



Full wwPDB EM Validation Report ⓘ

Apr 16, 2026 – 04:21 pm BST

PDB ID : 9QVX / pdb_00009qvx
EMDB ID : EMD-53414
Title : The targeting of non-fibrillar polyQ via distinct VCP-proteasome coupling
Authors : Zhao, D.Y.; Mi, C.C.
Deposited on : 2025-04-13
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

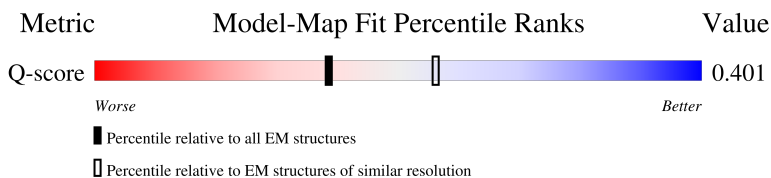
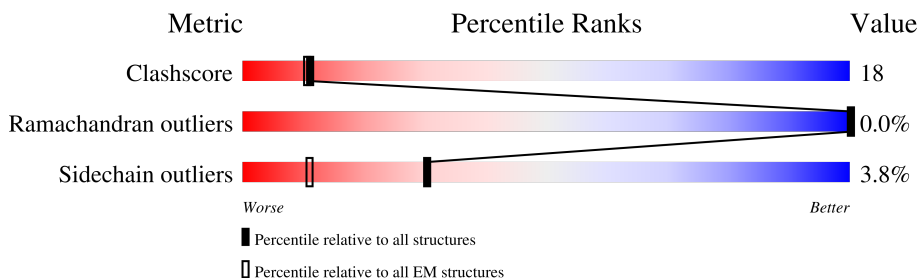
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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

Mol	Chain	Length	Quality of chain
1	A	240	<div> <div>19%</div> <div>61%</div> <div>38%</div> <div>.</div> </div>
1	O	240	<div> <div>18%</div> <div>65%</div> <div>34%</div> <div>.</div> </div>
2	B	229	<div> <div>.</div> <div>64%</div> <div>34%</div> <div>.</div> </div>
2	P	229	<div> <div>.</div> <div>63%</div> <div>36%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	247	
3	Q	247	
4	D	232	
4	R	232	
5	E	233	
5	S	233	
6	F	233	
6	T	233	
7	G	239	
7	U	239	
8	H	202	
8	V	202	
9	I	220	
9	W	220	
10	J	204	
10	X	204	
11	K	196	
11	Y	196	
12	L	200	
12	Z	200	
13	M	212	
13	a	212	
14	N	212	
14	b	212	
15	c	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	d	4	<div> <div></div> <div>75%</div> <div></div> <div>75%</div> <div>25%</div> </div>

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 45388 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	240	Total	C	N	O	S	0	0
			1734	1104	304	314	12		
1	O	240	Total	C	N	O	S	0	0
			1734	1104	304	314	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	229	Total	C	N	O	S	0	0
			1662	1080	288	288	6		
2	P	229	Total	C	N	O	S	0	0
			1670	1086	289	289	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	247	Total	C	N	O	S	0	0
			1786	1143	320	313	10		
3	Q	247	Total	C	N	O	S	0	0
			1786	1143	320	313	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	232	Total	C	N	O	S	0	0
			1633	1038	306	284	5		
4	R	232	Total	C	N	O	S	0	0
			1633	1038	306	284	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	233	Total	C	N	O	S	0	0
			1659	1056	287	305	11		
5	S	233	Total	C	N	O	S	0	0
			1659	1056	287	305	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	233	Total	C	N	O	S	0	0
			1704	1087	315	293	9		
6	T	233	Total	C	N	O	S	0	0
			1704	1087	315	293	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	239	Total	C	N	O	S	0	0
			1760	1131	308	311	10		
7	U	239	Total	C	N	O	S	0	0
			1760	1131	308	311	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	202	Total	C	N	O	S	0	0
			1465	926	256	271	12		
8	V	202	Total	C	N	O	S	0	0
			1465	926	256	271	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	220	Total	C	N	O	S	0	0
			1576	1003	272	292	9		
9	W	220	Total	C	N	O	S	0	0
			1576	1003	272	292	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	204	Total	C	N	O	S	0	0
			1534	987	262	267	18		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	204	Total	C	N	O	S	0	0
			1534	987	262	267	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	196	Total	C	N	O	S	0	0
			1506	973	259	266	8		
11	Y	196	Total	C	N	O	S	0	0
			1506	973	259	266	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	200	Total	C	N	O	S	0	0
			1500	954	270	267	9		
12	Z	200	Total	C	N	O	S	0	0
			1500	954	270	267	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	212	Total	C	N	O	S	0	0
			1583	1016	279	278	10		
13	a	212	Total	C	N	O	S	0	0
			1583	1016	279	278	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	212	Total	C	N	O	S	0	0
			1568	998	279	280	11		
14	b	212	Total	C	N	O	S	0	0
			1568	998	279	280	11		

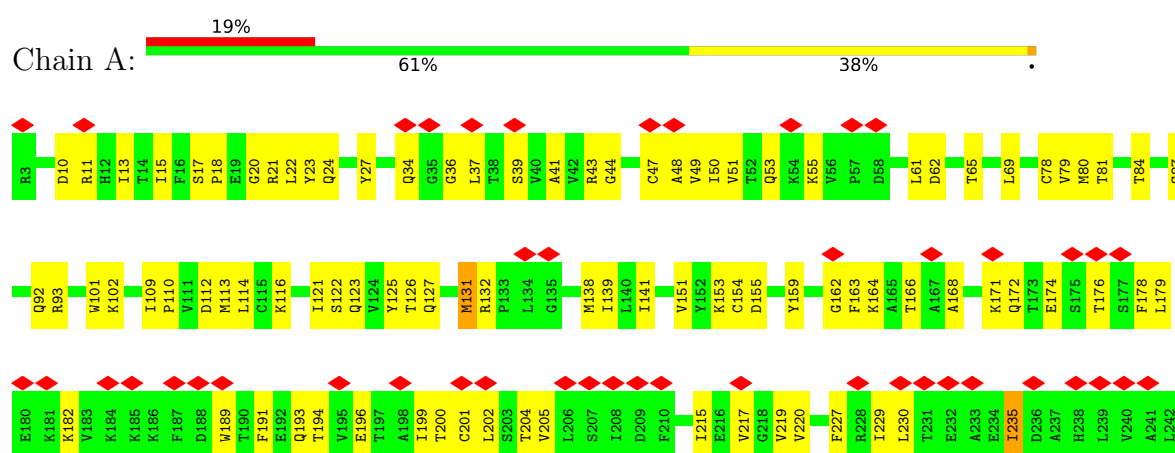
- Molecule 15 is a protein called polypeptide traced as poly-Ala.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	c	4	Total	C	N	O	0	0
			20	12	4	4		
15	d	4	Total	C	N	O	0	0
			20	12	4	4		

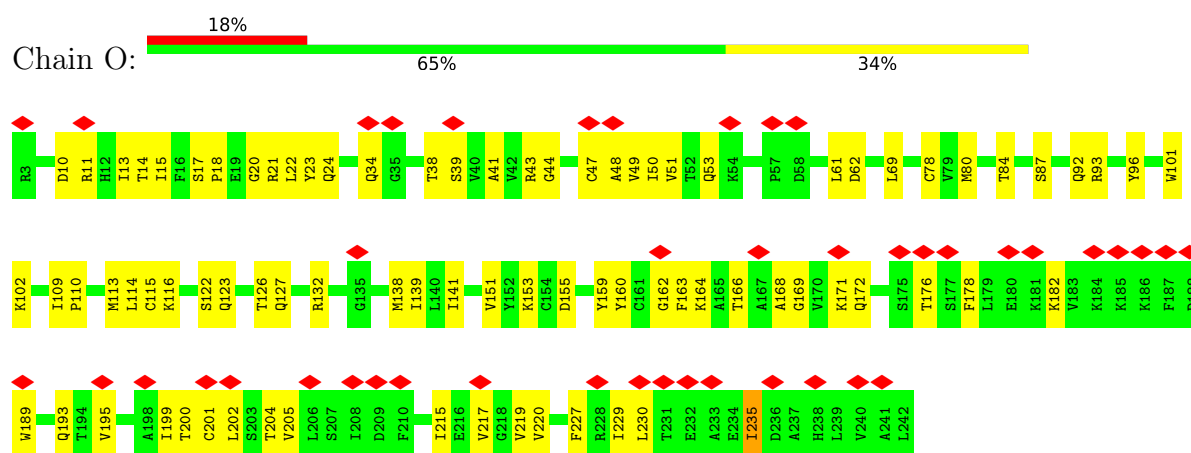
3 Residue-property plots

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

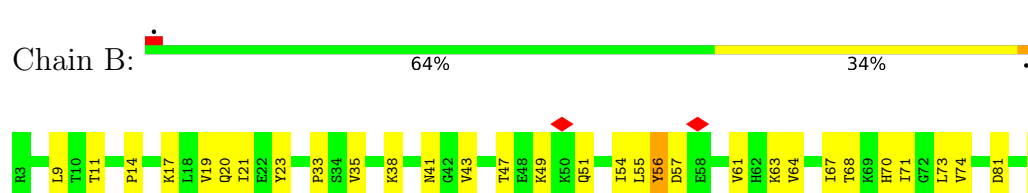
• Molecule 1: Proteasome subunit alpha type-6

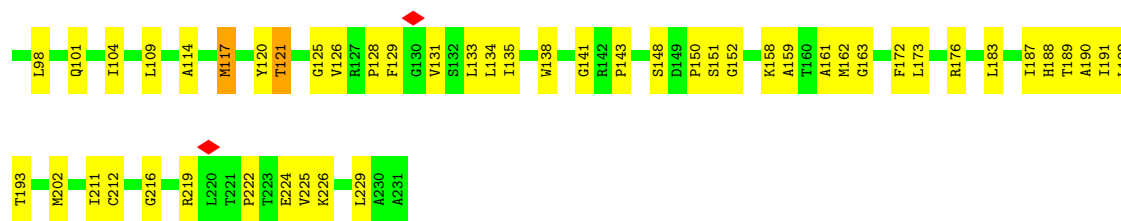


• Molecule 1: Proteasome subunit alpha type-6

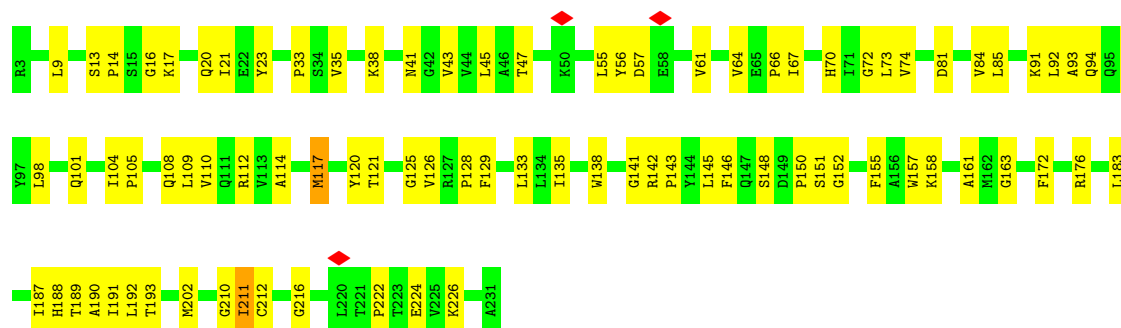


• Molecule 2: Proteasome subunit alpha type-2

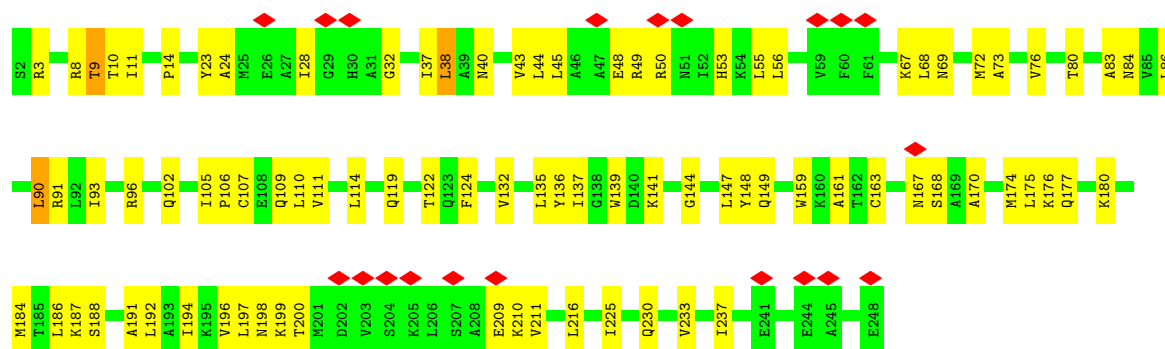




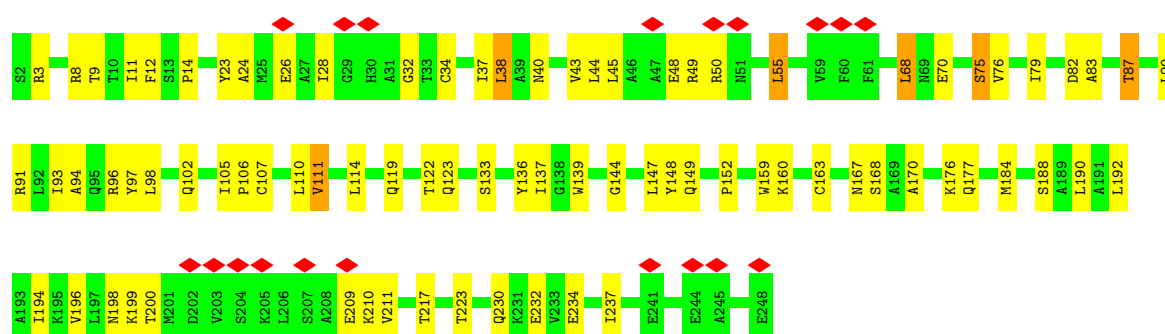
• Molecule 2: Proteasome subunit alpha type-2



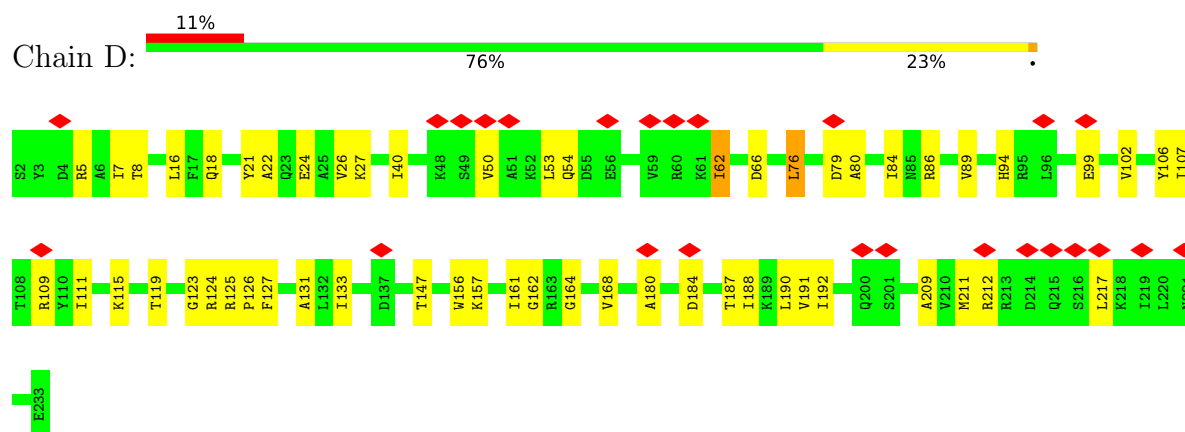
• Molecule 3: Proteasome subunit alpha type-4



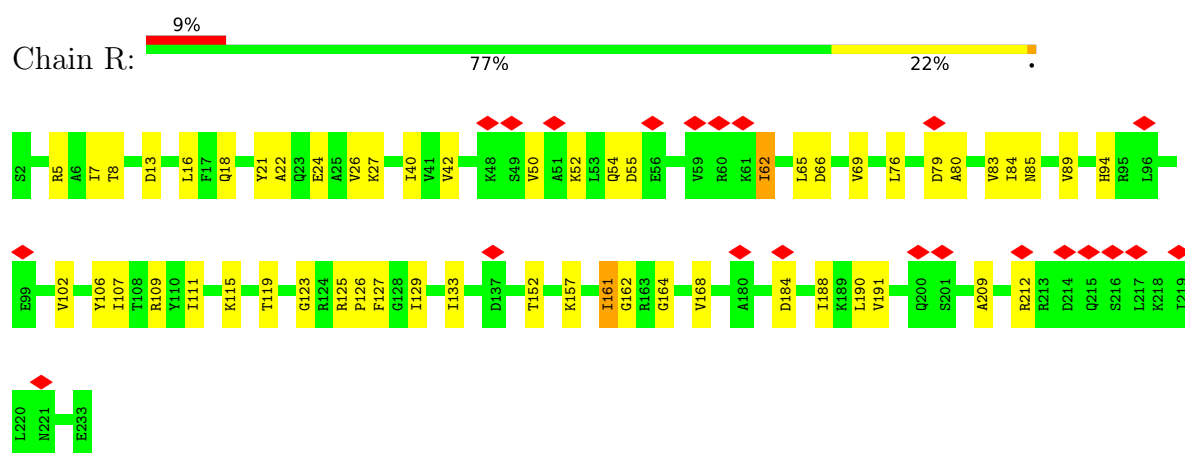
• Molecule 3: Proteasome subunit alpha type-4



- Molecule 4: Proteasome subunit alpha type-7



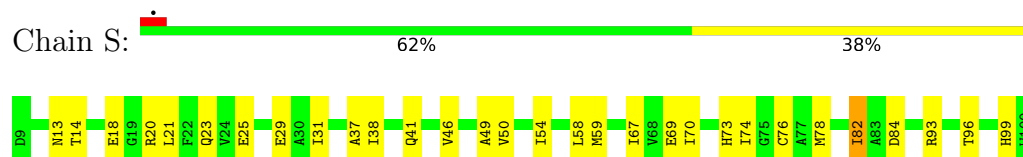
- Molecule 4: Proteasome subunit alpha type-7

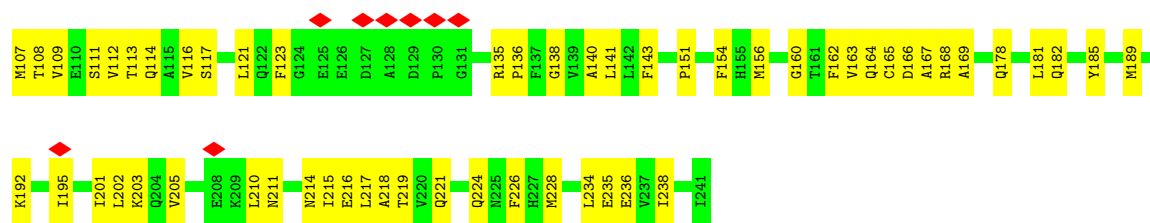


- Molecule 5: Proteasome subunit alpha type-5



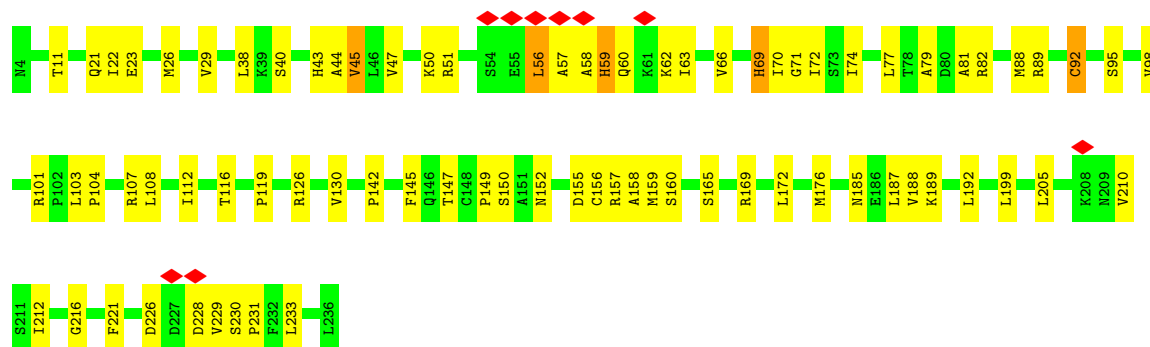
- Molecule 5: Proteasome subunit alpha type-5





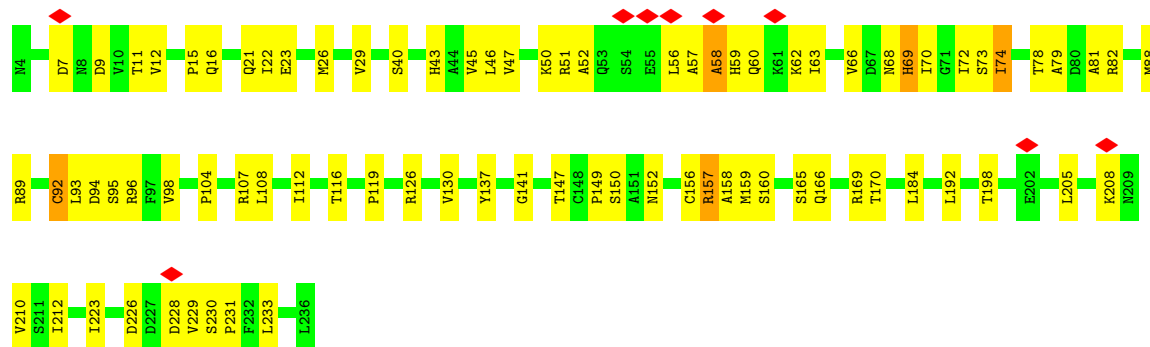
• Molecule 6: Proteasome subunit alpha type-1

Chain F: 66% 32% .



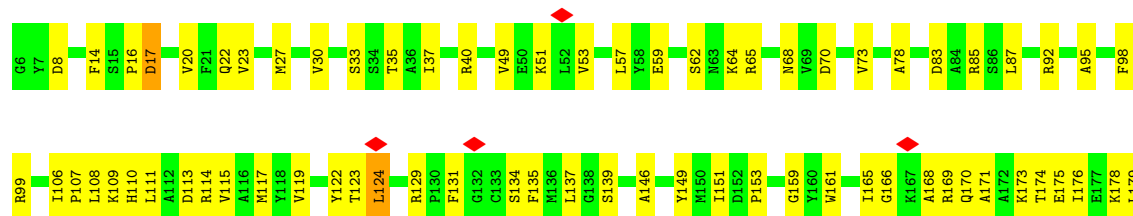
• Molecule 6: Proteasome subunit alpha type-1

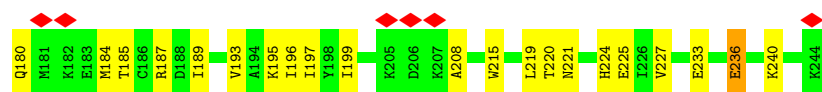
Chain T: 65% 33% .



• Molecule 7: Proteasome subunit alpha type-3

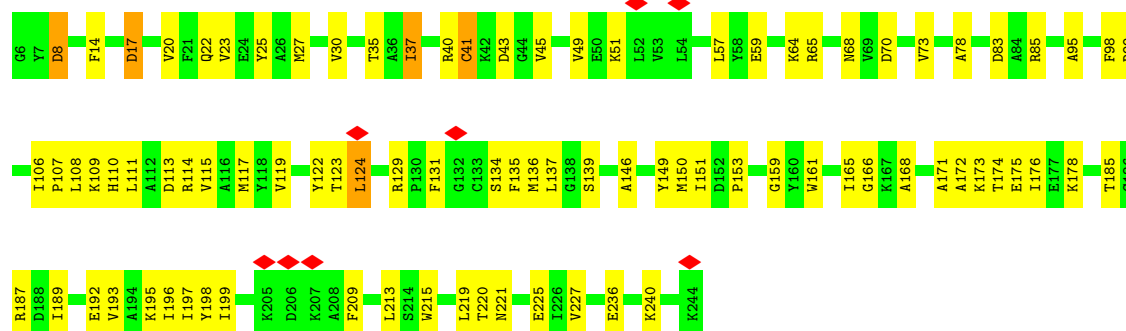
Chain G: 62% 37% .





• Molecule 7: Proteasome subunit alpha type-3

Chain U: 63% 35%



• Molecule 8: Proteasome subunit beta type-6

Chain H: 6% 64% 36%



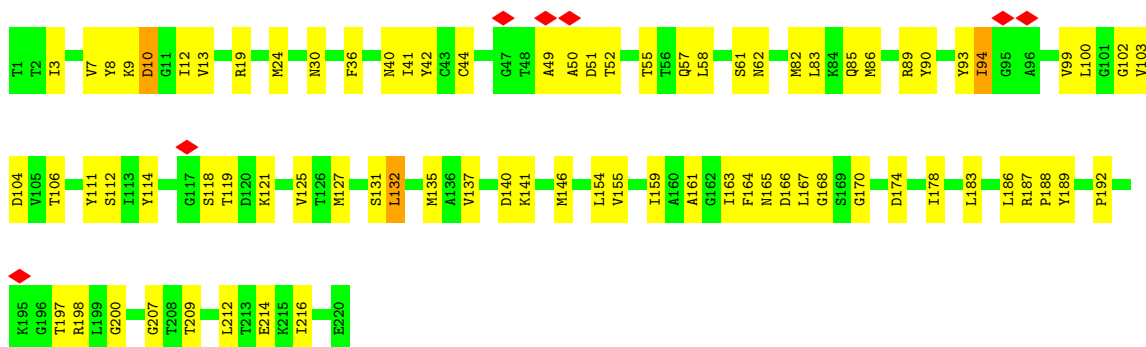
• Molecule 8: Proteasome subunit beta type-6

Chain V: 6% 64% 35%

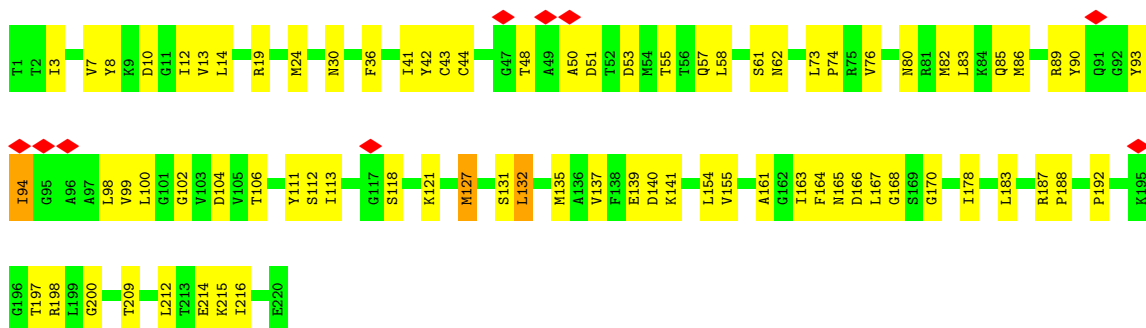


• Molecule 9: Proteasome subunit beta type-7

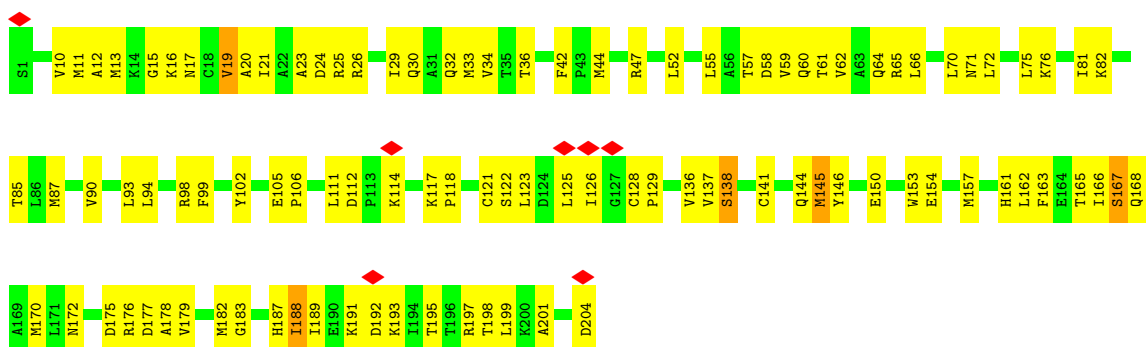
Chain I: 64% 35%



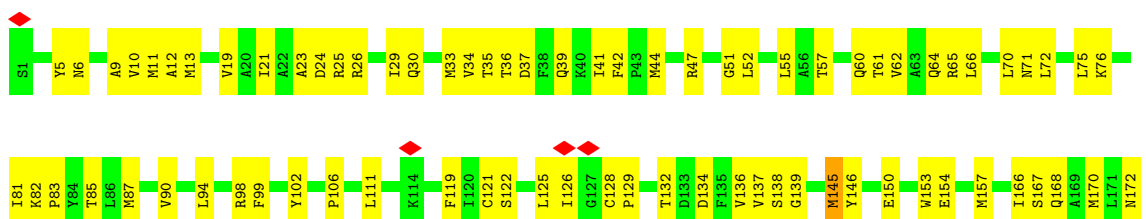
• Molecule 9: Proteasome subunit beta type-7

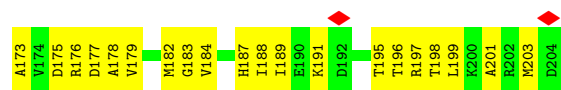


• Molecule 10: Proteasome subunit beta type-3

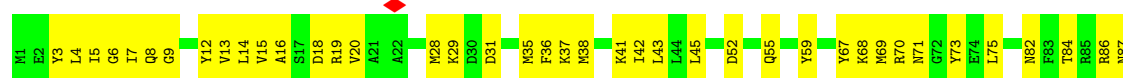


• Molecule 10: Proteasome subunit beta type-3

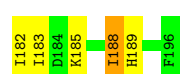
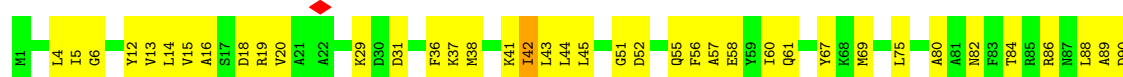




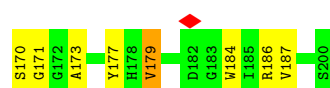
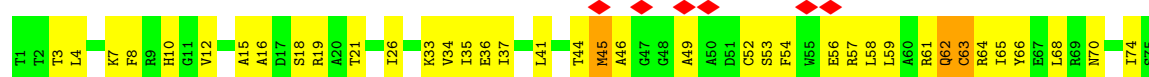
• Molecule 11: Proteasome subunit beta type-2



• Molecule 11: Proteasome subunit beta type-2

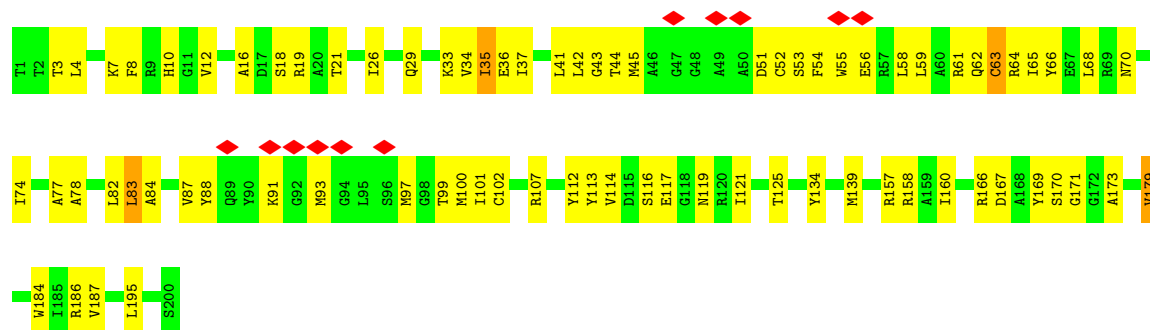


• Molecule 12: Proteasome subunit beta type-5



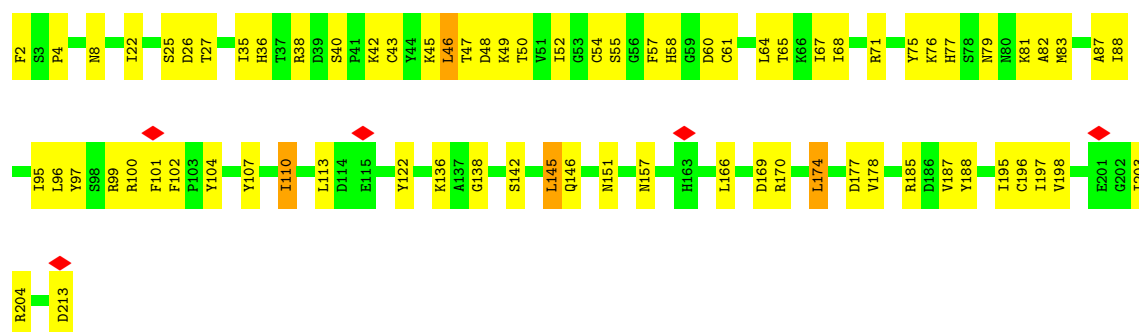
• Molecule 12: Proteasome subunit beta type-5





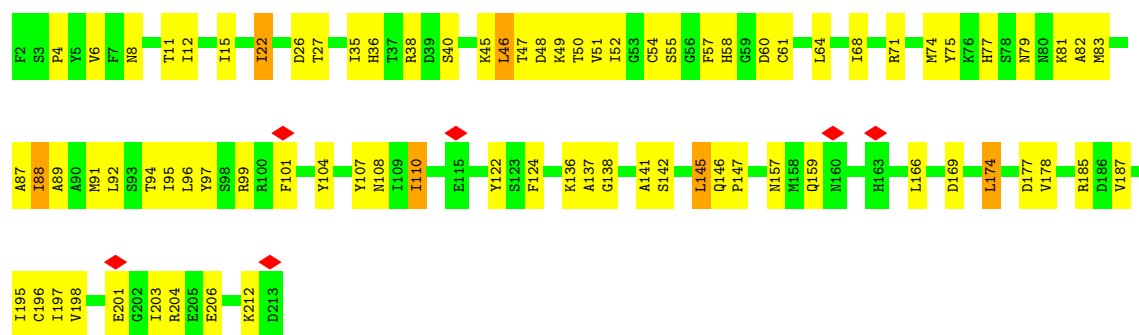
• Molecule 13: Proteasome subunit beta type-1

Chain M: 65% 33%



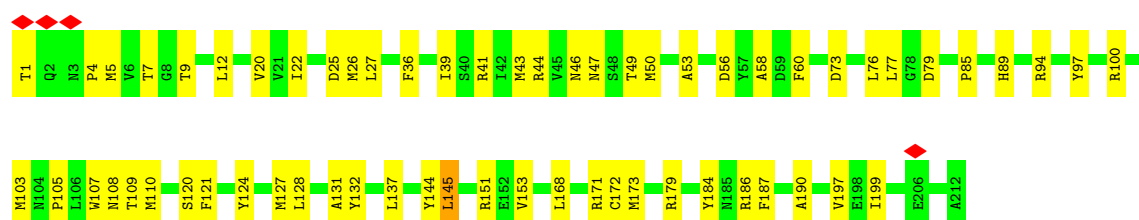
• Molecule 13: Proteasome subunit beta type-1

Chain a: 62% 35%

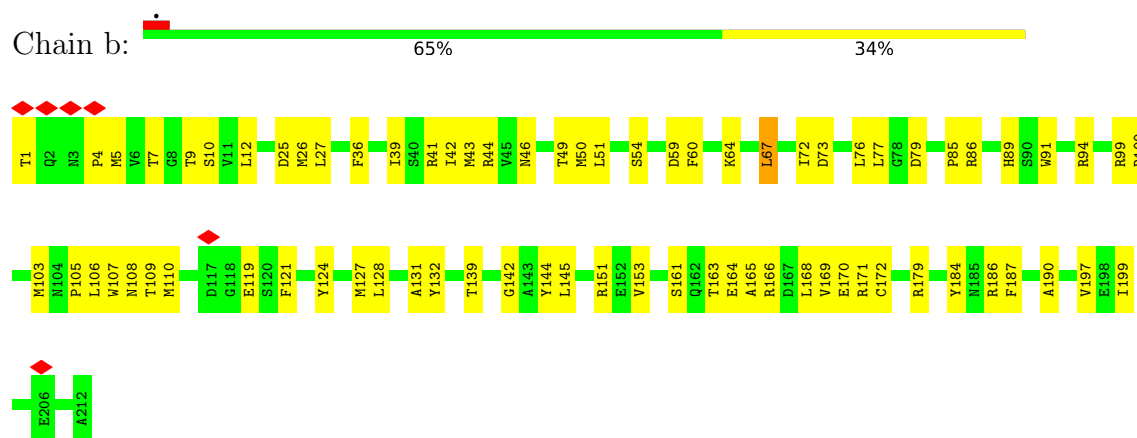


• Molecule 14: Proteasome subunit beta type-4

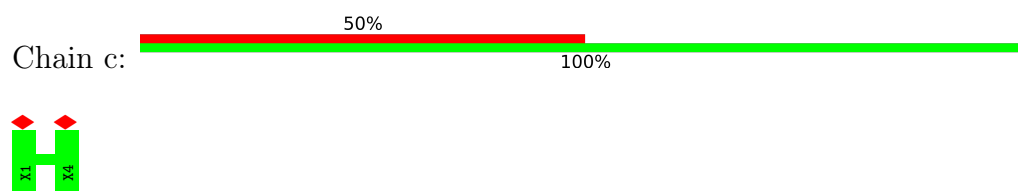
Chain N: 71% 29%



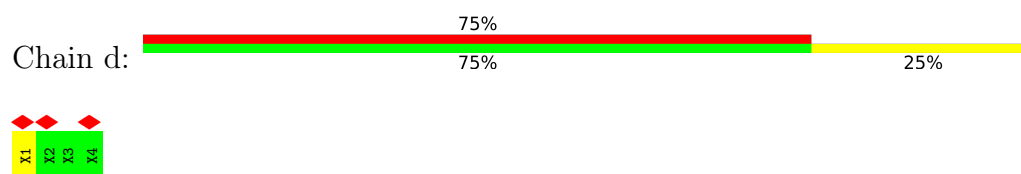
- Molecule 14: Proteasome subunit beta type-4



- Molecule 15: polypeptide traced as poly-Ala



- Molecule 15: polypeptide traced as poly-Ala



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	43227	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.140	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.035	Depositor
Map size (\AA)	209.56001, 209.56001, 209.56001	wwPDB
Map dimensions	124, 124, 124	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.69, 1.69, 1.69	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.18	0/1763	0.46	0/2393
1	O	0.18	0/1763	0.45	0/2393
2	B	0.20	0/1701	0.43	1/2318 (0.0%)
2	P	0.21	0/1709	0.40	0/2327
3	C	0.20	0/1815	0.43	0/2466
3	Q	0.21	0/1815	0.47	0/2466
4	D	0.19	0/1657	0.42	0/2261
4	R	0.18	0/1657	0.41	0/2261
5	E	0.20	0/1685	0.44	0/2290
5	S	0.20	0/1685	0.45	0/2290
6	F	0.25	0/1738	0.47	0/2364
6	T	0.21	0/1738	0.49	0/2364
7	G	0.18	0/1795	0.41	0/2434
7	U	0.18	0/1795	0.41	0/2434
8	H	0.21	0/1491	0.44	0/2021
8	V	0.21	0/1491	0.44	0/2021
9	I	0.20	0/1603	0.44	0/2180
9	W	0.21	0/1603	0.47	0/2180
10	J	0.22	0/1563	0.46	0/2113
10	X	0.22	0/1563	0.47	0/2113
11	K	0.21	0/1538	0.44	0/2088
11	Y	0.21	0/1538	0.46	0/2088
12	L	0.22	0/1531	0.51	0/2076
12	Z	0.23	0/1531	0.53	0/2076
13	M	0.21	0/1613	0.42	0/2178
13	a	0.21	0/1613	0.41	0/2178
14	N	0.21	0/1598	0.41	0/2170
14	b	0.21	0/1598	0.41	0/2170
All	All	0.21	0/46190	0.44	1/62713 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	T	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	54	ILE	N-CA-C	-5.18	108.24	113.47

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	T	58	ALA	Peptide

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	A	1734	0	1652	83	0
1	O	1734	0	1652	70	0
2	B	1662	0	1590	56	0
2	P	1670	0	1613	61	0
3	C	1786	0	1717	75	0
3	Q	1786	0	1717	66	0
4	D	1633	0	1518	41	0
4	R	1633	0	1518	44	0
5	E	1659	0	1589	70	0
5	S	1659	0	1589	71	0
6	F	1704	0	1638	59	0
6	T	1704	0	1638	63	0
7	G	1760	0	1680	74	0
7	U	1760	0	1680	73	0
8	H	1465	0	1419	58	0
8	V	1465	0	1419	62	0
9	I	1576	0	1558	63	0
9	W	1576	0	1558	61	0
10	J	1534	0	1539	86	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	X	1534	0	1539	76	0
11	K	1506	0	1475	69	0
11	Y	1506	0	1475	65	0
12	L	1500	0	1441	82	0
12	Z	1500	0	1441	73	0
13	M	1583	0	1579	53	0
13	a	1583	0	1579	63	0
14	N	1568	0	1513	56	0
14	b	1568	0	1513	62	0
15	c	20	0	8	0	0
15	d	20	0	6	1	0
All	All	45388	0	43853	1623	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 18.

All (1623) 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)
8:H:3:ILE:HD13	8:H:44:CYS:HB3	1.54	0.89
11:Y:14:LEU:HD21	11:Y:160:LEU:HD12	1.55	0.88
11:K:19:ARG:HH12	11:K:193:ASN:HD22	1.22	0.86
12:Z:4:LEU:HB2	12:Z:160:ILE:HD11	1.55	0.86
8:V:3:ILE:HD13	8:V:44:CYS:HB3	1.55	0.86
1:A:15:ILE:HB	2:B:20:GLN:HE22	1.41	0.86
6:T:50:LYS:HA	6:T:62:LYS:HZ3	1.41	0.86
4:D:109:ARG:NH2	12:L:70:ASN:OD1	2.11	0.83
4:R:66:ASP:HA	11:Y:69:MET:HE1	1.59	0.83
9:W:163:ILE:HG12	9:W:170:GLY:HA2	1.60	0.83
1:O:15:ILE:HB	2:P:20:GLN:HE22	1.43	0.82
4:R:109:ARG:NH2	12:Z:70:ASN:OD1	2.11	0.82
14:N:73:ASP:HA	14:N:76:LEU:HD12	1.59	0.81
9:I:163:ILE:HG12	9:I:170:GLY:HA2	1.61	0.81
5:S:99:HIS:HB2	5:S:107:MET:HE2	1.63	0.81
12:Z:12:VAL:HG21	12:Z:102:CYS:HB3	1.63	0.80
13:a:35:ILE:O	14:b:151:ARG:NH2	2.15	0.80
10:J:87:MET:HE1	10:J:129:PRO:HB3	1.63	0.80
12:L:4:LEU:HB2	12:L:160:ILE:HD11	1.63	0.80
12:Z:91:LYS:HE2	12:Z:91:LYS:HA	1.64	0.80
13:M:35:ILE:O	14:N:151:ARG:NH2	2.15	0.80
10:J:141:CYS:HB2	10:J:144:GLN:HE22	1.46	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:80:MET:HE1	1:O:138:MET:HB2	1.64	0.79
7:U:175:GLU:N	7:U:175:GLU:OE1	2.15	0.79
3:C:105:ILE:HG12	3:C:110:LEU:HD13	1.64	0.77
1:A:80:MET:HE1	1:A:138:MET:HB2	1.66	0.76
5:S:70:ILE:HD11	5:S:76:CYS:HB2	1.68	0.76
5:S:69:GLU:O	5:S:93:ARG:NH1	2.20	0.75
11:K:171:PHE:HE1	11:K:173:LEU:HB2	1.50	0.75
12:L:100:MET:HE3	12:L:100:MET:HA	1.69	0.75
5:E:70:ILE:HD11	5:E:76:CYS:HB2	1.69	0.75
12:L:12:VAL:HG21	12:L:102:CYS:HB3	1.67	0.75
12:Z:125:THR:HG23	12:Z:139:MET:HE3	1.68	0.74
3:Q:119:GLN:HE22	4:R:79:ASP:HA	1.52	0.74
14:b:73:ASP:HA	14:b:76:LEU:HD12	1.71	0.73
10:J:11:MET:HE2	10:J:170:MET:HE3	1.70	0.73
12:Z:100:MET:HE3	12:Z:100:MET:HA	1.70	0.73
12:L:33:LYS:HE3	12:L:45:MET:HB3	1.71	0.73
9:W:198:ARG:NH2	10:X:150:GLU:O	2.21	0.73
2:B:104:ILE:HG12	2:B:109:LEU:HB2	1.71	0.73
8:V:95:MET:HA	8:V:116:MET:HE1	1.70	0.73
11:K:4:LEU:HB2	11:K:132:HIS:HB2	1.69	0.72
2:B:101:GLN:HE21	9:I:57:GLN:HE22	1.34	0.72
8:H:107:GLU:N	8:H:107:GLU:OE1	2.23	0.72
11:K:8:GLN:NE2	11:K:9:GLY:O	2.22	0.72
6:T:50:LYS:NZ	6:T:208:LYS:O	2.14	0.72
7:G:8:ASP:O	7:G:22:GLN:NE2	2.23	0.72
14:b:43:MET:HB3	14:b:51:LEU:HB3	1.72	0.72
13:a:81:LYS:NZ	13:a:82:ALA:O	2.22	0.71
13:a:57:PHE:HZ	14:b:128:LEU:HB3	1.55	0.71
3:C:45:LEU:HD21	3:C:137:ILE:HG12	1.71	0.71
5:S:181:LEU:HD22	5:S:201:ILE:HD12	1.71	0.71
12:Z:83:LEU:HD11	12:Z:114:VAL:HG21	1.73	0.70
7:G:175:GLU:OE2	7:G:175:GLU:N	2.24	0.70
11:Y:111:GLU:N	11:Y:111:GLU:OE1	2.24	0.70
6:F:66:VAL:HG21	6:F:72:ILE:HG23	1.74	0.70
2:B:64:VAL:O	2:B:219:ARG:NH2	2.24	0.70
11:Y:4:LEU:HB2	11:Y:132:HIS:HB2	1.72	0.70
1:O:13:ILE:HG13	1:O:15:ILE:HG23	1.73	0.70
3:Q:90:LEU:HD11	3:Q:114:LEU:HB2	1.72	0.70
3:Q:91:ARG:HH21	10:X:75:LEU:HB3	1.57	0.70
6:F:69:HIS:HD1	6:F:70:ILE:HG13	1.55	0.69
10:J:72:LEU:O	10:J:76:LYS:HG2	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:155:ASP:OD1	1:O:159:TYR:N	2.22	0.69
3:C:194:ILE:O	3:C:198:ASN:ND2	2.24	0.69
8:H:116:MET:HB3	14:N:5:MET:HG3	1.73	0.69
8:H:192:ASP:HA	8:H:196:LYS:HZ1	1.57	0.69
12:L:158:ARG:HD3	11:Y:145:ARG:HD3	1.75	0.69
1:A:101:TRP:CD1	1:A:109:ILE:HB	2.27	0.69
7:G:35:THR:HA	7:G:166:GLY:HA3	1.75	0.69
13:M:81:LYS:NZ	13:M:82:ALA:O	2.26	0.69
5:E:182:GLN:HG2	6:F:56:LEU:HG	1.75	0.69
5:E:31:ILE:HD13	5:E:140:ALA:HB2	1.75	0.69
10:J:32:GLN:OE1	12:Z:134:TYR:OH	2.10	0.69
11:K:55:GLN:HG2	12:L:88:TYR:HE2	1.57	0.69
14:N:85:PRO:HB2	14:N:121:PHE:HD2	1.58	0.69
10:X:61:THR:O	10:X:65:ARG:HG2	1.93	0.69
5:E:167:ALA:HB3	6:F:56:LEU:HD13	1.75	0.69
6:T:88:MET:HG3	6:T:108:LEU:HD11	1.72	0.69
14:b:153:VAL:HG11	14:b:168:LEU:HD11	1.74	0.68
12:L:95:LEU:HD21	12:L:97:MET:HG2	1.75	0.68
1:O:101:TRP:CD1	1:O:109:ILE:HB	2.29	0.68
11:Y:52:ASP:OD2	12:Z:88:TYR:OH	2.09	0.68
5:E:69:GLU:O	5:E:93:ARG:NH1	2.25	0.68
13:M:57:PHE:HZ	14:N:128:LEU:HB3	1.57	0.68
9:I:93:TYR:HB3	10:J:99:PHE:HZ	1.59	0.68
1:A:155:ASP:OD1	1:A:159:TYR:N	2.20	0.68
1:A:13:ILE:HG13	1:A:15:ILE:HG23	1.76	0.68
10:J:16:LYS:O	10:J:17:ASN:ND2	2.26	0.68
5:S:164:GLN:HB3	6:T:58:ALA:HB3	1.74	0.68
11:K:14:LEU:HD21	11:K:160:LEU:HD22	1.76	0.67
6:T:159:MET:HE3	6:T:160:SER:H	1.59	0.67
12:L:125:THR:HG23	12:L:139:MET:HE3	1.76	0.67
14:N:153:VAL:HG11	14:N:168:LEU:HD11	1.75	0.67
6:F:159:MET:HE3	6:F:160:SER:H	1.59	0.67
12:L:91:LYS:HA	12:L:91:LYS:HE2	1.76	0.67
5:E:52:LYS:HE3	5:E:216:GLU:HB2	1.77	0.67
6:T:66:VAL:HG21	6:T:72:ILE:HG23	1.76	0.67
7:U:35:THR:HA	7:U:166:GLY:HA3	1.75	0.67
11:Y:41:LYS:NZ	11:Y:185:LYS:O	2.28	0.67
3:Q:40:ASN:ND2	3:Q:184:MET:O	2.28	0.67
13:M:57:PHE:HD1	13:M:60:ASP:H	1.43	0.67
2:B:225:VAL:O	2:B:229:LEU:HG	1.95	0.66
3:C:32:GLY:HA2	3:C:50:ARG:HH21	1.60	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:144:TYR:HB3	9:W:132:LEU:HG	1.77	0.66
7:U:20:VAL:HG12	7:U:23:VAL:H	1.59	0.66
10:J:61:THR:O	10:J:65:ARG:HG2	1.95	0.66
3:Q:68:LEU:HD11	3:Q:90:LEU:HD23	1.75	0.66
6:F:165:SER:OG	6:F:169:ARG:NH2	2.28	0.66
3:C:40:ASN:ND2	3:C:184:MET:O	2.28	0.66
5:E:210:LEU:HA	5:E:214:ASN:HD21	1.60	0.66
1:A:127:GLN:NE2	2:B:81:ASP:OD2	2.28	0.66
11:K:52:ASP:OD2	12:L:88:TYR:OH	2.14	0.66
2:P:35:VAL:HG23	2:P:161:ALA:HB2	1.77	0.66
5:S:31:ILE:HD13	5:S:140:ALA:HB2	1.78	0.66
5:S:215:ILE:HG23	5:S:234:LEU:HD21	1.76	0.66
11:K:145:ARG:HD3	12:Z:158:ARG:HD3	1.78	0.66
2:B:133:LEU:HD23	2:B:135:ILE:HD11	1.78	0.66
7:U:174:THR:O	7:U:178:LYS:NZ	2.30	0.65
3:C:102:GLN:NE2	10:J:64:GLN:OE1	2.29	0.65
9:I:51:ASP:O	9:I:55:THR:HG23	1.95	0.65
1:A:141:ILE:HG22	1:A:151:VAL:HG12	1.78	0.65
9:W:51:ASP:O	9:W:55:THR:HG23	1.96	0.65
1:A:51:VAL:HG22	1:A:217:VAL:HG22	1.78	0.65
11:Y:171:PHE:HE1	11:Y:173:LEU:HB2	1.60	0.65
7:U:8:ASP:O	7:U:22:GLN:NE2	2.30	0.65
1:A:80:MET:HG3	1:A:87:SER:HB2	1.77	0.65
14:N:53:ALA:HA	14:N:110:MET:HA	1.79	0.65
3:Q:149:GLN:HB3	3:Q:159:TRP:HE1	1.62	0.65
11:K:41:LYS:NZ	11:K:185:LYS:O	2.28	0.65
2:B:101:GLN:HE21	9:I:57:GLN:NE2	1.95	0.65
4:D:8:THR:HG23	4:D:18:GLN:HB2	1.78	0.65
1:O:141:ILE:HG22	1:O:151:VAL:HG12	1.79	0.65
9:W:7:VAL:HG12	9:W:12:ILE:HG12	1.79	0.65
3:C:3:ARG:HB3	4:D:5:ARG:HH21	1.60	0.65
6:T:165:SER:OG	6:T:169:ARG:NH2	2.28	0.65
3:C:102:GLN:HB2	11:K:82:ASN:HD22	1.62	0.65
9:W:73:LEU:HD12	9:W:74:PRO:HD2	1.77	0.65
10:X:98:ARG:HG2	10:X:126:ILE:HD12	1.77	0.65
11:Y:89:ALA:HA	11:Y:92:LEU:HD23	1.79	0.65
6:T:46:LEU:HD21	6:T:73:SER:HB2	1.78	0.64
14:b:25:ASP:OD1	14:b:41:ARG:NH2	2.31	0.64
9:I:214:GLU:OE2	10:J:197:ARG:NH2	2.29	0.64
14:N:171:ARG:NH2	9:W:140:ASP:OD2	2.30	0.64
8:V:14:LEU:HD13	8:V:34:LEU:HD22	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:TRP:O	1:A:193:GLN:NE2	2.30	0.64
2:B:38:LYS:HA	2:B:43:VAL:HG12	1.80	0.64
9:I:132:LEU:HG	14:b:144:TYR:HB3	1.78	0.64
5:E:191:LEU:O	5:E:195:ILE:HG13	1.97	0.64
4:R:8:THR:HG23	4:R:18:GLN:HB2	1.79	0.64
7:U:68:ASN:HB3	14:b:76:LEU:HD23	1.78	0.64
14:b:163:THR:OG1	14:b:164:GLU:OE2	2.14	0.64
10:J:121:CYS:SG	10:J:122:SER:N	2.71	0.64
5:S:192:LYS:HA	5:S:195:ILE:HD12	1.80	0.64
13:a:174:LEU:O	13:a:178:VAL:HG12	1.96	0.64
7:U:17:ASP:OD2	7:U:17:ASP:N	2.27	0.64
11:Y:19:ARG:HH21	11:Y:31:ASP:HB3	1.63	0.64
2:B:21:ILE:HG21	2:B:151:SER:HB3	1.80	0.63
12:L:54:PHE:CE2	12:L:58:LEU:HD11	2.33	0.63
5:E:41:GLN:NE2	5:E:151:PRO:O	2.31	0.63
6:F:81:ALA:HB2	6:F:130:VAL:HG21	1.79	0.63
10:J:33:MET:O	12:Z:166:ARG:NH1	2.31	0.63
3:Q:102:GLN:HB2	11:Y:82:ASN:HD22	1.63	0.63
5:S:41:GLN:NE2	5:S:151:PRO:O	2.32	0.63
5:E:165:CYS:HA	6:F:57:ALA:HA	1.80	0.63
11:K:89:ALA:HA	11:K:92:LEU:HD23	1.79	0.63
2:P:21:ILE:HG21	2:P:151:SER:HB3	1.81	0.63
3:Q:105:ILE:HG21	3:Q:110:LEU:HD13	1.81	0.63
11:Y:181:ARG:HD3	11:Y:188:ILE:HD11	1.79	0.63
14:N:25:ASP:OD1	14:N:41:ARG:NH2	2.31	0.63
1:O:127:GLN:NE2	2:P:81:ASP:OD1	2.32	0.63
1:O:195:VAL:O	1:O:199:ILE:HG12	1.98	0.63
10:X:72:LEU:O	10:X:76:LYS:NZ	2.31	0.63
11:Y:55:GLN:HG2	12:Z:88:TYR:HE2	1.62	0.63
2:P:73:LEU:HD12	2:P:133:LEU:HG	1.80	0.63
2:P:133:LEU:HB2	2:P:148:SER:HB3	1.80	0.63
4:R:76:LEU:HB2	4:R:79:ASP:HB2	1.81	0.63
4:R:79:ASP:OD1	4:R:125:ARG:NH2	2.30	0.63
14:b:86:ARG:NH2	14:b:119:GLU:OE2	2.32	0.63
2:B:35:VAL:HG23	2:B:161:ALA:HB2	1.79	0.63
5:E:66:LYS:HG2	5:E:82:ILE:HD11	1.81	0.63
6:F:22:ILE:HD12	6:F:22:ILE:H	1.62	0.63
7:G:236:GLU:O	7:G:240:LYS:HG3	1.98	0.63
11:K:111:GLU:OE2	11:K:111:GLU:N	2.30	0.63
6:F:95:SER:HB3	6:F:103:LEU:HD12	1.79	0.63
3:Q:177:GLN:N	3:Q:177:GLN:OE1	2.32	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:LEU:HB2	2:B:148:SER:HB3	1.80	0.62
5:E:221:GLN:HG2	5:E:224:GLN:H	1.63	0.62
8:H:57:ASP:OD1	9:I:85:GLN:NE2	2.32	0.62
13:M:169:ASP:OD1	13:M:170:ARG:N	2.32	0.62
9:W:30:ASN:O	9:W:187:ARG:NH2	2.31	0.62
13:a:137:ALA:N	13:a:146:GLN:OE1	2.26	0.62
1:A:162:GLY:O	2:B:57:ASP:N	2.28	0.62
4:D:184:ASP:O	4:D:188:ILE:HG13	1.98	0.62
5:E:38:ILE:HD11	5:E:181:LEU:HD11	1.81	0.62
4:D:111:ILE:O	4:D:115:LYS:HG3	1.99	0.62
3:Q:3:ARG:HB3	4:R:5:ARG:HH21	1.64	0.62
11:Y:182:ILE:HG22	11:Y:189:HIS:HB2	1.81	0.62
2:B:33:PRO:HA	2:B:163:GLY:HA3	1.81	0.62
2:B:188:HIS:O	2:B:192:LEU:HG	1.98	0.62
7:G:174:THR:O	7:G:178:LYS:NZ	2.32	0.62
9:I:30:ASN:O	9:I:187:ARG:NH2	2.33	0.62
4:D:16:LEU:HD11	5:E:135:ARG:HE	1.63	0.62
6:T:26:MET:HA	6:T:149:PRO:HG2	1.82	0.62
12:Z:66:TYR:HD1	12:Z:70:ASN:HD22	1.46	0.62
11:K:19:ARG:HH21	11:K:31:ASP:HB3	1.64	0.62
6:T:47:VAL:HG23	6:T:212:ILE:HG12	1.81	0.62
11:Y:19:ARG:HB3	11:Y:31:ASP:HA	1.82	0.62
6:F:88:MET:HG3	6:F:108:LEU:HD11	1.81	0.62
12:L:97:MET:HA	12:L:97:MET:HE3	1.82	0.62
5:S:182:GLN:HG2	6:T:56:LEU:HG	1.81	0.62
8:V:181:GLU:H	8:V:181:GLU:CD	2.08	0.62
1:A:53:GLN:HG2	1:A:202:LEU:HD21	1.82	0.62
12:L:52:CYS:HA	12:L:97:MET:HE1	1.82	0.62
8:H:14:LEU:HD13	8:H:34:LEU:HD22	1.81	0.61
10:X:87:MET:HE1	10:X:129:PRO:HB3	1.82	0.61
12:L:58:LEU:HA	12:L:61:ARG:HG2	1.81	0.61
6:T:81:ALA:HB2	6:T:130:VAL:HG21	1.81	0.61
12:Z:58:LEU:HA	12:Z:61:ARG:HG2	1.82	0.61
9:I:207:GLY:O	13:a:159:GLN:NE2	2.33	0.61
1:O:51:VAL:HG22	1:O:217:VAL:HG22	1.81	0.61
5:S:165:CYS:HA	6:T:57:ALA:HA	1.82	0.61
7:G:215:TRP:CE3	7:G:227:VAL:HG22	2.35	0.61
8:V:57:ASP:OD2	9:W:85:GLN:NE2	2.33	0.61
1:A:200:THR:O	1:A:204:THR:HG23	2.01	0.61
7:U:215:TRP:CE3	7:U:227:VAL:HG22	2.36	0.61
3:Q:97:TYR:HE1	3:Q:106:PRO:HD2	1.65	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:196:ILE:HA	7:U:199:ILE:HG12	1.82	0.61
3:Q:32:GLY:HA2	3:Q:50:ARG:HH21	1.65	0.61
11:Y:80:ALA:O	11:Y:84:THR:HG23	2.01	0.61
1:A:219:VAL:HG22	1:A:230:LEU:HD21	1.83	0.61
13:M:185:ARG:HD3	10:X:146:TYR:HB3	1.82	0.61
1:O:43:ARG:HA	1:O:48:ALA:HA	1.83	0.61
1:O:189:TRP:O	1:O:193:GLN:NE2	2.34	0.61
6:T:62:LYS:HD2	6:T:74:ILE:HG22	1.82	0.61
8:H:57:ASP:OD2	8:H:58:ALA:N	2.34	0.60
13:M:27:THR:HB	13:M:40:SER:H	1.66	0.60
14:N:124:TYR:HB2	14:N:137:LEU:HD13	1.81	0.60
12:L:166:ARG:NH1	10:X:33:MET:O	2.33	0.60
2:P:188:HIS:O	2:P:192:LEU:HG	2.00	0.60
5:S:182:GLN:HA	6:T:56:LEU:HD11	1.83	0.60
5:S:211:ASN:N	5:S:214:ASN:OD1	2.31	0.60
11:Y:43:LEU:HD12	11:Y:183:ILE:HD11	1.83	0.60
1:A:110:PRO:HB2	1:A:113:MET:HE1	1.83	0.60
10:J:70:LEU:HD11	10:J:81:ILE:HG21	1.83	0.60
11:K:43:LEU:HD12	11:K:183:ILE:HD11	1.84	0.60
4:R:184:ASP:O	4:R:188:ILE:HG13	2.01	0.60
14:b:1:THR:N	14:b:105:PRO:O	2.34	0.60
12:L:35:ILE:HD11	12:L:45:MET:HE2	1.83	0.60
13:M:45:LYS:NZ	13:M:196:CYS:SG	2.65	0.60
8:V:57:ASP:OD1	8:V:58:ALA:N	2.34	0.60
14:b:145:LEU:HD21	14:b:179:ARG:HB2	1.83	0.60
2:B:222:PRO:O	2:B:226:LYS:HG3	2.02	0.60
1:O:10:ASP:OD1	1:O:17:SER:HA	2.02	0.60
10:X:33:MET:SD	10:X:34:VAL:N	2.75	0.60
10:X:121:CYS:SG	10:X:122:SER:N	2.75	0.60
2:B:43:VAL:HG23	2:B:212:CYS:HB3	1.84	0.60
12:L:19:ARG:NH1	12:L:170:SER:O	2.35	0.60
3:Q:107:CYS:O	3:Q:111:VAL:HG13	2.02	0.60
6:T:150:SER:OG	6:T:152:ASN:OD1	2.14	0.60
10:X:71:ASN:O	10:X:75:LEU:HG	2.01	0.60
13:a:27:THR:HB	13:a:40:SER:H	1.67	0.60
5:E:202:LEU:HA	5:E:205:VAL:HG22	1.82	0.60
13:M:145:LEU:HD22	13:M:178:VAL:HG22	1.83	0.60
11:Y:38:MET:HA	11:Y:38:MET:HE3	1.84	0.60
12:Z:19:ARG:NH1	12:Z:170:SER:O	2.34	0.60
13:a:46:LEU:HD11	13:a:52:ILE:HG12	1.84	0.60
2:B:51:GLN:HB2	2:B:56:TYR:HB3	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:THR:HG22	2:B:128:PRO:HB3	1.83	0.59
3:C:197:LEU:HD21	3:C:211:VAL:HG11	1.83	0.59
5:E:56:SER:H	5:E:59:MET:HE2	1.67	0.59
7:G:185:THR:O	7:G:189:ILE:HG12	2.02	0.59
10:J:47:ARG:HD3	10:J:111:LEU:HD12	1.82	0.59
14:N:60:PHE:HB2	14:N:108:ASN:ND2	2.16	0.59
12:Z:33:LYS:O	12:Z:45:MET:HB2	2.02	0.59
3:Q:163:CYS:C	3:Q:168:SER:HG	2.10	0.59
9:W:214:GLU:OE1	10:X:197:ARG:NH2	2.36	0.59
4:D:76:LEU:HB2	4:D:79:ASP:HB2	1.84	0.59
14:N:89:HIS:HE1	14:N:131:ALA:HB1	1.65	0.59
1:O:80:MET:HG3	1:O:87:SER:HB2	1.85	0.59
4:R:85:ASN:O	4:R:89:VAL:HG23	2.02	0.59
2:B:190:ALA:O	2:B:193:THR:OG1	2.20	0.59
8:H:112:TYR:HE1	8:H:122:ARG:HB2	1.68	0.59
10:J:11:MET:HE1	10:J:166:ILE:HG13	1.83	0.59
10:X:145:MET:SD	10:X:145:MET:N	2.72	0.59
14:b:89:HIS:HE1	14:b:131:ALA:HB1	1.68	0.59
14:b:103:MET:HE2	14:b:103:MET:HA	1.84	0.59
3:Q:194:ILE:O	3:Q:198:ASN:ND2	2.35	0.59
1:A:43:ARG:HA	1:A:48:ALA:HA	1.85	0.59
3:C:105:ILE:HD12	3:C:106:PRO:HD2	1.85	0.59
3:C:136:TYR:HB2	3:C:148:TYR:HB2	1.84	0.59
7:G:40:ARG:NE	7:G:146:ALA:O	2.30	0.59
9:I:140:ASP:OD2	14:b:171:ARG:NH2	2.36	0.59
1:O:44:GLY:N	1:O:47:CYS:O	2.31	0.59
2:P:38:LYS:HA	2:P:43:VAL:HG12	1.83	0.59
3:C:174:MET:SD	3:C:177:GLN:NE2	2.72	0.59
11:K:55:GLN:HG2	12:L:88:TYR:CE2	2.38	0.59
4:R:66:ASP:HB3	4:R:69:VAL:HG12	1.84	0.59
3:C:90:LEU:HD21	3:C:114:LEU:HD22	1.85	0.59
14:N:190:ALA:HB2	14:N:199:ILE:HG23	1.84	0.59
3:Q:38:LEU:HB2	3:Q:147:LEU:HG	1.84	0.59
1:A:10:ASP:OD1	1:A:17:SER:HA	2.03	0.59
1:A:44:GLY:N	1:A:47:CYS:O	2.32	0.59
1:A:141:ILE:HD12	1:A:220:VAL:HG12	1.85	0.59
3:C:233:VAL:O	3:C:237:ILE:HG13	2.03	0.59
6:F:45:VAL:HG21	6:F:188:VAL:HG12	1.85	0.59
13:M:174:LEU:O	13:M:178:VAL:HG12	2.01	0.59
8:V:119:MET:HE1	8:V:121:VAL:HB	1.85	0.59
10:X:5:TYR:HD2	10:X:6:ASN:ND2	2.00	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:47:VAL:HG23	6:F:212:ILE:HG12	1.84	0.59
7:G:20:VAL:HG12	7:G:23:VAL:H	1.67	0.59
8:H:46:SER:OG	8:H:97:GLY:O	2.20	0.59
12:L:33:LYS:O	12:L:45:MET:HB2	2.03	0.59
4:R:111:ILE:O	4:R:115:LYS:HG3	2.03	0.59
3:C:119:GLN:HE22	4:D:79:ASP:HA	1.67	0.58
1:A:36:GLY:O	1:A:55:LYS:NZ	2.36	0.58
13:M:46:LEU:HD11	13:M:52:ILE:HG12	1.83	0.58
2:P:43:VAL:HG23	2:P:212:CYS:HB3	1.85	0.58
10:X:70:LEU:HD11	10:X:81:ILE:HG21	1.85	0.58
5:E:55:THR:H	5:E:59:MET:HE1	1.69	0.58
14:N:22:ILE:HG12	14:N:50:MET:HE2	1.84	0.58
14:b:43:MET:HE1	14:b:64:LYS:HA	1.85	0.58
2:B:67:ILE:HD11	2:B:73:LEU:HD22	1.85	0.58
5:E:210:LEU:HD23	5:E:238:ILE:HD11	1.86	0.58
6:F:150:SER:OG	6:F:152:ASN:OD1	2.19	0.58
11:K:19:ARG:HB3	11:K:31:ASP:HA	1.84	0.58
9:W:3:ILE:HD12	9:W:44:CYS:HB3	1.84	0.58
1:A:217:VAL:HG23	1:A:235:ILE:HD11	1.84	0.58
4:D:188:ILE:O	4:D:192:ILE:HG23	2.04	0.58
11:K:7:ILE:HD11	11:K:143:LEU:HD21	1.85	0.58
11:Y:14:LEU:HB2	11:Y:182:ILE:HD12	1.86	0.58
8:H:181:GLU:CD	8:H:181:GLU:H	2.11	0.58
8:H:50:ALA:N	9:I:118:SER:HB3	2.19	0.58
9:I:7:VAL:HG12	9:I:12:ILE:HG12	1.85	0.58
11:K:182:ILE:HG22	11:K:189:HIS:HB2	1.86	0.58
4:R:16:LEU:HD11	5:S:135:ARG:HE	1.69	0.58
10:X:11:MET:HG3	10:X:137:VAL:HG12	1.86	0.58
12:Z:36:GLU:HG2	12:Z:184:TRP:CZ2	2.38	0.58
13:M:197:ILE:HG21	13:M:204:ARG:HH11	1.68	0.57
1:O:200:THR:O	1:O:204:THR:HG23	2.04	0.57
2:P:96:TYR:HD2	2:P:112:ARG:HH12	1.52	0.57
7:U:236:GLU:O	7:U:240:LYS:HG3	2.04	0.57
8:V:29:ARG:NH2	9:W:139:GLU:OE1	2.36	0.57
8:V:112:TYR:HE1	8:V:122:ARG:HB2	1.68	0.57
12:Z:51:ASP:OD1	13:a:97:TYR:OH	2.21	0.57
14:b:4:PRO:HG3	14:b:107:TRP:CG	2.38	0.57
9:I:24:MET:HE2	9:I:24:MET:HA	1.84	0.57
12:Z:100:MET:HE1	12:Z:113:TYR:HB2	1.86	0.57
5:S:70:ILE:HD12	5:S:74:ILE:HG22	1.85	0.57
13:a:57:PHE:HD1	13:a:60:ASP:H	1.52	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:70:ILE:HD12	5:E:74:ILE:HG22	1.86	0.57
5:E:141:LEU:HB3	5:E:156:MET:HB2	1.86	0.57
9:I:3:ILE:HD12	9:I:44:CYS:HB3	1.86	0.57
5:E:215:ILE:HG23	5:E:234:LEU:HD21	1.87	0.57
1:O:53:GLN:HG2	1:O:202:LEU:HD21	1.86	0.57
10:X:12:ALA:HB2	10:X:21:ILE:HD13	1.87	0.57
10:X:66:LEU:HD11	10:X:90:VAL:HG22	1.86	0.57
12:Z:62:GLN:HA	12:Z:65:ILE:HG12	1.86	0.57
9:I:167:LEU:HB3	13:a:187:VAL:HB	1.86	0.57
1:A:15:ILE:HB	2:B:20:GLN:NE2	2.16	0.57
7:U:185:THR:O	7:U:189:ILE:HG12	2.05	0.57
8:V:50:ALA:N	9:W:118:SER:HB3	2.19	0.57
7:G:173:LYS:HA	7:G:176:ILE:HG12	1.86	0.57
9:I:141:LYS:HB3	9:I:154:LEU:HD11	1.85	0.57
10:J:82:LYS:O	10:J:85:THR:OG1	2.17	0.57
10:J:144:GLN:HB3	13:a:147:PRO:HG2	1.86	0.57
2:P:202:MET:SD	2:P:202:MET:N	2.73	0.57
11:Y:56:PHE:O	11:Y:60:ILE:HG12	2.04	0.57
3:C:80:THR:O	3:C:84:ASN:ND2	2.38	0.57
9:I:164:PHE:HE1	13:a:212:LYS:HD2	1.68	0.57
3:Q:12:PHE:CE2	4:R:125:ARG:HD2	2.39	0.57
8:V:34:LEU:HB2	8:V:186:ARG:HH12	1.70	0.57
9:W:141:LYS:HB3	9:W:154:LEU:HD11	1.85	0.57
10:X:47:ARG:HD3	10:X:111:LEU:HD12	1.86	0.57
12:L:93:MET:HG3	13:M:101:PHE:CZ	2.39	0.57
3:C:174:MET:HG2	3:C:199:LYS:NZ	2.20	0.56
5:E:77:ALA:HB3	5:E:142:LEU:HB2	1.85	0.56
2:P:47:THR:HB	2:P:74:VAL:HG21	1.87	0.56
2:P:222:PRO:O	2:P:226:LYS:HG3	2.05	0.56
8:V:107:GLU:OE2	8:V:110:GLN:NE2	2.38	0.56
13:a:75:TYR:CD2	13:a:83:MET:HB2	2.40	0.56
8:H:4:MET:HE2	8:H:156:THR:HA	1.87	0.56
8:H:34:LEU:HB2	8:H:186:ARG:HH12	1.69	0.56
10:J:11:MET:HE1	10:J:166:ILE:CG1	2.34	0.56
11:K:12:TYR:OH	11:K:151:ILE:O	2.20	0.56
13:M:99:ARG:NH1	13:M:102:PHE:O	2.38	0.56
11:Y:55:GLN:HG2	12:Z:88:TYR:CE2	2.40	0.56
2:B:202:MET:SD	2:B:202:MET:N	2.77	0.56
3:C:73:ALA:HB3	3:C:137:ILE:HD11	1.86	0.56
3:C:177:GLN:O	3:C:180:LYS:NZ	2.38	0.56
8:H:84:LYS:HD3	8:H:120:MET:HB2	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:26:ARG:NH1	10:J:179:VAL:O	2.38	0.56
10:J:182:MET:HA	10:J:182:MET:HE3	1.87	0.56
5:S:41:GLN:HA	5:S:46:VAL:HG12	1.86	0.56
6:T:11:THR:HA	7:U:129:ARG:HD3	1.86	0.56
8:V:46:SER:OG	8:V:97:GLY:O	2.23	0.56
10:X:11:MET:HE1	10:X:166:ILE:HG13	1.86	0.56
11:Y:158:GLU:O	11:Y:162:LYS:HG2	2.05	0.56
12:Z:18:SER:OG	12:Z:29:GLN:O	2.21	0.56
12:Z:18:SER:HB3	12:Z:173:ALA:H	1.69	0.56
12:Z:93:MET:HG3	13:a:101:PHE:CZ	2.40	0.56
13:a:54:CYS:HB3	13:a:61:CYS:SG	2.45	0.56
11:K:116:TYR:HD2	11:K:124:LEU:HD11	1.71	0.56
13:M:45:LYS:N	13:M:45:LYS:HD3	2.20	0.56
2:P:33:PRO:HA	2:P:163:GLY:HA3	1.87	0.56
3:C:38:LEU:HB2	3:C:147:LEU:HG	1.88	0.56
6:T:92:CYS:O	6:T:95:SER:OG	2.21	0.56
8:V:161:ALA:HA	8:V:164:MET:HE3	1.88	0.56
4:D:50:VAL:O	4:D:54:GLN:HG2	2.06	0.56
4:D:119:THR:HG22	4:D:126:PRO:HB3	1.87	0.56
10:J:52:LEU:HB2	10:J:59:VAL:HG13	1.87	0.56
13:a:49:LYS:O	13:a:50:THR:OG1	2.21	0.56
6:F:38:LEU:HD23	6:F:172:LEU:HD21	1.87	0.56
13:M:110:ILE:HB	13:M:122:TYR:HB2	1.88	0.56
9:W:62:ASN:HB3	9:W:82:MET:HE3	1.87	0.56
8:H:162:LEU:HD11	8:V:141:ALA:HB2	1.87	0.56
12:L:66:TYR:HD1	12:L:70:ASN:HD22	1.53	0.56
1:O:217:VAL:HG23	1:O:235:ILE:HD11	1.86	0.56
5:S:73:HIS:CE1	5:S:106:THR:HB	2.41	0.56
6:T:52:ALA:HB2	6:T:59:HIS:CE1	2.41	0.56
9:W:24:MET:HE2	9:W:24:MET:HA	1.88	0.56
10:X:44:MET:HE3	10:X:70:LEU:HD22	1.87	0.56
7:G:23:VAL:O	7:G:27:MET:HG2	2.06	0.56
5:S:18:GLU:N	5:S:18:GLU:OE2	2.39	0.56
7:U:8:ASP:OD1	7:U:8:ASP:N	2.32	0.56
9:W:216:ILE:HD12	10:X:195:THR:HG22	1.88	0.56
10:X:29:ILE:HG22	10:X:30:GLN:H	1.70	0.56
1:O:53:GLN:HA	1:O:215:ILE:HG22	1.88	0.55
7:G:106:ILE:HD12	7:G:107:PRO:HD2	1.88	0.55
7:G:117:MET:HA	7:G:117:MET:HE2	1.88	0.55
7:G:196:ILE:HA	7:G:199:ILE:HG12	1.88	0.55
12:L:91:LYS:HE3	12:L:116:SER:O	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:23:VAL:O	7:U:27:MET:HG2	2.05	0.55
7:U:40:ARG:NE	7:U:146:ALA:O	2.31	0.55
11:Y:38:MET:HB2	11:Y:42:ILE:HG23	1.88	0.55
6:T:16:GLN:N	6:T:16:GLN:OE1	2.37	0.55
8:V:112:TYR:CE1	8:V:122:ARG:HB2	2.41	0.55
10:X:145:MET:HE3	10:X:173:ALA:HB1	1.87	0.55
11:Y:171:PHE:CE1	11:Y:173:LEU:HB2	2.41	0.55
3:C:196:VAL:HA	3:C:199:LYS:NZ	2.21	0.55
6:F:50:LYS:HD3	6:F:59:HIS:HB2	1.87	0.55
10:J:62:VAL:HG22	10:J:102:TYR:HD1	1.72	0.55
13:M:36:HIS:HB3	14:N:132:TYR:CZ	2.42	0.55
14:N:103:MET:HE2	14:N:103:MET:HA	1.89	0.55
1:O:219:VAL:HG22	1:O:230:LEU:HD21	1.88	0.55
2:P:67:ILE:HD11	2:P:73:LEU:HD22	1.89	0.55
3:Q:49:ARG:N	3:Q:210:LYS:O	2.37	0.55
3:Q:105:ILE:HD12	3:Q:105:ILE:H	1.72	0.55
12:Z:184:TRP:HZ3	12:Z:186:ARG:HB2	1.71	0.55
14:b:12:LEU:HD11	14:b:172:CYS:HB3	1.88	0.55
10:J:29:ILE:HG22	10:J:30:GLN:H	1.71	0.55
12:L:37:ILE:HD12	12:L:41:LEU:HD23	1.88	0.55
8:V:41:ILE:HD11	8:V:76:VAL:HG22	1.87	0.55
10:X:98:ARG:HH21	10:X:99:PHE:HE2	1.52	0.55
12:Z:44:THR:OG1	12:Z:100:MET:N	2.37	0.55
2:P:16:GLY:HA3	3:Q:26:GLU:OE2	2.06	0.55
8:V:28:ASN:OD1	8:V:29:ARG:N	2.40	0.55
9:W:50:ALA:HB2	10:X:128:CYS:HB2	1.88	0.55
13:a:197:ILE:HG21	13:a:204:ARG:HH11	1.72	0.55
3:C:174:MET:O	3:C:177:GLN:NE2	2.40	0.55
5:E:69:GLU:HG3	5:E:226:PHE:HD2	1.72	0.55
5:E:108:THR:O	5:E:112:VAL:HG23	2.05	0.55
8:H:112:TYR:CE1	8:H:122:ARG:HB2	2.41	0.55
6:F:44:ALA:HB2	6:F:142:PRO:HB3	1.89	0.55
3:Q:190:LEU:O	3:Q:194:ILE:HG12	2.07	0.55
9:W:19:ARG:NH1	9:W:167:LEU:O	2.37	0.55
13:a:195:ILE:HB	13:a:206:GLU:HB2	1.87	0.55
4:D:5:ARG:O	4:D:123:GLY:N	2.40	0.55
1:O:171:LYS:HE2	1:O:205:VAL:HB	1.89	0.55
10:X:47:ARG:NH2	10:X:191:LYS:O	2.39	0.55
3:C:49:ARG:N	3:C:210:LYS:O	2.33	0.54
9:I:19:ARG:NH1	9:I:167:LEU:O	2.37	0.54
14:N:145:LEU:HD21	14:N:179:ARG:HB2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:229:ILE:HD12	1:O:229:ILE:H	1.72	0.54
12:Z:21:THR:HG22	12:Z:26:ILE:HA	1.89	0.54
6:F:192:LEU:HD21	6:F:212:ILE:HD11	1.89	0.54
3:C:167:ASN:OD1	3:C:170:ALA:HB3	2.08	0.54
4:D:107:ILE:O	4:D:111:ILE:HG22	2.07	0.54
6:F:50:LYS:HD3	6:F:60:GLN:H	1.72	0.54
11:K:108:ASP:HB3	11:K:112:GLY:H	1.73	0.54
3:Q:70:GLU:O	3:Q:223:THR:OG1	2.26	0.54
10:X:44:MET:SD	10:X:44:MET:N	2.80	0.54
8:H:28:ASN:OD1	8:H:29:ARG:N	2.41	0.54
11:K:101:ASN:HB3	11:K:132:HIS:CE1	2.43	0.54
13:M:49:LYS:O	13:M:50:THR:OG1	2.21	0.54
5:S:108:THR:O	5:S:112:VAL:HG23	2.07	0.54
3:C:163:CYS:O	3:C:168:SER:OG	2.26	0.54
5:E:38:ILE:HD13	5:E:169:ALA:HB2	1.88	0.54
7:G:109:LYS:HA	7:G:149:TYR:HE2	1.72	0.54
5:S:69:GLU:HG3	5:S:226:PHE:HD2	1.70	0.54
13:a:36:HIS:HB3	14:b:132:TYR:CZ	2.42	0.54
12:L:35:ILE:HD13	12:L:56:GLU:HG2	1.90	0.54
13:M:187:VAL:HB	9:W:167:LEU:HB3	1.88	0.54
3:Q:163:CYS:O	3:Q:168:SER:OG	2.25	0.54
9:I:187:ARG:HB3	9:I:188:PRO:HD3	1.89	0.54
11:K:181:ARG:HD3	11:K:188:ILE:HD11	1.90	0.54
4:R:13:ASP:N	5:S:29:GLU:OE2	2.40	0.54
5:E:203:LYS:NZ	5:E:210:LEU:HB3	2.23	0.54
7:G:98:PHE:CG	7:G:106:ILE:HD13	2.43	0.54
9:I:62:ASN:HB3	9:I:82:MET:HE3	1.89	0.54
10:J:47:ARG:NH2	10:J:191:LYS:O	2.41	0.54
1:O:17:SER:OG	1:O:20:GLY:N	2.41	0.54
11:Y:16:ALA:HB2	11:Y:160:LEU:HD11	1.89	0.54
14:N:89:HIS:CE1	14:N:131:ALA:HB1	2.42	0.54
12:Z:55:TRP:CZ3	12:Z:58:LEU:HD21	2.43	0.54
4:D:66:ASP:HA	11:K:69:MET:HE1	1.90	0.54
11:K:18:ASP:HB2	11:K:175:LEU:HD12	1.90	0.54
2:P:93:ALA:HA	2:P:104:ILE:HD12	1.88	0.54
5:S:210:LEU:HD23	5:S:238:ILE:HD11	1.90	0.54
6:F:158:ALA:HB1	6:F:172:LEU:HD13	1.89	0.53
2:P:172:PHE:HA	2:P:176:ARG:HH21	1.73	0.53
3:Q:76:VAL:HG11	3:Q:83:ALA:HB1	1.89	0.53
10:X:11:MET:HE1	10:X:166:ILE:CG1	2.37	0.53
10:X:177:ASP:OD1	10:X:178:ALA:N	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:124:TYR:HE1	14:b:139:THR:HG22	1.72	0.53
2:B:67:ILE:HG21	2:B:109:LEU:HD11	1.90	0.53
8:H:119:MET:HE1	8:H:121:VAL:HB	1.90	0.53
1:O:39:SER:O	1:O:168:ALA:N	2.38	0.53
7:U:187:ARG:HH21	7:U:219:LEU:HD21	1.73	0.53
13:a:110:ILE:HB	13:a:122:TYR:HB2	1.90	0.53
2:B:222:PRO:HA	2:B:225:VAL:HG22	1.91	0.53
6:F:11:THR:HA	7:G:129:ARG:HD3	1.89	0.53
1:O:123:GLN:OE1	2:P:84:VAL:HG21	2.08	0.53
2:P:38:LYS:HE3	2:P:143:PRO:HG2	1.91	0.53
9:W:10:ASP:OD1	9:W:10:ASP:N	2.41	0.53
9:W:166:ASP:OD1	9:W:168:GLY:N	2.34	0.53
9:I:161:ALA:O	9:I:165:ASN:ND2	2.21	0.53
10:J:71:ASN:O	10:J:75:LEU:HG	2.08	0.53
12:L:62:GLN:HA	12:L:65:ILE:HG12	1.90	0.53
10:X:184:VAL:HB	10:X:199:LEU:HD11	1.90	0.53
10:J:11:MET:HG2	10:J:136:VAL:O	2.09	0.53
1:O:153:LYS:HE3	1:O:163:PHE:CE2	2.43	0.53
2:P:92:LEU:HD23	2:P:112:ARG:HB3	1.90	0.53
3:Q:198:ASN:HB2	3:Q:199:LYS:HZ2	1.72	0.53
3:C:196:VAL:HA	3:C:199:LYS:HZ3	1.74	0.53
6:F:50:LYS:CD	6:F:59:HIS:HB2	2.39	0.53
4:R:5:ARG:O	4:R:123:GLY:N	2.42	0.53
5:S:167:ALA:HB1	5:S:181:LEU:HD12	1.90	0.53
7:U:83:ASP:HB3	7:U:131:PHE:HD1	1.73	0.53
10:X:26:ARG:NH1	10:X:179:VAL:O	2.42	0.53
12:Z:63:CYS:HB2	12:Z:74:ILE:HG21	1.91	0.53
1:A:153:LYS:HE3	1:A:163:PHE:CE2	2.44	0.53
1:A:168:ALA:HA	1:A:172:GLN:HG3	1.91	0.53
4:D:164:GLY:O	4:D:168:VAL:HG12	2.09	0.53
10:J:44:MET:SD	10:J:44:MET:N	2.80	0.53
12:L:33:LYS:CE	12:L:45:MET:HB3	2.36	0.53
6:T:40:SER:HG	6:T:43:HIS:H	1.57	0.53
10:X:39:GLN:OE1	10:X:41:ILE:N	2.39	0.53
5:E:78:MET:SD	5:E:89:ILE:HD11	2.49	0.53
12:L:18:SER:HB2	12:L:173:ALA:H	1.73	0.53
6:T:192:LEU:HD21	6:T:212:ILE:HD11	1.90	0.53
8:V:115:PRO:HG3	14:b:36:PHE:CZ	2.44	0.53
5:E:67:ILE:HD12	5:E:216:GLU:HG3	1.89	0.52
6:F:26:MET:HA	6:F:149:PRO:HG2	1.91	0.52
8:H:141:ALA:HB2	8:V:162:LEU:HD11	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:161:ALA:HA	8:H:164:MET:HE3	1.90	0.52
12:L:34:VAL:HG22	12:L:44:THR:HG22	1.91	0.52
4:R:119:THR:HG22	4:R:126:PRO:HB3	1.91	0.52
11:Y:101:ASN:HB3	11:Y:132:HIS:CE1	2.44	0.52
12:Z:35:ILE:HD11	12:Z:45:MET:HG2	1.92	0.52
12:L:36:GLU:HG2	12:L:184:TRP:CZ2	2.44	0.52
13:M:177:ASP:OD1	9:W:200:GLY:N	2.34	0.52
1:O:132:ARG:NH1	7:U:124:LEU:HA	2.25	0.52
2:P:190:ALA:O	2:P:193:THR:OG1	2.24	0.52
12:Z:53:SER:O	12:Z:56:GLU:HG3	2.09	0.52
11:K:38:MET:HB2	11:K:42:ILE:HG23	1.91	0.52
12:L:45:MET:HE1	12:L:49:ALA:O	2.09	0.52
1:O:164:LYS:N	2:P:55:LEU:O	2.42	0.52
3:Q:167:ASN:OD1	3:Q:170:ALA:HB3	2.09	0.52
14:b:89:HIS:CE1	14:b:131:ALA:HB1	2.44	0.52
1:A:123:GLN:OE1	2:B:84:VAL:HG21	2.10	0.52
7:G:92:ARG:HD3	14:N:76:LEU:HD13	1.92	0.52
10:J:26:ARG:HB2	10:J:182:MET:HB2	1.91	0.52
5:S:218:ALA:HB1	5:S:226:PHE:HE1	1.75	0.52
11:Y:12:TYR:OH	11:Y:151:ILE:O	2.21	0.52
11:Y:60:ILE:HG21	11:Y:84:THR:HG22	1.90	0.52
12:Z:4:LEU:HD11	12:Z:139:MET:SD	2.50	0.52
14:b:190:ALA:HB2	14:b:199:ILE:HG23	1.91	0.52
1:A:113:MET:H	1:A:113:MET:HE3	1.74	0.52
10:J:19:VAL:HG13	10:J:189:ILE:HB	1.90	0.52
13:M:54:CYS:HB3	13:M:61:CYS:SG	2.50	0.52
1:A:132:ARG:NH1	7:G:124:LEU:HA	2.24	0.52
9:I:216:ILE:HD12	10:J:195:THR:HG22	1.90	0.52
10:J:175:ASP:OD1	10:J:175:ASP:N	2.40	0.52
12:L:179:VAL:HA	12:L:184:TRP:HA	1.91	0.52
6:T:59:HIS:O	6:T:60:GLN:HG2	2.10	0.52
12:L:4:LEU:HD11	12:L:139:MET:SD	2.49	0.52
6:T:137:TYR:HE2	6:T:141:GLY:HA2	1.75	0.52
11:Y:5:ILE:HD11	11:Y:143:LEU:HD11	1.92	0.52
12:Z:37:ILE:HD12	12:Z:41:LEU:HD23	1.92	0.52
13:a:145:LEU:HD22	13:a:178:VAL:HG22	1.92	0.52
2:B:172:PHE:HA	2:B:176:ARG:HH21	1.73	0.52
9:I:10:ASP:OD1	9:I:10:ASP:N	2.42	0.52
14:N:1:THR:N	14:N:105:PRO:O	2.35	0.52
7:U:117:MET:HA	7:U:117:MET:HE2	1.92	0.52
3:C:90:LEU:HD21	3:C:114:LEU:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:49:ALA:HB2	5:E:217:LEU:HD12	1.92	0.52
7:G:49:VAL:HG21	7:G:65:ARG:HB2	1.91	0.52
12:L:97:MET:HB2	12:L:116:SER:HA	1.92	0.52
4:R:107:ILE:O	4:R:111:ILE:HG22	2.09	0.52
10:X:42:PHE:HE2	10:X:52:LEU:HD13	1.75	0.52
7:G:65:ARG:HH21	7:G:78:ALA:HA	1.75	0.52
10:J:12:ALA:HB2	10:J:21:ILE:HD13	1.91	0.52
9:W:163:ILE:HD13	9:W:192:PRO:HG3	1.91	0.52
9:W:187:ARG:HB3	9:W:188:PRO:HD3	1.90	0.52
11:Y:96:THR:O	11:Y:96:THR:OG1	2.25	0.52
3:C:149:GLN:HB3	3:C:159:TRP:HE1	1.75	0.51
8:H:51:ASP:OD2	8:H:94:LEU:HB2	2.10	0.51
8:H:115:PRO:HG3	14:N:36:PHE:CZ	2.46	0.51
10:J:33:MET:SD	10:J:34:VAL:N	2.83	0.51
2:P:66:PRO:HA	2:P:72:GLY:HA2	1.91	0.51
1:A:61:LEU:HD12	1:A:61:LEU:H	1.74	0.51
3:C:93:ILE:HG23	3:C:110:LEU:HD11	1.92	0.51
12:L:100:MET:HE1	12:L:113:TYR:HB2	1.90	0.51
1:O:93:ARG:HH12	1:O:96:TYR:HD2	1.57	0.51
5:S:67:ILE:HG22	5:S:226:PHE:HZ	1.75	0.51
5:S:203:LYS:NZ	5:S:210:LEU:HB3	2.26	0.51
6:T:22:ILE:HD11	6:T:150:SER:HB3	1.91	0.51
7:U:109:LYS:HA	7:U:149:TYR:HE2	1.74	0.51
12:Z:7:LYS:HB3	12:Z:12:VAL:HG12	1.93	0.51
13:a:71:ARG:NE	13:a:91:MET:SD	2.83	0.51
5:E:41:GLN:HA	5:E:46:VAL:HG12	1.92	0.51
7:G:17:ASP:OD2	7:G:17:ASP:N	2.28	0.51
13:a:46:LEU:HD21	13:a:52:ILE:HD11	1.91	0.51
3:C:119:GLN:NE2	4:D:79:ASP:HA	2.25	0.51
4:D:62:ILE:HD13	4:D:209:ALA:HB3	1.92	0.51
7:G:187:ARG:HH21	7:G:219:LEU:HD21	1.75	0.51
1:A:93:ARG:HH11	1:A:93:ARG:HG2	1.76	0.51
1:A:164:LYS:N	2:B:55:LEU:O	2.42	0.51
1:A:229:ILE:HD12	1:A:229:ILE:H	1.75	0.51
14:N:4:PRO:HG3	14:N:107:TRP:CG	2.45	0.51
3:Q:122:THR:O	4:R:125:ARG:NH1	2.43	0.51
9:W:215:LYS:HB3	10:X:196:THR:HB	1.93	0.51
1:A:39:SER:HB3	1:A:168:ALA:HB3	1.91	0.51
3:C:76:VAL:HG11	3:C:83:ALA:HB1	1.92	0.51
10:J:44:MET:HE3	10:J:70:LEU:HD22	1.92	0.51
10:J:204:ASP:OD2	12:Z:19:ARG:NH2	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:135:PHE:CE1	7:G:151:ILE:HD12	2.46	0.51
8:H:43:CYS:SG	8:H:44:CYS:N	2.83	0.51
9:W:212:LEU:HB2	10:X:198:THR:HG23	1.92	0.51
14:b:85:PRO:HB2	14:b:121:PHE:HD2	1.76	0.51
2:B:47:THR:HB	2:B:74:VAL:HG21	1.92	0.51
8:H:19:ARG:CZ	8:H:171:GLY:HA3	2.41	0.51
8:V:43:CYS:SG	8:V:44:CYS:N	2.83	0.51
8:V:135:ILE:HD11	8:V:162:LEU:HB2	1.93	0.51
7:G:195:LYS:O	7:G:199:ILE:HG23	2.11	0.51
12:L:7:LYS:HB3	12:L:12:VAL:HG12	1.92	0.51
6:T:69:HIS:HE2	6:T:96:ARG:HH12	1.57	0.51
7:U:106:ILE:HD12	7:U:107:PRO:HD2	1.91	0.51
8:V:4:MET:HE2	8:V:156:THR:HA	1.93	0.51
5:E:121:LEU:HA	5:E:123:PHE:CE1	2.46	0.51
11:K:31:ASP:N	11:K:31:ASP:OD1	2.44	0.51
3:Q:192:LEU:O	3:Q:196:VAL:HG13	2.11	0.51
8:V:127:ILE:HG23	8:V:132:SER:HB2	1.91	0.51
10:J:125:LEU:HD12	10:J:126:ILE:HG23	1.93	0.50
2:P:70:HIS:CE1	2:P:138:TRP:HB3	2.46	0.50
6:T:78:THR:O	6:T:82:ARG:HG2	2.11	0.50
14:b:44:ARG:HB2	14:b:199:ILE:HD11	1.92	0.50
1:A:11:ARG:O	1:A:24:GLN:NE2	2.43	0.50
1:A:171:LYS:HE2	1:A:205:VAL:HB	1.93	0.50
9:I:212:LEU:HB2	10:J:198:THR:HG23	1.93	0.50
12:L:44:THR:OG1	12:L:100:MET:N	2.37	0.50
7:U:149:TYR:HD1	7:U:159:GLY:HA2	1.75	0.50
10:X:60:GLN:O	10:X:64:GLN:HG3	2.11	0.50
12:Z:34:VAL:HG22	12:Z:44:THR:HG22	1.93	0.50
1:A:51:VAL:HG12	1:A:202:LEU:HD22	1.94	0.50
2:B:70:HIS:CE1	2:B:216:GLY:HA2	2.47	0.50
8:H:12:VAL:HG21	8:H:101:ALA:HB1	1.93	0.50
8:H:174:ILE:HG12	8:H:194:ILE:HG22	1.92	0.50
12:L:61:ARG:O	12:L:65:ILE:HG12	2.11	0.50
7:U:173:LYS:HA	7:U:176:ILE:HG12	1.94	0.50
7:U:193:VAL:O	7:U:197:ILE:HG12	2.11	0.50
8:V:174:ILE:HG12	8:V:194:ILE:HG22	1.93	0.50
9:W:44:CYS:HB2	9:W:99:VAL:HB	1.92	0.50
6:F:51:ARG:H	6:F:62:LYS:NZ	2.10	0.50
9:I:163:ILE:HD13	9:I:192:PRO:HG3	1.94	0.50
14:N:20:VAL:HG23	14:N:120:SER:HB3	1.92	0.50
7:U:65:ARG:HH21	7:U:78:ALA:HA	1.75	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:HD11	1:A:69:LEU:HD13	1.94	0.50
3:C:209:GLU:HA	3:C:230:GLN:HE22	1.76	0.50
1:A:41:ALA:HB3	1:A:166:THR:HB	1.93	0.50
1:A:101:TRP:CG	1:A:109:ILE:HB	2.46	0.50
7:G:68:ASN:HB3	14:N:76:LEU:HD23	1.93	0.50
7:G:193:VAL:O	7:G:197:ILE:HG12	2.11	0.50
7:U:215:TRP:HZ3	7:U:227:VAL:HG13	1.76	0.50
10:X:21:ILE:HG23	10:X:187:HIS:HB2	1.94	0.50
1:A:153:LYS:HB3	1:A:163:PHE:HE2	1.77	0.50
3:C:187:LYS:HD2	3:C:188:SER:N	2.27	0.50
5:E:200:ILE:HG23	5:E:204:GLN:HE22	1.76	0.50
8:H:127:ILE:HG23	8:H:132:SER:HB2	1.94	0.50
9:I:135:MET:HE3	14:b:179:ARG:NH1	2.27	0.50
1:O:61:LEU:HD12	1:O:61:LEU:H	1.76	0.50
2:P:138:TRP:CH2	2:P:141:GLY:HA2	2.46	0.50
7:U:122:TYR:HD2	7:U:131:PHE:CE2	2.29	0.50
11:Y:31:ASP:OD1	11:Y:31:ASP:N	2.44	0.50
11:Y:37:LYS:HA	11:Y:43:LEU:HD23	1.93	0.50
12:Z:58:LEU:O	12:Z:61:ARG:HG2	2.11	0.50
1:A:11:ARG:NH1	1:A:23:TYR:OH	2.45	0.50
7:G:225:GLU:N	7:G:225:GLU:OE1	2.45	0.50
11:K:164:LEU:HA	11:K:167:LEU:HD23	1.93	0.50
14:N:12:LEU:HD11	14:N:172:CYS:HB3	1.93	0.50
1:A:69:LEU:HD11	1:A:227:PHE:CE2	2.47	0.50
1:A:122:SER:O	1:A:126:THR:HG23	2.11	0.50
12:L:93:MET:HG3	13:M:101:PHE:HZ	1.75	0.50
7:U:49:VAL:HG21	7:U:65:ARG:HB2	1.94	0.50
7:G:149:TYR:HD1	7:G:159:GLY:HA2	1.77	0.49
9:I:44:CYS:HB2	9:I:99:VAL:HB	1.94	0.49
1:O:41:ALA:HB3	1:O:166:THR:HB	1.94	0.49
5:S:163:VAL:HG13	5:S:165:CYS:SG	2.52	0.49
6:T:69:HIS:ND1	6:T:70:ILE:HG13	2.26	0.49
5:E:67:ILE:HG22	5:E:226:PHE:HZ	1.77	0.49
6:F:98:VAL:HA	14:N:94:ARG:HG3	1.94	0.49
8:H:41:ILE:HD11	8:H:76:VAL:HG22	1.94	0.49
12:L:78:ALA:O	12:L:82:LEU:HG	2.12	0.49
13:M:157:ASN:ND2	10:X:172:ASN:OD1	2.35	0.49
13:a:15:ILE:HB	13:a:22:ILE:HG23	1.94	0.49
9:I:198:ARG:NH2	10:J:150:GLU:O	2.45	0.49
12:L:54:PHE:O	12:L:58:LEU:HG	2.13	0.49
2:P:104:ILE:HG21	2:P:109:LEU:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:50:VAL:O	4:R:54:GLN:HG2	2.11	0.49
6:T:60:GLN:HB2	6:T:62:LYS:HZ1	1.77	0.49
7:U:135:PHE:CE1	7:U:151:ILE:HD12	2.47	0.49
14:b:25:ASP:HA	14:b:187:PHE:HA	1.94	0.49
12:L:66:TYR:HD1	12:L:70:ASN:ND2	2.10	0.49
13:M:79:ASN:OD1	13:M:81:LYS:HB3	2.12	0.49
14:N:108:ASN:OD1	14:N:109:THR:N	2.46	0.49
3:Q:24:ALA:O	3:Q:28:ILE:HG12	2.12	0.49
8:V:92:GLU:OE1	8:V:92:GLU:N	2.32	0.49
5:E:23:GLN:HB3	5:E:136:PRO:HG3	1.94	0.49
7:G:30:VAL:HG21	7:G:134:SER:OG	2.12	0.49
8:H:187:GLN:HE22	8:H:189:LEU:HG	1.77	0.49
1:O:153:LYS:HB3	1:O:163:PHE:CE2	2.47	0.49
4:R:62:ILE:HD13	4:R:209:ALA:HB3	1.95	0.49
2:B:91:LYS:O	2:B:94:GLN:HG3	2.13	0.49
9:I:58:LEU:O	9:I:62:ASN:ND2	2.45	0.49
10:J:177:ASP:OD1	10:J:178:ALA:N	2.46	0.49
12:L:21:THR:HG22	12:L:26:ILE:HA	1.95	0.49
10:X:82:LYS:O	10:X:85:THR:OG1	2.21	0.49
14:b:60:PHE:HB2	14:b:108:ASN:HD22	1.77	0.49
5:E:156:MET:SD	5:E:162:PHE:HB3	2.53	0.49
5:E:164:GLN:HB3	6:F:58:ALA:HB3	1.95	0.49
2:P:135:ILE:HB	2:P:146:PHE:HB2	1.95	0.49
5:S:114:GLN:HE22	6:T:82:ARG:HD3	1.77	0.49
12:Z:45:MET:SD	12:Z:52:CYS:HB2	2.53	0.49
11:K:4:LEU:HD22	11:K:45:LEU:HD23	1.94	0.49
1:O:122:SER:O	1:O:126:THR:HG23	2.12	0.49
14:b:25:ASP:O	14:b:41:ARG:NH2	2.45	0.49
3:C:24:ALA:O	3:C:28:ILE:HG12	2.13	0.49
5:E:218:ALA:HB1	5:E:226:PHE:HE1	1.78	0.49
7:G:108:LEU:HD11	7:G:137:LEU:HB3	1.94	0.49
8:H:115:PRO:HD2	8:H:119:MET:HG3	1.95	0.49
1:O:50:ILE:HD11	1:O:69:LEU:HD13	1.94	0.49
1:O:132:ARG:NH1	7:U:123:THR:O	2.46	0.49
2:P:70:HIS:CE1	2:P:216:GLY:HA2	2.48	0.49
11:Y:115:LEU:HD12	11:Y:116:TYR:H	1.77	0.49
13:a:51:VAL:HG21	13:a:196:CYS:HB3	1.95	0.49
1:A:93:ARG:NH1	1:A:121:ILE:HG21	2.28	0.49
1:A:132:ARG:NH1	7:G:123:THR:O	2.46	0.49
2:B:49:LYS:C	2:B:49:LYS:HD2	2.38	0.49
6:F:152:ASN:HA	7:G:85:ARG:HH21	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:166:GLN:NE2	6:T:170:THR:OG1	2.45	0.49
7:U:30:VAL:HG21	7:U:134:SER:OG	2.13	0.49
1:A:132:ARG:HG2	1:A:132:ARG:HH11	1.77	0.48
7:G:179:LEU:O	7:G:180:GLN:HG3	2.13	0.48
12:L:125:THR:CG2	12:L:139:MET:HE3	2.43	0.48
14:N:179:ARG:NE	9:W:139:GLU:OE2	2.45	0.48
1:O:101:TRP:CG	1:O:109:ILE:HB	2.47	0.48
3:Q:43:VAL:HG21	3:Q:137:ILE:HB	1.95	0.48
3:Q:94:ALA:HB1	3:Q:105:ILE:HD13	1.95	0.48
7:U:225:GLU:OE1	7:U:225:GLU:N	2.46	0.48
8:V:49:ALA:O	8:V:53:GLN:HG3	2.13	0.48
11:Y:38:MET:SD	11:Y:44:LEU:HB2	2.52	0.48
3:C:48:GLU:HA	3:C:211:VAL:HA	1.95	0.48
3:C:167:ASN:OD1	3:C:167:ASN:O	2.30	0.48
5:E:160:GLY:HA3	6:F:79:ALA:HB2	1.94	0.48
2:P:188:HIS:O	2:P:191:ILE:HG12	2.13	0.48
6:T:60:GLN:HB2	6:T:62:LYS:NZ	2.28	0.48
12:Z:93:MET:HG3	13:a:101:PHE:HZ	1.77	0.48
2:B:70:HIS:C	2:B:71:ILE:HD13	2.38	0.48
7:G:83:ASP:HB3	7:G:131:PHE:HD1	1.79	0.48
7:G:215:TRP:CD1	7:G:215:TRP:C	2.92	0.48
14:N:56:ASP:OD2	14:N:58:ALA:N	2.41	0.48
1:O:141:ILE:HD12	1:O:220:VAL:HG12	1.94	0.48
1:A:62:ASP:HA	7:G:161:TRP:CZ3	2.49	0.48
5:E:99:HIS:HB2	5:E:107:MET:HE2	1.94	0.48
6:F:71:GLY:HA3	6:F:221:PHE:CE2	2.48	0.48
1:O:115:CYS:SG	1:O:160:TYR:HB2	2.53	0.48
4:R:79:ASP:OD2	4:R:127:PHE:HD1	1.97	0.48
7:U:192:GLU:O	7:U:195:LYS:HG2	2.13	0.48
9:W:102:GLY:HA2	9:W:178:ILE:HD12	1.94	0.48
11:Y:102:LEU:HB2	11:Y:118:MET:HG3	1.95	0.48
3:C:174:MET:HG2	3:C:199:LYS:HZ3	1.79	0.48
3:C:184:MET:SD	3:C:184:MET:N	2.86	0.48
10:J:21:ILE:HG23	10:J:187:HIS:HB2	1.94	0.48
10:J:65:ARG:HB2	10:J:93:LEU:HD11	1.96	0.48
12:L:53:SER:O	12:L:56:GLU:HG3	2.13	0.48
7:U:198:TYR:OH	7:U:236:GLU:OE1	2.17	0.48
1:A:39:SER:O	1:A:168:ALA:N	2.41	0.48
6:F:62:LYS:C	6:F:63:ILE:HD13	2.39	0.48
1:O:113:MET:HA	1:O:116:LYS:HG2	1.95	0.48
10:X:11:MET:HG2	10:X:136:VAL:O	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:SER:OG	1:A:20:GLY:N	2.47	0.48
1:O:39:SER:HB3	1:O:168:ALA:HB3	1.96	0.48
1:O:153:LYS:HB3	1:O:163:PHE:HE2	1.79	0.48
2:P:91:LYS:O	2:P:94:GLN:HG3	2.13	0.48
2:P:101:GLN:NE2	9:W:57:GLN:OE1	2.46	0.48
5:S:164:GLN:O	6:T:58:ALA:N	2.46	0.48
6:T:26:MET:O	6:T:29:VAL:HG22	2.13	0.48
13:a:79:ASN:OD1	13:a:81:LYS:HB3	2.12	0.48
6:F:43:HIS:CD2	6:F:216:GLY:HA3	2.49	0.48
7:G:180:GLN:NE2	7:G:184:MET:SD	2.87	0.48
4:R:7:ILE:HG22	4:R:18:GLN:HE21	1.78	0.48
5:S:38:ILE:HD13	5:S:169:ALA:HB2	1.96	0.48
5:S:67:ILE:HD12	5:S:216:GLU:HG3	1.95	0.48
7:U:59:GLU:OE2	7:U:59:GLU:HA	2.14	0.48
8:V:55:VAL:HG22	8:V:86:MET:HE2	1.95	0.48
10:X:23:ALA:HB3	10:X:41:ILE:HD11	1.95	0.48
1:A:132:ARG:HD2	7:G:14:PHE:CE2	2.48	0.48
4:D:180:ALA:HB1	4:D:190:LEU:HD22	1.95	0.48
7:G:53:VAL:HG23	7:G:208:ALA:HB1	1.96	0.48
7:G:122:TYR:HD2	7:G:131:PHE:CE2	2.31	0.48
11:K:102:LEU:HB2	11:K:118:MET:HG3	1.96	0.48
1:O:62:ASP:HA	7:U:161:TRP:CZ3	2.49	0.48
3:Q:167:ASN:OD1	3:Q:167:ASN:O	2.31	0.48
5:S:121:LEU:HA	5:S:123:PHE:CE1	2.49	0.48
6:T:50:LYS:HG2	6:T:59:HIS:CB	2.43	0.48
8:V:84:LYS:HD3	8:V:120:MET:HB2	1.94	0.48
2:B:138:TRP:CH2	2:B:141:GLY:HA2	2.49	0.48
8:H:127:ILE:CG2	8:H:132:SER:HB2	2.43	0.48
9:I:36:PHE:HA	9:I:42:TYR:CE2	2.49	0.48
9:W:104:ASP:OD2	9:W:106:THR:N	2.45	0.48
10:X:182:MET:HE2	10:X:182:MET:HA	1.95	0.48
8:H:96:ALA:N	8:H:116:MET:SD	2.76	0.47
9:I:166:ASP:OD1	9:I:168:GLY:N	2.35	0.47
13:M:198:VAL:HG22	13:M:203:ILE:HD12	1.95	0.47
5:S:23:GLN:HB3	5:S:136:PRO:HG3	1.96	0.47
8:V:187:GLN:HE22	8:V:189:LEU:HG	1.78	0.47
9:W:161:ALA:O	9:W:165:ASN:ND2	2.23	0.47
3:Q:209:GLU:HG3	3:Q:230:GLN:NE2	2.29	0.47
6:T:98:VAL:HA	14:b:94:ARG:HG3	1.94	0.47
8:V:19:ARG:CZ	8:V:171:GLY:HA3	2.43	0.47
9:W:83:LEU:HD12	9:W:100:LEU:HD22	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:107:TRP:CD2	14:b:127:MET:HE1	2.49	0.47
1:O:11:ARG:O	1:O:24:GLN:NE2	2.47	0.47
1:O:69:LEU:HD11	1:O:227:PHE:CE2	2.49	0.47
1:O:168:ALA:HA	1:O:172:GLN:HG3	1.96	0.47
5:S:103:TYR:O	13:a:87:ALA:HA	2.14	0.47
3:C:9:THR:HG23	3:C:10:THR:HG23	1.97	0.47
9:I:164:PHE:O	13:a:38:ARG:NH2	2.47	0.47
12:L:114:VAL:HA	12:L:119:ASN:O	2.14	0.47
14:N:25:ASP:HA	14:N:187:PHE:HA	1.95	0.47
1:O:51:VAL:HG12	1:O:202:LEU:HD22	1.95	0.47
10:X:55:LEU:HG	10:X:57:THR:HG22	1.95	0.47
1:A:172:GLN:O	1:A:176:THR:HG22	2.14	0.47
4:D:80:ALA:O	4:D:84:ILE:HG12	2.14	0.47
5:E:112:VAL:O	5:E:116:VAL:HG12	2.13	0.47
7:G:111:LEU:O	7:G:115:VAL:HG12	2.15	0.47
1:O:15:ILE:HB	2:P:20:GLN:NE2	2.20	0.47
1:O:132:ARG:HD2	7:U:14:PHE:CE2	2.49	0.47
3:Q:199:LYS:HD3	3:Q:199:LYS:N	2.28	0.47
6:T:89:ARG:HG2	13:a:77:HIS:CE1	2.49	0.47
11:Y:18:ASP:HB2	11:Y:175:LEU:HD12	1.96	0.47
11:Y:154:GLU:O	11:Y:158:GLU:HG3	2.15	0.47
12:Z:78:ALA:O	12:Z:82:LEU:HG	2.15	0.47
13:a:198:VAL:HG22	13:a:203:ILE:HD12	1.95	0.47
10:J:20:ALA:HB2	10:J:188:ILE:HG23	1.97	0.47
11:K:171:PHE:CE1	11:K:173:LEU:HB2	2.39	0.47
7:U:108:LEU:HD11	7:U:137:LEU:HB3	1.95	0.47
12:Z:37:ILE:HG13	12:Z:42:LEU:HA	1.96	0.47
1:A:109:ILE:HG12	1:A:114:LEU:HB2	1.97	0.47
2:B:158:LYS:HG3	3:C:55:LEU:O	2.14	0.47
3:C:44:LEU:O	3:C:45:LEU:HD13	2.15	0.47
3:C:93:ILE:HD13	3:C:96:ARG:HH21	1.80	0.47
3:C:174:MET:HE3	3:C:199:LYS:HZ1	1.78	0.47
5:E:141:LEU:O	5:E:156:MET:N	2.44	0.47
6:F:26:MET:O	6:F:29:VAL:HG22	2.14	0.47
6:F:116:THR:O	6:F:119:PRO:HD2	2.15	0.47
8:H:164:MET:CG	8:H:171:GLY:HA2	2.45	0.47
9:I:50:ALA:HB3	10:J:126:ILE:HD11	1.96	0.47
4:R:106:TYR:HD1	4:R:109:ARG:NH2	2.12	0.47
5:S:107:MET:HG3	5:S:111:SER:OG	2.14	0.47
5:S:112:VAL:O	5:S:116:VAL:HG12	2.15	0.47
5:S:228:MET:SD	5:S:228:MET:N	2.87	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:94:ASP:N	6:T:94:ASP:OD2	2.46	0.47
6:T:205:LEU:HD22	6:T:210:VAL:HG21	1.97	0.47
7:U:111:LEU:O	7:U:115:VAL:HG12	2.15	0.47
8:V:51:ASP:OD2	8:V:94:LEU:HB2	2.15	0.47
9:W:89:ARG:HH12	9:W:90:TYR:HD2	1.62	0.47
14:b:107:TRP:HA	14:b:127:MET:HE3	1.96	0.47
2:B:134:LEU:HD21	2:B:162:MET:HG2	1.96	0.47
7:G:30:VAL:O	7:G:33:SER:OG	2.32	0.47
9:I:102:GLY:HA2	9:I:178:ILE:HD12	1.97	0.47
13:M:46:LEU:HD21	13:M:52:ILE:HD11	1.97	0.47
14:N:79:ASP:OD2	14:N:79:ASP:N	2.42	0.47
2:P:114:ALA:HB1	2:P:152:GLY:O	2.15	0.47
4:R:80:ALA:O	4:R:84:ILE:HG12	2.15	0.47
5:S:109:VAL:O	5:S:113:THR:HG23	2.15	0.47
6:T:51:ARG:H	6:T:62:LYS:NZ	2.13	0.47
7:U:37:ILE:HD13	7:U:196:ILE:HG21	1.97	0.47
8:V:12:VAL:HG21	8:V:101:ALA:HB1	1.95	0.47
8:V:51:ASP:OD2	8:V:95:MET:N	2.48	0.47
10:X:10:VAL:HG22	10:X:23:ALA:HB2	1.97	0.47
13:a:57:PHE:CZ	14:b:128:LEU:HB3	2.43	0.47
2:B:114:ALA:HB1	2:B:152:GLY:O	2.15	0.47
7:G:51:LYS:HZ1	7:G:64:LYS:HA	1.80	0.47
13:M:48:ASP:O	13:M:49:LYS:HD3	2.15	0.47
14:N:53:ALA:HB2	14:N:110:MET:HB3	1.96	0.47
2:P:121:THR:HG22	2:P:128:PRO:HB3	1.97	0.47
7:U:215:TRP:CD1	7:U:215:TRP:C	2.92	0.47
7:G:95:ALA:HB2	7:G:111:LEU:HD21	1.97	0.47
5:S:160:GLY:HA3	6:T:79:ALA:HB2	1.97	0.47
10:X:62:VAL:HG22	10:X:102:TYR:HD2	1.80	0.47
13:a:83:MET:HG2	13:a:88:ILE:HG23	1.97	0.47
13:a:91:MET:O	13:a:94:THR:OG1	2.25	0.47
1:A:196:GLU:HA	1:A:199:ILE:HG12	1.96	0.46
3:C:176:LYS:HD2	4:D:53:LEU:HD23	1.97	0.46
4:D:161:ILE:HG22	4:D:162:GLY:H	1.80	0.46
5:E:228:MET:SD	5:E:228:MET:N	2.88	0.46
6:F:26:MET:HG2	6:F:149:PRO:HD2	1.97	0.46
6:F:92:CYS:O	6:F:95:SER:OG	2.27	0.46
9:I:155:VAL:O	9:I:159:ILE:HG22	2.15	0.46
10:J:192:ASP:OD2	10:J:193:LYS:N	2.49	0.46
13:M:22:ILE:HD11	13:M:195:ILE:HG23	1.95	0.46
1:O:110:PRO:HB2	1:O:113:MET:HE1	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:232:GLU:CD	3:Q:232:GLU:H	2.22	0.46
5:S:168:ARG:HD2	5:S:178:GLN:OE1	2.14	0.46
10:X:154:GLU:O	10:X:157:MET:HG3	2.16	0.46
13:a:4:PRO:HB3	14:b:103:MET:HE1	1.97	0.46
14:b:108:ASN:OD1	14:b:109:THR:N	2.49	0.46
2:B:38:LYS:HE3	2:B:143:PRO:HG2	1.96	0.46
3:C:107:CYS:O	3:C:111:VAL:HG13	2.15	0.46
5:E:197:SER:O	5:E:201:ILE:HG13	2.16	0.46
9:I:127:MET:C	9:I:131:SER:HB3	2.41	0.46
10:J:112:ASP:OD1	10:J:114:LYS:N	2.47	0.46
5:S:49:ALA:HB2	5:S:217:LEU:HD12	1.96	0.46
5:S:202:LEU:HA	5:S:205:VAL:HG22	1.95	0.46
2:B:47:THR:HG21	2:B:63:LYS:HB3	1.97	0.46
10:J:13:MET:SD	10:J:153:TRP:HD1	2.39	0.46
10:J:177:ASP:OD1	10:J:179:VAL:N	2.44	0.46
3:Q:91:ARG:NH2	10:X:75:LEU:HB3	2.26	0.46
8:V:127:ILE:CG2	8:V:132:SER:HB2	2.45	0.46
7:G:73:VAL:HG13	7:G:108:LEU:HD12	1.98	0.46
11:K:3:TYR:N	11:K:18:ASP:OD2	2.42	0.46
7:U:110:HIS:HA	7:U:113:ASP:OD1	2.15	0.46
9:W:209:THR:OG1	10:X:168:GLN:OE1	2.34	0.46
10:X:11:MET:HE2	10:X:170:MET:HE3	1.95	0.46
12:Z:61:ARG:O	12:Z:65:ILE:HG12	2.14	0.46
9:I:90:TYR:CE1	9:I:94:ILE:HG23	2.50	0.46
10:J:24:ASP:C	10:J:24:ASP:OD1	2.58	0.46
13:M:55:SER:OG	13:M:107:TYR:HB2	2.15	0.46
14:N:26:MET:HE1	14:N:186:ARG:HB3	1.97	0.46
14:b:27:LEU:HD13	14:b:184:TYR:HB2	1.98	0.46
6:F:157:ARG:HH21	7:G:59:GLU:HA	1.81	0.46
8:H:55:VAL:HG22	8:H:86:MET:HE2	1.97	0.46
11:K:86:ARG:NH2	11:K:90:ASP:OD2	2.39	0.46
13:M:71:ARG:HD3	13:M:95:ILE:HD11	1.98	0.46
1:O:50:ILE:O	1:O:50:ILE:HG13	2.16	0.46
1:O:132:ARG:HG2	1:O:132:ARG:HH11	1.80	0.46
2:P:14:PRO:HA	3:Q:23:TYR:CE1	2.51	0.46
1:A:113:MET:HA	1:A:116:LYS:HG2	1.98	0.46
6:F:11:THR:HB	7:G:129:ARG:HB3	1.98	0.46
8:H:25:TYR:HE2	14:b:179:ARG:HB3	1.80	0.46
9:I:100:LEU:HD12	9:I:100:LEU:HA	1.75	0.46
10:J:66:LEU:HD11	10:J:90:VAL:HG22	1.98	0.46
13:M:67:ILE:HD12	13:M:67:ILE:HA	1.82	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:43:VAL:HG21	3:C:137:ILE:HB	1.98	0.46
4:D:94:HIS:ND1	4:D:102:VAL:HG12	2.31	0.46
10:J:154:GLU:O	10:J:157:MET:HG3	2.15	0.46
12:L:8:PHE:CE2	12:L:10:HIS:HB2	2.51	0.46
14:N:108:ASN:OD1	14:N:110:MET:HE2	2.15	0.46
6:T:43:HIS:CG	6:T:184:LEU:HD13	2.51	0.46
3:C:163:CYS:C	3:C:168:SER:HG	2.24	0.46
4:D:211:MET:SD	4:D:217:LEU:HB2	2.56	0.46
3:Q:87:THR:O	3:Q:91:ARG:HG3	2.16	0.46
4:D:7:ILE:HG22	4:D:18:GLN:HE21	1.81	0.46
7:G:193:VAL:O	7:G:196:ILE:HG22	2.16	0.46
7:G:215:TRP:HE1	7:G:220:THR:CG2	2.29	0.46
12:L:37:ILE:H	12:L:37:ILE:HG13	1.58	0.46
14:N:94:ARG:NE	14:N:94:ARG:HA	2.31	0.46
3:Q:184:MET:SD	3:Q:184:MET:N	2.88	0.46
9:W:36:PHE:HA	9:W:42:TYR:CE1	2.51	0.46
9:W:48:THR:HG22	9:W:51:ASP:H	1.81	0.46
12:Z:8:PHE:CE2	12:Z:10:HIS:HB2	2.51	0.46
13:a:48:ASP:C	13:a:49:LYS:HD3	2.41	0.46
1:A:27:TYR:CE1	7:G:16:PRO:HA	2.51	0.45
3:C:124:PHE:HB3	4:D:124:ARG:HG2	1.97	0.45
4:D:211:MET:HG2	4:D:217:LEU:HD12	1.97	0.45
12:L:4:LEU:N	12:L:15:ALA:O	2.46	0.45
13:M:43:CYS:SG	13:M:45:LYS:NZ	2.89	0.45
13:M:75:TYR:CD2	13:M:83:MET:HB2	2.51	0.45
3:Q:114:LEU:HD23	3:Q:136:TYR:OH	2.16	0.45
8:V:164:MET:HG2	8:V:171:GLY:HA2	1.98	0.45
10:X:183:GLY:HA2	10:X:201:ALA:HB3	1.98	0.45
14:b:94:ARG:HA	14:b:94:ARG:NE	2.30	0.45
4:D:22:ALA:O	4:D:26:VAL:HG23	2.16	0.45
4:D:79:ASP:OD2	4:D:125:ARG:NH2	2.46	0.45
9:I:114:TYR:HD2	9:I:118:SER:HG	1.64	0.45
13:M:60:ASP:OD2	13:M:104:TYR:HA	2.16	0.45
3:Q:44:LEU:O	3:Q:45:LEU:HD13	2.16	0.45
3:Q:160:LYS:NZ	4:R:52:LYS:O	2.48	0.45
10:X:132:THR:HG22	10:X:134:ASP:H	1.81	0.45
13:a:48:ASP:O	13:a:49:LYS:HD3	2.17	0.45
5:E:231:LYS:HB3	5:E:231:LYS:HE3	1.64	0.45
10:J:112:ASP:HB3	10:J:117:LYS:H	1.80	0.45
11:K:16:ALA:HB2	11:K:160:LEU:HD21	1.97	0.45
14:N:44:ARG:HB2	14:N:199:ILE:HD11	1.96	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:85:PRO:HB2	14:N:121:PHE:CD2	2.46	0.45
5:S:166:ASP:HB3	5:S:185:TYR:CZ	2.51	0.45
8:V:8:PHE:HB3	8:V:152:CYS:SG	2.56	0.45
8:V:81:SER:O	8:V:85:GLU:HG2	2.16	0.45
12:Z:12:VAL:HG22	12:Z:179:VAL:HG22	1.99	0.45
7:G:110:HIS:HA	7:G:113:ASP:OD2	2.16	0.45
9:I:50:ALA:HB3	10:J:126:ILE:CD1	2.46	0.45
13:M:8:ASN:HD22	13:M:58:HIS:HB2	1.81	0.45
14:N:25:ASP:O	14:N:41:ARG:NH2	2.50	0.45
3:Q:136:TYR:HB2	3:Q:148:TYR:HB2	1.98	0.45
7:U:193:VAL:O	7:U:196:ILE:HG22	2.16	0.45
11:Y:154:GLU:CD	11:Y:154:GLU:H	2.24	0.45
6:F:157:ARG:HG2	7:G:57:LEU:O	2.17	0.45
7:G:168:ALA:HB1	7:G:171:ALA:HB3	1.98	0.45
8:H:135:ILE:O	8:H:139:VAL:HG22	2.17	0.45
10:J:25:ARG:HB3	10:J:36:THR:O	2.16	0.45
10:J:163:PHE:O	10:J:167:SER:OG	2.27	0.45
13:M:25:SER:HB2	13:M:42:LYS:HB2	1.97	0.45
14:N:179:ARG:CZ	9:W:135:MET:HE3	2.47	0.45
1:O:38:THR:HA	1:O:169:GLY:HA3	1.97	0.45
3:Q:8:ARG:HD2	3:Q:11:ILE:HG21	1.99	0.45
5:S:20:ARG:HG3	5:S:25:GLU:HB2	1.98	0.45
9:W:127:MET:C	9:W:131:SER:HB3	2.41	0.45
6:F:101:ARG:HH12	6:F:104:PRO:HD3	1.81	0.45
8:H:106:GLN:HB3	8:H:107:GLU:OE1	2.16	0.45
11:K:8:GLN:HB3	11:K:128:PRO:O	2.17	0.45
12:L:19:ARG:CZ	12:L:171:GLY:HA3	2.47	0.45
2:P:38:LYS:NZ	2:P:142:ARG:HH21	2.14	0.45
5:S:143:PHE:N	5:S:154:PHE:O	2.50	0.45
8:V:151:GLU:O	8:V:154:GLN:HG2	2.17	0.45
9:W:112:SER:O	9:W:113:ILE:HD13	2.16	0.45
10:X:5:TYR:HD2	10:X:6:ASN:HD21	1.65	0.45
12:Z:55:TRP:HE3	12:Z:58:LEU:HD11	1.82	0.45
12:Z:62:GLN:HE21	12:Z:82:LEU:HD13	1.81	0.45
5:E:21:LEU:HD12	5:E:21:LEU:HA	1.76	0.45
5:E:36:THR:HA	5:E:171:GLY:HA3	1.98	0.45
7:G:83:ASP:OD2	7:G:83:ASP:N	2.50	0.45
9:I:83:LEU:O	9:I:86:MET:HG3	2.17	0.45
9:I:104:ASP:OD1	9:I:106:THR:N	2.45	0.45
12:L:44:THR:HG21	12:L:100:MET:HB2	1.98	0.45
5:S:54:ILE:HA	5:S:59:MET:HE2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:213:LEU:HB3	7:U:227:VAL:HG21	1.98	0.45
12:Z:19:ARG:CZ	12:Z:171:GLY:HA3	2.47	0.45
12:Z:114:VAL:HA	12:Z:119:ASN:O	2.16	0.45
13:a:99:ARG:HD3	13:a:104:TYR:CE2	2.52	0.45
3:C:167:ASN:ND2	3:C:200:THR:HA	2.32	0.45
3:C:176:LYS:HB3	3:C:176:LYS:HE3	1.78	0.45
8:H:100:ILE:HG13	8:H:112:TYR:HB2	1.98	0.45
13:M:4:PRO:HB3	14:N:103:MET:HE1	1.98	0.45
14:N:27:LEU:HD13	14:N:184:TYR:HB2	1.98	0.45
2:P:96:TYR:HD2	2:P:112:ARG:NH1	2.14	0.45
2:P:120:TYR:HD2	2:P:129:PHE:CE2	2.33	0.45
6:T:11:THR:HB	7:U:129:ARG:HB3	1.98	0.45
8:V:164:MET:CG	8:V:171:GLY:HA2	2.46	0.45
13:a:8:ASN:HD22	13:a:58:HIS:HB2	1.81	0.45
4:D:156:TRP:CZ2	5:E:59:MET:HG2	2.52	0.45
12:L:83:LEU:CD2	12:L:114:VAL:HG21	2.46	0.45
5:S:69:GLU:HG3	5:S:226:PHE:CD2	2.51	0.45
11:Y:14:LEU:HB2	11:Y:182:ILE:CD1	2.46	0.45
1:A:43:ARG:HD3	1:A:151:VAL:HG22	1.99	0.45
1:A:153:LYS:HB3	1:A:163:PHE:CE2	2.51	0.45
2:B:14:PRO:HA	3:C:23:TYR:CE1	2.52	0.45
2:B:98:LEU:HD21	9:I:61:SER:OG	2.17	0.45
5:E:121:LEU:HD11	6:F:126:ARG:HE	1.80	0.45
8:H:7:GLN:NE2	8:H:109:GLY:O	2.48	0.45
8:H:81:SER:O	8:H:85:GLU:HG2	2.17	0.45
10:J:55:LEU:HG	10:J:57:THR:HG22	1.99	0.45
10:J:60:GLN:O	10:J:64:GLN:HG2	2.16	0.45
11:K:116:TYR:CE1	11:K:126:LYS:HG3	2.52	0.45
14:N:1:THR:H2	14:N:105:PRO:HD2	1.81	0.45
3:Q:97:TYR:HD1	3:Q:105:ILE:HG23	1.82	0.45
4:R:157:LYS:HG2	5:S:58:LEU:O	2.17	0.45
5:S:101:PHE:HZ	12:Z:54:PHE:CE1	2.35	0.45
7:U:95:ALA:HB2	7:U:111:LEU:HD21	1.99	0.45
8:V:135:ILE:O	8:V:139:VAL:HG22	2.16	0.45
12:Z:84:ALA:HA	12:Z:87:VAL:HG22	1.98	0.45
3:C:110:LEU:HA	3:C:110:LEU:HD12	1.73	0.44
5:E:103:TYR:O	13:M:87:ALA:HA	2.17	0.44
6:F:185:ASN:O	6:F:189:LYS:HE3	2.17	0.44
12:L:3:THR:HG23	12:L:16:ALA:HB2	1.98	0.44
13:M:64:LEU:HD11	13:M:96:LEU:HD11	1.99	0.44
14:N:77:LEU:HD12	14:N:77:LEU:H	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:139:ILE:HG12	1:O:153:LYS:HB2	1.98	0.44
2:P:9:LEU:HD21	2:P:125:GLY:HA2	1.99	0.44
2:P:158:LYS:HG3	3:Q:55:LEU:O	2.16	0.44
3:Q:123:GLN:HA	4:R:125:ARG:NH1	2.31	0.44
3:Q:159:TRP:N	4:R:55:ASP:OD1	2.50	0.44
5:S:221:GLN:HG2	5:S:224:GLN:H	1.82	0.44
6:T:229:VAL:HG22	6:T:233:LEU:HG	1.98	0.44
10:X:33:MET:SD	10:X:35:THR:N	2.90	0.44
4:D:184:ASP:O	4:D:187:THR:OG1	2.29	0.44
12:L:76:VAL:HG13	12:L:101:ILE:HG22	1.99	0.44
1:O:153:LYS:HE3	1:O:163:PHE:HE2	1.82	0.44
2:P:17:LYS:HB3	2:P:17:LYS:HE3	1.80	0.44
2:P:187:ILE:O	2:P:191:ILE:HG23	2.17	0.44
4:R:161:ILE:HG22	4:R:162:GLY:H	1.82	0.44
5:S:14:THR:HG23	6:T:21:GLN:HE22	1.81	0.44
11:Y:13:VAL:CG1	11:Y:105:ALA:HB1	2.47	0.44
12:Z:179:VAL:HA	12:Z:184:TRP:HA	1.98	0.44
2:B:120:TYR:HD2	2:B:129:PHE:CE2	2.34	0.44
4:D:24:GLU:HA	4:D:27:LYS:NZ	2.32	0.44
5:E:14:THR:HG23	6:F:21:GLN:HE22	1.81	0.44
9:I:112:SER:HB3	9:I:125:VAL:HG11	1.99	0.44
11:K:154:GLU:O	11:K:158:GLU:HG3	2.18	0.44
7:U:149:TYR:CD1	7:U:159:GLY:HA2	2.52	0.44
8:V:55:VAL:HA	8:V:86:MET:HE1	1.99	0.44
1:A:178:PHE:CZ	1:A:182:LYS:HD2	2.52	0.44
6:F:185:ASN:O	6:F:188:VAL:HG22	2.17	0.44
7:G:119:VAL:HG23	7:G:131:PHE:CD2	2.52	0.44
11:K:28:MET:HE1	12:L:113:TYR:CD1	2.52	0.44
5:S:78:MET:HE1	5:S:82:ILE:HA	1.99	0.44
6:F:89:ARG:HG2	13:M:77:HIS:CE1	2.53	0.44
7:G:149:TYR:CD1	7:G:159:GLY:HA2	2.53	0.44
8:H:41:ILE:HD13	8:H:41:ILE:HA	1.82	0.44
10:J:11:MET:HG3	10:J:137:VAL:HG12	2.00	0.44
11:K:154:GLU:CD	11:K:154:GLU:H	2.24	0.44
2:P:224:GLU:OE2	2:P:224:GLU:HA	2.18	0.44
4:R:24:GLU:HA	4:R:27:LYS:NZ	2.32	0.44
4:R:157:LYS:HG2	4:R:157:LYS:H	1.61	0.44
7:U:215:TRP:HE1	7:U:220:THR:HG23	1.83	0.44
11:Y:88:LEU:HD22	11:Y:122:ALA:HB2	1.99	0.44
12:Z:77:ALA:HA	12:Z:112:TYR:HE2	1.83	0.44
14:b:26:MET:HB3	14:b:39:ILE:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:O	1:A:50:ILE:HG13	2.16	0.44
2:B:9:LEU:HD21	2:B:125:GLY:HA2	2.00	0.44
9:I:186:LEU:HD12	9:I:189:TYR:HD1	1.83	0.44
3:Q:34:CYS:SG	3:Q:75:SER:OG	2.52	0.44
8:V:100:ILE:HG13	8:V:112:TYR:HB2	1.99	0.44
13:a:136:LYS:HD3	13:a:146:GLN:OE1	2.18	0.44
1:A:139:ILE:HG12	1:A:153:LYS:HB2	2.00	0.44
2:B:183:LEU:O	2:B:187:ILE:HG23	2.18	0.44
3:C:192:LEU:O	3:C:196:VAL:HG13	2.17	0.44
5:E:236:GLU:OE2	5:E:236:GLU:N	2.42	0.44
8:H:53:GLN:NE2	9:I:119:THR:O	2.43	0.44
8:H:151:GLU:O	8:H:154:GLN:HG2	2.16	0.44
14:N:107:TRP:O	14:N:127:MET:HE2	2.18	0.44
6:T:63:ILE:HG21	6:T:223:ILE:HD13	2.00	0.44
13:a:138:GLY:C	13:a:142:SER:HB3	2.43	0.44
1:A:37:LEU:HD23	1:A:81:THR:HG23	1.99	0.44
3:C:135:LEU:HD23	3:C:149:GLN:HB2	1.99	0.44
9:I:50:ALA:HB2	10:J:128:CYS:HB2	1.99	0.44
10:J:172:ASN:OD1	13:a:157:ASN:ND2	2.40	0.44
13:M:188:TYR:OH	9:W:24:MET:SD	2.60	0.44
6:T:107:ARG:NH1	14:b:79:ASP:OD2	2.51	0.44
6:T:152:ASN:HA	7:U:85:ARG:HH21	1.83	0.44
8:V:83:PHE:CD1	8:V:98:ILE:HG21	2.53	0.44
9:W:90:TYR:CE1	9:W:94:ILE:HG23	2.52	0.44
10:X:35:THR:HG22	10:X:37:ASP:H	1.83	0.44
11:Y:108:ASP:OD1	11:Y:109:GLU:N	2.51	0.44
1:A:21:ARG:HH12	1:A:23:TYR:HD1	1.65	0.44
3:C:114:LEU:HD23	3:C:136:TYR:OH	2.18	0.44
5:E:202:LEU:O	5:E:206:MET:HB2	2.17	0.44
3:Q:48:GLU:HA	3:Q:211:VAL:HA	1.99	0.44
10:X:26:ARG:HG3	10:X:33:MET:HE2	1.99	0.44
12:Z:91:LYS:HE3	12:Z:116:SER:O	2.18	0.44
13:a:64:LEU:O	13:a:68:ILE:HG22	2.18	0.44
10:J:58:ASP:O	10:J:62:VAL:HG23	2.17	0.43
12:L:37:ILE:HD13	12:L:59:LEU:HD21	1.99	0.43
12:L:66:TYR:CE2	12:L:74:ILE:HA	2.53	0.43
13:M:110:ILE:HD13	13:M:110:ILE:HA	1.90	0.43
14:N:46:ASN:OD1	14:N:49:THR:OG1	2.22	0.43
1:O:172:GLN:O	1:O:176:THR:HG22	2.17	0.43
1:O:178:PHE:CZ	1:O:182:LYS:HD2	2.53	0.43
2:P:135:ILE:O	2:P:145:LEU:HA	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:22:ALA:O	4:R:26:VAL:HG23	2.18	0.43
9:W:58:LEU:O	9:W:62:ASN:ND2	2.48	0.43
9:W:93:TYR:HB3	10:X:99:PHE:HZ	1.83	0.43
10:X:167:SER:HB3	10:X:199:LEU:HD22	1.99	0.43
12:Z:82:LEU:HD12	12:Z:83:LEU:N	2.33	0.43
13:a:71:ARG:CD	13:a:95:ILE:HD11	2.48	0.43
14:b:46:ASN:OD1	14:b:49:THR:OG1	2.21	0.43
14:b:50:MET:HE3	14:b:197:VAL:HG13	1.99	0.43
8:H:4:MET:SD	8:H:127:ILE:HD11	2.58	0.43
11:K:103:LEU:HD13	11:K:132:HIS:CD2	2.53	0.43
12:L:166:ARG:NE	11:Y:144:ASP:OD1	2.41	0.43
4:R:164:GLY:O	4:R:168:VAL:HG12	2.19	0.43
8:V:90:TYR:HB2	8:V:94:LEU:HD23	2.00	0.43
11:Y:115:LEU:HD12	11:Y:116:TYR:N	2.32	0.43
12:Z:3:THR:HG23	12:Z:16:ALA:HB2	2.00	0.43
1:A:191:PHE:H	1:A:194:THR:HG23	1.81	0.43
5:E:101:PHE:HD1	12:L:57:ARG:HG2	1.82	0.43
11:K:35:MET:CE	11:K:181:ARG:HE	2.31	0.43
1:O:34:GLN:NE2	7:U:17:ASP:O	2.51	0.43
1:O:109:ILE:HG12	1:O:114:LEU:HB2	2.00	0.43
3:Q:198:ASN:HB2	3:Q:199:LYS:NZ	2.33	0.43
5:S:141:LEU:HB2	5:S:156:MET:HB2	1.99	0.43
5:S:236:GLU:OE2	5:S:236:GLU:N	2.42	0.43
11:Y:67:TYR:CD2	11:Y:75:LEU:HG	2.53	0.43
11:Y:164:LEU:HA	11:Y:167:LEU:HD23	2.00	0.43
12:Z:58:LEU:O	12:Z:62:GLN:HG2	2.18	0.43
2:B:73:LEU:HD12	2:B:133:LEU:HG	1.99	0.43
2:B:224:GLU:OE2	2:B:224:GLU:HA	2.18	0.43
3:C:139:TRP:HA	3:C:144:GLY:O	2.18	0.43
4:D:79:ASP:OD1	4:D:127:PHE:HD1	2.01	0.43
5:E:20:ARG:HG3	5:E:25:GLU:HB2	2.01	0.43
6:F:212:ILE:HD12	6:F:229:VAL:HG23	1.99	0.43
7:G:233:GLU:HA	7:G:236:GLU:OE1	2.18	0.43
9:I:135:MET:HE3	14:b:179:ARG:HH12	1.82	0.43
7:U:168:ALA:HB1	7:U:171:ALA:HB3	2.00	0.43
8:V:103:TRP:CZ2	8:V:181:GLU:HB3	2.54	0.43
8:V:116:MET:HB3	14:b:5:MET:HG3	1.98	0.43
11:Y:146:TYR:HB2	11:Y:159:LEU:HD11	2.00	0.43
13:a:64:LEU:HD11	13:a:96:LEU:HD11	2.00	0.43
1:A:49:VAL:HG22	1:A:219:VAL:HG12	2.00	0.43
7:G:87:LEU:HD23	7:G:87:LEU:HA	1.80	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:34:LEU:HB2	8:H:186:ARG:NH1	2.33	0.43
8:H:103:TRP:CZ2	8:H:181:GLU:HB3	2.53	0.43
9:I:49:ALA:O	9:I:52:THR:OG1	2.32	0.43
11:K:59:TYR:HE2	11:K:87:ASN:HD22	1.67	0.43
1:O:14:THR:HG22	1:O:24:GLN:HB3	2.00	0.43
2:P:110:VAL:HG21	2:P:146:PHE:CD2	2.53	0.43
5:S:84:ASP:OD2	5:S:138:GLY:N	2.43	0.43
7:U:119:VAL:HG23	7:U:131:PHE:CD2	2.54	0.43
10:X:94:LEU:HD11	10:X:106:PRO:HG3	2.00	0.43
1:A:65:THR:HG21	7:G:149:TYR:CE1	2.53	0.43
9:I:111:TYR:CE2	9:I:121:LYS:HB2	2.54	0.43
9:I:209:THR:OG1	10:J:168:GLN:OE1	2.37	0.43
12:L:63:CYS:HB2	12:L:74:ILE:HG21	2.01	0.43
12:L:162:GLN:OE1	11:Y:144:ASP:HB3	2.18	0.43
1:O:22:LEU:HD23	1:O:22:LEU:HA	1.85	0.43
2:P:101:GLN:OE1	9:W:57:GLN:NE2	2.51	0.43
3:Q:79:ILE:HG22	3:Q:82:ASP:H	1.84	0.43
6:T:157:ARG:HD2	7:U:59:GLU:OE2	2.17	0.43
7:U:175:GLU:HB2	7:U:196:ILE:HD11	1.99	0.43
12:Z:157:ARG:HB3	12:Z:195:LEU:HD21	2.01	0.43
13:a:55:SER:OG	13:a:107:TYR:HB2	2.18	0.43
1:A:78:CYS:SG	1:A:138:MET:HG2	2.59	0.43
4:D:86:ARG:HA	4:D:89:VAL:HG12	1.99	0.43
8:H:70:LEU:O	8:H:70:LEU:HD12	2.19	0.43
8:H:164:MET:HG2	8:H:171:GLY:HA2	2.00	0.43
9:I:90:TYR:HD1	9:I:94:ILE:HG12	1.83	0.43
11:K:96:THR:O	11:K:96:THR:OG1	2.25	0.43
11:K:175:LEU:HD13	11:K:175:LEU:HA	1.82	0.43
1:O:178:PHE:CE1	1:O:201:CYS:HA	2.53	0.43
3:Q:196:VAL:O	3:Q:200:THR:HG23	2.19	0.43
6:T:50:LYS:HG2	6:T:59:HIS:HB2	2.00	0.43
1:A:112:ASP:OD2	1:A:113:MET:HE3	2.19	0.43
8:H:55:VAL:HA	8:H:86:MET:HE1	2.01	0.43
1:O:78:CYS:SG	1:O:138:MET:HG2	2.58	0.43
2:P:98:LEU:HD21	9:W:61:SER:OG	2.18	0.43
7:U:215:TRP:HE3	7:U:227:VAL:HG22	1.84	0.43
13:a:4:PRO:O	14:b:100:ARG:NH2	2.48	0.43
1:A:18:PRO:HA	2:B:23:TYR:CD1	2.54	0.43
2:B:17:LYS:HB3	2:B:17:LYS:HE3	1.72	0.43
3:C:196:VAL:O	3:C:200:THR:HG23	2.18	0.43
5:E:123:PHE:CE1	5:E:136:PRO:HB3	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:178:LYS:HE3	7:G:178:LYS:HB3	1.70	0.43
10:J:146:TYR:CD1	13:a:185:ARG:HD3	2.54	0.43
11:K:67:TYR:CD2	11:K:75:LEU:HG	2.52	0.43
1:O:17:SER:C	1:O:20:GLY:H	2.26	0.43
6:T:9:ASP:HB2	6:T:12:VAL:HG13	1.99	0.43
10:X:11:MET:HB3	10:X:170:MET:HE3	2.01	0.43
10:J:176:ARG:HG2	13:a:147:PRO:HG3	2.00	0.43
12:L:95:LEU:CD2	12:L:97:MET:HG2	2.47	0.43
13:M:38:ARG:NH2	9:W:164:PHE:O	2.50	0.43
1:O:18:PRO:HA	2:P:23:TYR:CD1	2.54	0.43
1:O:49:VAL:HG22	1:O:219:VAL:HG12	2.01	0.43
2:P:96:TYR:CG	2:P:104:ILE:HG13	2.54	0.43
2:P:120:TYR:CD1	2:P:126:VAL:HG11	2.54	0.43
3:Q:209:GLU:HA	3:Q:230:GLN:HE22	1.82	0.43
5:S:21:LEU:HD12	5:S:21:LEU:HA	1.75	0.43
7:U:73:VAL:HG13	7:U:108:LEU:HD12	2.00	0.43
7:U:178:LYS:HE3	7:U:178:LYS:HB3	1.72	0.43
7:U:196:ILE:HG13	7:U:199:ILE:HD11	2.01	0.43
9:W:42:TYR:CE2	9:W:183:LEU:HD11	2.54	0.43
13:a:11:THR:HG21	13:a:141:ALA:HB3	2.00	0.43
1:A:154:CYS:HA	1:A:159:TYR:O	2.19	0.42
2:B:68:THR:OG1	2:B:71:ILE:HG12	2.19	0.42
11:K:36:PHE:CD1	11:K:36:PHE:N	2.87	0.42
11:K:114:ALA:HB1	11:K:116:TYR:HE1	1.83	0.42
11:K:116:TYR:HB3	11:K:124:LEU:HD11	2.01	0.42
12:L:167:ASP:OD2	12:L:169:TYR:N	2.52	0.42
5:S:235:GLU:HG3	5:S:236:GLU:OE2	2.19	0.42
6:T:50:LYS:HE3	6:T:50:LYS:HB3	1.86	0.42
8:V:84:LYS:HG3	8:V:118:GLY:O	2.19	0.42
9:W:83:LEU:O	9:W:86:MET:HG3	2.19	0.42
1:A:171:LYS:HE3	1:A:174:GLU:HB2	2.00	0.42
2:B:85:LEU:HD11	2:B:117:MET:SD	2.59	0.42
6:F:107:ARG:NH2	14:N:77:LEU:HD13	2.34	0.42
11:K:70:ARG:HG3	11:K:71:ASN:ND2	2.34	0.42
12:L:12:VAL:HG22	12:L:179:VAL:HG22	2.00	0.42
12:L:104:TRP:CD1	12:L:109:PRO:HA	2.53	0.42
3:Q:93:ILE:HD13	3:Q:96:ARG:HH21	1.84	0.42
4:R:83:VAL:HG21	4:R:129:ILE:HD11	2.00	0.42
10:X:9:ALA:HA	10:X:139:GLY:HA3	2.01	0.42
6:F:229:VAL:HG22	6:F:233:LEU:HG	2.01	0.42
7:G:169:ARG:HG3	7:G:170:GLN:NE2	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:76:VAL:HG23	8:H:104:ASP:OD2	2.19	0.42
9:I:200:GLY:N	13:a:177:ASP:OD1	2.45	0.42
10:J:55:LEU:O	10:J:59:VAL:HG23	2.19	0.42
11:K:3:TYR:O	11:K:4:LEU:HD23	2.18	0.42
14:N:26:MET:HB3	14:N:39:ILE:O	2.19	0.42
14:N:43:MET:HB3	14:N:43:MET:HE2	1.77	0.42
14:N:56:ASP:OD2	14:N:56:ASP:C	2.62	0.42
14:N:179:ARG:HB3	8:V:25:TYR:HE2	1.83	0.42
2:P:64:VAL:HG22	2:P:74:VAL:HB	2.02	0.42
6:T:116:THR:O	6:T:119:PRO:HD2	2.18	0.42
11:Y:51:GLY:HA3	12:Z:117:GLU:O	2.19	0.42
14:b:10:SER:OG	14:b:142:GLY:N	2.52	0.42
14:b:124:TYR:CE1	14:b:139:THR:HG22	2.54	0.42
1:A:22:LEU:HD23	1:A:22:LEU:HA	1.80	0.42
1:A:153:LYS:HE3	1:A:163:PHE:HE2	1.84	0.42
2:B:117:MET:HE3	2:B:150:PRO:HA	2.00	0.42
3:C:105:ILE:HD11	3:C:109:GLN:OE1	2.18	0.42
5:E:52:LYS:HA	5:E:66:LYS:NZ	2.35	0.42
6:F:108:LEU:O	6:F:112:ILE:HG12	2.19	0.42
6:F:226:ASP:O	6:F:229:VAL:HG12	2.20	0.42
10:J:10:VAL:HG22	10:J:23:ALA:HB2	2.01	0.42
10:J:15:GLY:HA3	10:J:162:LEU:HD22	2.01	0.42
11:K:182:ILE:HD12	11:K:182:ILE:HA	1.87	0.42
13:M:113:LEU:HD13	13:M:198:VAL:HG12	2.01	0.42
3:Q:14:PRO:HA	4:R:21:TYR:CD1	2.55	0.42
3:Q:234:GLU:HA	3:Q:237:ILE:HG12	2.02	0.42
5:S:37:ALA:HB2	5:S:50:VAL:HG23	1.99	0.42
5:S:123:PHE:CE1	5:S:136:PRO:HB3	2.55	0.42
8:V:34:LEU:HB2	8:V:186:ARG:NH1	2.34	0.42
12:Z:64:ARG:O	12:Z:68:LEU:HD23	2.20	0.42
14:b:26:MET:HE1	14:b:186:ARG:HB3	2.00	0.42
14:b:166:ARG:HG2	14:b:170:GLU:OE2	2.20	0.42
1:A:17:SER:C	1:A:20:GLY:H	2.27	0.42
1:A:78:CYS:SG	1:A:79:VAL:N	2.92	0.42
1:A:92:GLN:HE22	8:H:65:PHE:HZ	1.66	0.42
3:C:68:LEU:HD13	3:C:90:LEU:HB3	2.01	0.42
4:D:40:ILE:HD12	4:D:212:ARG:HG2	2.02	0.42
5:E:189:MET:HE3	5:E:189:MET:HB2	1.73	0.42
6:F:158:ALA:O	7:G:57:LEU:HB3	2.19	0.42
6:F:205:LEU:HD22	6:F:210:VAL:HG21	2.02	0.42
11:K:13:VAL:HG12	11:K:13:VAL:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:36:GLU:N	12:Z:36:GLU:OE1	2.53	0.42
14:b:108:ASN:OD1	14:b:108:ASN:C	2.62	0.42
14:b:161:SER:OG	14:b:164:GLU:HG2	2.20	0.42
1:A:34:GLN:NE2	7:G:17:ASP:O	2.52	0.42
2:B:183:LEU:HD11	2:B:211:ILE:HD11	2.01	0.42
5:E:101:PHE:CD1	12:L:57:ARG:HG2	2.54	0.42
11:K:6:GLY:HA2	11:K:15:VAL:HA	2.02	0.42
13:M:151:ASN:HB2	10:X:172:ASN:ND2	2.35	0.42
2:P:183:LEU:O	2:P:187:ILE:HG23	2.20	0.42
6:T:108:LEU:O	6:T:112:ILE:HG12	2.19	0.42
9:W:43:CYS:SG	9:W:98:LEU:HB3	2.60	0.42
10:X:35:THR:CG2	10:X:37:ASP:H	2.32	0.42
11:Y:44:LEU:HD23	11:Y:45:LEU:N	2.34	0.42
13:a:92:LEU:HD23	13:a:124:PHE:CE2	2.54	0.42
13:a:212:LYS:H	13:a:212:LYS:HG3	1.53	0.42
14:b:108:ASN:OD1	14:b:110:MET:HG3	2.19	0.42
1:A:178:PHE:CE1	1:A:201:CYS:HA	2.55	0.42
3:C:216:LEU:HD12	3:C:225:ILE:HG12	2.02	0.42
5:E:66:LYS:O	5:E:78:MET:HE2	2.20	0.42
7:G:92:ARG:HE	7:G:92:ARG:HB2	1.65	0.42
10:J:33:MET:HE3	10:J:182:MET:HG3	2.02	0.42
10:J:176:ARG:HD2	10:J:176:ARG:HA	1.81	0.42
12:L:64:ARG:O	12:L:68:LEU:HD23	2.19	0.42
7:U:114:ARG:HE	7:U:114:ARG:HB3	1.63	0.42
8:V:160:LEU:HD23	8:V:160:LEU:HA	1.77	0.42
9:W:80:ASN:OD1	9:W:80:ASN:N	2.53	0.42
7:G:175:GLU:HB2	7:G:196:ILE:HD12	2.02	0.42
8:H:135:ILE:HA	8:H:135:ILE:HD13	1.76	0.42
11:K:37:LYS:HA	11:K:43:LEU:HD23	2.01	0.42
1:O:43:ARG:HD3	1:O:151:VAL:HG22	2.01	0.42
2:P:96:TYR:CD2	2:P:104:ILE:HG13	2.55	0.42
2:P:155:PHE:HB2	2:P:157:TRP:NE1	2.34	0.42
7:U:51:LYS:HZ1	7:U:64:LYS:HA	1.84	0.42
8:V:7:GLN:HA	8:V:12:VAL:HG12	2.02	0.42
8:V:41:ILE:CD1	8:V:76:VAL:HG22	2.48	0.42
10:X:87:MET:CE	10:X:129:PRO:HB3	2.50	0.42
11:Y:108:ASP:HB3	11:Y:112:GLY:H	1.84	0.42
3:C:8:ARG:HD2	3:C:11:ILE:HG21	2.01	0.42
5:E:73:HIS:CE1	5:E:106:THR:HB	2.55	0.42
8:H:8:PHE:HB3	8:H:152:CYS:SG	2.60	0.42
8:H:83:PHE:CD1	8:H:98:ILE:HG21	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:42:PHE:HE2	10:J:52:LEU:HD13	1.84	0.42
1:O:21:ARG:HH12	1:O:23:TYR:HE1	1.67	0.42
5:S:189:MET:HE3	5:S:189:MET:HB2	1.70	0.42
6:T:158:ALA:O	7:U:57:LEU:HB3	2.20	0.42
8:V:149:LYS:NZ	8:V:153:LEU:HD11	2.35	0.42
10:X:25:ARG:HB3	10:X:36:THR:O	2.19	0.42
14:b:99:ARG:CZ	14:b:106:LEU:HD21	2.49	0.42
7:G:215:TRP:HZ3	7:G:227:VAL:HG13	1.84	0.42
9:I:89:ARG:HH12	9:I:90:TYR:HD2	1.68	0.42
10:J:111:LEU:HD23	10:J:118:PRO:HA	2.01	0.42
11:K:38:MET:HA	11:K:38:MET:HE2	2.01	0.42
11:K:52:ASP:OD2	11:K:52:ASP:N	2.53	0.42
12:L:7:LYS:HA	12:L:12:VAL:HA	2.02	0.42
7:U:110:HIS:O	7:U:114:ARG:HG2	2.20	0.42
11:Y:164:LEU:HD13	11:Y:178:PHE:CD2	2.55	0.42
12:Z:4:LEU:HD12	12:Z:4:LEU:HA	1.87	0.42
12:Z:99:THR:OG1	12:Z:100:MET:N	2.53	0.42
12:Z:107:ARG:HE	12:Z:107:ARG:HB3	1.65	0.42
14:b:42:ILE:HD12	14:b:51:LEU:O	2.20	0.42
14:b:59:ASP:OD1	14:b:59:ASP:N	2.53	0.42
5:E:93:ARG:HD3	12:L:68:LEU:HB3	2.02	0.41
9:I:214:GLU:HG3	10:J:197:ARG:HG2	2.02	0.41
12:L:44:THR:CG2	12:L:100:MET:HB2	2.50	0.41
14:N:97:TYR:HA	14:N:100:ARG:HG2	2.02	0.41
7:U:172:ALA:O	7:U:176:ILE:HG12	2.20	0.41
10:X:175:ASP:OD1	10:X:175:ASP:C	2.63	0.41
12:Z:35:ILE:HD11	12:Z:45:MET:HE2	2.02	0.41
14:b:77:LEU:HD12	14:b:77:LEU:H	1.85	0.41
3:C:10:THR:O	4:D:125:ARG:HD2	2.20	0.41
3:C:67:LYS:O	3:C:91:ARG:NH1	2.53	0.41
5:E:99:HIS:CG	5:E:107:MET:SD	3.13	0.41
8:H:135:ILE:HG12	8:H:163:ALA:HB2	2.01	0.41
9:I:166:ASP:OD1	9:I:167:LEU:N	2.53	0.41
10:J:105:GLU:HB3	10:J:138:SER:OG	2.19	0.41
11:K:5:ILE:HD11	11:K:143:LEU:HD11	2.02	0.41
11:K:104:LEU:HD12	11:K:104:LEU:HA	1.83	0.41
12:L:107:ARG:HE	12:L:107:ARG:HB3	1.67	0.41
1:O:123:GLN:CD	1:O:123:GLN:C	2.88	0.41
1:O:162:GLY:O	2:P:57:ASP:N	2.41	0.41
5:S:211:ASN:O	5:S:215:ILE:HG22	2.20	0.41
6:T:230:SER:N	6:T:231:PRO:HD2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:53:GLN:HG3	8:V:53:GLN:H	1.71	0.41
9:W:53:ASP:OD1	9:W:53:ASP:C	2.63	0.41
9:W:111:TYR:CE2	9:W:121:LYS:HB2	2.55	0.41
10:X:51:GLY:C	10:X:52:LEU:HD12	2.45	0.41
14:b:107:TRP:CE3	14:b:127:MET:HE1	2.55	0.41
3:C:119:GLN:HA	3:C:122:THR:HG23	2.02	0.41
9:I:40:ASN:O	9:I:41:ILE:HD13	2.20	0.41
10:J:172:ASN:CG	13:a:157:ASN:HD22	2.25	0.41
11:K:8:GLN:HE22	11:K:113:PRO:HB2	1.85	0.41
12:L:82:LEU:HD12	12:L:83:LEU:N	2.34	0.41
13:M:138:GLY:C	13:M:142:SER:HB3	2.45	0.41
11:Y:13:VAL:HB	11:Y:183:ILE:HB	2.02	0.41
11:Y:29:LYS:HB2	12:Z:121:ILE:HD12	2.02	0.41
12:Z:33:LYS:HE3	12:Z:45:MET:HB3	2.03	0.41
3:C:69:ASN:HB3	3:C:72:MET:HG2	2.02	0.41
4:D:106:TYR:HD2	4:D:109:ARG:NH2	2.18	0.41
4:D:131:ALA:HB3	4:D:147:THR:HB	2.02	0.41
6:F:40:SER:HB3	6:F:187:LEU:HD22	2.01	0.41
10:J:114:LYS:HE2	10:J:114:LYS:HB2	1.79	0.41
11:K:108:ASP:OD1	11:K:109:GLU:N	2.53	0.41
13:M:76:LYS:HE2	13:M:76:LYS:HB2	1.85	0.41
13:M:97:TYR:O	13:M:100:ARG:HB3	2.21	0.41
2:P:45:LEU:O	2:P:210:GLY:N	2.29	0.41
4:R:65:LEU:HD12	4:R:65:LEU:H	1.85	0.41
4:R:66:ASP:HA	11:Y:69:MET:CE	2.39	0.41
4:R:106:TYR:HD1	4:R:109:ARG:HH22	1.68	0.41
5:S:235:GLU:O	5:S:238:ILE:HG22	2.21	0.41
6:T:7:ASP:OD2	6:T:7:ASP:N	2.33	0.41
7:U:73:VAL:HG22	7:U:139:SER:HB3	2.01	0.41
7:U:136:MET:HE2	7:U:136:MET:HB2	1.82	0.41
8:V:135:ILE:HA	8:V:135:ILE:HD13	1.77	0.41
12:Z:43:GLY:HA2	12:Z:100:MET:O	2.20	0.41
12:Z:167:ASP:OD2	12:Z:169:TYR:N	2.53	0.41
2:B:120:TYR:CD1	2:B:126:VAL:HG11	2.55	0.41
3:C:53:HIS:HB2	3:C:56:LEU:HG	2.02	0.41
3:C:174:MET:HA	3:C:177:GLN:HE21	1.86	0.41
6:F:145:PHE:HD1	6:F:155:ASP:HA	1.86	0.41
6:F:230:SER:N	6:F:231:PRO:HD2	2.36	0.41
7:G:114:ARG:HE	7:G:114:ARG:HB3	1.63	0.41
10:J:157:MET:HE2	10:J:161:HIS:HB3	2.02	0.41
11:K:124:LEU:HG	11:K:125:ALA:N	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:2:PHE:CE1	14:N:105:PRO:HG3	2.56	0.41
3:Q:139:TRP:HA	3:Q:144:GLY:O	2.20	0.41
12:Z:18:SER:OG	12:Z:18:SER:O	2.37	0.41
13:a:45:LYS:HD3	13:a:45:LYS:N	2.34	0.41
1:A:53:GLN:HA	1:A:215:ILE:HG22	2.02	0.41
2:B:188:HIS:O	2:B:191:ILE:HG13	2.20	0.41
3:C:186:LEU:HD23	3:C:187:LYS:H	1.86	0.41
10:J:161:HIS:O	10:J:165:THR:HG23	2.21	0.41
11:K:13:VAL:O	11:K:13:VAL:CG1	2.68	0.41
12:L:58:LEU:O	12:L:61:ARG:HG2	2.20	0.41
12:L:77:ALA:HA	12:L:112:TYR:HE2	1.86	0.41
12:L:128:VAL:C	12:L:132:SER:HB3	2.46	0.41
13:M:22:ILE:HD13	13:M:197:ILE:HB	2.02	0.41
3:Q:32:GLY:HA2	3:Q:50:ARG:NH2	2.34	0.41
10:X:13:MET:SD	10:X:153:TRP:HD1	2.43	0.41
11:Y:43:LEU:HD11	11:Y:188:ILE:HD13	2.03	0.41
11:Y:107:TYR:HB2	11:Y:183:ILE:HG22	2.01	0.41
12:Z:62:GLN:HG2	12:Z:62:GLN:H	1.76	0.41
13:a:6:VAL:HG12	13:a:57:PHE:CE2	2.56	0.41
13:a:74:MET:HE3	13:a:74:MET:HA	2.03	0.41
13:a:201:GLU:OE1	13:a:201:GLU:N	2.53	0.41
14:b:67:LEU:HG	14:b:91:TRP:CZ3	2.55	0.41
1:A:37:LEU:HA	1:A:55:LYS:HZ1	1.85	0.41
1:A:171:LYS:HA	1:A:171:LYS:HD2	1.90	0.41
4:D:106:TYR:HD2	4:D:109:ARG:HH22	1.69	0.41
5:E:69:GLU:HG3	5:E:226:PHE:CD2	2.52	0.41
11:K:116:TYR:CD2	11:K:124:LEU:HD11	2.53	0.41
12:L:4:LEU:HD12	12:L:4:LEU:HA	1.62	0.41
12:L:83:LEU:O	12:L:86:MET:HG2	2.21	0.41
2:P:105:PRO:HB2	2:P:108:GLN:HG2	2.02	0.41
3:Q:188:SER:O	3:Q:192:LEU:HD13	2.20	0.41
5:S:58:LEU:HD12	5:S:58:LEU:H	1.84	0.41
5:S:156:MET:SD	5:S:162:PHE:HB3	2.61	0.41
9:W:8:TYR:CE1	9:W:13:VAL:HG23	2.56	0.41
9:W:104:ASP:OD2	9:W:104:ASP:C	2.62	0.41
12:Z:7:LYS:HA	12:Z:12:VAL:HA	2.02	0.41
1:A:125:TYR:CE1	1:A:131:MET:HE2	2.56	0.41
3:C:141:LYS:HE2	11:K:110:HIS:ND1	2.36	0.41
8:H:108:GLY:O	8:H:110:GLN:NE2	2.54	0.41
11:K:29:LYS:HB2	12:L:121:ILE:HD12	2.03	0.41
11:K:68:LYS:HA	11:K:73:TYR:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:46:ALA:HB3	12:L:98:GLY:O	2.21	0.41
2:P:117:MET:HE3	2:P:150:PRO:HA	2.02	0.41
4:R:42:VAL:HG11	4:R:191:VAL:HG21	2.02	0.41
4:R:94:HIS:ND1	4:R:102:VAL:HG12	2.36	0.41
5:S:117:SER:HB3	5:S:156:MET:SD	2.61	0.41
5:S:154:PHE:HD1	5:S:164:GLN:HA	1.85	0.41
8:V:135:ILE:HG12	8:V:163:ALA:HB2	2.01	0.41
2:B:14:PRO:HA	3:C:23:TYR:CD1	2.56	0.41
3:C:14:PRO:HA	4:D:21:TYR:CD1	2.55	0.41
4:D:157:LYS:NZ	5:E:57:PRO:O	2.51	0.41
8:H:120:MET:SD	8:H:121:VAL:N	2.94	0.41
9:I:8:TYR:CE1	9:I:13:VAL:HG23	2.56	0.41
9:I:42:TYR:CE1	9:I:183:LEU:HD11	2.55	0.41
9:I:174:ASP:OD2	9:I:187:ARG:HA	2.21	0.41
10:J:98:ARG:HH12	10:J:126:ILE:HG21	1.86	0.41
10:J:167:SER:HB3	10:J:199:LEU:HD22	2.02	0.41
10:J:183:GLY:HA2	10:J:201:ALA:HB3	2.02	0.41
12:L:58:LEU:HB2	12:L:86:MET:HE1	2.03	0.41
13:M:65:THR:HA	13:M:68:ILE:HG22	2.03	0.41
13:M:213:ASP:O	9:W:19:ARG:NH2	2.51	0.41
2:P:67:ILE:HG21	2:P:109:LEU:HD11	2.03	0.41
3:Q:98:LEU:HD23	3:Q:102:GLN:HA	2.02	0.41
3:Q:176:LYS:HE3	3:Q:176:LYS:HB3	1.84	0.41
4:R:40:ILE:HD12	4:R:212:ARG:HG2	2.03	0.41
4:R:115:LYS:O	4:R:119:THR:HG23	2.20	0.41
4:R:190:LEU:HD12	4:R:190:LEU:HA	1.88	0.41
5:S:121:LEU:O	5:S:121:LEU:HD12	2.20	0.41
6:T:26:MET:HG2	6:T:149:PRO:HD2	2.01	0.41
6:T:92:CYS:SG	6:T:93:LEU:N	2.93	0.41
7:U:27:MET:HA	7:U:153:PRO:HG2	2.02	0.41
10:X:125:LEU:HD12	10:X:126:ILE:HG12	2.03	0.41
10:X:177:ASP:OD1	10:X:179:VAL:N	2.49	0.41
11:Y:86:ARG:NH2	11:Y:90:ASP:OD2	2.36	0.41
11:Y:182:ILE:CG2	11:Y:189:HIS:HB2	2.50	0.41
12:Z:125:THR:CG2	12:Z:139:MET:HE3	2.44	0.41
13:a:136:LYS:HB2	13:a:136:LYS:HE2	1.86	0.41
13:a:169:ASP:OD1	13:a:169:ASP:C	2.63	0.41
14:b:72:ILE:O	14:b:76:LEU:HD12	2.21	0.41
1:A:179:LEU:O	1:A:179:LEU:HD12	2.21	0.41
3:C:161:ALA:HB1	3:C:175:LEU:HD21	2.03	0.41
4:D:99:GLU:OE2	4:D:99:GLU:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:78:MET:HE2	5:E:78:MET:HB2	1.90	0.41
8:H:174:ILE:HB	8:H:189:LEU:HB2	2.02	0.41
13:M:136:LYS:HB2	13:M:136:LYS:HE2	1.82	0.41
1:O:159:TYR:OH	15:d:1:UNK:O	2.31	0.41
3:Q:159:TRP:HZ3	4:R:54:GLN:OE1	2.03	0.41
5:S:13:ASN:HB3	6:T:126:ARG:HB3	2.03	0.41
7:U:98:PHE:CE2	7:U:106:ILE:HA	2.56	0.41
8:V:90:TYR:HB2	8:V:94:LEU:CD2	2.50	0.41
9:W:41:ILE:HD11	9:W:76:VAL:HG22	2.02	0.41
10:X:175:ASP:OD1	10:X:176:ARG:N	2.54	0.41
12:Z:37:ILE:HD13	12:Z:59:LEU:HD21	2.03	0.41
14:b:54:SER:OG	14:b:139:THR:OG1	2.28	0.41
1:A:123:GLN:CD	1:A:123:GLN:C	2.88	0.40
5:E:114:GLN:OE1	6:F:82:ARG:NH1	2.53	0.40
9:I:9:LYS:HG2	9:I:146:MET:O	2.21	0.40
10:J:122:SER:C	10:J:123:LEU:HD22	2.46	0.40
11:K:14:LEU:HB2	11:K:182:ILE:CD1	2.51	0.40
11:K:114:ALA:HB1	11:K:116:TYR:CE1	2.56	0.40
12:L:177:TYR:HE1	12:L:186:ARG:HG3	1.84	0.40
3:Q:167:ASN:ND2	3:Q:200:THR:HA	2.36	0.40
6:T:15:PRO:HA	7:U:25:TYR:CE1	2.56	0.40
7:U:41:CYS:SG	7:U:43:ASP:N	2.94	0.40
7:U:70:ASP:OD1	7:U:99:ARG:NH2	2.55	0.40
8:V:120:MET:SD	8:V:121:VAL:N	2.94	0.40
11:Y:104:LEU:HA	11:Y:104:LEU:HD12	1.77	0.40
13:a:89:ALA:HB1	13:a:124:PHE:HZ	1.85	0.40
2:B:159:ALA:HB1	2:B:173:LEU:HD23	2.03	0.40
5:E:101:PHE:HZ	12:L:54:PHE:CE1	2.39	0.40
6:F:59:HIS:O	6:F:60:GLN:HG2	2.21	0.40
7:G:70:ASP:OD1	7:G:99:ARG:NH2	2.55	0.40
7:G:110:HIS:O	7:G:114:ARG:HG2	2.22	0.40
9:I:104:ASP:OD1	9:I:104:ASP:C	2.64	0.40
10:J:11:MET:CG	10:J:137:VAL:HG12	2.51	0.40
14:N:47:ASN:O	14:N:197:VAL:HG23	2.22	0.40
5:S:46:VAL:O	5:S:219:THR:OG1	2.36	0.40
8:V:34:LEU:HB2	8:V:186:ARG:HH22	1.86	0.40
9:W:13:VAL:HG11	9:W:155:VAL:HG11	2.03	0.40
9:W:93:TYR:O	10:X:98:ARG:NH2	2.54	0.40
11:Y:6:GLY:HA2	11:Y:15:VAL:HA	2.03	0.40
11:Y:36:PHE:HD1	11:Y:57:ALA:CB	2.35	0.40
11:Y:58:GLU:HA	11:Y:61:GLN:HG2	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:103:LEU:HD13	11:Y:132:HIS:CD2	2.56	0.40
11:Y:124:LEU:HG	11:Y:125:ALA:N	2.37	0.40
1:A:229:ILE:HD12	1:A:229:ILE:N	2.36	0.40
3:C:114:LEU:O	3:C:114:LEU:HD12	2.22	0.40
3:C:191:ALA:O	3:C:194:ILE:HG22	2.21	0.40
5:E:18:GLU:OE2	5:E:18:GLU:N	2.51	0.40
6:F:70:ILE:HD13	6:F:108:LEU:HD22	2.03	0.40
7:G:68:ASN:OD1	7:G:224:HIS:ND1	2.51	0.40
10:J:93:LEU:C	10:J:93:LEU:HD23	2.47	0.40
3:Q:133:SER:HB2	3:Q:152:PRO:HD3	2.03	0.40
3:Q:139:TRP:CD1	3:Q:144:GLY:HA2	2.56	0.40
8:V:125:PHE:C	8:V:125:PHE:CD2	2.99	0.40
14:b:165:ALA:O	14:b:169:VAL:HG22	2.22	0.40
5:E:195:ILE:HG13	5:E:195:ILE:H	1.65	0.40
5:E:235:GLU:O	5:E:238:ILE:HG22	2.21	0.40
6:F:157:ARG:HD2	6:F:176:MET:SD	2.61	0.40
7:G:27:MET:HA	7:G:153:PRO:HG2	2.03	0.40
7:G:51:LYS:NZ	7:G:62:SER:O	2.51	0.40
7:G:73:VAL:HG22	7:G:139:SER:HB3	2.03	0.40
10:J:94:LEU:HD11	10:J:106:PRO:HG3	2.02	0.40
2:P:211:ILE:HD13	2:P:211:ILE:HA	1.96	0.40
5:S:113:THR:HG21	5:S:154:PHE:HD2	1.87	0.40
6:T:104:PRO:HB2	6:T:107:ARG:HG3	2.03	0.40
6:T:226:ASP:O	6:T:229:VAL:HG12	2.21	0.40
7:U:98:PHE:CG	7:U:106:ILE:HD13	2.56	0.40
9:W:100:LEU:HD12	9:W:100:LEU:HA	1.74	0.40
10:X:19:VAL:HG22	10:X:189:ILE:HB	2.04	0.40
3:C:91:ARG:NH2	10:J:75:LEU:HB3	2.36	0.40
6:F:199:LEU:H	6:F:199:LEU:HD12	1.86	0.40
10:J:141:CYS:HB2	10:J:144:GLN:NE2	2.25	0.40
10:J:145:MET:SD	10:J:145:MET:N	2.89	0.40
11:K:13:VAL:CG1	11:K:105:ALA:HB1	2.52	0.40
14:N:25:ASP:OD1	14:N:25:ASP:N	2.44	0.40
14:N:53:ALA:HB1	14:N:108:ASN:OD1	2.22	0.40
1:O:92:GLN:HE22	8:V:65:PHE:HZ	1.69	0.40
5:S:109:VAL:HG12	5:S:154:PHE:CD2	2.57	0.40
7:U:189:ILE:HG12	7:U:189:ILE:H	1.72	0.40
7:U:198:TYR:HE1	7:U:209:PHE:CZ	2.40	0.40
10:X:24:ASP:OD2	10:X:26:ARG:N	2.46	0.40
10:X:83:PRO:HB2	10:X:119:PHE:CD2	2.57	0.40
10:X:83:PRO:HB2	10:X:119:PHE:HD2	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:68:ILE:HA	13:a:71:ARG:HG2	2.03	0.40
14:b:25:ASP:OD1	14:b:25:ASP:N	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	238/240 (99%)	231 (97%)	7 (3%)	0	100	100
1	O	238/240 (99%)	231 (97%)	7 (3%)	0	100	100
2	B	227/229 (99%)	220 (97%)	7 (3%)	0	100	100
2	P	227/229 (99%)	223 (98%)	4 (2%)	0	100	100
3	C	245/247 (99%)	235 (96%)	10 (4%)	0	100	100
3	Q	245/247 (99%)	237 (97%)	8 (3%)	0	100	100
4	D	230/232 (99%)	222 (96%)	8 (4%)	0	100	100
4	R	230/232 (99%)	225 (98%)	5 (2%)	0	100	100
5	E	231/233 (99%)	223 (96%)	8 (4%)	0	100	100
5	S	231/233 (99%)	225 (97%)	6 (3%)	0	100	100
6	F	231/233 (99%)	224 (97%)	6 (3%)	1 (0%)	30	64
6	T	231/233 (99%)	222 (96%)	9 (4%)	0	100	100
7	G	237/239 (99%)	235 (99%)	2 (1%)	0	100	100
7	U	237/239 (99%)	234 (99%)	3 (1%)	0	100	100
8	H	200/202 (99%)	197 (98%)	3 (2%)	0	100	100
8	V	200/202 (99%)	195 (98%)	5 (2%)	0	100	100
9	I	218/220 (99%)	209 (96%)	9 (4%)	0	100	100
9	W	218/220 (99%)	210 (96%)	8 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	202/204 (99%)	191 (95%)	11 (5%)	0	100	100
10	X	202/204 (99%)	192 (95%)	10 (5%)	0	100	100
11	K	194/196 (99%)	184 (95%)	10 (5%)	0	100	100
11	Y	194/196 (99%)	183 (94%)	11 (6%)	0	100	100
12	L	198/200 (99%)	191 (96%)	7 (4%)	0	100	100
12	Z	198/200 (99%)	190 (96%)	8 (4%)	0	100	100
13	M	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
13	a	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
14	N	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
14	b	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
All	All	6142/6198 (99%)	5948 (97%)	193 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	59	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	163/205 (80%)	159 (98%)	4 (2%)	42	62
1	O	163/205 (80%)	160 (98%)	3 (2%)	51	67
2	B	150/188 (80%)	140 (93%)	10 (7%)	15	41
2	P	153/188 (81%)	145 (95%)	8 (5%)	21	46
3	C	160/207 (77%)	154 (96%)	6 (4%)	29	52
3	Q	160/207 (77%)	151 (94%)	9 (6%)	19	45
4	D	136/196 (69%)	132 (97%)	4 (3%)	37	58
4	R	136/196 (69%)	132 (97%)	4 (3%)	37	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	158/195 (81%)	156 (99%)	2 (1%)	61	71
5	S	158/195 (81%)	156 (99%)	2 (1%)	61	71
6	F	160/199 (80%)	150 (94%)	10 (6%)	16	42
6	T	160/199 (80%)	149 (93%)	11 (7%)	14	40
7	G	162/197 (82%)	156 (96%)	6 (4%)	30	53
7	U	162/197 (82%)	153 (94%)	9 (6%)	19	45
8	H	140/157 (89%)	139 (99%)	1 (1%)	76	78
8	V	140/157 (89%)	139 (99%)	1 (1%)	76	78
9	I	157/181 (87%)	151 (96%)	6 (4%)	29	52
9	W	157/181 (87%)	151 (96%)	6 (4%)	29	52
10	J	155/173 (90%)	150 (97%)	5 (3%)	34	56
10	X	155/173 (90%)	151 (97%)	4 (3%)	40	60
11	K	148/167 (89%)	142 (96%)	6 (4%)	27	51
11	Y	148/167 (89%)	143 (97%)	5 (3%)	32	55
12	L	138/156 (88%)	133 (96%)	5 (4%)	31	54
12	Z	138/156 (88%)	131 (95%)	7 (5%)	21	46
13	M	158/177 (89%)	149 (94%)	9 (6%)	18	44
13	a	158/177 (89%)	147 (93%)	11 (7%)	14	40
14	N	149/175 (85%)	145 (97%)	4 (3%)	39	60
14	b	149/175 (85%)	146 (98%)	3 (2%)	48	65
All	All	4271/5146 (83%)	4110 (96%)	161 (4%)	30	52

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	THR
1	A	102	LYS
1	A	131	MET
1	A	235	ILE
2	B	11	THR
2	B	19	VAL
2	B	41	ASN
2	B	56	TYR
2	B	61	VAL
2	B	85	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	117	MET
2	B	121	THR
2	B	131	VAL
2	B	189	THR
3	C	9	THR
3	C	37	ILE
3	C	38	LEU
3	C	86	LEU
3	C	90	LEU
3	C	132	VAL
4	D	62	ILE
4	D	76	LEU
4	D	133	ILE
4	D	191	VAL
5	E	96	THR
5	E	238	ILE
6	F	23	GLU
6	F	45	VAL
6	F	56	LEU
6	F	69	HIS
6	F	74	ILE
6	F	77	LEU
6	F	92	CYS
6	F	147	THR
6	F	156	CYS
6	F	228	ASP
7	G	17	ASP
7	G	37	ILE
7	G	124	LEU
7	G	165	ILE
7	G	221	ASN
7	G	236	GLU
8	H	68	ILE
9	I	10	ASP
9	I	94	ILE
9	I	103	VAL
9	I	132	LEU
9	I	137	VAL
9	I	197	THR
10	J	19	VAL
10	J	138	SER
10	J	145	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	167	SER
10	J	188	ILE
11	K	20	VAL
11	K	84	THR
11	K	115	LEU
11	K	139	THR
11	K	150	THR
11	K	175	LEU
12	L	45	MET
12	L	62	GLN
12	L	63	CYS
12	L	179	VAL
12	L	187	VAL
13	M	26	ASP
13	M	46	LEU
13	M	47	THR
13	M	88	ILE
13	M	110	ILE
13	M	145	LEU
13	M	146	GLN
13	M	166	LEU
13	M	174	LEU
14	N	7	THR
14	N	9	THR
14	N	145	LEU
14	N	173	MET
1	O	84	THR
1	O	102	LYS
1	O	235	ILE
2	P	13	SER
2	P	41	ASN
2	P	56	TYR
2	P	61	VAL
2	P	85	LEU
2	P	117	MET
2	P	189	THR
2	P	211	ILE
3	Q	9	THR
3	Q	37	ILE
3	Q	38	LEU
3	Q	55	LEU
3	Q	68	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Q	75	SER
3	Q	87	THR
3	Q	111	VAL
3	Q	217	THR
4	R	62	ILE
4	R	133	ILE
4	R	152	THR
4	R	161	ILE
5	S	82	ILE
5	S	96	THR
6	T	23	GLU
6	T	45	VAL
6	T	68	ASN
6	T	69	HIS
6	T	74	ILE
6	T	92	CYS
6	T	147	THR
6	T	156	CYS
6	T	157	ARG
6	T	198	THR
6	T	228	ASP
7	U	8	ASP
7	U	17	ASP
7	U	37	ILE
7	U	41	CYS
7	U	45	VAL
7	U	124	LEU
7	U	150	MET
7	U	165	ILE
7	U	221	ASN
8	V	135	ILE
9	W	14	LEU
9	W	94	ILE
9	W	127	MET
9	W	132	LEU
9	W	137	VAL
9	W	197	THR
10	X	138	SER
10	X	145	MET
10	X	188	ILE
10	X	203	MET
11	Y	20	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	Y	42	ILE
11	Y	150	THR
11	Y	175	LEU
11	Y	188	ILE
12	Z	35	ILE
12	Z	63	CYS
12	Z	83	LEU
12	Z	97	MET
12	Z	101	ILE
12	Z	179	VAL
12	Z	187	VAL
13	a	12	ILE
13	a	22	ILE
13	a	26	ASP
13	a	46	LEU
13	a	47	THR
13	a	88	ILE
13	a	108	ASN
13	a	110	ILE
13	a	145	LEU
13	a	166	LEU
13	a	174	LEU
14	b	7	THR
14	b	9	THR
14	b	67	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	75	ASN
2	B	101	GLN
2	B	111	GLN
3	C	119	GLN
3	C	230	GLN
4	D	175	ASN
6	F	43	HIS
6	F	59	HIS
6	F	60	GLN
6	F	65	HIS
7	G	97	ASN
7	G	201	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	110	GLN
9	I	57	GLN
9	I	62	ASN
10	J	17	ASN
11	K	61	GLN
11	K	71	ASN
11	K	99	HIS
11	K	132	HIS
11	K	193	ASN
13	M	151	ASN
14	N	89	HIS
14	N	185	ASN
1	O	34	GLN
1	O	75	ASN
1	O	100	ASN
2	P	111	GLN
3	Q	30	HIS
3	Q	119	GLN
3	Q	230	GLN
6	T	59	HIS
6	T	60	GLN
6	T	65	HIS
6	T	121	GLN
6	T	166	GLN
9	W	62	ASN
11	Y	71	ASN
11	Y	132	HIS
11	Y	186	ASN
14	b	89	HIS
14	b	185	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

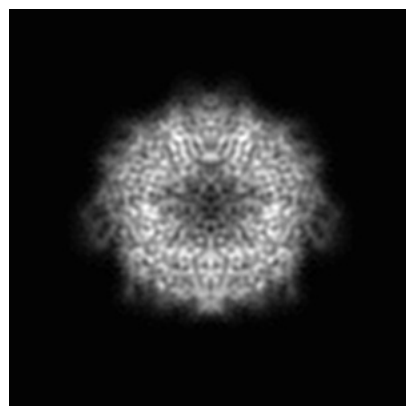
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53414. These allow visual inspection of the internal detail of the map and identification of artifacts.

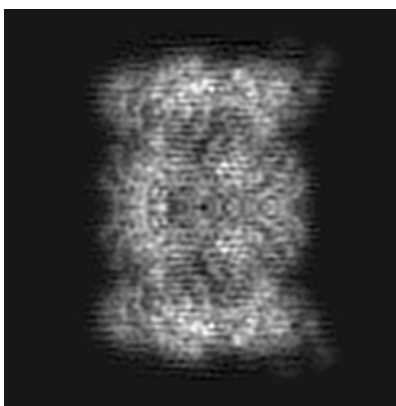
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

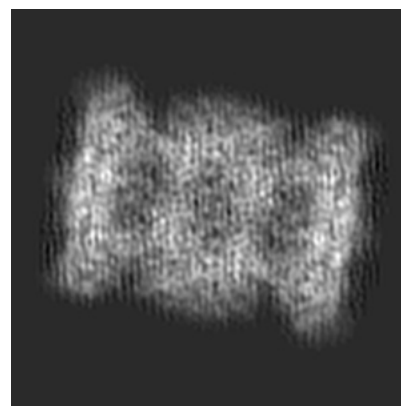
6.1.1 Primary map



X

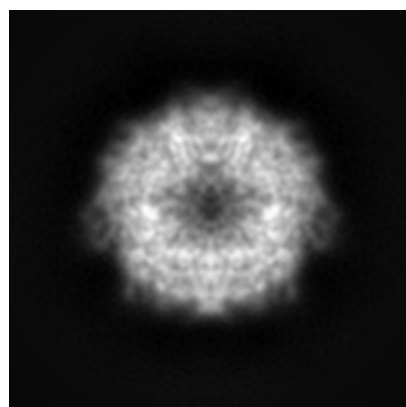


Y

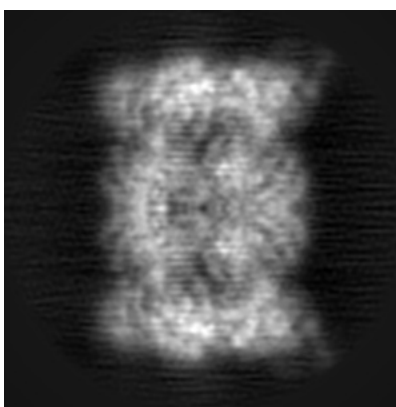


Z

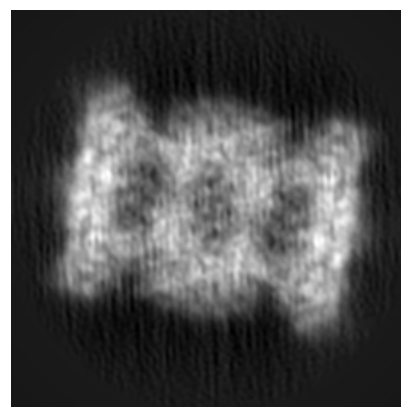
6.1.2 Raw map



X



Y

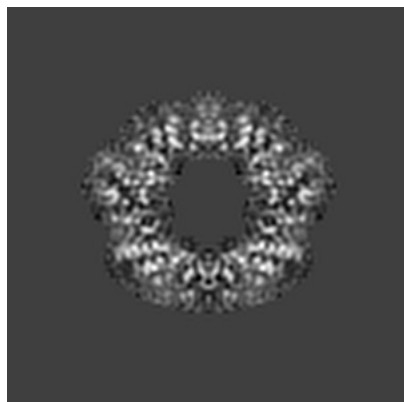


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 62

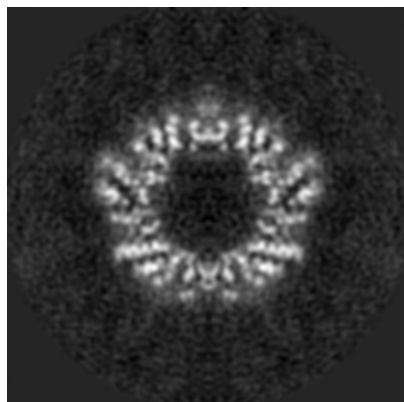


Y Index: 62

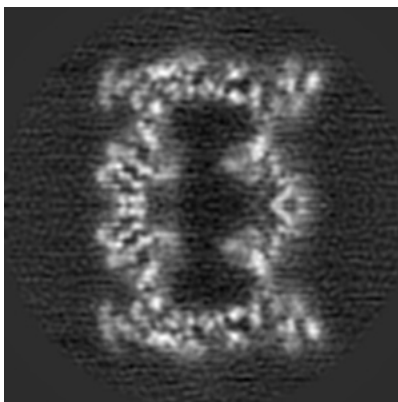


Z Index: 62

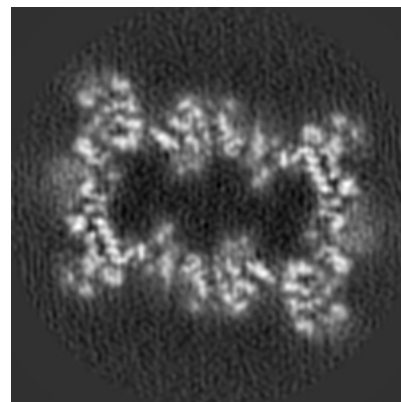
6.2.2 Raw map



X Index: 62



Y Index: 62

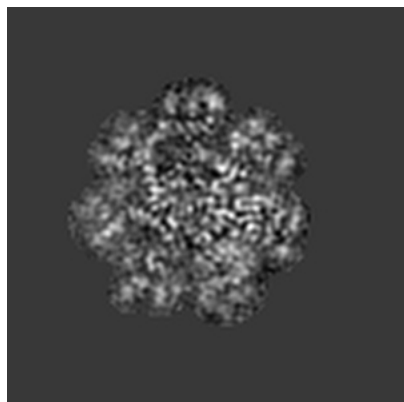


Z Index: 62

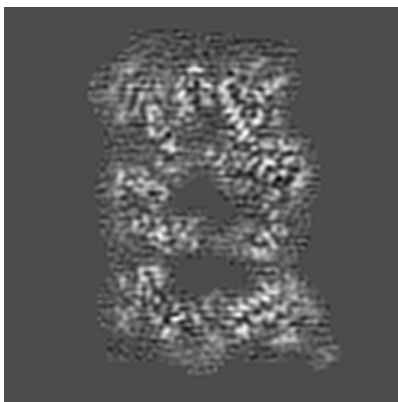
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

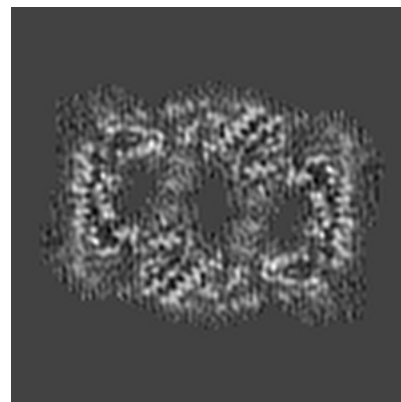
6.3.1 Primary map



X Index: 99

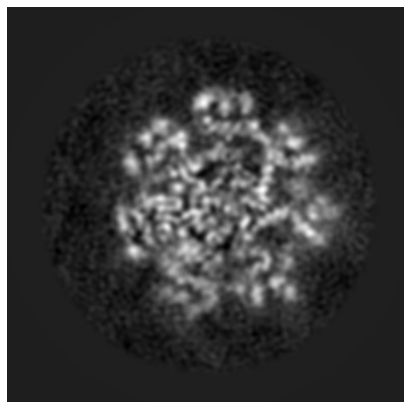


Y Index: 71

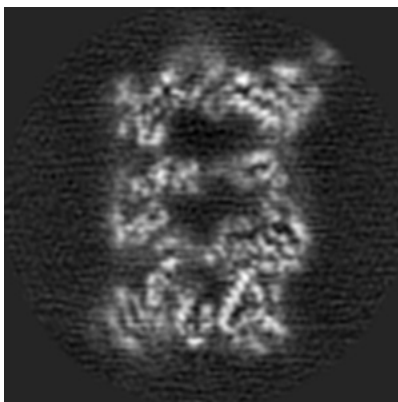


Z Index: 72

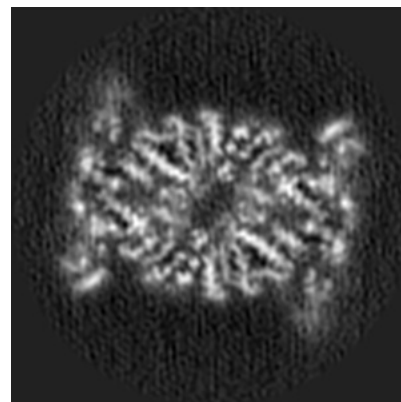
6.3.2 Raw map



X Index: 25



Y Index: 53



Z Index: 48

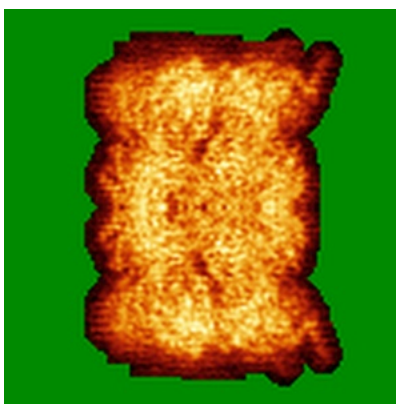
The images above show the largest variance slices of the map in three orthogonal directions.

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

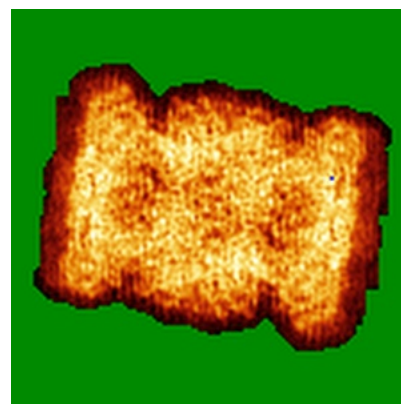
6.4.1 Primary map



X

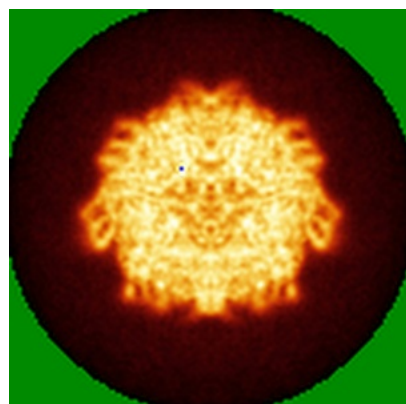


Y

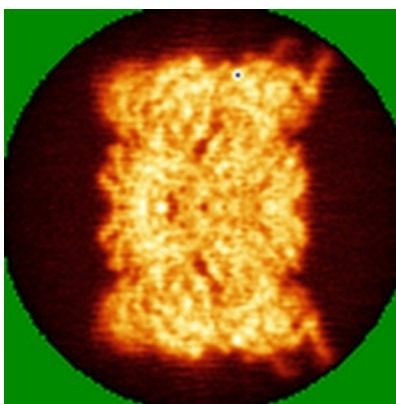


Z

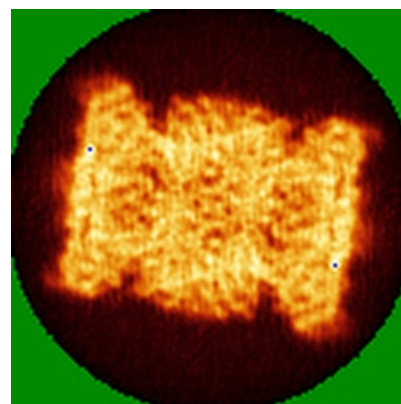
6.4.2 Raw map



X



Y

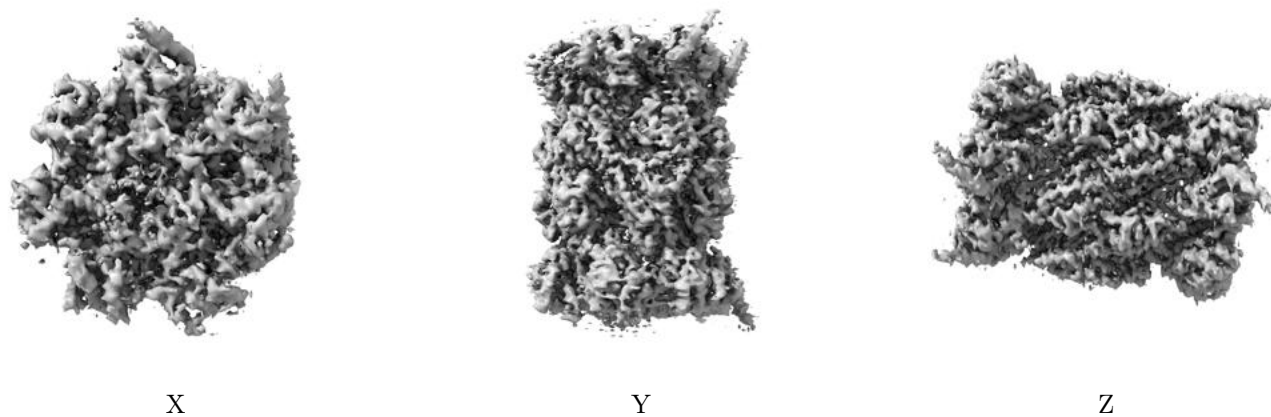


Z

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.

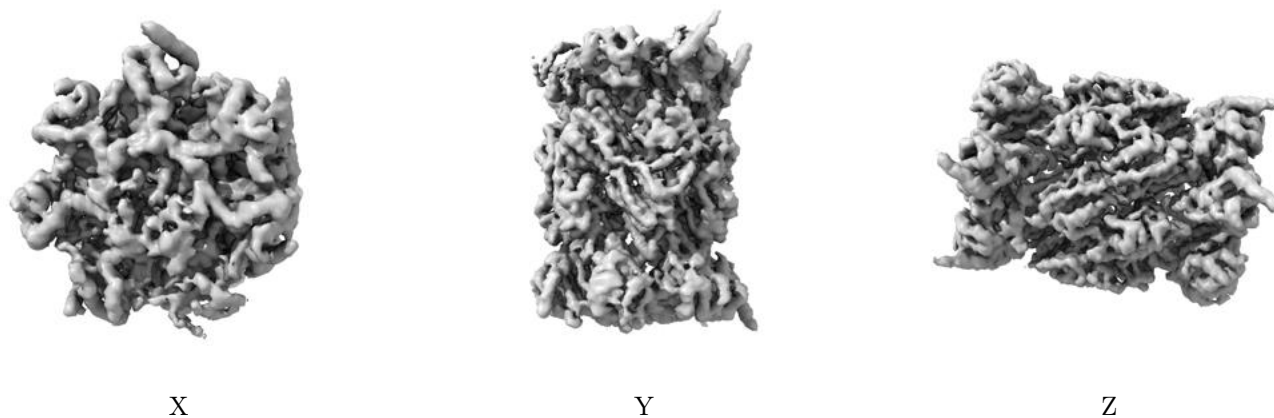
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. 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



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.

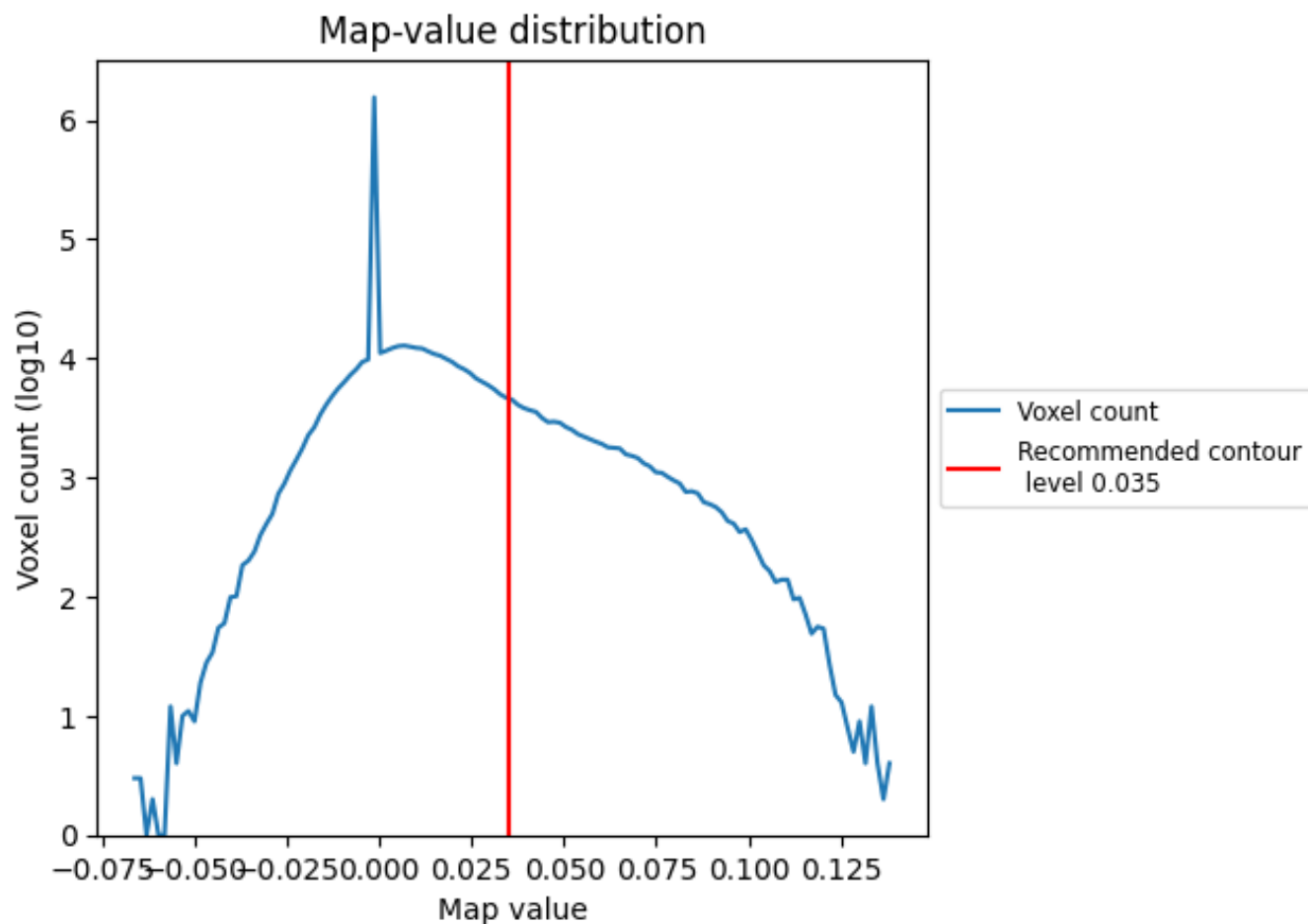
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

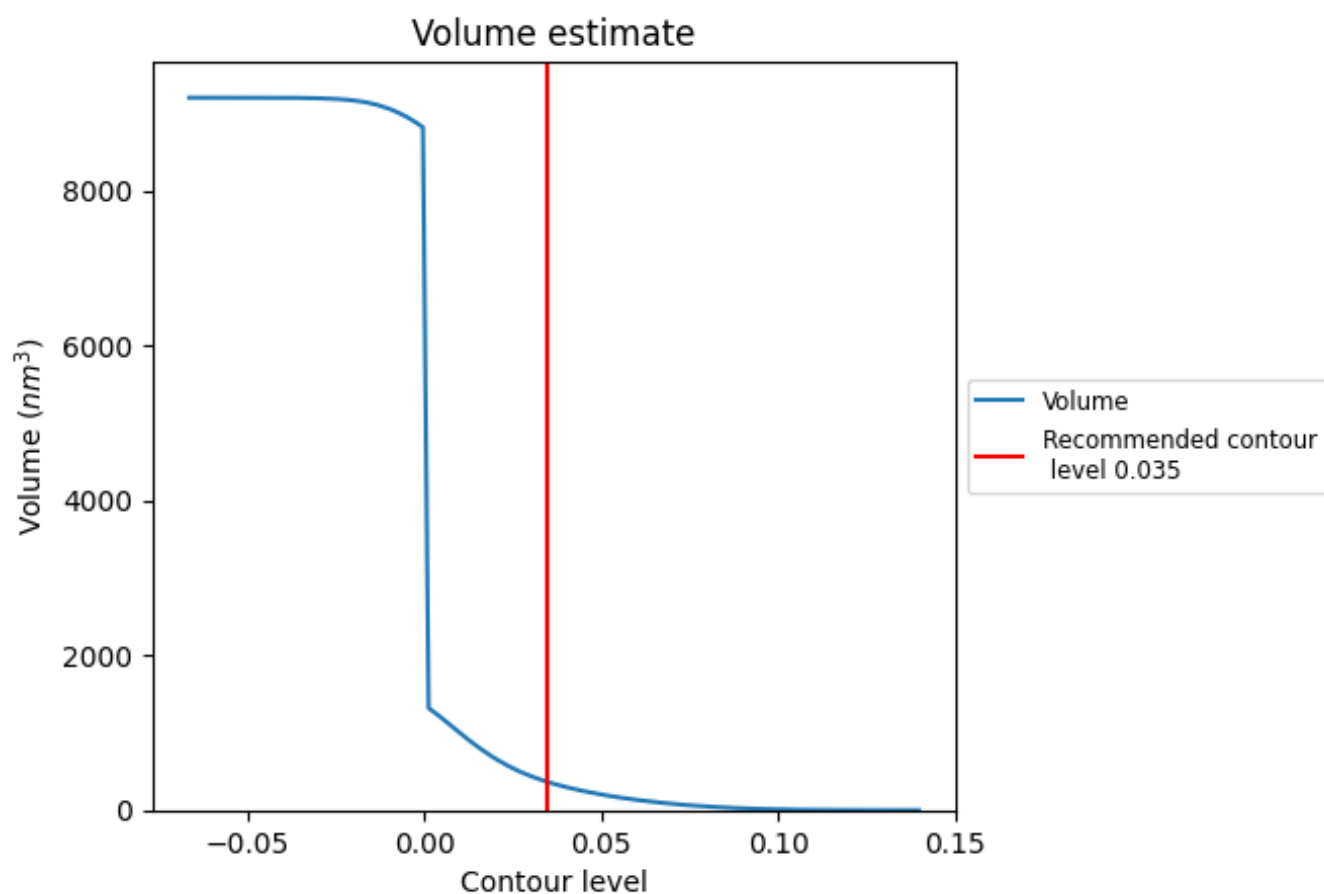
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

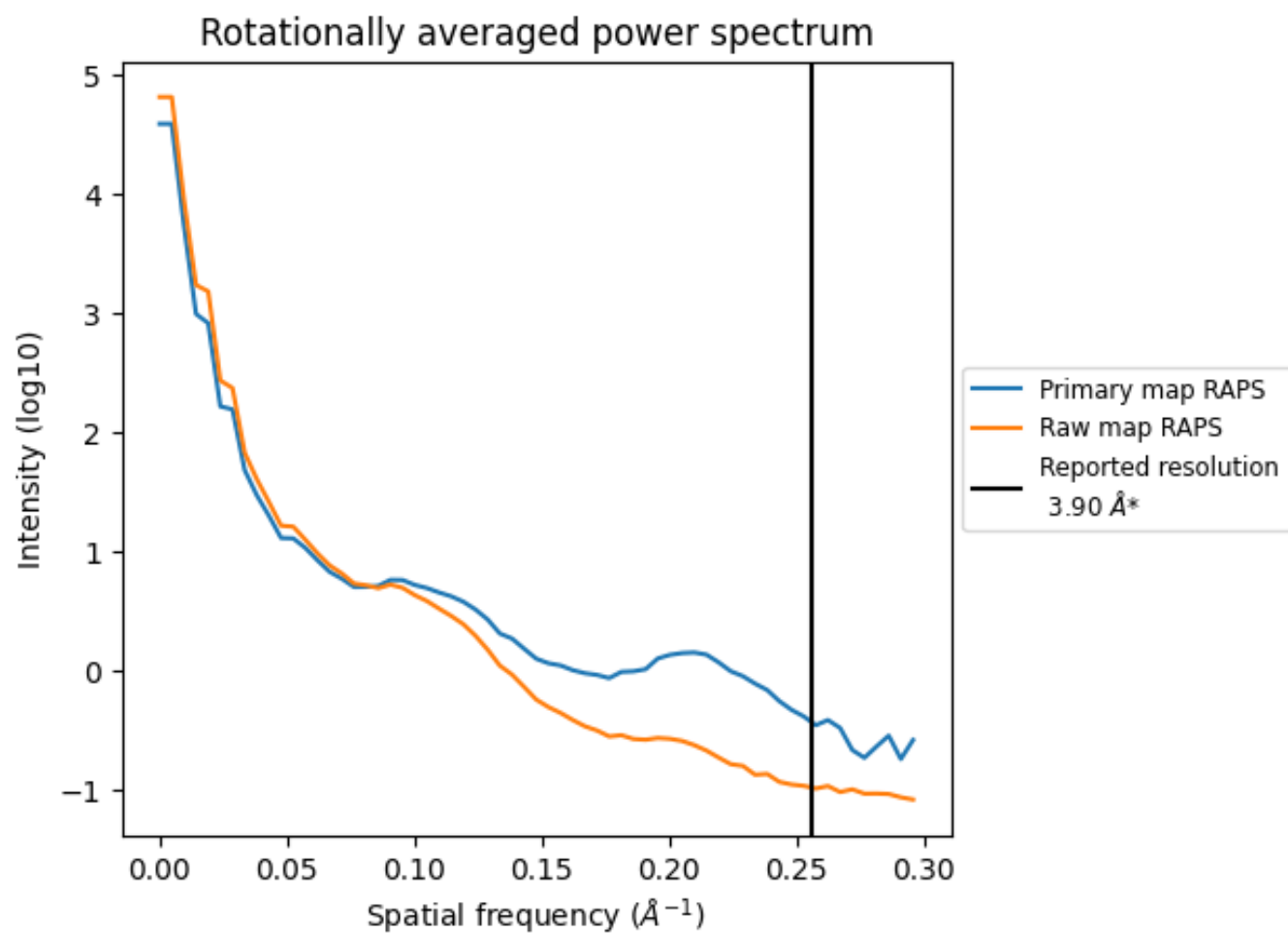
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 364 nm^3 ; this corresponds to an approximate mass of 329 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

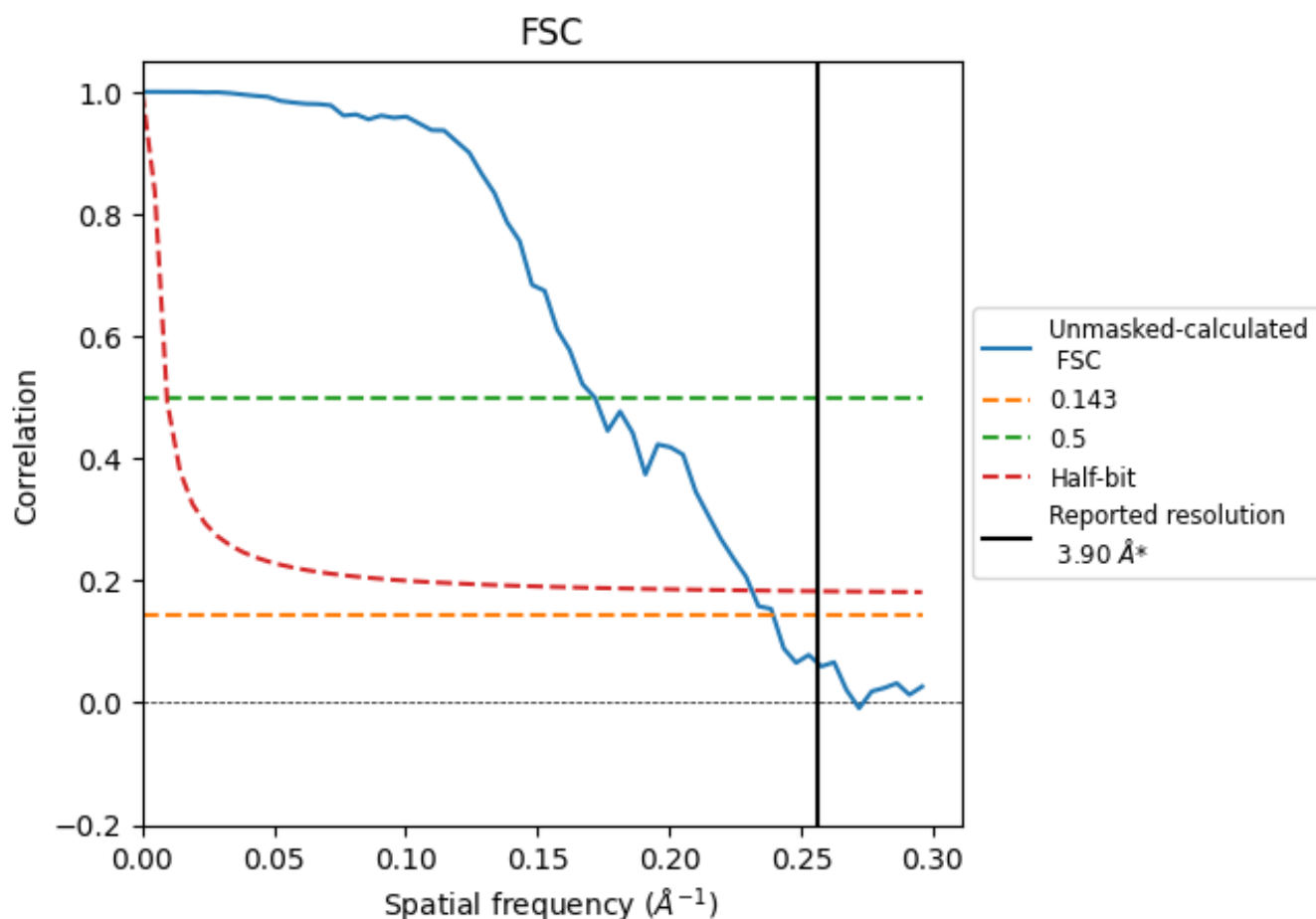


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 \AA^{-1}

8.2 Resolution estimates [i](#)

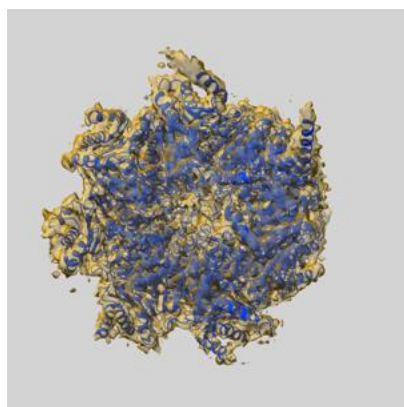
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.18	5.83	4.32

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

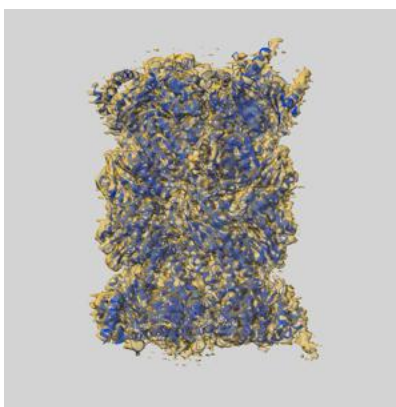
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53414 and PDB model 9QVX. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

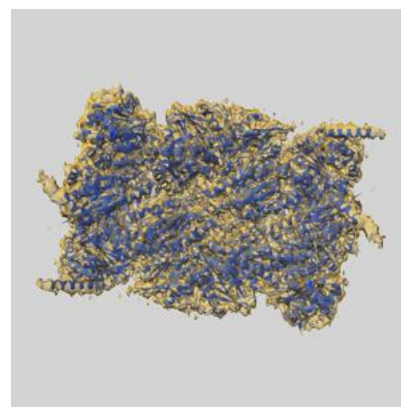
9.1 Map-model overlay [i](#)



X



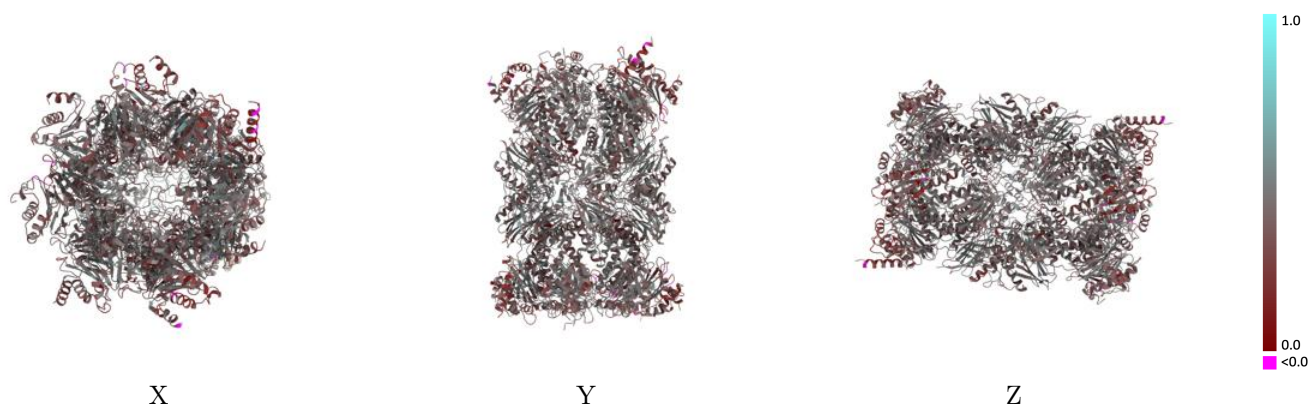
Y



Z

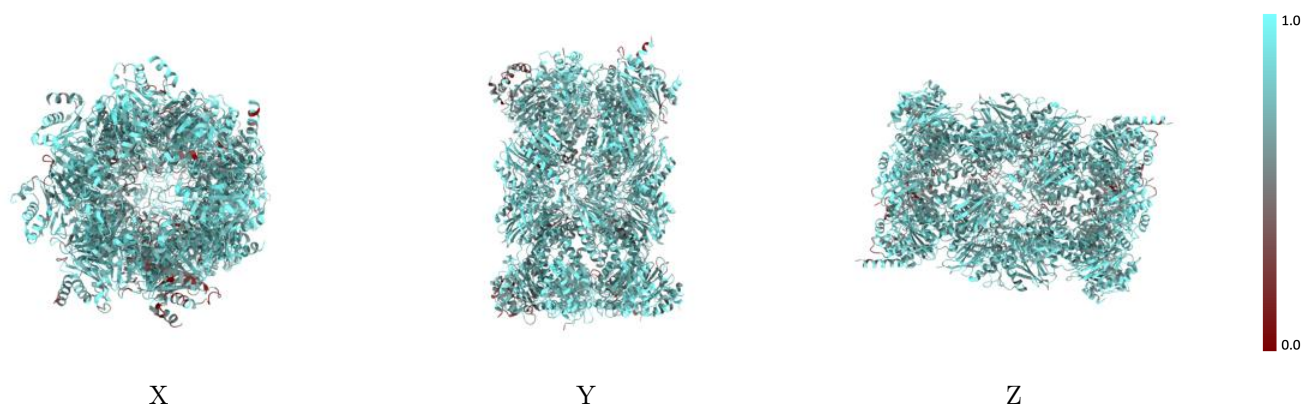
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



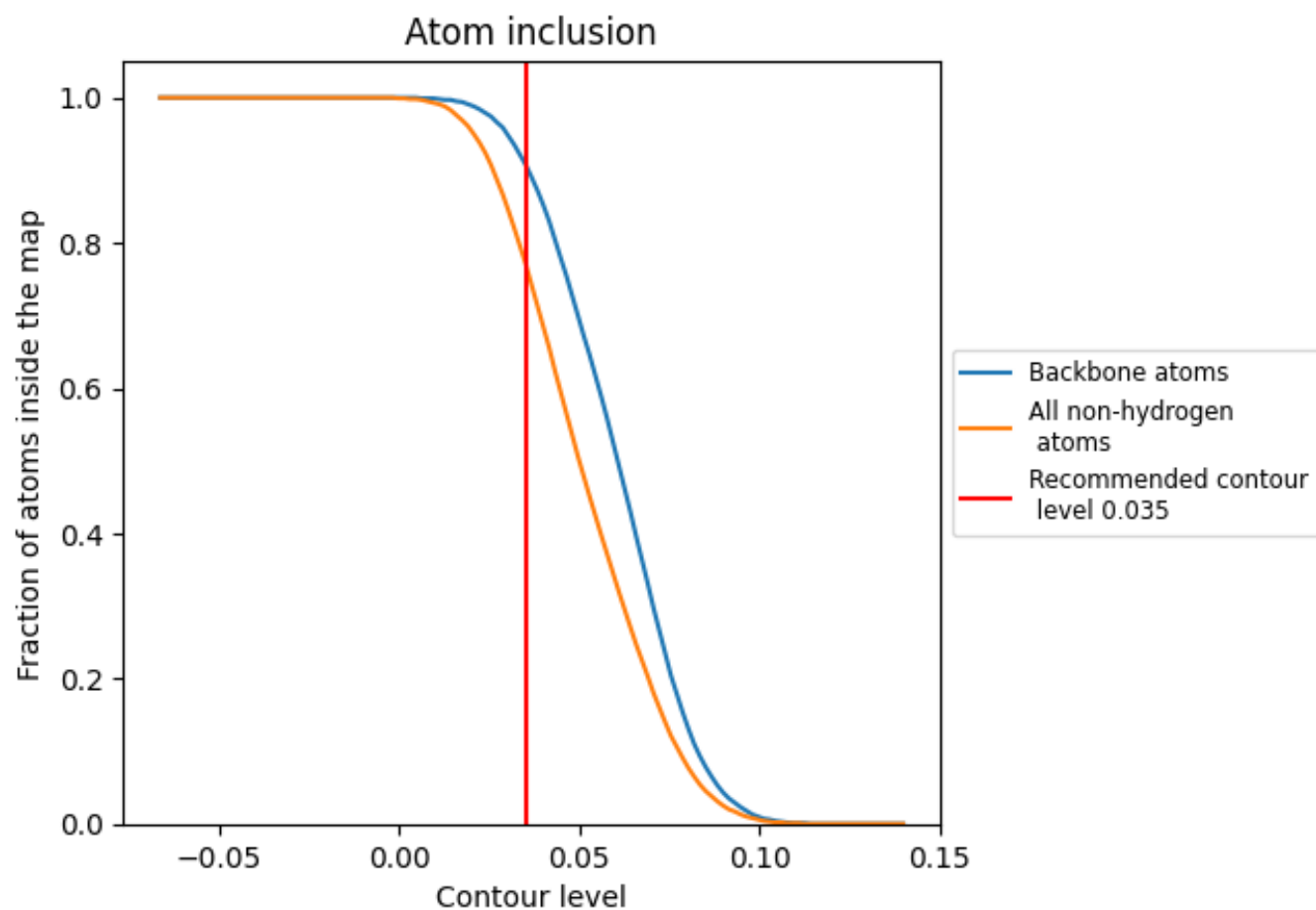
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).































































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 77% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7720	 0.4010
A	 0.6570	 0.3720
B	 0.8140	 0.4160
C	 0.7730	 0.3640
D	 0.7530	 0.3590
E	 0.7970	 0.4180
F	 0.7820	 0.3880
G	 0.7610	 0.3980
H	 0.7790	 0.4000
I	 0.7630	 0.3990
J	 0.7890	 0.4310
K	 0.7920	 0.4230
L	 0.7680	 0.4000
M	 0.7760	 0.4200
N	 0.8260	 0.4340
O	 0.6560	 0.3720
P	 0.8080	 0.4170
Q	 0.7730	 0.3640
R	 0.7550	 0.3600
S	 0.7950	 0.4110
T	 0.7790	 0.3920
U	 0.7610	 0.4010
V	 0.7840	 0.3990
W	 0.7670	 0.3990
X	 0.7840	 0.4310
Y	 0.7960	 0.4220
Z	 0.7700	 0.3970
a	 0.7730	 0.4170
b	 0.8230	 0.4380
c	 0.4500	 0.5120
d	 0.3000	 0.4310

