144

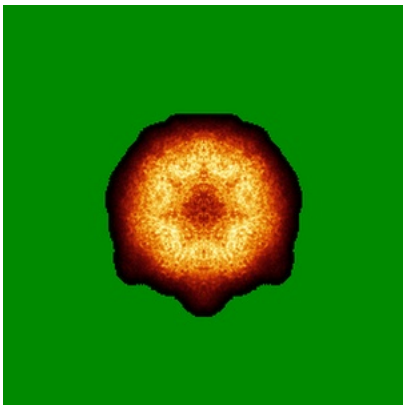


Z Index: 148

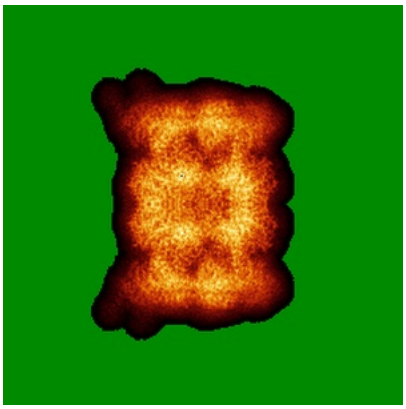
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

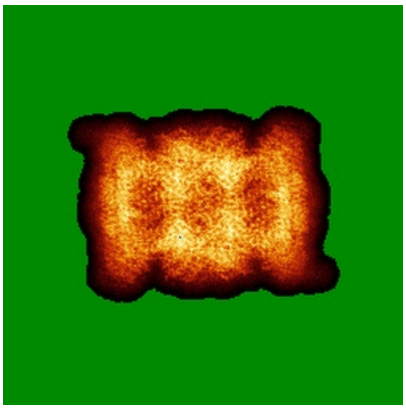
6.4.1 Primary map



X

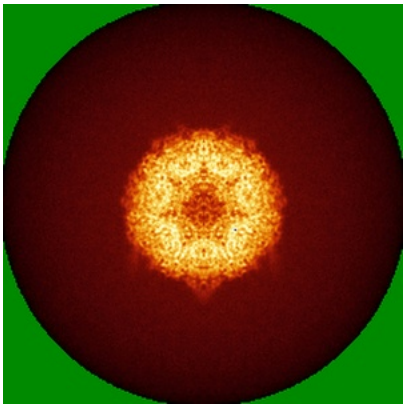


Y

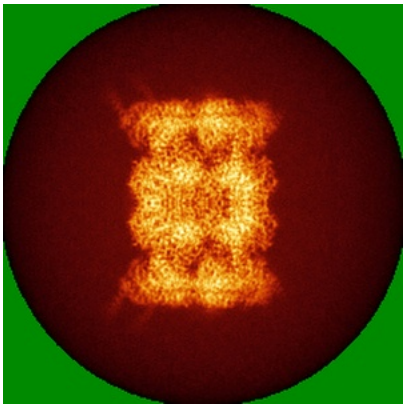


Z

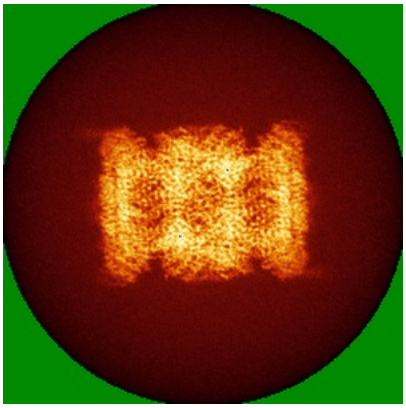
6.4.2 Raw map



X



Y

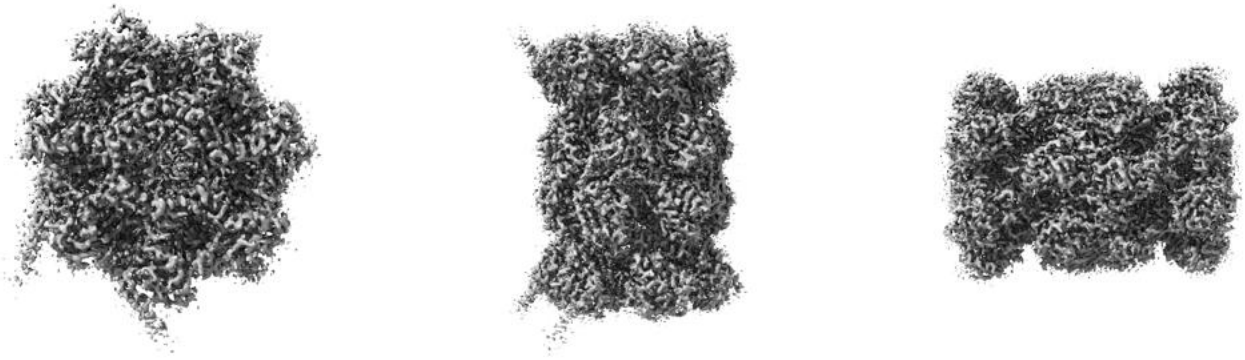


Z

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

6.5 Orthogonal surface views (i)

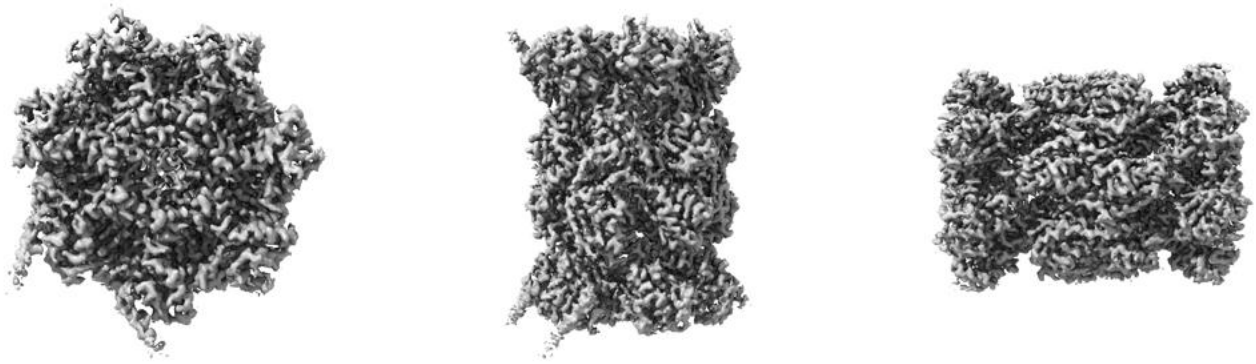
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0282. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

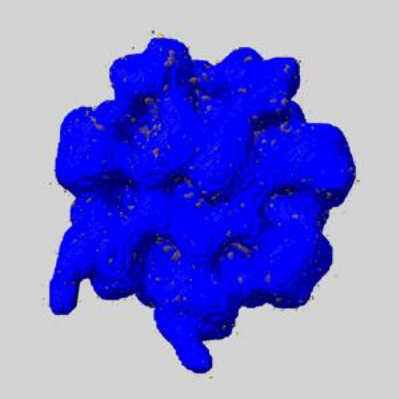
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

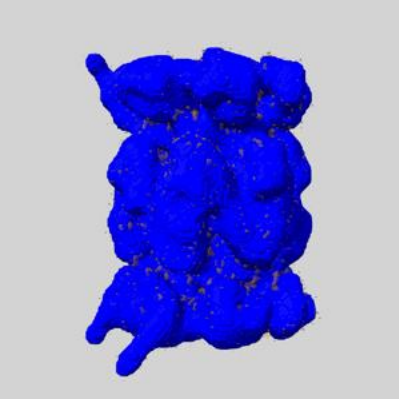
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

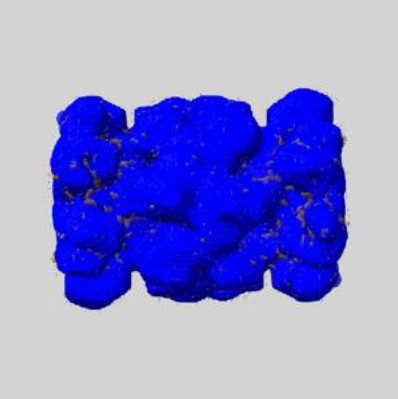
6.6.1 emd_39612_msk_1.map



X



Y

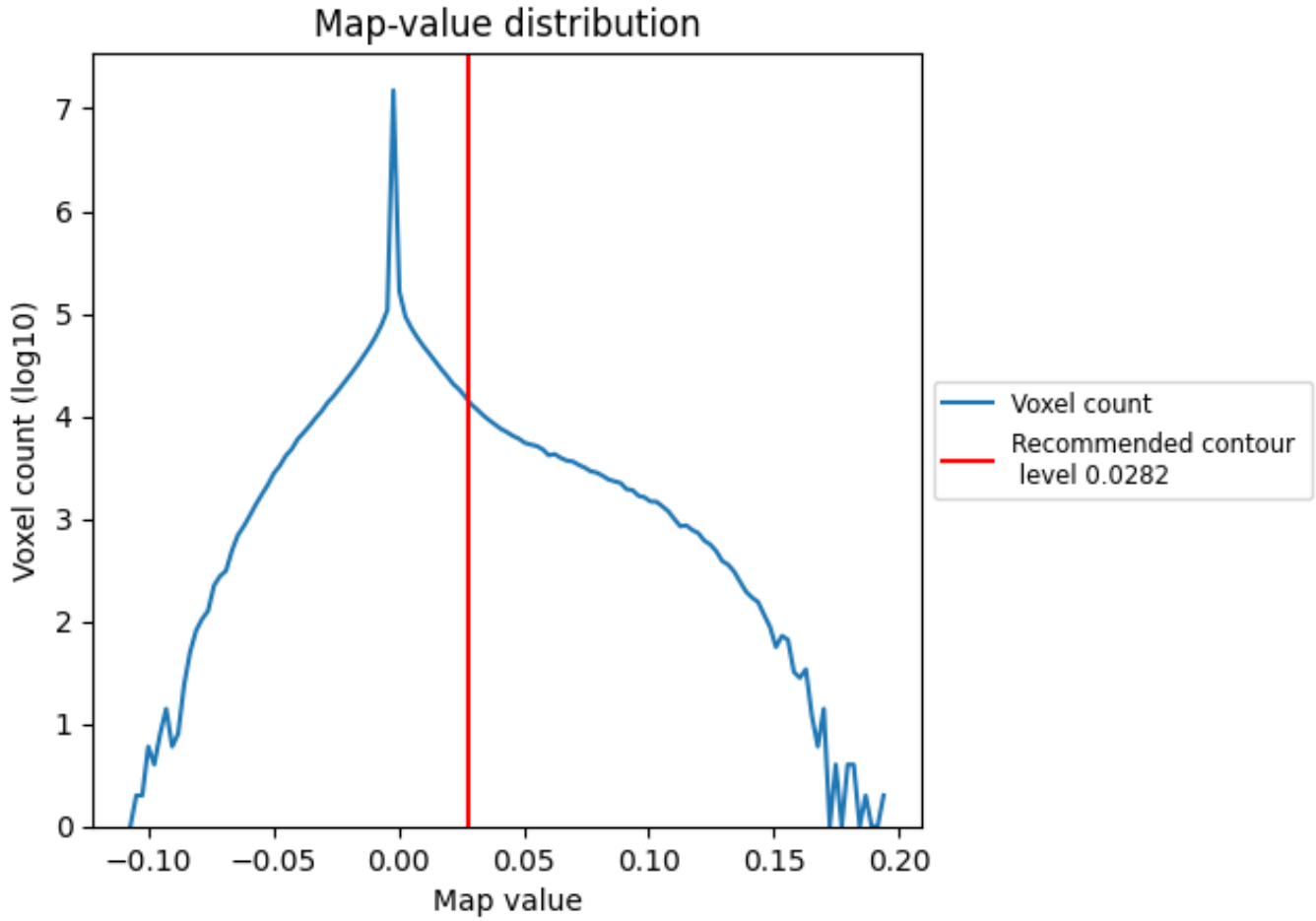


Z

7 Map analysis

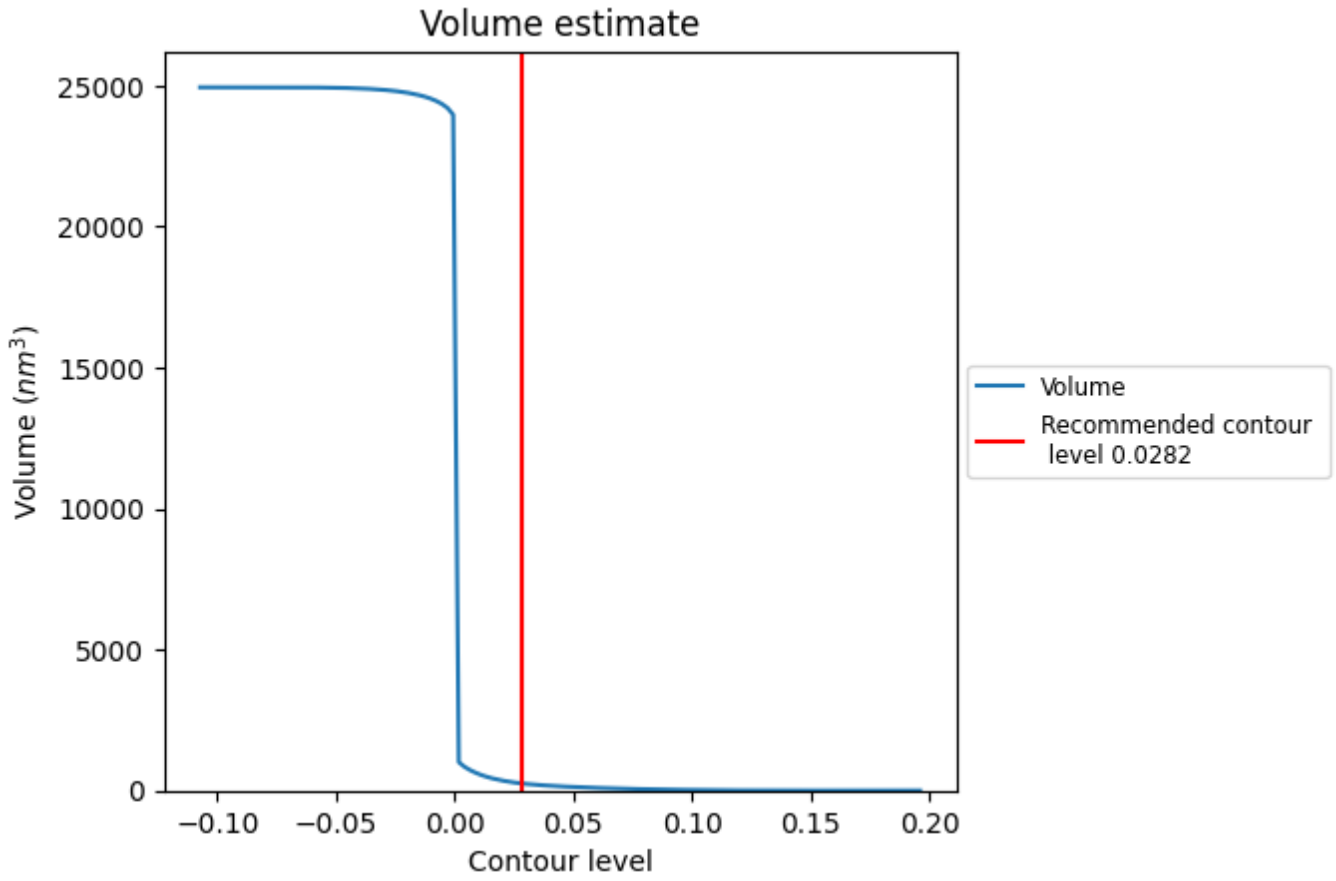
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

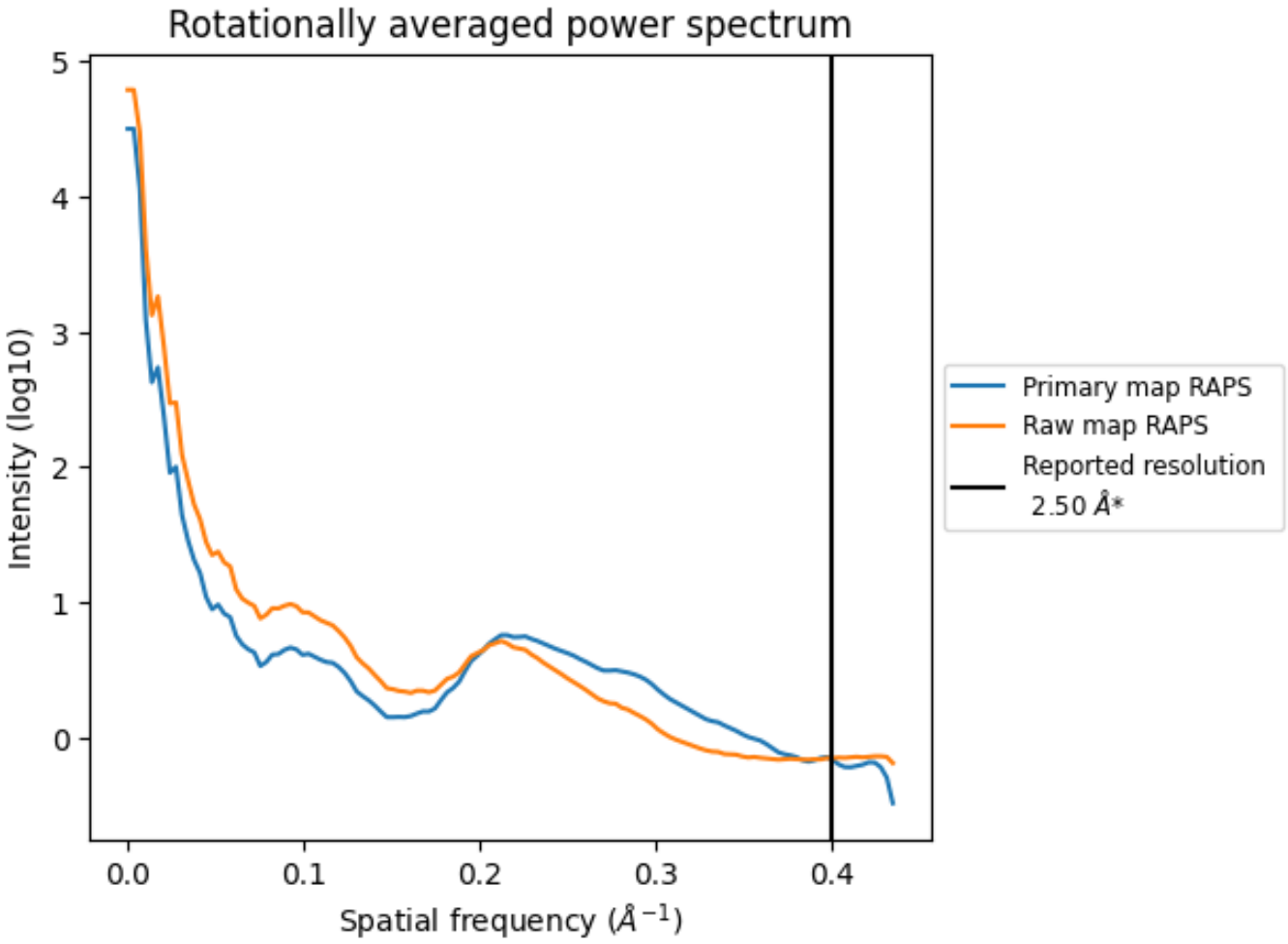
7.2 Volume estimate



The volume at the recommended contour level is 254 nm^3; this corresponds to an approximate mass of 230 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 (i)

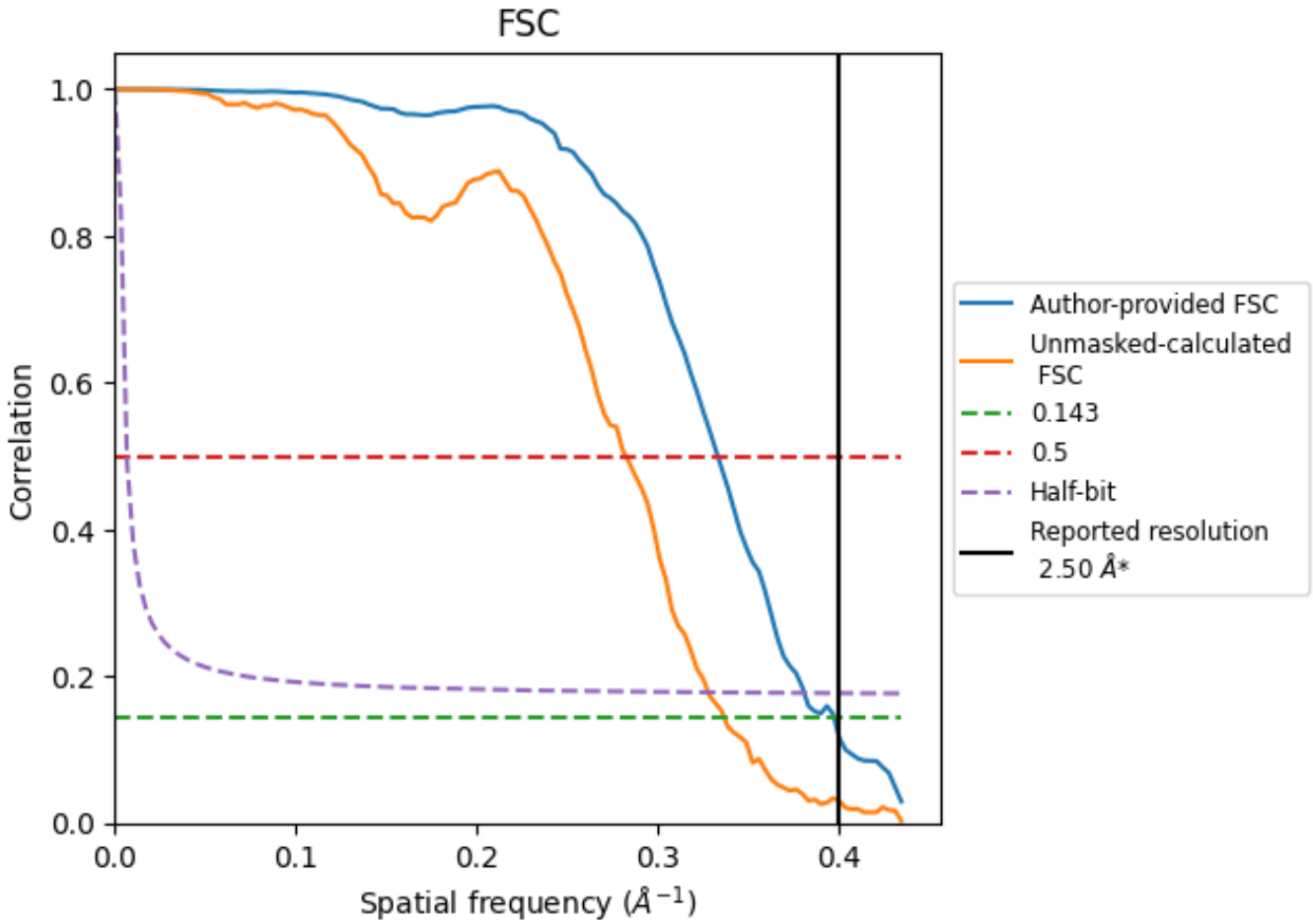


*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8.2 Resolution estimates (i)

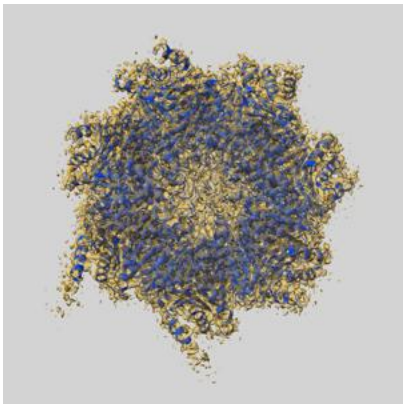
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.52	3.00	2.62
Unmasked-calculated*	2.97	3.54	3.05

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.97 differs from the reported value 2.5 by more than 10 %

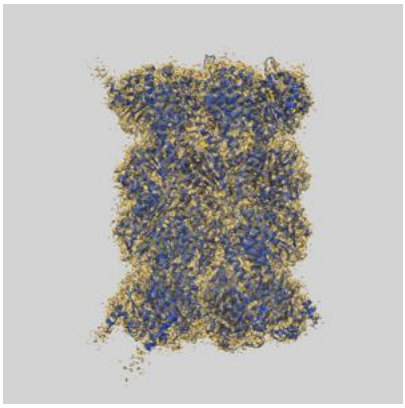
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-39612 and PDB model 8YVP. Per-residue inclusion information can be found in section 3 on page 8.

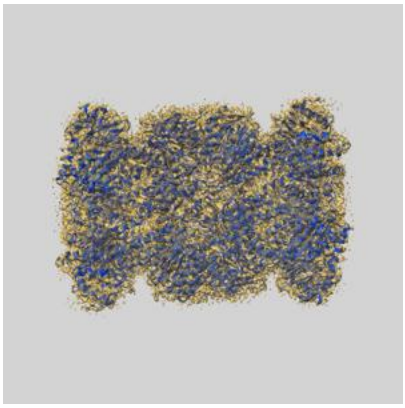
9.1 Map-model overlay



X



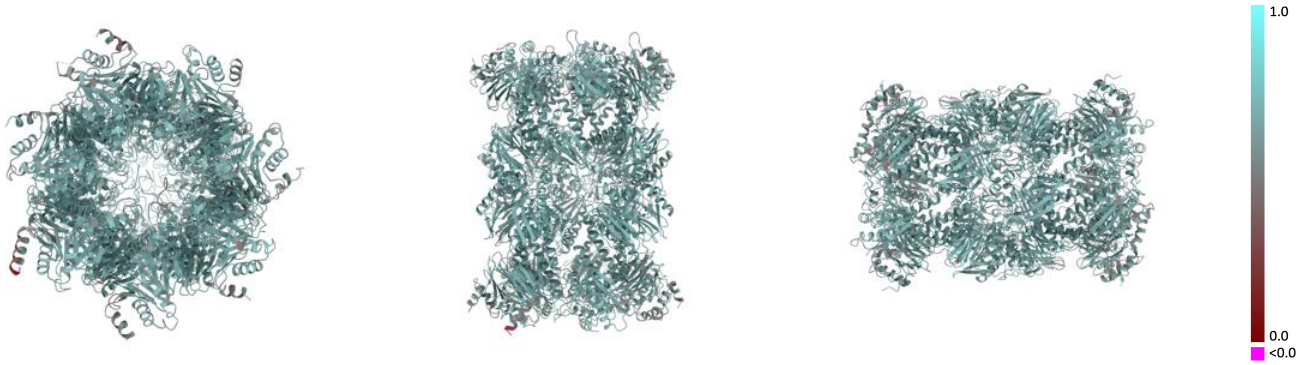
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0282 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.

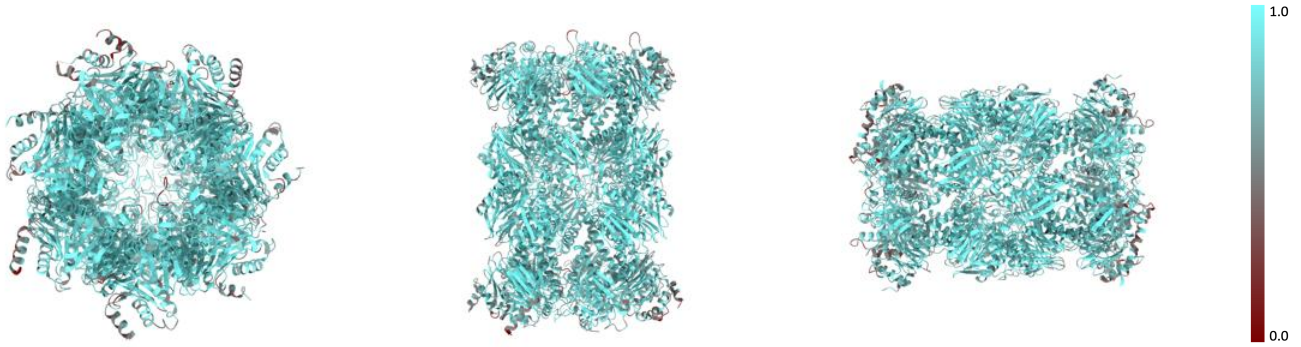
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

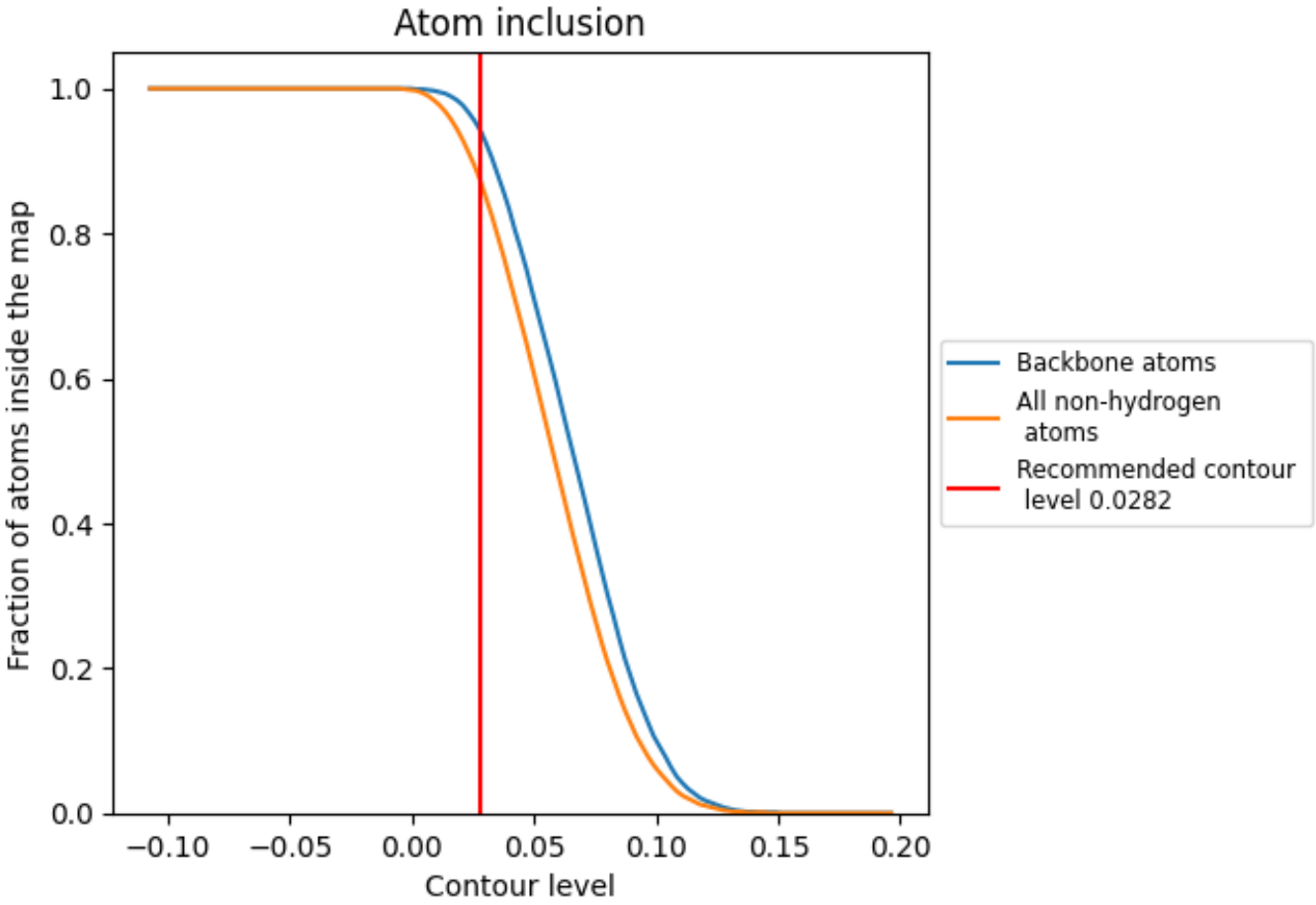
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0282).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 87% 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 (0.0282) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8710	0.6400
A	0.9160	0.6590
B	0.9050	0.6530
C	0.9250	0.6600
D	0.9230	0.6590
E	0.9070	0.6550
F	0.9170	0.6610
G	0.8460	0.6250
H	0.8320	0.6270
I	0.8230	0.6140
J	0.8070	0.6250
K	0.7930	0.6190
L	0.8460	0.6270
M	0.8280	0.6280
N	0.8250	0.6150
O	0.8330	0.6150
P	0.8430	0.6280
Q	0.8070	0.6220
R	0.7910	0.6150
S	0.9210	0.6570
T	0.9290	0.6680
U	0.9360	0.6690
V	0.9270	0.6670
W	0.9330	0.6630
X	0.9210	0.6560
Y	0.9370	0.6700
Z	0.8320	0.6170
a	0.9330	0.6620
b	0.8410	0.6300