



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 08:38 PM UTC

PDB ID : 7QVE / pdb_00007qve
EMDB ID : EMD-14175
Title : Spinach 20S proteasome
Authors : Kandolf, S.; Grishkovskaya, I.; Meinhart, A.; Haselbach, D.
Deposited on : 2022-01-21
Resolution : 3.30 Å (reported)
Based on initial model : 6MSB

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:

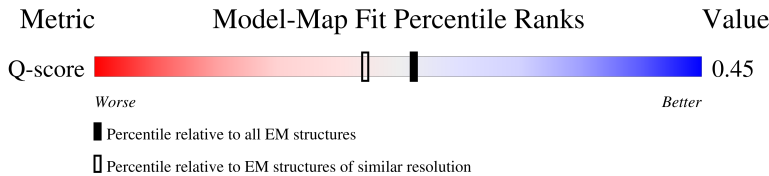
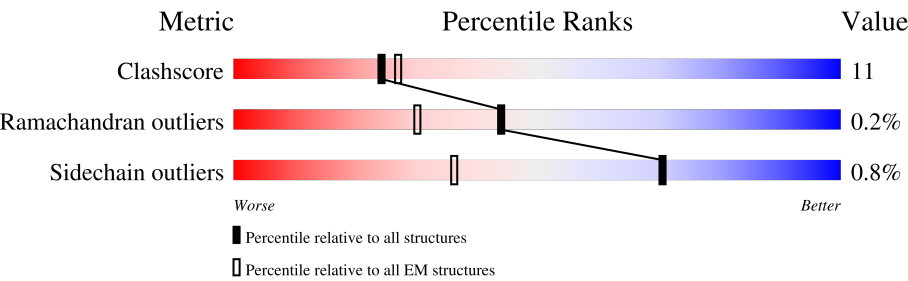
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.30 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.



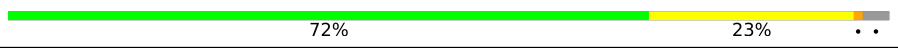
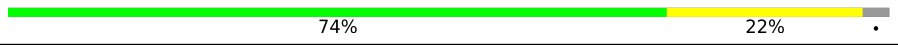
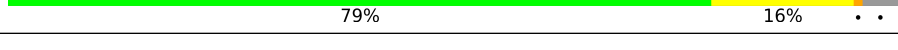
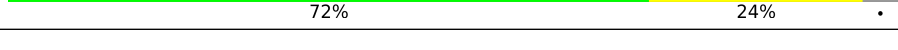
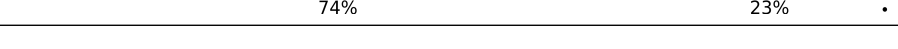
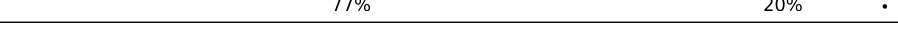
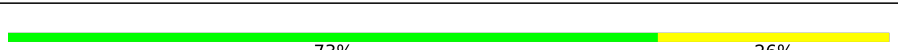
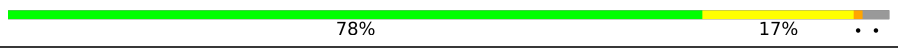
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	C	235	
1	i	235	
2	D	250	
2	j	250	

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Mol	Chain	Length	Quality of chain
3	E	247	
3	k	247	
4	F	237	
4	l	237	
5	G	274	
5	m	274	
6	X	249	
6	n	249	
7	B	246	
7	h	246	
8	a	236	
8	o	236	
9	b	274	
9	p	274	
10	c	204	
10	q	204	
11	d	209	
11	r	209	
12	e	272	
12	s	272	
13	f	223	
13	t	223	
14	g	240	
14	u	240	

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 48322 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	i	229	Total	C	N	O	S	0	0
			1754	1117	291	342	4		
1	C	229	Total	C	N	O	S	0	0
			1754	1117	291	342	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	j	249	Total	C	N	O	S	0	0
			1920	1209	322	380	9		
2	D	249	Total	C	N	O	S	0	0
			1920	1209	322	380	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	k	240	Total	C	N	O	S	0	0
			1845	1157	327	358	3		
3	E	240	Total	C	N	O	S	0	0
			1845	1157	327	358	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	l	230	Total	C	N	O	S	0	0
			1763	1104	294	357	8		
4	F	230	Total	C	N	O	S	0	0
			1763	1104	294	357	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	m	231	Total	C	N	O	S	0	0
			1794	1129	312	345	8		
5	G	231	Total	C	N	O	S	0	0
			1794	1129	312	345	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	n	239	Total	C	N	O	S	0	0
			1842	1164	320	347	11		
6	X	239	Total	C	N	O	S	0	0
			1842	1164	320	347	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	238	Total	C	N	O	S	0	0
			1861	1180	319	356	6		
7	h	238	Total	C	N	O	S	0	0
			1861	1180	319	356	6		

- Molecule 8 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	o	212	Total	C	N	O	S	0	0
			1617	1024	273	317	3		
8	a	212	Total	C	N	O	S	0	0
			1617	1024	273	317	3		

- Molecule 9 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	p	220	Total	C	N	O	S	0	0
			1648	1033	286	320	9		
9	b	220	Total	C	N	O	S	0	0
			1648	1033	286	320	9		

- Molecule 10 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	q	203	Total	C	N	O	S	0	0
			1593	1010	269	303	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	c	203	Total	C	N	O	S	0	0
			1593	1010	269	303	11		

- Molecule 11 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	r	196	Total	C	N	O	S	0	0
			1524	972	260	284	8		
11	d	196	Total	C	N	O	S	0	0
			1524	972	260	284	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	s	203	Total	C	N	O	S	0	0
			1553	985	270	288	10		
12	e	203	Total	C	N	O	S	0	0
			1553	985	270	288	10		

- Molecule 13 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	t	217	Total	C	N	O	S	0	0
			1695	1074	286	325	10		
13	f	217	Total	C	N	O	S	0	0
			1695	1074	286	325	10		

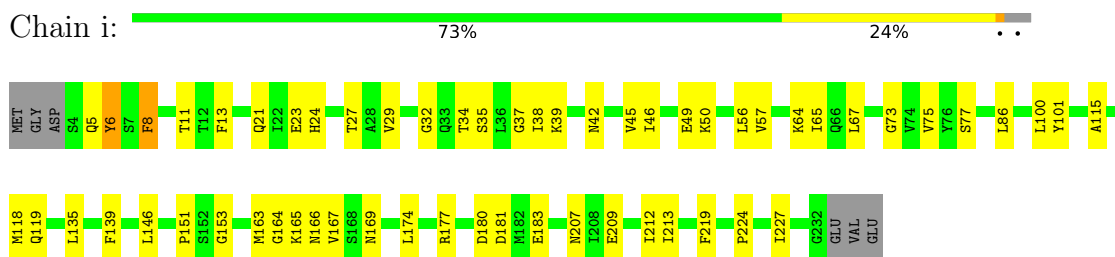
- Molecule 14 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	u	221	Total	C	N	O	S	0	0
			1752	1120	300	326	6		
14	g	221	Total	C	N	O	S	0	0
			1752	1120	300	326	6		

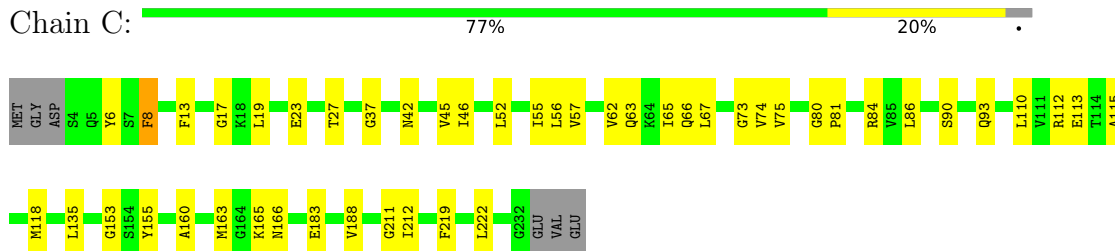
3 Residue-property plots

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

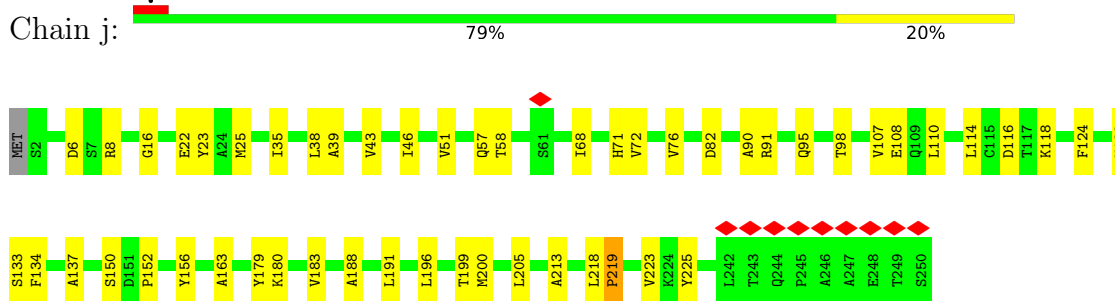
- Molecule 1: Proteasome subunit alpha type



- Molecule 1: Proteasome subunit alpha type

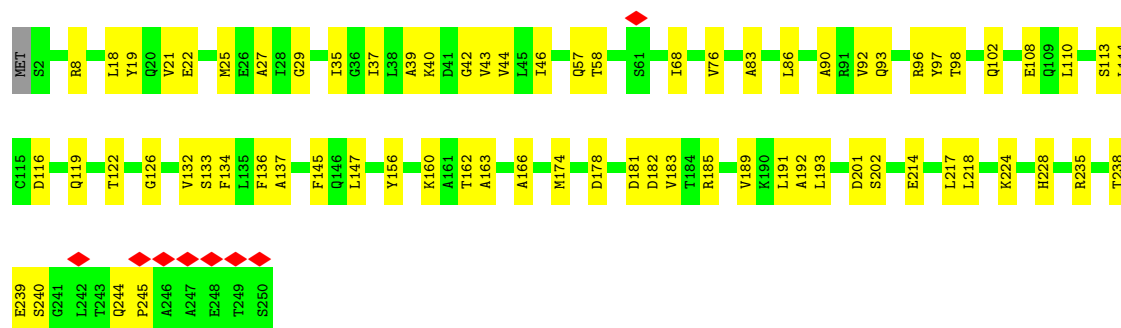


- Molecule 2: Proteasome subunit alpha type



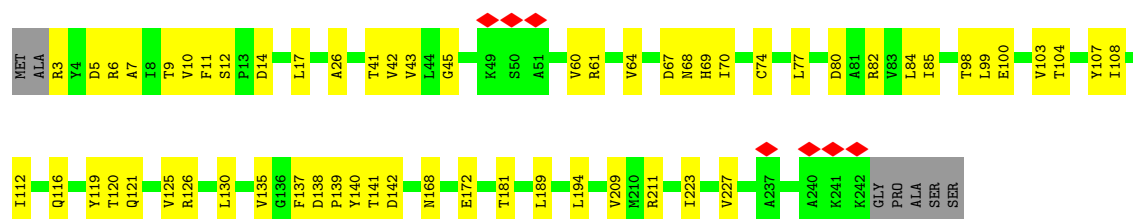
- Molecule 2: Proteasome subunit alpha type





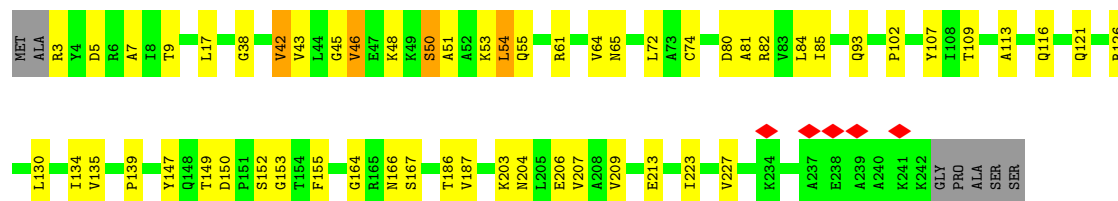
- Molecule 3: Proteasome subunit alpha type

Chain k: 73% 24%



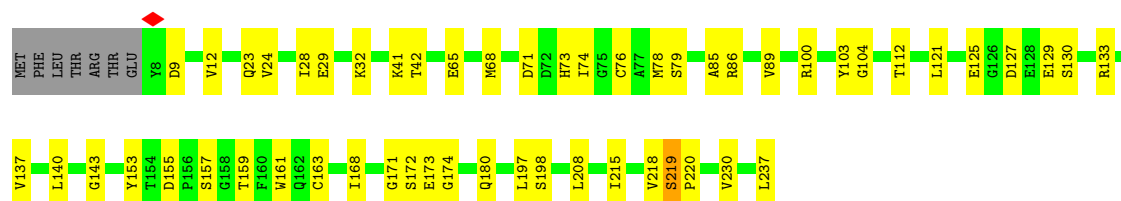
- Molecule 3: Proteasome subunit alpha type

Chain E: 74% 21%



- Molecule 4: Proteasome subunit alpha type

Chain I: 74% 22%



- Molecule 4: Proteasome subunit alpha type

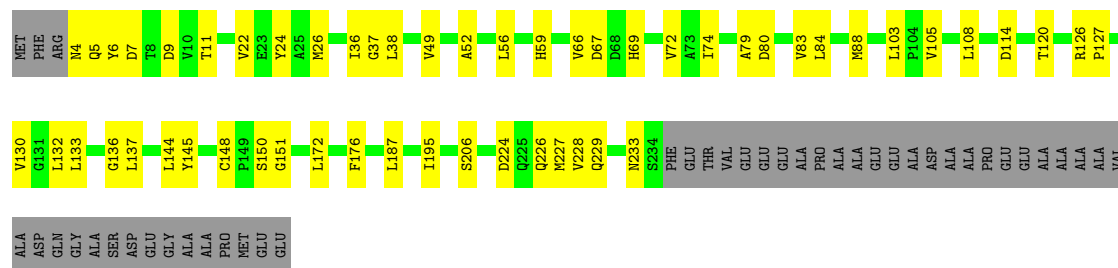
Chain F: 72% 23%





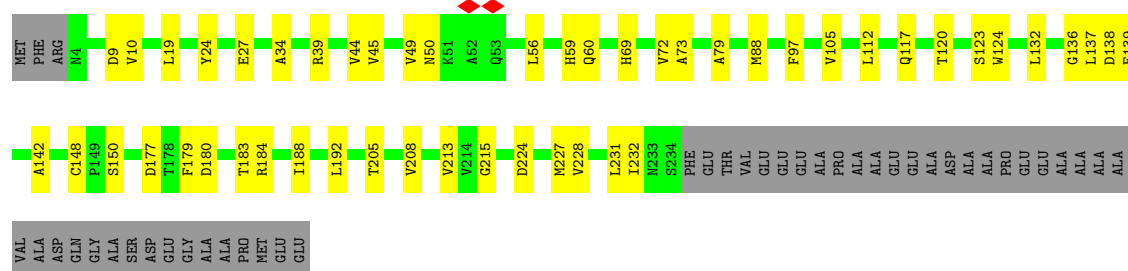
• Molecule 5: Proteasome subunit alpha type

Chain m: 65% 20% 16%



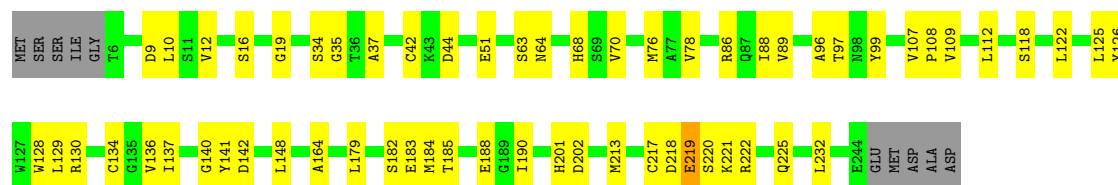
• Molecule 5: Proteasome subunit alpha type

Chain G: 66% 18% 16%



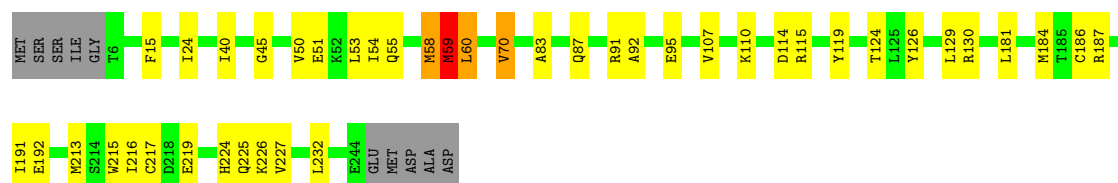
• Molecule 6: Proteasome subunit alpha type-3

Chain n: 72% 24% 4%



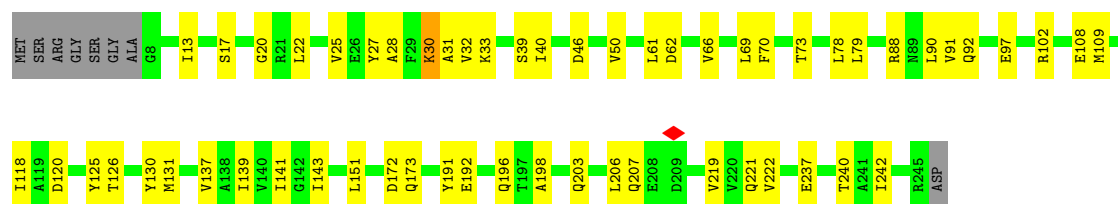
• Molecule 6: Proteasome subunit alpha type-3

Chain X: 79% 16% 5%



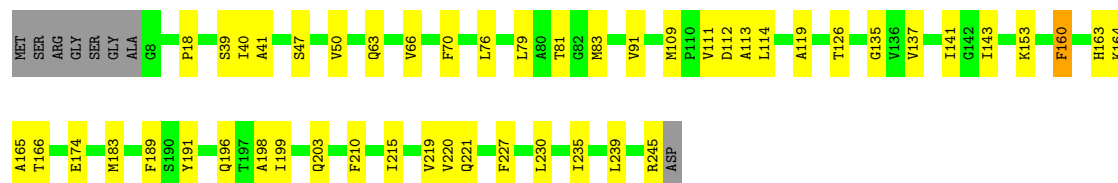
• Molecule 7: Proteasome subunit alpha type

Chain B:  74% 23% .



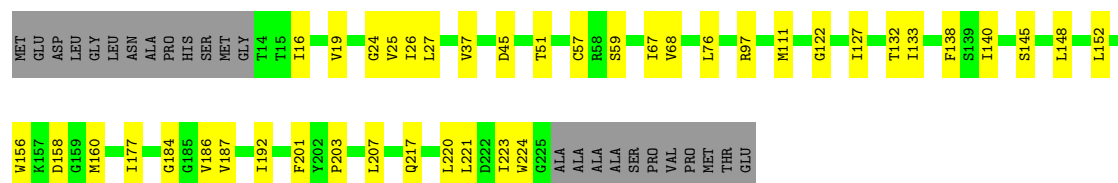
- Molecule 7: Proteasome subunit alpha type

Chain h:  77% 20% .



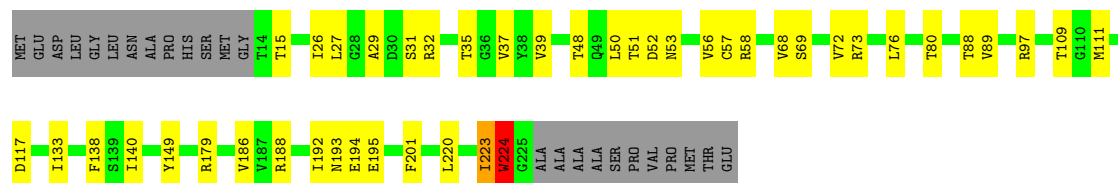
- Molecule 8: Proteasome subunit beta

Chain o:  72% 17% 10%



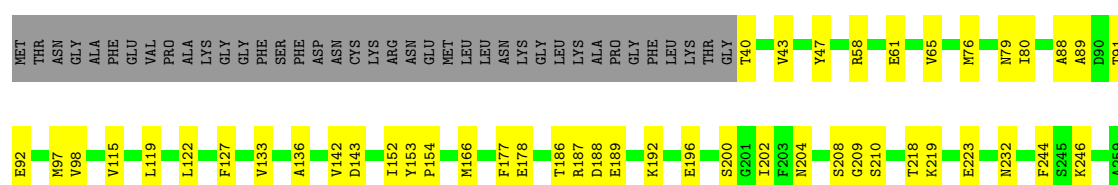
- Molecule 8: Proteasome subunit beta

Chain a:  71% 18% 10%



- Molecule 9: Proteasome subunit beta

Chain p:  63% 17% 20%



GLN
ARG
ALA
VAL
THR
GLU
ARG
GLY
ASP
ALA
MET
GLU
GLU

• Molecule 9: Proteasome subunit beta

Chain b: 

MET THR ASN GLY ALA VAL PHE THR GLU VAL PRO PRO ALA LYS GLY GLY PHE SER PHE ASP ASN CYS LYS ARG ASN ASN GLU MET LEU LEU ASN LYS GLY LEU LYS LYS ALA PRO GLY PHE LEU LYS THR GLY T40 V43 Q44 D56 T57 R58 V65 K72 M76 Y81 A85 G86 T87

D90 T91 V94 V98 L102 H105 T109 R114 A118 L119 H125 V133 S134 A135 A136 D143 V144 I152 Y153 P154 T165 M166 F177 E178 R182 E189 I198 G209 S210 N211 V212 D213 V214 T217 T218 V222 R226 N227 R234

T235 Y236 T237 T248 E249 V250 T253 T256 A259 GLN ARG ALA VAL VAL THR GLU ARG GLY ASP MET LEU GLU GLU

• Molecule 10: Proteasome subunit beta

Chain q: 

MET S2 E5 M14 V15 I20 D25 R26 R27 V30 Q31 Q33 T34 T35 A36 T37 D38 B41 T45 L49 F50 G55 S58 F69 R70 H71 K72 L73 M82 K83 P84 E85 T86 F87 L90 V91 P107 G111 I120 G121 M123 M124

S125 K129 E130 L131 D134 F135 V136 E150 Y153 V166 S167 Q168 V174 D175 R176 D177 C178 G181 V189 R202 M203 D204

• Molecule 10: Proteasome subunit beta

Chain c: 

MET S2 V12 I20 G23 S24 D25 R26 R27 L28 G29 V30 Q31 T34 I42 H46 L49 R70 H71 K72 L73 Y74 Q75 L76 R77 E78 D81 M82 A88 I94 A110 D114 P118 T122 M123 D124 S125 L131 D134 F135 V136 V137

M152 Y153 K154 P155 D156 M157 E158 P159 E160 F161 L162 F163 E164 S167 Q168 L179 S180 G181 H185 E196 D204

• Molecule 11: Proteasome subunit beta

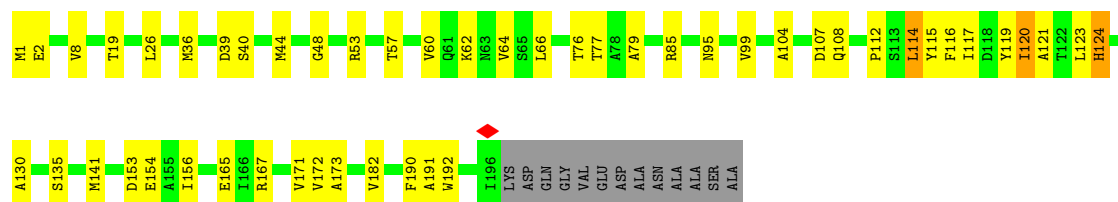
Chain r: 

H1 M10 G11 A21 V22 V27 H28 K29 T30 K37 L38 L43 M44 E49 D52 Q61 V64 F116 I117 D118 Y119 I120 A121 T122 L123 H124 K125 V126 D127 R128 A129 A130 F131 Y136 M141 M142 D143 Y146 S151 E154 R167 V171 V172

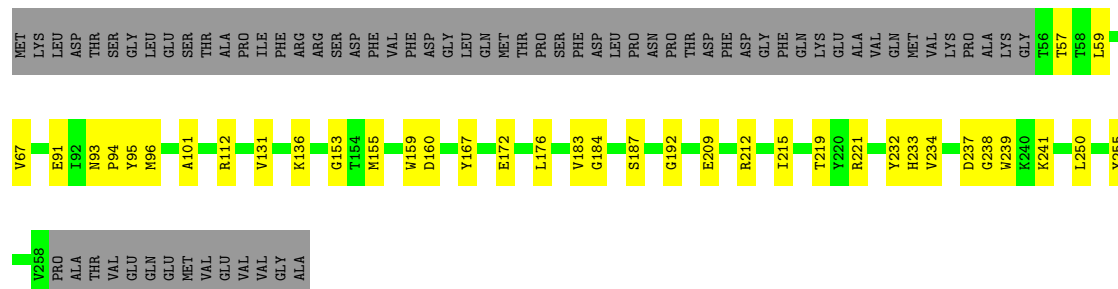
A173 P174 P175 V182 W192 R193 Q194 S195 I196 LYS ASP GLN GLY VAL GLU GLU ASP ALA ASN ALA ALA SER ALA

• Molecule 11: Proteasome subunit beta

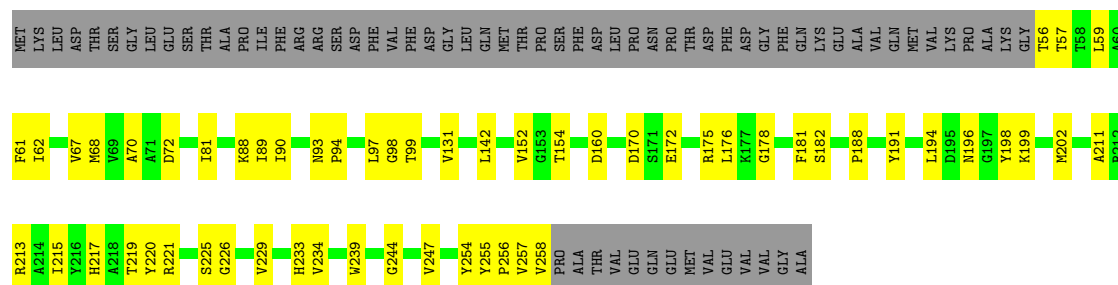
Chain d: 



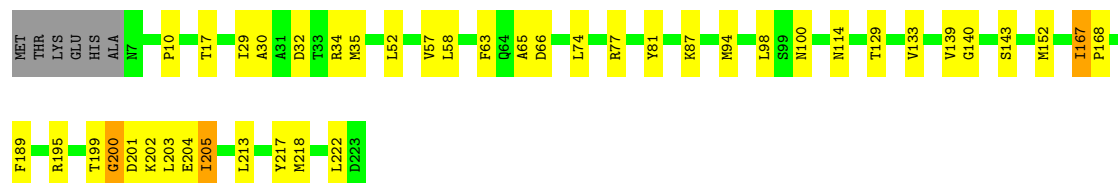
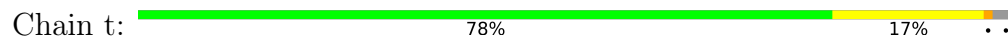
• Molecule 12: Proteasome subunit beta type-5



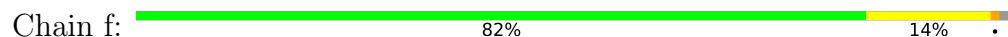
• Molecule 12: Proteasome subunit beta type-5



• Molecule 13: Proteasome subunit beta



• Molecule 13: Proteasome subunit beta

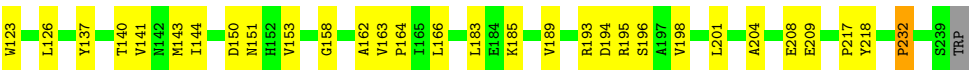
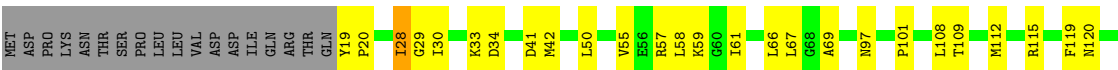




● Molecule 14: Proteasome subunit beta



● Molecule 14: Proteasome subunit beta



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	951422	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80, 50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k), FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.932	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.0168	Depositor
Map size ($\text{\AA}$)	541.696, 541.696, 541.696	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.2311273, 1.2311273, 1.2311273	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	C	0.35	0/1785	0.45	2/2414 (0.1%)
1	i	0.36	0/1785	0.50	1/2414 (0.0%)
2	D	0.33	0/1953	0.40	0/2640
2	j	0.40	0/1953	0.52	0/2640
3	E	0.45	0/1870	0.60	1/2526 (0.0%)
3	k	0.35	0/1870	0.45	0/2526
4	F	0.49	0/1794	0.71	3/2428 (0.1%)
4	l	0.55	0/1794	0.62	0/2428
5	G	0.37	0/1827	0.45	0/2470
5	m	0.46	0/1827	0.55	0/2470
6	X	0.40	0/1876	0.55	1/2529 (0.0%)
6	n	0.41	0/1876	0.57	1/2529 (0.0%)
7	B	0.49	0/1897	0.68	3/2565 (0.1%)
7	h	0.48	0/1897	0.61	1/2565 (0.0%)
8	a	0.58	1/1648 (0.1%)	0.64	0/2238
8	o	0.58	0/1648	0.71	0/2238
9	b	0.59	0/1679	0.75	1/2282 (0.0%)
9	p	0.51	0/1679	0.66	0/2282
10	c	0.52	0/1624	0.64	1/2189 (0.0%)
10	q	0.55	0/1624	0.82	1/2189 (0.0%)
11	d	0.54	0/1553	0.72	3/2099 (0.1%)
11	r	0.49	0/1553	0.58	0/2099
12	e	0.49	0/1589	0.59	1/2146 (0.0%)
12	s	0.45	0/1589	0.53	1/2146 (0.0%)
13	f	0.58	0/1730	0.70	1/2340 (0.0%)
13	t	0.57	0/1730	0.66	2/2340 (0.1%)
14	g	0.54	0/1792	0.70	1/2422 (0.0%)
14	u	0.49	0/1792	0.55	0/2422
All	All	0.48	1/49234 (0.0%)	0.61	25/66576 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	a	31	SER	CA-CB	-7.25	1.47	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	s	255	TYR	CB-CA-C	8.72	119.72	110.65
4	F	70	ILE	N-CA-C	-7.21	103.94	111.58
12	e	255	TYR	CB-CA-C	7.10	118.03	110.65
4	F	123	PHE	CA-CB-CG	6.25	120.05	113.80
7	B	30	LYS	CA-C-N	6.20	130.12	120.82
7	B	30	LYS	C-N-CA	6.20	130.12	120.82
1	C	8	PHE	CA-CB-CG	6.03	119.83	113.80
10	c	159	PRO	CA-C-O	-6.01	114.96	121.27
13	t	168	PRO	N-CA-C	-5.91	100.30	112.47
13	f	168	PRO	N-CA-C	-5.71	100.71	112.47
3	E	155	PHE	CA-CB-CG	5.59	119.39	113.80
11	d	120	ILE	N-CA-C	-5.56	100.31	108.54
7	B	30	LYS	CA-C-O	-5.54	114.53	121.02
7	h	160	PHE	CA-CB-CG	5.54	119.33	113.80
4	F	74	ILE	N-CA-C	5.46	116.30	108.93
11	d	116	PHE	CA-CB-CG	5.36	119.16	113.80
13	t	200	GLY	CA-C-O	-5.30	116.35	121.86
11	d	119	TYR	CB-CA-C	5.30	119.28	110.81
1	C	6	TYR	CB-CA-C	5.23	118.15	111.40
6	X	70	VAL	N-CA-C	-5.20	108.77	113.71
1	i	6	TYR	CB-CA-C	5.20	119.75	111.95
9	b	165	THR	CB-CA-C	-5.17	101.01	109.80
14	g	232	PRO	N-CA-C	-5.12	103.06	111.15
6	n	219	GLU	N-CA-C	-5.01	105.90	111.36
10	q	69	PHE	CA-CB-CG	5.01	118.81	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1754	0	1775	30	0
1	i	1754	0	1775	43	0
2	D	1920	0	1910	52	0
2	j	1920	0	1910	41	0
3	E	1845	0	1872	53	0
3	k	1845	0	1872	44	0
4	F	1763	0	1728	58	0
4	l	1763	0	1728	48	0
5	G	1794	0	1769	41	0
5	m	1794	0	1769	42	0
6	X	1842	0	1847	39	0
6	n	1842	0	1847	42	0
7	B	1861	0	1848	48	0
7	h	1861	0	1848	35	0
8	a	1617	0	1594	39	0
8	o	1617	0	1594	34	0
9	b	1648	0	1640	38	0
9	p	1648	0	1640	38	0
10	c	1593	0	1570	37	0
10	q	1593	0	1570	48	0
11	d	1524	0	1520	34	0
11	r	1524	0	1520	35	0
12	e	1553	0	1518	46	0
12	s	1553	0	1518	27	0
13	f	1695	0	1665	29	0
13	t	1695	0	1665	32	0
14	g	1752	0	1732	44	0
14	u	1752	0	1732	50	0
All	All	48322	0	47976	1034	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 11.

All (1034) 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)
5:m:6:TYR:OH	6:n:9:ASP:OD2	1.61	1.15
14:u:213:THR:HG22	8:a:224:TRP:CZ2	1.81	1.15
3:E:50:SER:CB	3:E:53:LYS:HD3	1.79	1.11
4:F:78:MET:HB3	4:F:139:LEU:CD2	1.87	1.03
3:E:50:SER:HB3	3:E:53:LYS:HD3	1.38	1.03
14:u:213:THR:HG22	8:a:224:TRP:HZ2	1.28	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:p:232:ASN:ND2	13:f:223:ASP:OD1	1.97	0.97
12:e:57:THR:HG22	12:e:72:ASP:OD2	1.67	0.95
8:o:156:TRP:NE1	8:o:158:ASP:OD1	1.99	0.94
4:F:85:ALA:HB2	4:F:137:VAL:HG11	1.50	0.93
3:E:46:VAL:HG12	3:E:206:GLU:HB3	1.48	0.93
4:l:219:SER:OG	4:l:220:PRO:CD	2.17	0.93
3:k:3:ARG:NH1	3:k:5:ASP:OD1	2.03	0.92
12:e:72:ASP:OD1	12:e:215:ILE:CG2	2.18	0.92
5:m:114:ASP:OD1	6:n:86:ARG:NH1	2.04	0.91
7:B:31:ALA:HB2	6:X:15:PHE:HZ	1.36	0.91
12:e:57:THR:CG2	12:e:72:ASP:OD2	2.19	0.89
5:m:148:CYS:SG	5:m:150:SER:OG	2.30	0.89
2:D:116:ASP:OD1	3:E:82:ARG:NH1	2.07	0.88
4:F:78:MET:HB3	4:F:139:LEU:HD23	1.54	0.87
3:k:100:GLU:OE2	12:s:136:LYS:NZ	2.07	0.87
3:E:61:ARG:NH2	3:E:206:GLU:OE2	2.08	0.87
12:e:72:ASP:OD1	12:e:215:ILE:HG23	1.75	0.87
13:f:206:LEU:HD21	13:f:213:LEU:HD12	1.59	0.85
7:h:196:GLN:OE1	7:h:245:ARG:NH2	2.10	0.84
11:r:127:ASP:OD1	11:r:146:TYR:OH	1.95	0.84
6:X:83:ALA:O	6:X:87:GLN:NE2	2.10	0.84
5:m:120:THR:O	6:n:130:ARG:NH1	2.11	0.84
3:E:121:GLN:HG3	4:F:133:ARG:HG2	1.61	0.83
2:D:214:GLU:OE2	2:D:228:HIS:NE2	2.11	0.82
7:B:25:VAL:HG21	7:B:126:THR:HG23	1.60	0.82
12:e:99:THR:O	12:e:154:THR:OG1	1.96	0.81
6:n:96:ALA:HA	6:n:107:VAL:HG21	1.63	0.81
1:C:46:ILE:HD12	1:C:75:VAL:HG23	1.63	0.81
3:E:72:LEU:HD22	3:E:85:ILE:HD11	1.63	0.81
14:u:41:ASP:OD1	14:u:57:ARG:NH2	2.14	0.79
2:j:22:GLU:HA	2:j:25:MET:HE2	1.64	0.78
9:p:79:ASN:ND2	9:p:143:ASP:OD1	2.16	0.78
9:p:187:ARG:NH2	9:p:223:GLU:OE1	2.16	0.78
5:G:72:VAL:HG21	5:G:88:MET:HE1	1.66	0.78
10:c:75:GLN:NE2	10:c:81:ASP:OD1	2.16	0.78
10:q:83:LYS:NZ	10:q:85:GLU:OE1	2.16	0.78
4:l:219:SER:OG	4:l:220:PRO:HD2	1.83	0.77
10:c:25:ASP:OD2	10:c:181:GLY:N	2.17	0.77
9:p:186:THR:HG22	9:p:189:GLU:OE1	1.84	0.77
7:B:39:SER:HB3	7:B:79:LEU:HD21	1.67	0.77
2:D:185:ARG:NH2	2:D:214:GLU:OE1	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:l:85:ALA:HB2	4:l:137:VAL:HG21	1.67	0.76
11:d:156:ILE:HD13	11:d:190:PHE:CE2	2.21	0.76
9:p:188:ASP:OD1	9:p:189:GLU:N	2.19	0.76
14:u:105:HIS:HD1	14:u:137:TYR:HH	1.30	0.76
14:u:157:PHE:HE2	14:u:161:LEU:HD12	1.52	0.75
5:m:151:GLY:O	6:n:86:ARG:NH2	2.19	0.75
4:F:208:LEU:HD13	4:F:213:VAL:HG21	1.69	0.75
9:p:244:PHE:HB3	10:q:168:GLN:NE2	2.02	0.75
14:g:50:LEU:HD13	14:g:198:VAL:HG12	1.68	0.74
7:B:31:ALA:HB2	6:X:15:PHE:CZ	2.20	0.74
6:X:215:TRP:HE1	6:X:227:VAL:HG13	1.52	0.74
8:a:193:ASN:OD1	8:a:194:GLU:N	2.19	0.73
4:l:219:SER:OG	4:l:220:PRO:HD3	1.88	0.73
13:f:89:MET:CE	13:f:94:MET:HE2	2.18	0.73
7:B:130:TYR:OH	1:C:8:PHE:CZ	2.38	0.73
11:d:171:VAL:HG13	11:d:172:VAL:HG13	1.70	0.73
1:i:42:ASN:ND2	1:i:183:GLU:OE1	2.21	0.73
8:o:186:VAL:HG21	8:o:201:PHE:CE1	2.24	0.73
8:a:32:ARG:HG3	8:a:39:VAL:HG13	1.68	0.73
6:n:9:ASP:OD1	6:n:10:LEU:CD2	2.37	0.73
7:B:125:TYR:CE1	7:B:131:MET:HE2	2.23	0.73
4:F:197:LEU:HD11	4:F:215:ILE:HD11	1.69	0.73
5:G:148:CYS:SG	5:G:150:SER:OG	2.47	0.72
1:C:42:ASN:ND2	1:C:183:GLU:OE2	2.21	0.72
11:r:27:VAL:HG11	11:r:30:THR:HG22	1.71	0.72
4:l:103:TYR:OH	13:t:77:ARG:NH2	2.22	0.72
5:G:228:VAL:O	5:G:232:ILE:HD12	1.88	0.72
3:E:9:THR:HG22	3:E:17:LEU:HD12	1.72	0.72
14:u:213:THR:O	8:a:224:TRP:CH2	2.43	0.72
10:q:202:ARG:NH2	10:q:204:ASP:OD2	2.23	0.72
1:i:32:GLY:O	1:i:165:LYS:N	2.24	0.71
2:D:201:ASP:OD1	2:D:202:SER:N	2.24	0.71
11:d:39:ASP:OD1	11:d:40:SER:N	2.22	0.71
7:B:125:TYR:CD1	7:B:131:MET:HE2	2.25	0.70
6:X:215:TRP:CD1	6:X:227:VAL:HG22	2.26	0.70
4:F:78:MET:CB	4:F:139:LEU:HD23	2.21	0.70
5:G:97:PHE:O	13:f:72:LYS:NZ	2.23	0.70
6:n:44:ASP:OD2	6:n:185:THR:OG1	2.08	0.70
3:E:164:GLY:N	3:E:167:SER:OG	2.25	0.70
1:i:164:GLY:O	1:i:167:VAL:HG23	1.92	0.69
5:m:67:ASP:OD1	5:m:69:HIS:ND1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:l:155:ASP:OD1	4:l:157:SER:OG	2.11	0.69
10:q:41:ARG:NH2	10:q:55:GLY:O	2.26	0.69
4:l:65:GLU:OE2	4:l:86:ARG:NH1	2.25	0.68
12:e:72:ASP:OD2	12:e:225:SER:HB3	1.93	0.68
9:p:136:ALA:HB1	9:p:166:MET:HE1	1.76	0.68
2:j:180:LYS:O	2:j:183:VAL:HG23	1.92	0.68
7:h:50:VAL:HG22	7:h:79:LEU:HD22	1.76	0.68
7:h:40:ILE:HD11	7:h:198:ALA:O	1.92	0.68
10:q:123:MET:HG2	10:q:129:LYS:HA	1.73	0.68
2:D:235:ARG:O	2:D:238:THR:OG1	2.08	0.67
14:g:115:ARG:NH2	14:g:120:ASN:OD1	2.27	0.67
11:d:77:THR:OG1	11:d:107:ASP:OD1	2.10	0.67
5:G:60:GLN:N	5:G:60:GLN:OE1	2.28	0.67
14:u:157:PHE:CE2	14:u:161:LEU:HD12	2.29	0.67
1:i:56:LEU:HD13	7:h:165:ALA:HB3	1.75	0.67
3:E:3:ARG:NE	3:E:5:ASP:OD1	2.27	0.67
11:d:104:ALA:HB2	11:d:114:LEU:HD12	1.76	0.67
2:D:108:GLU:OE2	2:D:156:TYR:OH	2.05	0.67
2:D:122:THR:O	3:E:126:ARG:NH1	2.28	0.67
5:m:38:LEU:CD1	5:m:187:LEU:HD22	2.24	0.66
13:t:34:ARG:NH2	13:t:222:LEU:O	2.28	0.66
4:F:193:GLU:OE2	4:F:225:TYR:OH	2.10	0.66
7:B:102:ARG:NH1	7:B:108:GLU:OE1	2.28	0.66
4:F:85:ALA:CB	4:F:137:VAL:HG11	2.25	0.66
11:r:172:VAL:HG12	11:r:172:VAL:O	1.95	0.66
6:n:220:SER:HB2	6:n:225:GLN:HG2	1.76	0.66
8:o:24:GLY:HA2	8:o:122:GLY:HA3	1.78	0.66
4:l:68:MET:HE3	4:l:89:VAL:HG11	1.77	0.66
1:i:11:THR:HG23	1:i:21:GLN:HB3	1.78	0.66
8:o:19:VAL:HG13	8:o:156:TRP:CZ3	2.31	0.66
1:i:46:ILE:HD12	1:i:75:VAL:HG23	1.76	0.65
3:E:38:GLY:HA3	3:E:186:THR:HG21	1.78	0.65
8:a:186:VAL:HG11	8:a:201:PHE:CE1	2.30	0.65
3:E:50:SER:HB3	3:E:53:LYS:CD	2.21	0.65
8:o:19:VAL:HG13	8:o:156:TRP:HZ3	1.61	0.65
3:k:7:ALA:N	4:l:125:GLU:OE2	2.27	0.65
7:h:109:MET:HE3	7:h:114:LEU:HB2	1.78	0.65
7:B:73:THR:HG21	7:B:102:ARG:HH12	1.62	0.65
4:l:74:ILE:CD1	4:l:112:THR:HG21	2.27	0.65
6:n:9:ASP:C	6:n:10:LEU:HD22	2.22	0.65
6:n:185:THR:HG22	6:n:188:GLU:OE1	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:u:229:PHE:O	8:a:188:ARG:NH2	2.28	0.65
5:G:138:ASP:OD1	14:g:97:ASN:ND2	2.29	0.64
3:k:67:ASP:OD1	3:k:68:ASN:N	2.30	0.64
4:l:153:TYR:OH	4:l:161:TRP:NE1	2.30	0.64
3:E:72:LEU:HD21	3:E:74:CYS:SG	2.37	0.64
12:s:112:ARG:NH2	13:t:100:ASN:OD1	2.30	0.64
14:u:25:THR:HG22	14:u:26:SER:H	1.63	0.64
5:m:72:VAL:CG2	5:m:88:MET:HE1	2.28	0.64
2:j:68:ILE:HG21	2:j:110:LEU:HD21	1.80	0.63
3:k:69:HIS:NE2	3:k:137:PHE:O	2.32	0.63
2:D:160:LYS:HB2	3:E:54:LEU:HB3	1.80	0.63
3:E:50:SER:HB2	3:E:53:LYS:HD3	1.77	0.63
3:E:113:ALA:HB1	3:E:153:GLY:O	1.99	0.63
12:s:184:GLY:O	12:s:187:SER:OG	2.10	0.63
1:i:56:LEU:O	7:h:164:LYS:N	2.29	0.63
2:j:6:ASP:OD2	3:k:6:ARG:NE	2.29	0.63
2:D:44:VAL:HG21	2:D:189:VAL:HG22	1.81	0.63
10:q:131:LEU:HD22	10:q:131:LEU:H	1.64	0.63
10:q:20:ILE:HD11	10:q:120:ILE:CG2	2.29	0.63
6:n:9:ASP:OD1	6:n:10:LEU:HD22	1.99	0.62
3:E:7:ALA:HB2	4:F:12:VAL:CG2	2.29	0.62
11:r:167:ARG:HA	11:r:173:ALA:HB1	1.80	0.62
9:b:119:LEU:HD12	9:b:152:ILE:HD11	1.80	0.62
8:a:50:LEU:O	8:a:51:THR:OG1	2.12	0.62
2:D:174:MET:HE3	2:D:178:ASP:OD2	1.99	0.62
12:s:237:ASP:OD1	12:s:238:GLY:N	2.31	0.62
14:u:25:THR:HG22	14:u:26:SER:N	2.14	0.62
9:p:115:VAL:N	9:p:143:ASP:OD2	2.27	0.62
5:G:9:ASP:OD1	5:G:10:VAL:N	2.32	0.62
7:B:50:VAL:CG1	7:B:79:LEU:HD22	2.30	0.61
2:D:76:VAL:HG21	2:D:83:ALA:HB1	1.82	0.61
5:G:72:VAL:HG21	5:G:88:MET:CE	2.30	0.61
11:d:53:ARG:HA	11:d:99:VAL:HG11	1.81	0.61
13:t:143:SER:HB3	13:t:152:MET:HE3	1.81	0.61
7:B:88:ARG:O	7:B:92:GLN:OE1	2.17	0.61
2:j:43:VAL:HG11	2:j:137:ALA:HB1	1.81	0.61
1:C:115:ALA:HB1	1:C:153:GLY:O	2.01	0.61
11:r:10:ASN:OD1	11:r:11:GLY:N	2.33	0.61
14:u:215:SER:HB3	8:a:220:LEU:HD11	1.83	0.61
14:u:213:THR:O	8:a:224:TRP:CZ2	2.54	0.61
6:n:118:SER:O	6:n:122:LEU:HD23	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:76:VAL:HG21	2:D:83:ALA:CB	2.30	0.61
13:t:30:ALA:HB2	13:t:205:ILE:HG23	1.83	0.60
3:k:11:PHE:CZ	4:l:133:ARG:NH2	2.69	0.60
3:k:42:VAL:HG11	3:k:135:VAL:HG13	1.81	0.60
6:n:190:ILE:HG23	6:n:213:MET:HE1	1.82	0.60
4:F:85:ALA:HB2	4:F:137:VAL:CG1	2.28	0.60
6:X:215:TRP:HD1	6:X:227:VAL:HG22	1.66	0.60
11:d:19:THR:HG21	11:d:192:TRP:CH2	2.37	0.60
8:o:68:VAL:HG11	8:o:111:MET:HE1	1.83	0.60
4:F:21:LEU:HD13	4:F:123:PHE:HZ	1.66	0.60
13:t:30:ALA:HB1	13:t:203:LEU:HD11	1.82	0.60
5:G:49:VAL:O	5:G:49:VAL:HG13	2.01	0.60
9:b:119:LEU:CD1	9:b:152:ILE:HD11	2.31	0.60
6:n:213:MET:HE2	6:n:232:LEU:HD13	1.84	0.60
2:D:57:GLN:O	2:D:58:THR:OG1	2.17	0.60
13:t:35:MET:HE1	14:u:146:VAL:HG13	1.84	0.60
3:k:17:LEU:HD21	4:l:133:ARG:HH21	1.67	0.60
6:X:58:MET:O	6:X:59:MET:C	2.44	0.60
12:s:232:TYR:CE1	12:s:241:LYS:HG3	2.37	0.59
3:k:181:THR:HG21	3:k:189:LEU:HD13	1.84	0.59
4:F:218:VAL:O	4:F:218:VAL:HG13	2.02	0.59
11:r:21:ALA:HB1	12:s:176:LEU:HD21	1.84	0.59
8:a:195:GLU:N	8:a:195:GLU:OE1	2.35	0.59
7:B:120:ASP:OD1	1:C:84:ARG:NH1	2.28	0.59
14:u:61:ILE:CD1	14:u:83:LEU:HD13	2.32	0.59
11:d:95:ASN:OD1	11:d:95:ASN:O	2.20	0.59
9:p:119:LEU:HD12	9:p:152:ILE:HD11	1.83	0.59
12:s:131:VAL:HG23	12:s:160:ASP:OD1	2.02	0.59
10:c:25:ASP:OD1	10:c:26:ARG:N	2.33	0.59
11:d:167:ARG:HA	11:d:173:ALA:HB1	1.84	0.59
3:k:80:ASP:OD2	3:k:126:ARG:NH2	2.35	0.59
6:X:40:ILE:HG23	6:X:181:LEU:CD1	2.32	0.59
5:G:112:LEU:HD21	5:G:132:LEU:HD22	1.83	0.59
14:u:213:THR:O	8:a:224:TRP:HH2	1.84	0.59
10:c:46:HIS:CD2	10:c:49:LEU:HD23	2.38	0.59
2:j:72:VAL:CG2	2:j:107:VAL:HG22	2.33	0.59
2:j:124:PHE:HB3	3:k:125:VAL:HG23	1.85	0.58
8:a:186:VAL:HG11	8:a:201:PHE:CZ	2.38	0.58
14:g:42:MET:SD	14:g:217:PRO:HB3	2.42	0.58
2:j:35:ILE:HG22	2:j:163:ALA:CB	2.33	0.58
10:q:87:PHE:O	10:q:91:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:u:50:LEU:HD22	14:u:198:VAL:CG1	2.33	0.58
9:b:76:MET:HE3	9:b:98:VAL:HG13	1.84	0.58
11:r:118:ASP:OD1	11:r:119:TYR:N	2.36	0.58
4:F:197:LEU:HD12	4:F:233:VAL:HG12	1.84	0.58
8:o:186:VAL:HG12	8:o:203:PRO:HA	1.85	0.58
7:h:174:GLU:OE1	7:h:174:GLU:N	2.33	0.58
8:a:48:THR:OG1	8:a:58:ARG:NE	2.34	0.58
3:k:9:THR:HG22	3:k:17:LEU:HD22	1.84	0.58
9:p:58:ARG:HB3	9:p:209:GLY:H	1.68	0.58
14:u:166:LEU:HD23	14:u:182:LEU:HD21	1.85	0.58
8:a:27:LEU:HB3	8:a:57:CYS:SG	2.44	0.58
12:e:131:VAL:HG23	12:e:160:ASP:OD1	2.03	0.58
4:l:198:SER:HB3	4:l:237:LEU:HD11	1.86	0.58
7:B:46:ASP:O	7:B:222:VAL:HG23	2.04	0.58
6:X:187:ARG:NH2	6:X:219:GLU:OE2	2.37	0.58
10:q:38:ASP:OD1	11:r:124:HIS:NE2	2.33	0.57
11:d:36:MET:HE3	11:d:57:THR:HB	1.86	0.57
11:d:156:ILE:HD13	11:d:190:PHE:CZ	2.39	0.57
1:i:45:VAL:HG13	1:i:212:ILE:HG22	1.86	0.57
4:F:219:SER:OG	4:F:220:PRO:CD	2.52	0.57
6:X:187:ARG:NH1	6:X:219:GLU:OE1	2.38	0.57
11:d:153:ASP:OD1	11:d:154:GLU:N	2.37	0.57
6:n:68:HIS:ND1	6:n:89:VAL:HG21	2.19	0.57
4:F:123:PHE:HD1	4:F:123:PHE:H	1.52	0.57
14:u:105:HIS:ND1	14:u:137:TYR:OH	2.18	0.57
14:u:105:HIS:CE1	14:u:137:TYR:HH	2.21	0.57
13:f:49:ILE:HG21	13:f:206:LEU:HD13	1.86	0.57
2:j:71:HIS:ND1	2:j:72:VAL:HG23	2.19	0.57
7:B:69:LEU:HD23	7:B:79:LEU:HB2	1.87	0.57
9:p:178:GLU:OE2	14:g:193:ARG:NH1	2.35	0.57
10:c:70:ARG:HD2	10:c:94:ILE:HD11	1.87	0.56
5:G:138:ASP:OD1	5:G:139:GLU:N	2.38	0.56
4:l:74:ILE:HD13	4:l:112:THR:HG21	1.86	0.56
4:F:99:HIS:HB2	4:F:107:MET:HE3	1.86	0.56
8:o:97:ARG:CG	8:o:133:ILE:HD11	2.35	0.56
14:g:67:LEU:HD13	14:g:126:LEU:HD12	1.86	0.56
1:i:224:PRO:HA	1:i:227:ILE:HG22	1.87	0.56
7:B:192:GLU:O	7:B:196:GLN:HG2	2.04	0.56
14:u:61:ILE:HD13	14:u:83:LEU:HD13	1.87	0.56
12:e:142:LEU:HD21	12:e:152:VAL:CG1	2.35	0.56
12:e:182:SER:HB3	12:e:191:TYR:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:k:223:ILE:O	3:k:227:VAL:HG23	2.06	0.56
4:F:208:LEU:CD1	4:F:213:VAL:HG21	2.34	0.56
7:h:191:TYR:HE1	7:h:219:VAL:HG21	1.70	0.56
7:B:28:ALA:HA	6:X:15:PHE:CE2	2.41	0.56
14:u:140:THR:HB	14:u:153:VAL:HG11	1.88	0.56
6:n:99:TYR:HB3	6:n:107:VAL:HG22	1.88	0.56
7:B:61:LEU:HD23	7:B:62:ASP:N	2.21	0.56
12:e:70:ALA:HB2	12:e:211:ALA:HB1	1.87	0.56
3:E:164:GLY:C	3:E:167:SER:HG	2.14	0.55
7:h:76:LEU:CD2	7:h:111:VAL:HG22	2.36	0.55
2:j:43:VAL:CG1	2:j:137:ALA:HB1	2.35	0.55
3:E:7:ALA:CB	4:F:12:VAL:CG2	2.85	0.55
4:F:92:ALA:HB2	4:F:116:LEU:HD11	1.88	0.55
5:m:36:ILE:HG22	5:m:37:GLY:N	2.21	0.55
1:C:135:LEU:HG	1:C:163:MET:HE2	1.88	0.55
6:X:40:ILE:HG23	6:X:181:LEU:HD12	1.88	0.55
6:X:216:ILE:HG13	6:X:224:HIS:HA	1.88	0.55
2:j:116:ASP:OD1	3:k:82:ARG:NH1	2.40	0.55
7:B:40:ILE:HD11	7:B:198:ALA:O	2.07	0.55
12:s:172:GLU:OE1	12:s:172:GLU:N	2.39	0.55
10:q:14:MET:HE2	10:q:166:VAL:HG22	1.87	0.55
10:q:20:ILE:HD11	10:q:120:ILE:HG21	1.89	0.55
11:d:85:ARG:HG2	11:d:121:ALA:HB1	1.86	0.55
14:g:28:ILE:HG22	14:g:166:LEU:HD11	1.87	0.55
5:m:74:ILE:HG22	5:m:132:LEU:CD2	2.36	0.55
12:s:215:ILE:O	12:s:219:THR:HG23	2.05	0.55
10:q:26:ARG:HG2	10:q:38:ASP:HA	1.88	0.55
8:o:25:VAL:HG22	8:o:192:ILE:HB	1.89	0.55
9:b:143:ASP:CG	9:b:144:VAL:H	2.15	0.55
3:E:51:ALA:HB3	3:E:203:LYS:HD3	1.88	0.55
3:k:168:ASN:O	3:k:172:GLU:OE1	2.26	0.54
14:u:51:ARG:O	8:a:179:ARG:NH1	2.40	0.54
1:C:65:ILE:HG12	1:C:75:VAL:HG22	1.89	0.54
4:F:178:SER:HB3	4:F:199:ILE:HD11	1.88	0.54
5:G:224:ASP:OD1	5:G:227:MET:N	2.34	0.54
10:q:178:CYS:HB3	12:e:81:ILE:HD11	1.89	0.54
14:g:55:VAL:HG13	14:g:55:VAL:O	2.08	0.54
5:m:38:LEU:HD13	5:m:187:LEU:HD22	1.89	0.54
1:C:112:ARG:NE	1:C:155:TYR:OH	2.40	0.54
10:c:25:ASP:OD1	10:c:181:GLY:O	2.26	0.54
4:l:215:ILE:HD11	4:l:230:VAL:HG13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:n:97:THR:HG21	14:u:89:TYR:CE1	2.42	0.54
7:B:50:VAL:HG13	7:B:79:LEU:HD22	1.88	0.54
9:p:133:VAL:HG23	9:p:133:VAL:O	2.07	0.54
13:t:52:LEU:HB3	13:t:94:MET:HE3	1.90	0.54
6:X:184:MET:HE1	6:X:192:GLU:HG3	1.90	0.54
10:q:174:VAL:HG11	10:q:181:GLY:HA2	1.90	0.54
11:r:27:VAL:HG11	11:r:30:THR:CG2	2.37	0.54
3:E:72:LEU:HD23	3:E:72:LEU:C	2.32	0.54
10:q:124:ASP:OD1	10:q:125:SER:N	2.38	0.54
3:E:80:ASP:OD2	3:E:126:ARG:NH2	2.40	0.54
8:o:217:GLN:HE22	8:o:223:ILE:HG12	1.73	0.54
5:G:227:MET:HE3	5:G:231:LEU:HD11	1.90	0.53
6:X:110:LYS:O	6:X:114:ASP:OD2	2.26	0.53
14:g:150:ASP:OD1	14:g:151:ASN:N	2.37	0.53
2:D:39:ALA:HB1	2:D:183:VAL:O	2.08	0.53
2:D:189:VAL:O	2:D:193:LEU:HD23	2.08	0.53
14:g:58:LEU:HD13	14:g:204:ALA:HB2	1.90	0.53
5:m:229:GLN:NE2	5:m:233:ASN:OD1	2.42	0.53
14:g:208:GLU:O	14:g:209:GLU:HG3	2.07	0.53
5:m:7:ASP:OD2	5:m:24:TYR:OH	2.21	0.53
5:m:126:ARG:NH1	5:m:127:PRO:O	2.42	0.53
2:D:43:VAL:HG11	2:D:137:ALA:HB1	1.89	0.53
4:F:92:ALA:CB	4:F:116:LEU:HD11	2.39	0.53
4:F:121:LEU:HD12	5:G:79:ALA:HB3	1.90	0.53
9:b:237:THR:O	9:b:237:THR:HG22	2.08	0.53
2:D:8:ARG:HH12	4:F:8:TYR:N	2.07	0.53
1:C:86:LEU:HD21	1:C:118:MET:HG2	1.91	0.53
12:s:241:LYS:HB3	13:t:167:ILE:HD11	1.90	0.53
14:g:57:ARG:HD2	14:g:69:ALA:O	2.09	0.53
1:i:64:LYS:N	1:i:209:GLU:OE2	2.41	0.53
6:n:9:ASP:O	6:n:10:LEU:HD22	2.08	0.53
7:B:17:SER:O	7:B:20:GLY:N	2.36	0.53
2:D:40:LYS:NZ	2:D:182:ASP:HA	2.24	0.53
11:r:192:TRP:CD1	11:r:194:GLN:HE21	2.27	0.53
13:t:133:VAL:HG12	13:t:133:VAL:O	2.09	0.53
13:f:29:ILE:HD12	13:f:29:ILE:H	1.73	0.53
4:l:85:ALA:CB	4:l:137:VAL:HG21	2.38	0.53
1:C:45:VAL:HG21	1:C:188:VAL:HG22	1.91	0.53
2:j:91:ARG:HB3	10:q:73:LEU:HD11	1.91	0.52
5:G:137:LEU:HD11	5:G:215:GLY:O	2.08	0.52
6:X:24:ILE:HD11	6:X:124:THR:HG23	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:u:66:LEU:HD22	14:u:206:ILE:HB	1.91	0.52
9:b:85:ALA:O	9:b:91:THR:HG21	2.09	0.52
7:B:27:TYR:C	6:X:15:PHE:HE2	2.18	0.52
6:X:124:THR:O	6:X:124:THR:HG22	2.09	0.52
13:t:81:TYR:OH	13:t:87:LYS:NZ	2.31	0.52
8:a:76:LEU:O	8:a:80:THR:HG22	2.09	0.52
10:c:30:VAL:O	10:c:31:GLN:C	2.52	0.52
10:c:88:ALA:O	10:c:123:MET:HE1	2.09	0.52
4:l:197:LEU:HD11	4:l:215:ILE:HD13	1.91	0.52
1:i:119:GLN:NE2	2:j:82:ASP:OD1	2.39	0.52
11:d:44:MET:HE1	11:d:60:VAL:HG11	1.90	0.52
4:F:180:GLN:HA	5:G:56:LEU:HD21	1.91	0.52
6:X:53:LEU:H	6:X:53:LEU:HD23	1.75	0.52
8:o:97:ARG:HG3	8:o:133:ILE:HD11	1.92	0.52
7:B:50:VAL:HG12	7:B:69:LEU:HD21	1.92	0.52
14:u:42:MET:SD	14:u:217:PRO:HB3	2.50	0.52
4:F:202:GLN:NE2	4:F:203:VAL:HG23	2.25	0.52
4:F:78:MET:HA	4:F:139:LEU:HD23	1.92	0.52
8:a:220:LEU:HD21	8:a:224:TRP:CE3	2.45	0.52
1:i:181:ASP:C	1:i:181:ASP:OD1	2.53	0.52
12:e:97:LEU:HD11	12:e:239:TRP:CG	2.45	0.52
10:c:30:VAL:HG12	10:c:31:GLN:H	1.73	0.51
14:g:61:ILE:HD11	14:g:67:LEU:HG	1.92	0.51
3:E:43:VAL:HG13	3:E:209:VAL:HG12	1.92	0.51
11:d:8:VAL:HG13	11:d:112:PRO:HB2	1.92	0.51
9:p:88:ALA:O	9:p:92:GLU:OE1	2.28	0.51
11:r:116:PHE:CE1	11:r:131:PHE:CZ	2.98	0.51
11:d:60:VAL:O	11:d:64:VAL:HG23	2.10	0.51
4:F:76:CYS:SG	4:F:139:LEU:HB3	2.50	0.51
10:q:71:HIS:HD2	10:q:82:MET:HE3	1.75	0.51
9:b:250:VAL:HG11	9:b:253:THR:HG22	1.91	0.51
9:b:43:VAL:CG1	9:b:177:PHE:CZ	2.94	0.51
12:e:142:LEU:HD23	12:e:170:ASP:O	2.11	0.51
14:g:185:LYS:O	14:g:189:VAL:HG23	2.11	0.51
1:i:65:ILE:HG12	1:i:75:VAL:CG2	2.41	0.51
4:F:73:HIS:ND1	4:F:74:ILE:HG13	2.25	0.51
10:q:34:THR:OG1	12:e:221:ARG:HA	2.11	0.51
4:l:180:GLN:HG2	5:m:56:LEU:HG	1.92	0.51
8:a:223:ILE:HG23	8:a:224:TRP:H	1.76	0.51
14:g:194:ASP:O	14:g:195:ARG:HG2	2.11	0.51
1:i:57:VAL:HA	7:h:163:HIS:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:126:TYR:HD2	6:X:129:LEU:HD12	1.75	0.51
3:k:138:ASP:O	3:k:141:THR:OG1	2.24	0.50
2:D:235:ARG:O	2:D:239:GLU:OE1	2.29	0.50
12:e:172:GLU:N	12:e:172:GLU:OE1	2.43	0.50
13:f:162:PRO:HB3	13:f:166:LEU:HD12	1.93	0.50
2:D:35:ILE:HG22	2:D:163:ALA:CB	2.41	0.50
10:q:2:SER:HG	10:q:5:GLU:CD	2.17	0.50
1:i:67:LEU:HD23	1:i:67:LEU:H	1.77	0.50
4:l:153:TYR:HH	4:l:161:TRP:NE1	2.07	0.50
13:f:49:ILE:HG21	13:f:206:LEU:CD1	2.41	0.50
3:k:84:LEU:HD11	3:k:112:ILE:HG23	1.93	0.50
5:m:49:VAL:CG2	5:m:195:ILE:HD12	2.42	0.50
5:G:228:VAL:HG22	5:G:232:ILE:CD1	2.42	0.50
11:r:27:VAL:CG1	11:r:30:THR:HG22	2.38	0.50
11:r:120:ILE:O	11:r:121:ALA:HB3	2.12	0.50
11:r:142:MET:O	11:r:146:TYR:N	2.41	0.50
2:D:93:GLN:OE1	2:D:113:SER:OG	2.28	0.50
5:G:188:ILE:O	5:G:192:LEU:HD23	2.11	0.50
8:o:51:THR:HG23	8:o:76:LEU:CD2	2.41	0.50
10:q:25:ASP:OD2	10:q:181:GLY:N	2.40	0.50
9:b:182:ARG:NH2	9:b:189:GLU:OE2	2.44	0.50
10:c:74:TYR:CE2	10:c:78:GLU:OE2	2.64	0.50
9:p:61:GLU:O	9:p:61:GLU:HG3	2.12	0.50
9:p:88:ALA:O	9:p:89:ALA:C	2.55	0.50
14:u:50:LEU:HD13	14:u:198:VAL:HG12	1.93	0.50
9:b:76:MET:HE1	9:b:118:ALA:HB1	1.94	0.50
13:f:209:ASN:OD1	13:f:210:LYS:N	2.37	0.50
2:D:18:LEU:O	2:D:19:TYR:C	2.53	0.50
11:r:43:LEU:HD12	11:r:182:VAL:HG23	1.94	0.50
1:i:67:LEU:HA	1:i:73:GLY:HA2	1.93	0.50
9:p:244:PHE:HB3	10:q:168:GLN:HE21	1.77	0.50
13:f:98:LEU:HD12	13:f:98:LEU:O	2.12	0.50
2:j:35:ILE:HG22	2:j:163:ALA:HB1	1.93	0.49
2:j:200:MET:HG3	2:j:205:LEU:HD21	1.94	0.49
7:B:130:TYR:OH	1:C:8:PHE:CE1	2.61	0.49
3:E:48:LYS:N	3:E:204:ASN:O	2.42	0.49
8:o:25:VAL:CG2	8:o:192:ILE:HB	2.42	0.49
11:d:36:MET:HE3	11:d:57:THR:CB	2.42	0.49
7:h:41:ALA:HB2	7:h:50:VAL:HG23	1.93	0.49
8:a:53:ASN:O	8:a:192:ILE:HG21	2.12	0.49
2:D:162:THR:HG22	2:D:163:ALA:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:19:LEU:N	5:G:19:LEU:HD12	2.27	0.49
11:d:130:ALA:HB1	11:d:135:SER:HA	1.95	0.49
2:j:95:GLN:HE21	10:q:69:PHE:HA	1.77	0.49
3:k:5:ASP:OD2	4:l:127:ASP:N	2.45	0.49
4:F:85:ALA:N	4:F:137:VAL:HG21	2.27	0.49
14:u:215:SER:OG	8:a:220:LEU:HD21	2.13	0.49
7:B:97:GLU:HG3	7:B:109:MET:HE1	1.95	0.49
10:q:50:PHE:CE1	10:q:189:VAL:HG21	2.47	0.49
3:k:141:THR:O	3:k:142:ASP:OD1	2.31	0.49
4:F:197:LEU:HD11	4:F:215:ILE:CD1	2.38	0.49
12:s:57:THR:HG23	12:s:57:THR:O	2.12	0.49
8:a:68:VAL:O	8:a:72:VAL:HG12	2.12	0.49
10:c:27:ARG:NH2	10:c:179:LEU:O	2.45	0.49
2:D:46:ILE:HG21	2:D:192:ALA:HB1	1.95	0.49
2:D:92:VAL:HG12	2:D:96:ARG:NH1	2.28	0.49
12:e:62:ILE:O	12:e:198:TYR:OH	2.22	0.49
2:j:16:GLY:O	3:k:26:ALA:HB2	2.13	0.49
7:B:90:LEU:HD11	7:B:118:ILE:HD12	1.95	0.49
7:B:203:GLN:O	7:B:207:GLN:N	2.45	0.49
9:p:65:VAL:O	9:p:65:VAL:HG23	2.12	0.49
7:h:70:PHE:CD2	7:h:91:VAL:HG21	2.48	0.49
1:i:101:TYR:HB3	10:q:86:THR:HG23	1.95	0.48
7:B:32:VAL:HG21	7:B:137:VAL:HG23	1.95	0.48
2:D:21:VAL:O	2:D:25:MET:HG2	2.12	0.48
3:E:48:LYS:HD3	3:E:206:GLU:HB2	1.95	0.48
13:f:103:TYR:O	13:f:106:ARG:N	2.46	0.48
4:l:85:ALA:HB2	4:l:137:VAL:CG2	2.42	0.48
8:o:186:VAL:HG11	8:o:201:PHE:CZ	2.47	0.48
12:s:212:ARG:HE	12:s:250:LEU:HD21	1.77	0.48
9:b:87:THR:OG1	9:b:134:SER:HB3	2.13	0.48
9:b:136:ALA:HB1	9:b:166:MET:HE1	1.94	0.48
2:j:191:LEU:HD23	2:j:191:LEU:O	2.13	0.48
8:o:27:LEU:HB3	8:o:57:CYS:SG	2.54	0.48
10:c:124:ASP:OD1	10:c:125:SER:N	2.44	0.48
5:m:49:VAL:HG22	5:m:195:ILE:HG23	1.95	0.48
6:n:76:MET:HA	6:n:137:ILE:O	2.13	0.48
9:b:105:HIS:O	9:b:109:THR:HG22	2.13	0.48
6:n:16:SER:O	6:n:19:GLY:N	2.44	0.48
10:q:107:PRO:HG2	10:q:123:MET:HE3	1.95	0.48
9:b:81:TYR:CE1	9:b:222:VAL:HG11	2.49	0.48
9:b:98:VAL:HG22	9:b:102:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:e:90:ILE:N	12:e:98:GLY:O	2.42	0.48
4:l:79:SER:OG	4:l:168:ILE:HD12	2.13	0.48
7:B:139:ILE:O	7:B:139:ILE:HG22	2.13	0.48
2:D:44:VAL:HG23	2:D:214:GLU:HG2	1.94	0.48
9:b:234:ARG:HD2	9:b:237:THR:OG1	2.14	0.48
7:h:63:GLN:OE1	7:h:63:GLN:N	2.44	0.48
3:k:119:TYR:CE2	3:k:125:VAL:HG21	2.48	0.48
6:n:70:VAL:HG11	6:n:112:LEU:HD21	1.96	0.48
9:b:90:ASP:HB3	9:b:133:VAL:CG1	2.44	0.48
12:e:178:GLY:HA3	12:e:181:PHE:CE2	2.49	0.48
4:l:29:GLU:OE2	4:l:32:LYS:NZ	2.34	0.48
4:l:173:GLU:HG2	4:l:174:GLY:N	2.29	0.48
6:n:88:ILE:HD12	6:n:134:CYS:SG	2.54	0.48
1:C:66:GLN:O	1:C:74:VAL:HG12	2.14	0.48
5:G:123:SER:O	5:G:124:TRP:CD2	2.67	0.48
8:o:127:ILE:HA	8:o:132:THR:O	2.13	0.48
12:e:219:THR:HG21	12:e:247:VAL:HG11	1.96	0.48
13:f:213:LEU:HD23	13:f:213:LEU:H	1.77	0.48
3:k:9:THR:CG2	3:k:17:LEU:HD22	2.44	0.48
8:o:67:ILE:HD13	9:p:127:PHE:CE1	2.49	0.48
12:e:213:ARG:HD2	12:e:217:HIS:NE2	2.28	0.48
14:g:140:THR:HG22	14:g:141:VAL:N	2.29	0.48
2:j:95:GLN:HG3	10:q:73:LEU:HD13	1.95	0.48
1:C:17:GLY:O	2:D:27:ALA:HB2	2.14	0.48
4:F:8:TYR:CD2	4:F:9:ASP:N	2.80	0.48
5:G:19:LEU:HD21	6:X:130:ARG:CD	2.44	0.48
6:X:213:MET:HB3	6:X:227:VAL:HG21	1.96	0.48
9:p:47:TYR:OH	9:p:218:THR:HG22	2.14	0.48
11:r:37:LYS:O	11:r:61:GLN:NE2	2.46	0.48
13:t:213:LEU:HD12	13:t:213:LEU:C	2.39	0.48
1:i:23:GLU:O	1:i:27:THR:HG23	2.14	0.47
3:k:98:THR:C	3:k:99:LEU:HD12	2.39	0.47
10:q:2:SER:N	10:q:5:GLU:OE2	2.46	0.47
9:p:188:ASP:OD1	9:p:188:ASP:C	2.57	0.47
14:u:22:VAL:HG13	14:u:22:VAL:O	2.14	0.47
11:d:141:MET:HE3	11:d:165:GLU:HB2	1.96	0.47
12:e:175:ARG:C	12:e:176:LEU:HD12	2.38	0.47
12:e:219:THR:HG23	12:e:226:GLY:HA2	1.96	0.47
13:f:8:TRP:HZ2	14:g:119:PHE:HA	1.78	0.47
2:j:76:VAL:HG22	2:j:134:PHE:CE1	2.49	0.47
2:j:132:VAL:HG12	2:j:133:SER:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:m:144:LEU:HD23	5:m:145:TYR:N	2.28	0.47
6:n:179:LEU:HB3	6:n:184:MET:HE1	1.96	0.47
5:G:44:VAL:HG23	5:G:142:ALA:HB1	1.95	0.47
11:r:38:LEU:HD23	11:r:64:VAL:HG21	1.97	0.47
9:b:198:ILE:HG21	9:b:212:VAL:HG13	1.96	0.47
14:g:28:ILE:CG2	14:g:166:LEU:HD11	2.43	0.47
7:h:126:THR:HG22	7:h:126:THR:O	2.15	0.47
1:i:115:ALA:HB1	1:i:153:GLY:O	2.13	0.47
3:k:10:VAL:HG12	3:k:11:PHE:N	2.28	0.47
4:l:121:LEU:HD22	5:m:79:ALA:HB3	1.96	0.47
5:m:9:ASP:OD2	5:m:11:THR:OG1	2.27	0.47
7:B:69:LEU:CD2	7:B:79:LEU:HB2	2.43	0.47
4:F:184:ARG:O	4:F:185:LYS:HB3	2.14	0.47
8:a:51:THR:HG22	8:a:52:ASP:N	2.30	0.47
10:c:122:THR:HG22	10:c:136:VAL:HG13	1.97	0.47
10:c:134:ASP:OD1	10:c:135:PHE:N	2.44	0.47
14:g:163:VAL:N	14:g:164:PRO:CD	2.77	0.47
5:m:224:ASP:OD1	5:m:226:GLN:N	2.48	0.47
13:t:32:ASP:OD2	13:t:199:THR:HA	2.14	0.47
8:a:186:VAL:HG21	8:a:201:PHE:HE1	1.78	0.47
3:k:116:GLN:O	3:k:120:THR:HG23	2.13	0.47
3:k:139:PRO:O	3:k:140:TYR:HB2	2.14	0.47
3:k:142:ASP:OD1	3:k:142:ASP:C	2.57	0.47
7:B:172:ASP:OD1	7:B:173:GLN:N	2.48	0.47
3:E:81:ALA:O	3:E:85:ILE:HG12	2.15	0.47
6:X:95:GLU:OE1	6:X:115:ARG:HB3	2.14	0.47
10:c:162:LEU:O	10:c:163:PHE:C	2.56	0.47
3:k:17:LEU:HD21	4:l:133:ARG:NH2	2.28	0.47
5:m:72:VAL:HG21	5:m:88:MET:HE1	1.97	0.47
7:B:66:VAL:HG13	7:B:66:VAL:O	2.15	0.47
1:C:90:SER:OG	1:C:110:LEU:HD11	2.14	0.47
3:E:7:ALA:HB2	4:F:12:VAL:HG21	1.97	0.47
4:F:70:ILE:HD13	4:F:89:VAL:HG13	1.97	0.47
8:o:37:VAL:O	14:g:195:ARG:HG2	2.15	0.47
9:p:142:VAL:HG11	9:p:219:LYS:HA	1.96	0.47
11:r:120:ILE:O	11:r:120:ILE:HG22	2.14	0.47
9:b:153:TYR:HB3	9:b:154:PRO:HD2	1.96	0.47
14:g:67:LEU:C	14:g:67:LEU:HD12	2.39	0.47
1:i:100:LEU:HD21	10:q:90:LEU:HD13	1.97	0.47
4:F:219:SER:OG	4:F:220:PRO:HD3	2.15	0.47
8:o:37:VAL:O	8:o:37:VAL:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:t:202:LYS:HA	13:t:218:MET:O	2.14	0.47
2:j:218:LEU:HG	2:j:219:PRO:HD2	1.96	0.47
2:D:145:PHE:CZ	2:D:217:LEU:HD13	2.50	0.47
13:t:167:ILE:HD13	13:t:167:ILE:HA	1.70	0.47
1:i:213:ILE:HD11	1:i:219:PHE:HD2	1.80	0.47
13:t:202:LYS:HE3	13:t:217:TYR:CD1	2.50	0.47
13:f:89:MET:HE3	13:f:94:MET:HE2	1.96	0.47
6:n:182:SER:OG	6:n:183:GLU:OE2	2.21	0.46
2:D:244:GLN:HB2	2:D:245:PRO:HD3	1.97	0.46
6:X:45:GLY:HA3	6:X:217:CYS:HB3	1.97	0.46
13:t:63:PHE:CZ	13:t:65:ALA:HB3	2.50	0.46
11:d:107:ASP:O	11:d:108:GLN:C	2.58	0.46
12:e:142:LEU:HD21	12:e:152:VAL:HG13	1.95	0.46
1:i:139:PHE:HB3	1:i:213:ILE:HG21	1.95	0.46
4:l:140:LEU:HD23	4:l:153:TYR:HB3	1.97	0.46
7:B:126:THR:O	7:B:126:THR:HG22	2.15	0.46
2:D:119:GLN:HA	2:D:122:THR:HG22	1.98	0.46
8:o:177:ILE:HG23	8:o:184:GLY:HA2	1.97	0.46
9:p:43:VAL:HG13	9:p:177:PHE:CE2	2.50	0.46
10:q:91:VAL:CG1	10:q:123:MET:HE1	2.45	0.46
14:u:67:LEU:C	14:u:67:LEU:HD12	2.40	0.46
7:B:50:VAL:HG11	7:B:79:LEU:HB2	1.97	0.46
8:o:67:ILE:CD1	9:p:127:PHE:CZ	2.99	0.46
11:d:85:ARG:CG	11:d:121:ALA:HB1	2.45	0.46
14:g:194:ASP:C	14:g:196:SER:H	2.24	0.46
2:j:118:LYS:NZ	2:j:150:SER:OG	2.46	0.46
3:k:74:CYS:SG	3:k:130:LEU:HD22	2.55	0.46
5:m:7:ASP:OD1	5:m:7:ASP:O	2.34	0.46
5:G:177:ASP:N	5:G:177:ASP:OD1	2.45	0.46
11:r:141:MET:HE3	12:e:196:ASN:OD1	2.16	0.46
13:t:213:LEU:HD12	13:t:213:LEU:O	2.16	0.46
5:G:19:LEU:HD21	6:X:130:ARG:HD2	1.98	0.46
10:q:129:LYS:HE2	10:q:131:LEU:HD11	1.98	0.46
13:t:30:ALA:HB1	13:t:203:LEU:CD1	2.45	0.46
10:c:12:VAL:HG23	10:c:137:VAL:HG12	1.98	0.46
14:g:30:ILE:HD12	14:g:183:LEU:HB2	1.98	0.46
7:h:50:VAL:HG22	7:h:79:LEU:CD2	2.43	0.46
1:i:135:LEU:HG	1:i:163:MET:CE	2.46	0.46
3:k:41:THR:HG22	3:k:211:ARG:HD2	1.98	0.46
4:l:121:LEU:HD22	5:m:79:ALA:CB	2.46	0.46
5:G:72:VAL:CG2	5:G:88:MET:HE1	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:215:TRP:CZ3	6:X:217:CYS:SG	3.08	0.46
10:q:30:VAL:HG23	10:q:35:ILE:HD11	1.96	0.46
11:r:136:TYR:HB3	12:e:188:PRO:HB2	1.96	0.46
7:h:39:SER:HB2	7:h:79:LEU:HD21	1.97	0.46
4:l:24:VAL:O	4:l:28:ILE:HG13	2.16	0.46
5:m:7:ASP:OD1	5:m:24:TYR:CE2	2.68	0.46
1:C:8:PHE:HA	2:D:126:GLY:O	2.16	0.46
2:D:218:LEU:CD2	2:D:224:LYS:HB2	2.46	0.46
13:f:89:MET:HE1	13:f:97:LEU:HD23	1.98	0.46
7:B:191:TYR:OH	7:B:219:VAL:HG21	2.15	0.46
2:D:68:ILE:HG21	2:D:110:LEU:HD21	1.98	0.46
3:E:38:GLY:CA	3:E:186:THR:HG21	2.45	0.46
11:r:126:VAL:HG21	11:r:129:ALA:HB2	1.97	0.46
12:e:68:MET:HE1	12:e:233:HIS:HB2	1.98	0.46
5:m:66:VAL:HG21	5:m:88:MET:HE2	1.97	0.46
5:m:224:ASP:OD1	5:m:227:MET:N	2.32	0.46
6:n:12:VAL:HG12	6:n:12:VAL:O	2.15	0.46
4:F:187:LEU:HD22	4:F:191:GLU:OE1	2.15	0.46
9:p:43:VAL:HG13	9:p:177:PHE:CZ	2.51	0.46
7:B:50:VAL:CG2	7:B:141:ILE:HG21	2.46	0.46
4:F:78:MET:CA	4:F:139:LEU:HD23	2.46	0.46
10:c:159:PRO:O	10:c:160:GLU:HB2	2.16	0.46
11:d:182:VAL:O	11:d:182:VAL:HG13	2.15	0.46
14:g:57:ARG:HG2	14:g:57:ARG:O	2.16	0.46
1:i:100:LEU:HD22	1:i:101:TYR:CZ	2.51	0.45
5:m:105:VAL:HG23	5:m:137:LEU:O	2.15	0.45
3:E:84:LEU:HD12	3:E:130:LEU:HD13	1.98	0.45
8:a:89:VAL:HG23	8:a:117:ASP:OD2	2.17	0.45
2:j:57:GLN:O	2:j:58:THR:OG1	2.20	0.45
2:D:132:VAL:HG12	2:D:133:SER:N	2.31	0.45
5:G:72:VAL:HG12	5:G:73:ALA:N	2.30	0.45
10:q:176:ARG:NH1	12:e:81:ILE:O	2.49	0.45
12:s:93:ASN:HB3	12:s:96:MET:HB3	1.98	0.45
13:t:74:LEU:HD11	13:t:98:LEU:HD13	1.98	0.45
8:a:50:LEU:HD22	8:a:72:VAL:HG13	1.97	0.45
11:d:190:PHE:O	11:d:191:ALA:C	2.58	0.45
2:j:72:VAL:HG22	2:j:107:VAL:HG22	1.99	0.45
4:F:91:HIS:O	4:F:94:VAL:HG12	2.15	0.45
13:t:30:ALA:HA	13:t:204:GLU:O	2.17	0.45
14:u:152:HIS:HB2	14:u:166:LEU:HD13	1.97	0.45
12:e:142:LEU:HD21	12:e:152:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:86:LEU:HD11	1:i:118:MET:SD	2.56	0.45
6:n:128:TRP:CZ3	6:n:129:LEU:HD21	2.52	0.45
5:G:39:ARG:NH1	6:X:60:LEU:HD11	2.32	0.45
5:G:117:GLN:O	5:G:120:THR:N	2.49	0.45
10:q:122:THR:HB	10:q:136:VAL:HG11	1.98	0.45
14:u:162:ALA:O	14:u:165:ILE:N	2.49	0.45
14:u:213:THR:CG2	8:a:224:TRP:CZ2	2.75	0.45
3:k:64:VAL:HG11	3:k:85:ILE:HD13	1.98	0.45
3:E:45:GLY:HA2	3:E:207:VAL:HA	1.98	0.45
11:r:27:VAL:CG1	11:r:30:THR:CG2	2.95	0.45
8:a:97:ARG:CB	8:a:133:ILE:HD11	2.46	0.45
8:a:220:LEU:HG	8:a:224:TRP:HB2	1.99	0.45
1:C:166:ASN:OD1	1:C:166:ASN:C	2.60	0.45
9:p:202:ILE:HG23	9:p:209:GLY:HA2	1.98	0.45
9:b:90:ASP:HB3	9:b:133:VAL:HG13	1.98	0.45
12:e:257:VAL:O	12:e:258:VAL:C	2.58	0.45
1:i:39:LYS:HG3	1:i:39:LYS:O	2.17	0.45
5:m:22:VAL:O	5:m:26:MET:HG3	2.16	0.45
5:m:84:LEU:HD13	5:m:132:LEU:HD11	1.98	0.45
8:o:37:VAL:HA	14:g:195:ARG:HD3	1.99	0.45
12:s:59:LEU:C	12:s:59:LEU:HD12	2.42	0.45
1:i:65:ILE:HG12	1:i:75:VAL:HG22	1.97	0.45
3:E:64:VAL:HG22	3:E:65:ASN:N	2.31	0.45
4:F:178:SER:O	4:F:182:GLN:HG2	2.17	0.45
6:X:107:VAL:HG13	6:X:107:VAL:O	2.17	0.45
6:X:191:ILE:HD12	6:X:191:ILE:H	1.82	0.45
8:o:140:ILE:HG22	8:o:145:SER:CB	2.47	0.45
9:p:80:ILE:HG12	9:p:115:VAL:HG22	1.99	0.45
8:a:97:ARG:HB2	8:a:133:ILE:HD11	1.98	0.45
14:g:29:GLY:N	14:g:153:VAL:O	2.49	0.45
14:g:67:LEU:HD13	14:g:126:LEU:CD1	2.47	0.45
6:n:141:TYR:CD2	6:n:222:ARG:HG2	2.52	0.45
2:D:18:LEU:O	2:D:22:GLU:OE1	2.34	0.45
2:D:37:ILE:O	2:D:43:VAL:HG23	2.16	0.45
10:q:14:MET:CE	10:q:166:VAL:HG22	2.46	0.45
12:e:93:ASN:OD1	12:e:94:PRO:HD2	2.16	0.45
14:g:41:ASP:OD1	14:g:57:ARG:NH2	2.44	0.45
7:h:235:ILE:O	7:h:239:LEU:HD23	2.16	0.45
3:E:149:THR:HG22	3:E:150:ASP:N	2.32	0.44
11:d:1:MET:HE3	11:d:172:VAL:HB	1.99	0.44
11:d:2:GLU:OE2	11:d:48:GLY:O	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:g:201:LEU:HD11	14:g:218:TYR:CZ	2.51	0.44
10:q:5:GLU:OE1	10:q:5:GLU:N	2.49	0.44
9:b:226:ARG:O	9:b:227:ASN:C	2.60	0.44
6:n:34:SER:OG	6:n:35:GLY:N	2.50	0.44
7:B:196:GLN:NE2	7:B:242:ILE:HG13	2.32	0.44
1:C:62:VAL:O	1:C:62:VAL:HG13	2.17	0.44
1:C:165:LYS:O	1:C:166:ASN:OD1	2.35	0.44
8:o:148:LEU:HB3	8:o:152:LEU:HD23	2.00	0.44
10:q:14:MET:SD	10:q:153:TYR:HD1	2.41	0.44
11:r:143:ASP:OD2	12:e:221:ARG:HD3	2.17	0.44
12:s:91:GLU:HG2	12:s:239:TRP:CZ2	2.52	0.44
11:d:115:TYR:HB3	11:d:123:LEU:HD11	1.99	0.44
4:l:171:GLY:O	4:l:172:SER:C	2.59	0.44
5:G:179:PHE:O	5:G:180:ASP:C	2.60	0.44
9:b:56:ASP:OD1	9:b:72:LYS:NZ	2.51	0.44
13:f:8:TRP:CZ2	14:g:119:PHE:HA	2.52	0.44
7:B:22:LEU:HD12	7:B:22:LEU:HA	1.79	0.44
4:F:92:ALA:HB2	4:F:116:LEU:CD1	2.47	0.44
10:q:15:VAL:HG22	10:q:20:ILE:CD1	2.48	0.44
14:u:25:THR:CG2	14:u:26:SER:H	2.29	0.44
9:b:94:VAL:HG22	9:b:125:HIS:CD2	2.53	0.44
12:e:67:VAL:HG13	12:e:234:VAL:HB	2.00	0.44
7:h:141:ILE:HD11	7:h:227:PHE:CE1	2.53	0.44
7:h:210:PHE:CE1	7:h:215:ILE:HG21	2.52	0.44
1:i:35:SER:HB2	1:i:75:VAL:HG11	1.99	0.44
3:k:69:HIS:CE1	3:k:103:VAL:O	2.70	0.44
1:C:55:ILE:HG13	1:C:56:LEU:HD12	2.00	0.44
3:E:164:GLY:O	3:E:167:SER:OG	2.33	0.44
4:F:78:MET:HB3	4:F:139:LEU:HD22	1.91	0.44
10:q:27:ARG:HD2	10:q:34:THR:HG22	1.99	0.44
7:h:112:ASP:OD1	7:h:113:ALA:N	2.50	0.44
7:B:27:TYR:O	6:X:15:PHE:HE2	2.01	0.44
7:B:237:GLU:O	7:B:240:THR:HG22	2.16	0.44
14:u:41:ASP:O	14:u:57:ARG:NH2	2.46	0.44
8:a:56:VAL:CG2	8:a:111:MET:HE3	2.48	0.44
10:c:185:HIS:NE2	10:c:196:GLU:OE2	2.44	0.44
12:e:254:TYR:O	12:e:256:PRO:HD3	2.17	0.44
4:l:103:TYR:OH	13:t:77:ARG:CZ	2.66	0.44
3:E:84:LEU:HD12	3:E:130:LEU:CD1	2.48	0.44
6:X:50:VAL:HG12	6:X:51:GLU:N	2.33	0.44
14:g:19:TYR:CG	14:g:20:PRO:HD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:38:LEU:O	2:j:179:TYR:OH	2.30	0.44
1:C:212:ILE:HG12	1:C:222:LEU:HD21	2.00	0.44
2:D:29:GLY:O	2:D:166:ALA:HA	2.17	0.44
3:E:50:SER:HA	3:E:204:ASN:OD1	2.17	0.44
11:d:124:HIS:HD1	11:d:124:HIS:HA	1.70	0.44
1:i:180:ASP:O	1:i:181:ASP:OD1	2.35	0.43
2:j:51:VAL:HG23	2:j:51:VAL:O	2.18	0.43
4:l:100:ARG:O	4:l:104:GLY:N	2.45	0.43
6:n:78:VAL:HG12	6:n:136:VAL:HG12	2.00	0.43
2:D:90:ALA:HB2	2:D:114:LEU:HD13	1.99	0.43
13:t:17:THR:HG23	13:t:189:PHE:CE1	2.53	0.43
9:b:143:ASP:CG	9:b:144:VAL:N	2.76	0.43
12:e:229:VAL:HG23	12:e:247:VAL:HG23	1.99	0.43
5:m:80:ASP:O	5:m:83:VAL:HG12	2.18	0.43
1:C:63:GLN:OE1	1:C:63:GLN:N	2.43	0.43
1:C:67:LEU:HA	1:C:73:GLY:HA2	1.99	0.43
3:E:102:PRO:HG2	3:E:139:PRO:HB3	2.00	0.43
6:X:91:ARG:NH1	6:X:119:TYR:CD1	2.86	0.43
9:p:97:MET:HE2	9:p:98:VAL:HG23	2.00	0.43
12:e:56:THR:CB	12:e:88:LYS:HZ3	2.29	0.43
7:B:78:LEU:O	7:B:78:LEU:HD23	2.18	0.43
1:C:93:GLN:OE1	1:C:113:GLU:HB3	2.17	0.43
6:X:70:VAL:HG21	6:X:92:ALA:HB1	1.99	0.43
8:a:56:VAL:O	8:a:56:VAL:HG13	2.18	0.43
10:c:122:THR:CG2	10:c:136:VAL:HG13	2.49	0.43
12:e:244:GLY:O	13:f:166:LEU:HA	2.18	0.43
4:l:78:MET:SD	4:l:85:ALA:HB1	2.59	0.43
4:l:121:LEU:HG	4:l:121:LEU:O	2.18	0.43
4:l:129:GLU:OE2	4:l:130:SER:N	2.52	0.43
3:E:121:GLN:HG3	4:F:133:ARG:CG	2.40	0.43
4:F:155:ASP:HB2	4:F:156:PRO:CD	2.48	0.43
4:F:214:ASP:OD1	4:F:224:LEU:HD11	2.18	0.43
14:u:61:ILE:HD12	14:u:67:LEU:CD2	2.48	0.43
8:a:50:LEU:C	8:a:51:THR:HG1	2.17	0.43
8:a:140:ILE:HD11	8:a:149:TYR:CE1	2.53	0.43
10:c:30:VAL:HG12	10:c:31:GLN:N	2.31	0.43
10:c:157:MET:HE3	10:c:157:MET:HB2	1.74	0.43
12:e:61:PHE:CD2	12:e:194:LEU:HD11	2.53	0.43
7:h:119:ALA:HB2	7:h:160:PHE:HB3	2.00	0.43
1:i:8:PHE:HB3	2:j:6:ASP:OD1	2.18	0.43
2:D:43:VAL:CG1	2:D:137:ALA:HB1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:p:40:THR:HA	9:p:208:SER:HB3	1.99	0.43
12:s:209:GLU:OE1	12:s:212:ARG:NH2	2.50	0.43
14:u:163:VAL:N	14:u:164:PRO:CD	2.81	0.43
12:e:220:TYR:CD2	12:e:221:ARG:HD2	2.53	0.43
7:h:219:VAL:CG1	7:h:230:LEU:HD11	2.49	0.43
5:m:84:LEU:HD12	5:m:130:VAL:CG1	2.49	0.43
6:n:42:CYS:SG	6:n:184:MET:HG3	2.59	0.43
2:D:181:ASP:O	2:D:182:ASP:HB2	2.18	0.43
5:G:39:ARG:NH2	5:G:142:ALA:O	2.43	0.43
9:p:200:SER:O	9:p:204:ASN:ND2	2.49	0.43
12:s:233:HIS:O	12:s:239:TRP:HA	2.18	0.43
13:t:63:PHE:HZ	14:u:144:ILE:HG22	1.82	0.43
13:t:195:ARG:HA	9:b:65:VAL:CG1	2.49	0.43
3:E:43:VAL:HG11	3:E:187:VAL:HA	2.01	0.43
4:F:70:ILE:HD12	4:F:92:ALA:HB3	1.99	0.43
5:G:227:MET:HE3	5:G:231:LEU:CD1	2.48	0.43
12:s:192:GLY:O	11:d:141:MET:CE	2.66	0.43
1:i:29:VAL:HG23	1:i:77:SER:O	2.18	0.43
1:i:57:VAL:HG22	7:h:163:HIS:ND1	2.33	0.43
6:n:63:SER:O	6:n:64:ASN:C	2.62	0.43
8:o:16:ILE:HD13	8:o:59:SER:HB2	1.99	0.43
10:q:73:LEU:HD12	10:q:73:LEU:HA	1.79	0.43
9:b:43:VAL:CG1	9:b:177:PHE:HZ	2.31	0.43
2:j:8:ARG:NH1	4:l:9:ASP:OD2	2.52	0.43
2:j:90:ALA:HB2	2:j:114:LEU:HD13	2.01	0.43
2:j:213:ALA:HB1	2:j:225:TYR:CE1	2.53	0.43
1:C:37:GLY:O	1:C:160:ALA:HA	2.19	0.43
6:X:124:THR:O	6:X:124:THR:CG2	2.66	0.43
9:b:98:VAL:O	9:b:102:LEU:HD13	2.18	0.43
10:c:72:LYS:O	10:c:76:LEU:HD23	2.18	0.43
7:h:143:ILE:CD1	7:h:221:GLN:C	2.92	0.43
1:i:38:ILE:HD11	1:i:174:LEU:CD2	2.49	0.43
2:j:196:LEU:O	2:j:200:MET:HG2	2.18	0.43
1:C:13:PHE:CE1	1:C:19:LEU:HD11	2.53	0.43
3:E:150:ASP:C	3:E:152:SER:N	2.75	0.43
8:o:67:ILE:HD13	9:p:127:PHE:CZ	2.53	0.43
8:o:97:ARG:HG3	8:o:133:ILE:CD1	2.49	0.43
10:q:150:GLU:OE1	13:f:195:ARG:NH2	2.43	0.43
14:u:112:MET:HE3	14:u:143:MET:HA	2.01	0.43
9:b:217:ILE:HG23	9:b:222:VAL:HG22	1.99	0.43
14:g:109:THR:HG22	14:g:141:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:m:133:LEU:O	5:m:133:LEU:HD23	2.19	0.42
7:B:70:PHE:CD2	7:B:91:VAL:HG21	2.54	0.42
6:X:55:GLN:OE1	6:X:55:GLN:N	2.52	0.42
6:X:186:CYS:O	6:X:187:ARG:HB2	2.19	0.42
13:t:29:ILE:CD1	13:t:57:VAL:HB	2.49	0.42
10:c:20:ILE:HD11	10:c:118:PRO:HB2	2.01	0.42
13:f:201:ASP:O	13:f:202:LYS:HB2	2.18	0.42
6:n:202:ASP:N	6:n:202:ASP:OD1	2.52	0.42
1:C:46:ILE:HD11	1:C:219:PHE:HZ	1.84	0.42
2:D:191:LEU:C	2:D:191:LEU:HD23	2.44	0.42
4:F:188:SER:O	4:F:189:PHE:C	2.62	0.42
13:t:139:VAL:HG22	13:t:140:GLY:N	2.34	0.42
10:c:122:THR:HB	10:c:136:VAL:CG1	2.50	0.42
7:h:199:ILE:HG23	7:h:210:PHE:HZ	1.84	0.42
4:l:71:ASP:O	4:l:73:HIS:N	2.52	0.42
7:B:78:LEU:HD23	7:B:78:LEU:C	2.44	0.42
4:F:66:LYS:O	4:F:78:MET:HG2	2.18	0.42
4:F:73:HIS:O	4:F:218:VAL:HG21	2.19	0.42
4:F:236:ARG:O	4:F:237:LEU:C	2.62	0.42
9:p:153:TYR:HB3	9:p:154:PRO:HD2	2.01	0.42
10:q:37:THR:OG1	10:q:203:MET:HE1	2.19	0.42
10:q:45:ILE:CD1	10:q:87:PHE:CZ	3.02	0.42
14:u:108:LEU:HA	14:u:111:VAL:HG12	2.01	0.42
14:u:195:ARG:O	14:u:195:ARG:HG2	2.19	0.42
9:b:256:THR:O	9:b:256:THR:HG22	2.18	0.42
10:c:23:GLY:C	10:c:42:ILE:HD11	2.44	0.42
12:e:89:ILE:HG21	12:e:97:LEU:HD23	2.02	0.42
7:h:153:LYS:HB3	7:h:163:HIS:CD2	2.54	0.42
1:i:13:PHE:HB3	2:j:23:TYR:HB3	2.02	0.42
5:m:206:SER:CB	5:m:228:VAL:HG13	2.49	0.42
6:n:51:GLU:OE2	6:n:201:HIS:ND1	2.50	0.42
1:C:80:GLY:N	1:C:81:PRO:CD	2.83	0.42
5:G:34:ALA:HB3	5:G:49:VAL:CG1	2.50	0.42
10:q:70:ARG:HE	10:q:90:LEU:HD11	1.84	0.42
11:r:27:VAL:O	11:r:28:HIS:C	2.62	0.42
14:u:163:VAL:CG2	14:u:164:PRO:HD3	2.49	0.42
14:g:33:LYS:O	14:g:34:ASP:CG	2.63	0.42
1:i:77:SER:HB2	1:i:163:MET:HG3	2.00	0.42
2:j:25:MET:SD	2:j:152:PRO:HG2	2.59	0.42
5:m:52:ALA:HA	5:m:59:HIS:HA	2.00	0.42
2:D:98:THR:O	2:D:102:GLN:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:93:GLN:HG3	11:d:66:LEU:HG	2.01	0.42
4:F:131:MET:HB2	4:F:131:MET:HE2	1.67	0.42
8:o:138:PHE:CD1	8:o:138:PHE:C	2.96	0.42
8:o:186:VAL:HG21	8:o:201:PHE:HE1	1.76	0.42
11:d:26:LEU:HD21	12:e:191:TYR:CE2	2.55	0.42
7:h:83:MET:HE2	7:h:135:GLY:HA3	2.01	0.42
1:i:177:ARG:O	1:i:177:ARG:HG3	2.18	0.42
2:j:199:THR:O	2:j:199:THR:HG22	2.19	0.42
3:k:12:SER:O	3:k:14:ASP:N	2.52	0.42
1:C:23:GLU:O	1:C:27:THR:HG23	2.19	0.42
2:D:160:LYS:HD2	3:E:54:LEU:HD12	2.01	0.42
3:E:107:TYR:CD1	3:E:107:TYR:C	2.97	0.42
11:r:38:LEU:HD13	11:r:44:MET:HB2	2.02	0.42
11:r:171:VAL:HG23	11:r:172:VAL:HG23	2.01	0.42
12:e:59:LEU:HD12	12:e:59:LEU:C	2.45	0.42
4:l:76:CYS:HA	4:l:140:LEU:O	2.19	0.42
5:m:4:ASN:O	5:m:5:GLN:HB3	2.19	0.42
6:n:99:TYR:CD1	6:n:107:VAL:HG22	2.54	0.42
6:n:126:TYR:HD2	6:n:129:LEU:HD12	1.84	0.42
2:D:97:TYR:CD1	2:D:97:TYR:C	2.96	0.42
3:E:213:GLU:N	3:E:213:GLU:OE1	2.53	0.42
5:G:45:VAL:HG22	5:G:213:VAL:HG22	2.02	0.42
11:r:21:ALA:CB	12:s:176:LEU:HD21	2.48	0.42
11:r:49:GLU:OE1	11:r:52:ASP:N	2.43	0.42
14:u:25:THR:CG2	14:u:26:SER:N	2.81	0.42
9:b:226:ARG:HG3	9:b:227:ASN:N	2.35	0.42
12:e:89:ILE:CG2	12:e:97:LEU:HD23	2.50	0.42
13:f:167:ILE:HD13	13:f:167:ILE:HA	1.88	0.42
3:E:42:VAL:HB	3:E:135:VAL:HG11	2.02	0.42
11:r:22:VAL:HG12	11:r:27:VAL:HA	2.02	0.42
12:s:93:ASN:OD1	12:s:94:PRO:HD2	2.19	0.42
12:s:159:TRP:CD1	12:s:160:ASP:O	2.72	0.42
14:u:58:LEU:HD13	14:u:204:ALA:HB2	2.01	0.42
13:f:126:CYS:O	13:f:127:VAL:HG23	2.18	0.42
13:f:129:THR:OG1	13:f:142:SER:OG	2.22	0.42
14:g:57:ARG:CD	14:g:69:ALA:O	2.67	0.42
1:i:166:ASN:OD1	1:i:169:ASN:HB2	2.19	0.42
2:j:35:ILE:HG12	2:j:46:ILE:CG2	2.50	0.42
4:l:153:TYR:HD1	4:l:163:CYS:HG	1.66	0.42
6:n:219:GLU:C	6:n:221:LYS:H	2.28	0.42
7:B:125:TYR:CE1	7:B:131:MET:CE	2.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:36:THR:HG21	4:F:203:VAL:HG11	2.01	0.42
5:G:69:HIS:HB2	5:G:137:LEU:HD12	2.01	0.42
11:r:27:VAL:C	11:r:29:LYS:N	2.76	0.42
10:c:152:MET:HE1	10:c:168:GLN:CB	2.50	0.42
11:d:77:THR:HG1	11:d:107:ASP:CG	2.17	0.42
12:e:67:VAL:CG1	12:e:234:VAL:HB	2.49	0.42
7:h:183:MET:HE3	7:h:189:PHE:CE2	2.55	0.42
3:k:69:HIS:CE1	3:k:139:PRO:HD3	2.55	0.42
5:m:105:VAL:HG21	5:m:136:GLY:C	2.45	0.42
7:B:13:ILE:HD11	7:B:130:TYR:CD1	2.55	0.42
3:E:166:ASN:O	3:E:166:ASN:CG	2.62	0.42
9:p:246:LYS:HB3	9:p:246:LYS:HE2	1.89	0.42
10:q:204:ASP:HB2	12:e:219:THR:CG2	2.50	0.42
12:s:101:ALA:HB3	12:s:153:GLY:O	2.19	0.42
12:s:155:MET:HA	12:s:167:TYR:O	2.20	0.42
13:t:32:ASP:HB2	13:t:200:GLY:O	2.20	0.42
9:b:43:VAL:HG12	9:b:44:GLY:N	2.34	0.42
14:g:101:PRO:HB2	14:g:137:TYR:HB3	2.02	0.42
3:k:42:VAL:CG1	3:k:135:VAL:HG13	2.48	0.41
3:k:43:VAL:HG22	3:k:209:VAL:HG12	2.02	0.41
3:k:104:THR:HG23	3:k:107:TYR:H	1.85	0.41
4:l:12:VAL:HG23	4:l:23:GLN:HG3	2.01	0.41
4:l:208:LEU:HD23	4:l:208:LEU:HA	1.84	0.41
6:n:137:ILE:CG2	6:n:148:LEU:HD11	2.50	0.41
5:G:205:THR:O	5:G:208:VAL:HG22	2.20	0.41
6:X:54:ILE:CG2	6:X:55:GLN:N	2.83	0.41
10:q:58:SER:N	11:r:122:THR:HG22	2.35	0.41
14:u:128:LEU:C	14:u:128:LEU:HD23	2.45	0.41
7:h:66:VAL:O	7:h:66:VAL:HG13	2.19	0.41
1:i:5:GLN:O	1:i:6:TYR:C	2.62	0.41
2:j:39:ALA:HB2	2:j:188:ALA:HB2	2.02	0.41
4:l:218:VAL:O	4:l:219:SER:C	2.63	0.41
10:q:49:LEU:HA	10:q:111:GLY:HA3	2.01	0.41
10:q:134:ASP:OD1	10:q:134:ASP:N	2.49	0.41
11:r:172:VAL:O	11:r:172:VAL:CG1	2.65	0.41
8:a:69:SER:O	8:a:73:ARG:HG3	2.20	0.41
14:g:143:MET:HG3	14:g:144:ILE:HG23	2.01	0.41
2:j:68:ILE:HA	2:j:91:ARG:HG2	2.01	0.41
6:n:217:CYS:HB2	6:n:218:ASP:H	1.60	0.41
7:B:141:ILE:HG22	7:B:151:LEU:HD13	2.02	0.41
8:o:51:THR:HG23	8:o:76:LEU:HD23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:q:25:ASP:CG	10:q:181:GLY:H	2.28	0.41
11:r:151:SER:O	11:r:154:GLU:N	2.53	0.41
9:b:250:VAL:CG1	9:b:253:THR:HG22	2.50	0.41
10:c:27:ARG:HD2	10:c:28:LEU:C	2.46	0.41
7:h:203:GLN:HG2	7:h:210:PHE:HE2	1.85	0.41
3:k:70:ILE:HD13	3:k:108:ILE:HG21	2.02	0.41
5:m:49:VAL:HG23	5:m:195:ILE:HD12	2.01	0.41
2:D:76:VAL:HG21	2:D:83:ALA:HB2	2.00	0.41
2:D:86:LEU:HD23	2:D:134:PHE:HE2	1.86	0.41
3:E:46:VAL:N	3:E:206:GLU:O	2.52	0.41
4:F:37:ALA:HB3	4:F:168:ILE:HG13	2.02	0.41
5:G:50:ASN:ND2	5:G:59:HIS:CG	2.87	0.41
8:o:45:ASP:HB2	14:g:232:PRO:HG2	2.02	0.41
8:o:160:MET:HE3	8:o:160:MET:HB2	1.83	0.41
13:t:66:ASP:OD1	14:u:113:TYR:OH	2.35	0.41
9:b:58:ARG:CZ	9:b:209:GLY:HA3	2.50	0.41
3:k:67:ASP:O	3:k:70:ILE:O	2.39	0.41
6:n:37:ALA:O	6:n:164:ALA:HA	2.21	0.41
6:n:122:LEU:HD13	6:n:125:LEU:HD12	2.01	0.41
1:C:45:VAL:HA	1:C:211:GLY:O	2.21	0.41
2:D:93:GLN:CD	2:D:113:SER:HG	2.26	0.41
2:D:136:PHE:O	2:D:147:LEU:HA	2.21	0.41
4:F:73:HIS:O	4:F:222:TYR:HB2	2.20	0.41
5:G:34:ALA:HB3	5:G:49:VAL:HG12	2.02	0.41
5:G:105:VAL:HG21	5:G:136:GLY:CA	2.51	0.41
13:t:10:PRO:O	14:u:116:ARG:NH2	2.49	0.41
10:c:20:ILE:HG21	10:c:110:ALA:HB1	2.02	0.41
13:f:159:LEU:HD23	13:f:159:LEU:HA	1.94	0.41
1:i:24:HIS:CE1	7:h:18:PRO:HA	2.55	0.41
1:i:118:MET:HE3	1:i:151:PRO:HA	2.03	0.41
4:l:41:LYS:HG2	4:l:42:THR:N	2.34	0.41
3:E:116:GLN:OE1	3:E:149:THR:HG21	2.21	0.41
4:F:73:HIS:CD2	4:F:73:HIS:H	2.37	0.41
5:G:183:THR:O	5:G:184:ARG:C	2.62	0.41
9:p:76:MET:HE1	9:p:122:LEU:HD11	2.01	0.41
9:p:88:ALA:O	9:p:91:THR:N	2.53	0.41
9:p:136:ALA:HB1	9:p:166:MET:CE	2.48	0.41
10:c:162:LEU:C	10:c:164:GLU:N	2.76	0.41
2:j:95:GLN:HA	2:j:98:THR:HG22	2.03	0.41
2:j:108:GLU:OE2	2:j:156:TYR:OH	2.26	0.41
3:k:121:GLN:HA	4:l:133:ARG:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:g:59:LYS:O	14:g:66:LEU:HD12	2.20	0.41
7:h:81:THR:O	7:h:137:VAL:N	2.54	0.41
7:B:206:LEU:O	7:B:207:GLN:HG3	2.20	0.41
3:E:109:THR:HG21	3:E:147:TYR:HB3	2.02	0.41
4:F:95:GLU:HG3	4:F:107:MET:HE1	2.03	0.41
6:X:225:GLN:OE1	6:X:226:LYS:O	2.39	0.41
13:t:129:THR:O	13:t:129:THR:HG23	2.20	0.41
9:b:58:ARG:HG3	9:b:65:VAL:HG23	2.03	0.41
9:b:248:THR:HG21	10:c:167:SER:HB3	2.02	0.41
10:c:131:LEU:HD12	10:c:131:LEU:H	1.85	0.41
14:g:50:LEU:HD13	14:g:198:VAL:CG1	2.46	0.41
3:k:45:GLY:HA3	3:k:194:LEU:HD11	2.02	0.41
5:m:67:ASP:OD1	5:m:67:ASP:C	2.64	0.41
5:m:105:VAL:CG2	5:m:137:LEU:N	2.84	0.41
6:n:108:PRO:HA	6:n:142:ASP:OD2	2.21	0.41
7:B:143:ILE:CD1	7:B:221:GLN:C	2.94	0.41
2:D:39:ALA:O	2:D:42:GLY:O	2.39	0.41
5:G:24:TYR:O	5:G:27:GLU:N	2.52	0.41
12:s:95:TYR:CD1	12:s:237:ASP:O	2.74	0.41
12:s:221:ARG:HA	10:c:34:THR:HG22	2.03	0.41
14:u:83:LEU:HD11	14:u:108:LEU:HD21	2.02	0.41
8:a:109:THR:HG23	8:a:109:THR:O	2.19	0.41
9:b:250:VAL:HG22	10:c:163:PHE:HZ	1.84	0.41
10:c:74:TYR:CD2	10:c:82:MET:HE2	2.55	0.41
11:d:76:THR:HG23	11:d:79:ALA:H	1.86	0.41
12:e:68:MET:HE2	12:e:233:HIS:ND1	2.35	0.41
14:g:50:LEU:CD1	14:g:198:VAL:HG12	2.45	0.41
7:h:47:SER:HB2	7:h:220:VAL:O	2.20	0.41
7:h:196:GLN:OE1	7:h:245:ARG:CZ	2.66	0.41
7:B:30:LYS:HD2	7:B:33:LYS:HD2	2.02	0.41
3:E:134:ILE:HG22	3:E:135:VAL:N	2.35	0.41
3:E:223:ILE:O	3:E:227:VAL:HG23	2.21	0.41
6:X:227:VAL:HG21	6:X:232:LEU:HD21	2.02	0.41
11:r:120:ILE:O	11:r:120:ILE:CG2	2.69	0.41
8:a:15:THR:O	8:a:29:ALA:HA	2.21	0.41
13:f:14:ASN:HA	13:f:36:SER:O	2.20	0.41
14:g:20:PRO:HB3	14:g:123:TRP:NE1	2.36	0.41
14:g:140:THR:CG2	14:g:141:VAL:N	2.84	0.41
1:i:34:THR:HG22	1:i:49:GLU:CD	2.46	0.40
1:i:50:LYS:N	1:i:207:ASN:O	2.47	0.40
3:E:43:VAL:HG22	3:E:209:VAL:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:188:ILE:HG21	5:G:231:LEU:CD2	2.51	0.40
10:c:46:HIS:HD2	10:c:49:LEU:HD23	1.85	0.40
11:d:8:VAL:CG2	11:d:114:LEU:HB2	2.51	0.40
13:f:89:MET:HE2	13:f:94:MET:HE2	1.99	0.40
14:g:108:LEU:O	14:g:112:MET:HG2	2.21	0.40
14:g:158:GLY:O	14:g:162:ALA:HB3	2.21	0.40
7:h:210:PHE:HE1	7:h:215:ILE:HG21	1.86	0.40
3:k:60:VAL:O	3:k:61:ARG:CZ	2.69	0.40
3:E:93:GLN:HB3	11:d:62:LYS:HG3	2.02	0.40
9:p:65:VAL:HG22	13:f:195:ARG:HA	2.03	0.40
9:p:115:VAL:HG23	9:p:143:ASP:OD2	2.22	0.40
11:r:167:ARG:NH2	11:r:175:PRO:O	2.54	0.40
12:s:183:VAL:HG12	12:s:184:GLY:N	2.36	0.40
13:t:58:LEU:HD11	13:t:114:ASN:HB3	2.02	0.40
13:f:129:THR:OG1	13:f:142:SER:CB	2.69	0.40
13:f:214:ARG:NH1	13:f:216:GLU:OE2	2.38	0.40
2:j:35:ILE:HG22	2:j:163:ALA:HB2	2.00	0.40
3:k:77:LEU:HD12	3:k:77:LEU:N	2.37	0.40
5:m:103:LEU:HD22	5:m:108:LEU:HB2	2.03	0.40
1:C:52:LEU:HD13	1:C:57:VAL:CG1	2.51	0.40
9:p:192:LYS:O	9:p:196:GLU:HG2	2.21	0.40
12:s:67:VAL:HG13	12:s:234:VAL:HB	2.03	0.40
14:u:144:ILE:HG22	14:u:144:ILE:O	2.21	0.40
8:a:88:THR:HG22	8:a:89:VAL:N	2.37	0.40
4:l:157:SER:OG	4:l:159:THR:HG22	2.22	0.40
4:F:53:ARG:O	4:F:53:ARG:HG3	2.21	0.40
8:o:187:VAL:HG23	8:o:207:LEU:HD11	2.02	0.40
14:u:153:VAL:HG12	14:u:154:ALA:N	2.35	0.40
8:a:138:PHE:CD1	8:a:138:PHE:C	2.99	0.40
9:b:114:ARG:HA	9:b:143:ASP:CG	2.46	0.40
9:b:178:GLU:OE1	9:b:178:GLU:HA	2.21	0.40
10:c:27:ARG:HH22	10:c:179:LEU:HA	1.87	0.40
10:c:114:ASP:OD1	10:c:114:ASP:N	2.54	0.40
12:e:199:LYS:O	12:e:202:MET:HG2	2.21	0.40
1:i:37:GLY:HA3	1:i:146:LEU:HD11	2.04	0.40
4:l:73:HIS:O	4:l:143:GLY:HA2	2.22	0.40
4:l:197:LEU:HD11	4:l:215:ILE:CD1	2.51	0.40
5:m:172:LEU:O	5:m:176:PHE:N	2.54	0.40
6:n:109:VAL:HG21	6:n:140:GLY:HA3	2.03	0.40
2:D:8:ARG:HH12	4:F:8:TYR:CA	2.35	0.40
2:D:240:SER:O	2:D:244:GLN:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:o:67:ILE:HG13	8:o:68:VAL:N	2.37	0.40
14:u:61:ILE:HD12	14:u:67:LEU:HD23	2.03	0.40
13:f:63:PHE:O	13:f:67:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	227/235 (97%)	219 (96%)	8 (4%)	0	100	100
1	i	227/235 (97%)	214 (94%)	13 (6%)	0	100	100
2	D	247/250 (99%)	238 (96%)	9 (4%)	0	100	100
2	j	247/250 (99%)	234 (95%)	13 (5%)	0	100	100
3	E	238/247 (96%)	228 (96%)	9 (4%)	1 (0%)	30	60
3	k	238/247 (96%)	230 (97%)	8 (3%)	0	100	100
4	F	228/237 (96%)	213 (93%)	15 (7%)	0	100	100
4	l	228/237 (96%)	216 (95%)	11 (5%)	1 (0%)	30	60
5	G	229/274 (84%)	220 (96%)	9 (4%)	0	100	100
5	m	229/274 (84%)	218 (95%)	11 (5%)	0	100	100
6	X	237/249 (95%)	219 (92%)	17 (7%)	1 (0%)	30	60
6	n	237/249 (95%)	220 (93%)	17 (7%)	0	100	100
7	B	236/246 (96%)	225 (95%)	11 (5%)	0	100	100
7	h	236/246 (96%)	224 (95%)	12 (5%)	0	100	100
8	a	210/236 (89%)	191 (91%)	17 (8%)	2 (1%)	12	40
8	o	210/236 (89%)	196 (93%)	13 (6%)	1 (0%)	24	55
9	b	218/274 (80%)	199 (91%)	18 (8%)	1 (0%)	24	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	p	218/274 (80%)	205 (94%)	12 (6%)	1 (0%)	24	55
10	c	201/204 (98%)	184 (92%)	16 (8%)	1 (0%)	24	55
10	q	201/204 (98%)	178 (89%)	22 (11%)	1 (0%)	24	55
11	d	194/209 (93%)	179 (92%)	15 (8%)	0	100	100
11	r	194/209 (93%)	181 (93%)	13 (7%)	0	100	100
12	e	201/272 (74%)	193 (96%)	8 (4%)	0	100	100
12	s	201/272 (74%)	192 (96%)	9 (4%)	0	100	100
13	f	215/223 (96%)	198 (92%)	17 (8%)	0	100	100
13	t	215/223 (96%)	201 (94%)	13 (6%)	1 (0%)	24	55
14	g	219/240 (91%)	202 (92%)	17 (8%)	0	100	100
14	u	219/240 (91%)	198 (90%)	21 (10%)	0	100	100
All	All	6200/6792 (91%)	5815 (94%)	374 (6%)	11 (0%)	44	71

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	t	201	ASP
10	c	160	GLU
4	l	219	SER
8	a	224	TRP
9	p	210	SER
8	a	223	ILE
9	b	210	SER
3	E	50	SER
6	X	59	MET
8	o	224	TRP
10	q	31	GLN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	192/197 (98%)	192 (100%)	0	100	100
1	i	192/197 (98%)	191 (100%)	1 (0%)	81	83
2	D	208/209 (100%)	208 (100%)	0	100	100
2	j	208/209 (100%)	206 (99%)	2 (1%)	68	76
3	E	194/198 (98%)	190 (98%)	4 (2%)	47	67
3	k	194/198 (98%)	194 (100%)	0	100	100
4	F	194/201 (96%)	191 (98%)	3 (2%)	57	72
4	l	194/201 (96%)	194 (100%)	0	100	100
5	G	193/220 (88%)	193 (100%)	0	100	100
5	m	193/220 (88%)	193 (100%)	0	100	100
6	X	191/199 (96%)	188 (98%)	3 (2%)	55	72
6	n	191/199 (96%)	191 (100%)	0	100	100
7	B	199/204 (98%)	199 (100%)	0	100	100
7	h	199/204 (98%)	198 (100%)	1 (0%)	81	83
8	a	171/188 (91%)	167 (98%)	4 (2%)	44	66
8	o	171/188 (91%)	168 (98%)	3 (2%)	51	70
9	b	180/222 (81%)	176 (98%)	4 (2%)	45	66
9	p	180/222 (81%)	180 (100%)	0	100	100
10	c	171/172 (99%)	168 (98%)	3 (2%)	51	70
10	q	171/172 (99%)	170 (99%)	1 (1%)	78	81
11	d	160/168 (95%)	156 (98%)	4 (2%)	42	64
11	r	160/168 (95%)	160 (100%)	0	100	100
12	e	158/217 (73%)	158 (100%)	0	100	100
12	s	158/217 (73%)	158 (100%)	0	100	100
13	f	181/186 (97%)	178 (98%)	3 (2%)	53	71
13	t	181/186 (97%)	179 (99%)	2 (1%)	65	76
14	g	186/205 (91%)	185 (100%)	1 (0%)	81	83
14	u	186/205 (91%)	186 (100%)	0	100	100
All	All	5156/5572 (92%)	5117 (99%)	39 (1%)	70	79

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	i	8	PHE
2	j	219	PRO
2	j	223	VAL
3	E	42	VAL
3	E	46	VAL
3	E	54	LEU
3	E	55	GLN
4	F	123	PHE
4	F	131	MET
4	F	132	SER
6	X	58	MET
6	X	59	MET
6	X	60	LEU
8	o	26	ILE
8	o	220	LEU
8	o	221	LEU
10	q	33	GLN
13	t	167	ILE
13	t	205	ILE
8	a	26	ILE
8	a	35	THR
8	a	37	VAL
8	a	224	TRP
9	b	144	VAL
9	b	214	VAL
9	b	218	THR
9	b	226	ARG
10	c	154	LYS
10	c	155	PRO
10	c	158	GLU
11	d	114	LEU
11	d	117	ILE
11	d	120	ILE
11	d	124	HIS
13	f	7	ASN
13	f	162	PRO
13	f	167	ILE
14	g	28	ILE
7	h	166	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	i	96	GLN
2	j	95	GLN
2	j	102	GLN
2	j	172	GLN
3	k	31	ASN
3	k	166	ASN
4	l	91	HIS
1	C	5	GLN
2	D	146	GLN
3	E	31	ASN
3	E	65	ASN
4	F	223	HIS
5	G	5	GLN
5	G	43	HIS
6	X	147	GLN
8	o	49	GLN
8	o	78	GLN
8	o	85	GLN
8	o	108	GLN
8	o	217	GLN
9	p	101	GLN
9	p	211	ASN
10	q	33	GLN
10	q	71	HIS
10	q	75	GLN
11	r	63	ASN
13	t	121	ASN
13	t	157	ASN
14	u	159	ASN
14	u	202	GLN
8	a	66	GLN
8	a	78	GLN
8	a	103	ASN
9	b	101	GLN
9	b	221	ASN
9	b	228	HIS
10	c	33	GLN
10	c	40	GLN
12	e	108	GLN
13	f	114	ASN
14	g	152	HIS
7	h	150	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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-14175. These allow visual inspection of the internal detail of the map and identification of artifacts.

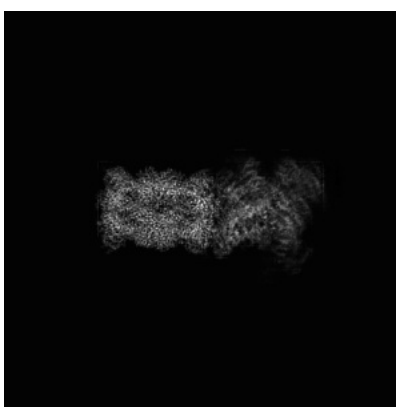
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

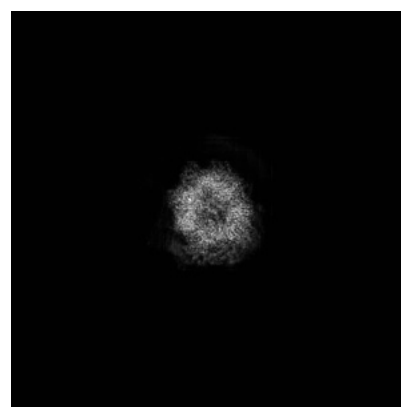
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 220



Y Index: 220



Z Index: 220

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

6.3 Largest variance slices [i](#)

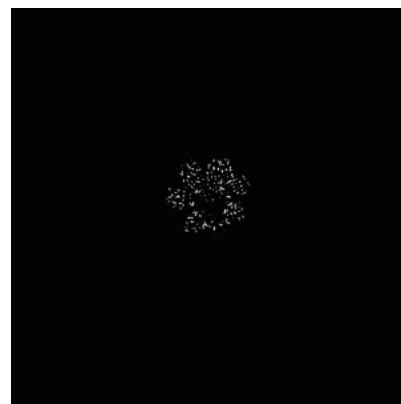
6.3.1 Primary map



X Index: 199



Y Index: 200



Z Index: 210

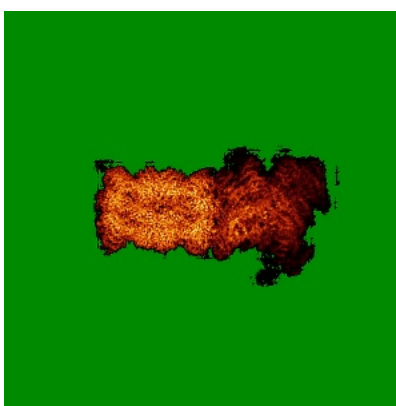
The images above show the largest variance slices of the map in three orthogonal directions.

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

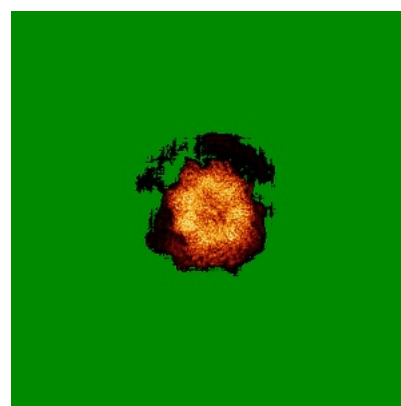
6.4.1 Primary map



X



Y

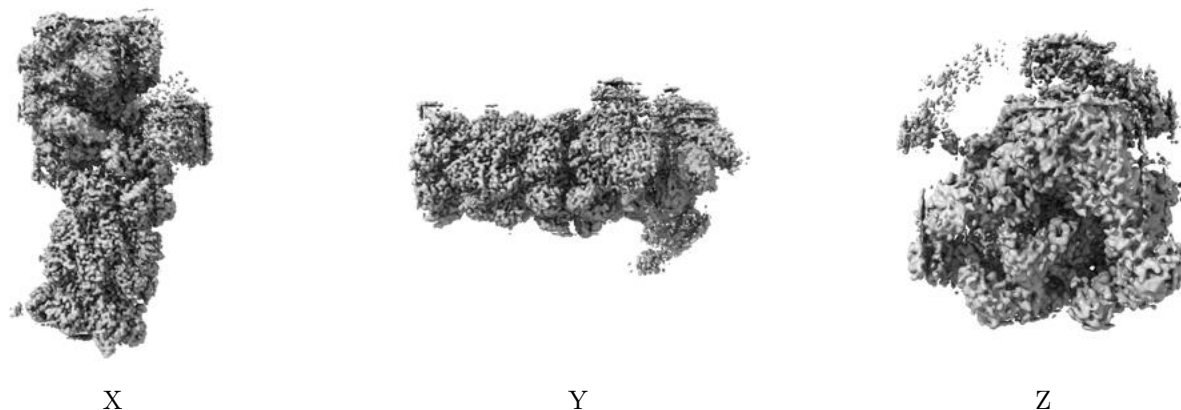


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0168. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

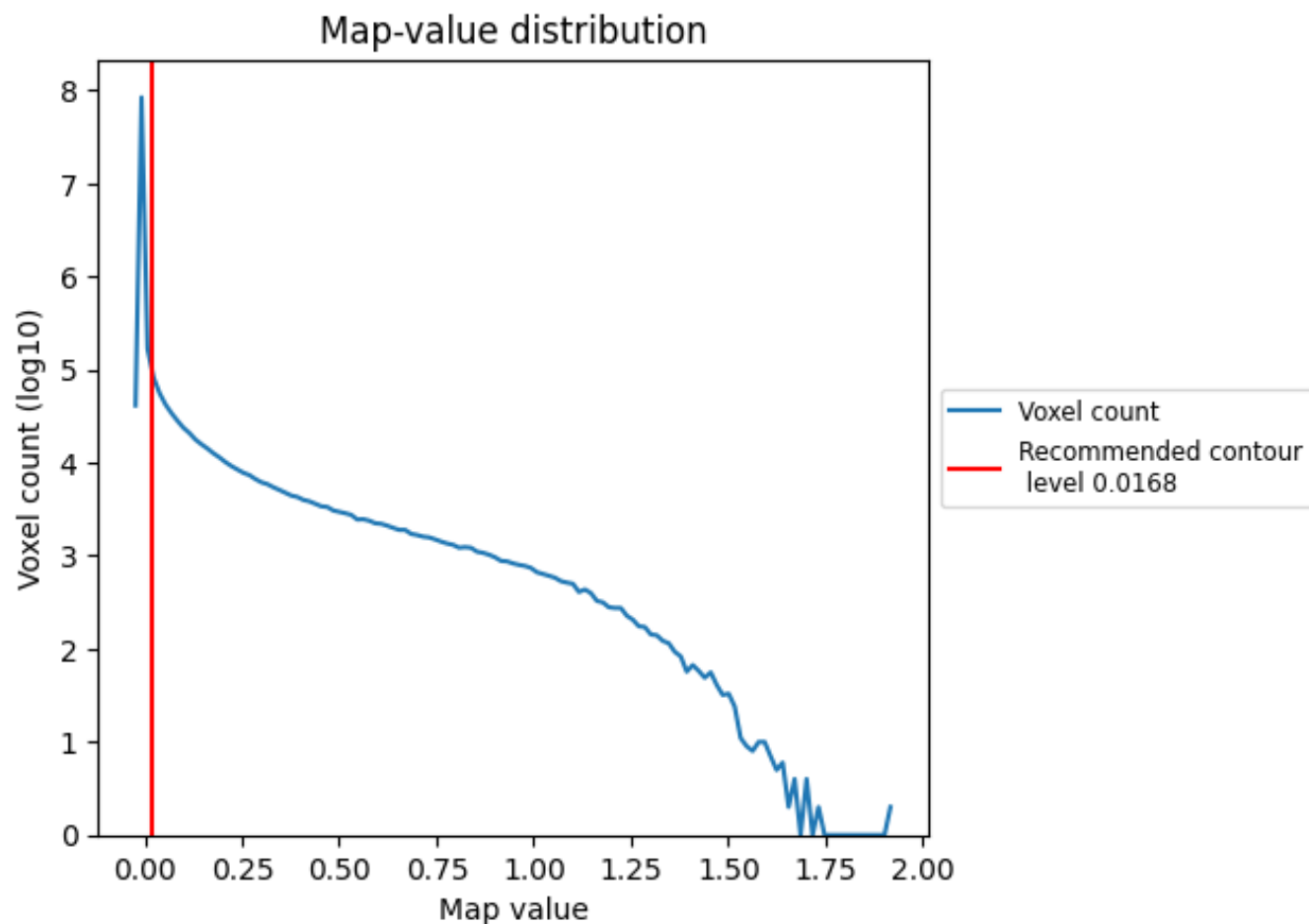
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

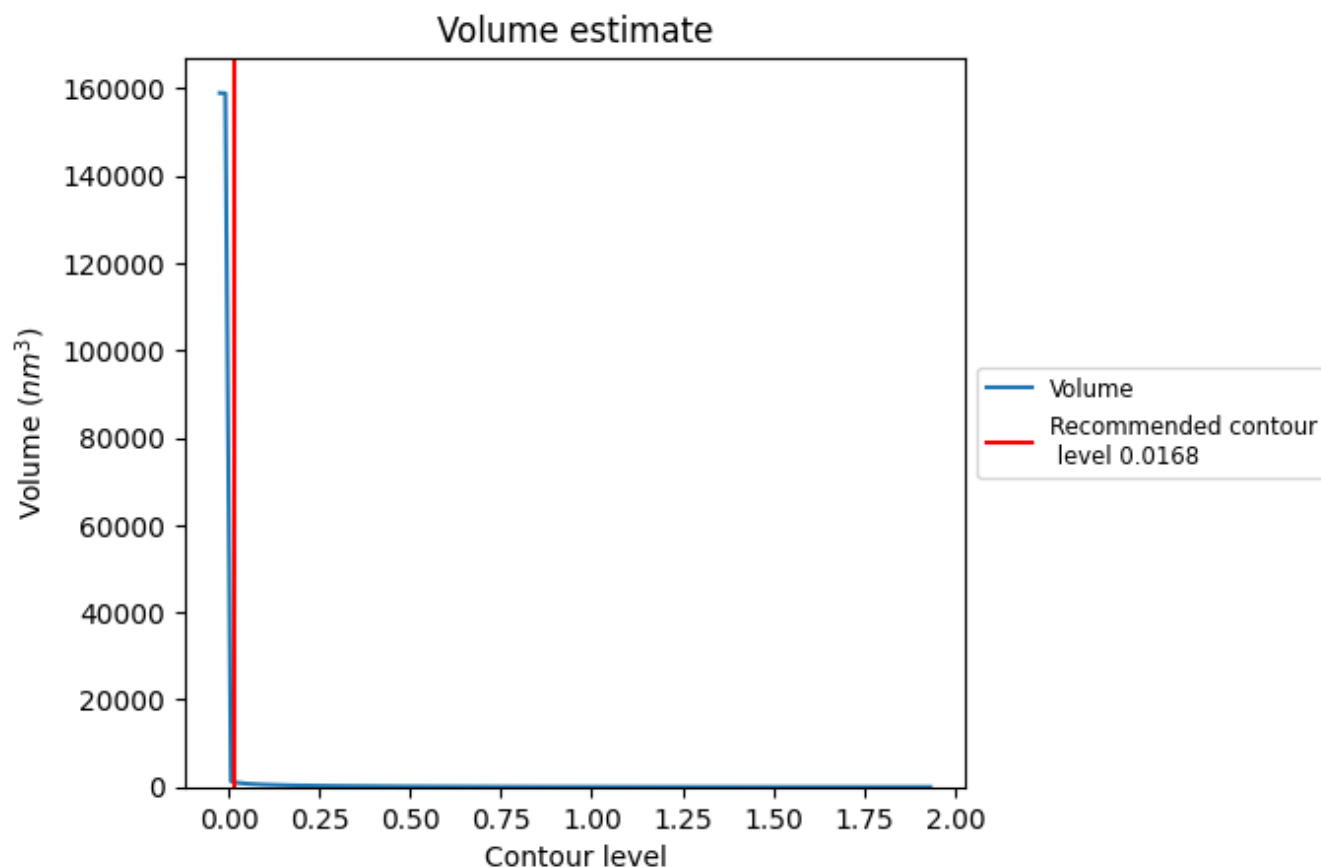
This section contains the results of statistical analysis of the map.

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.

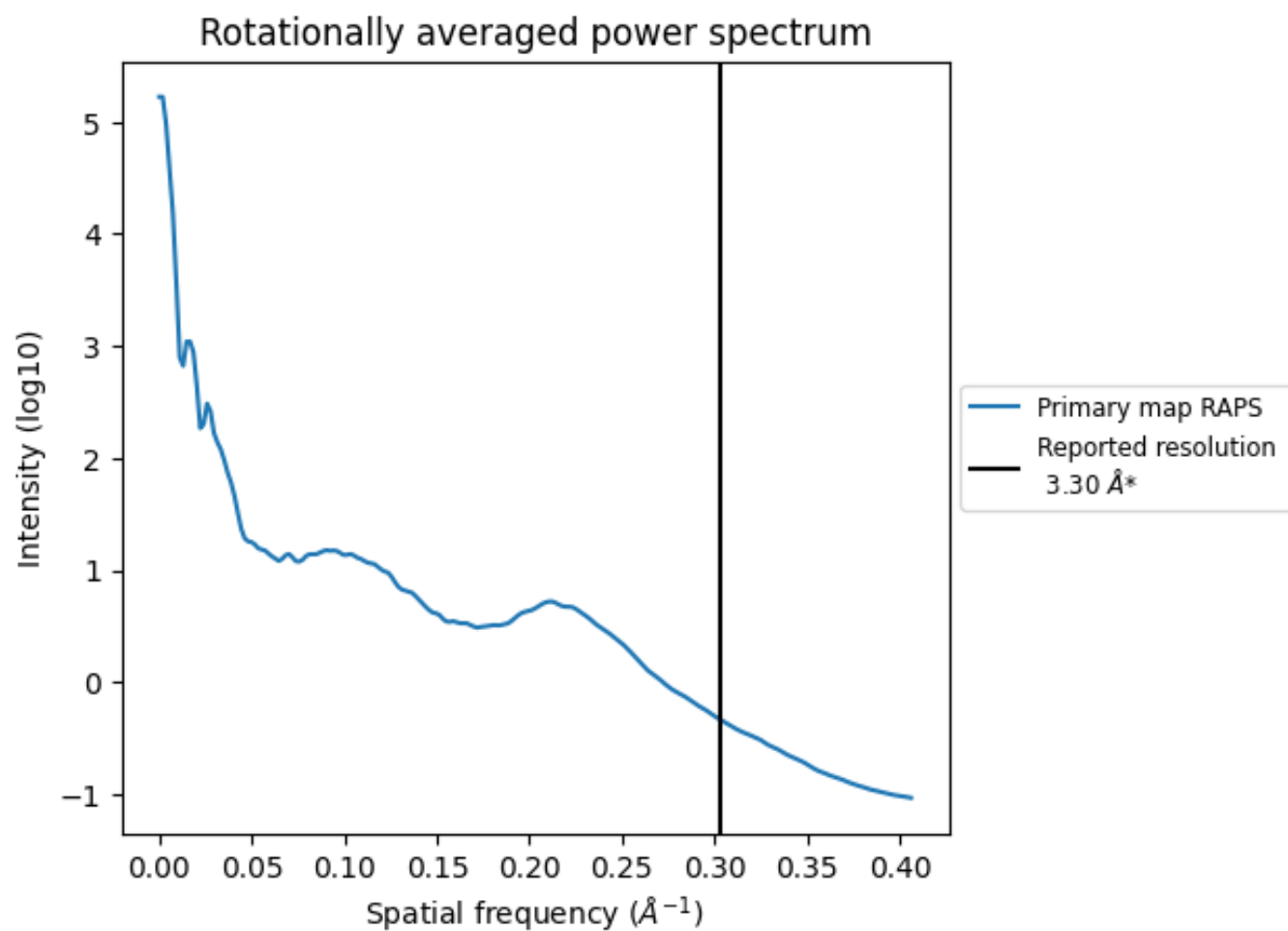
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1112 nm^3 ; this corresponds to an approximate mass of 1004 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 0.303 Å⁻¹

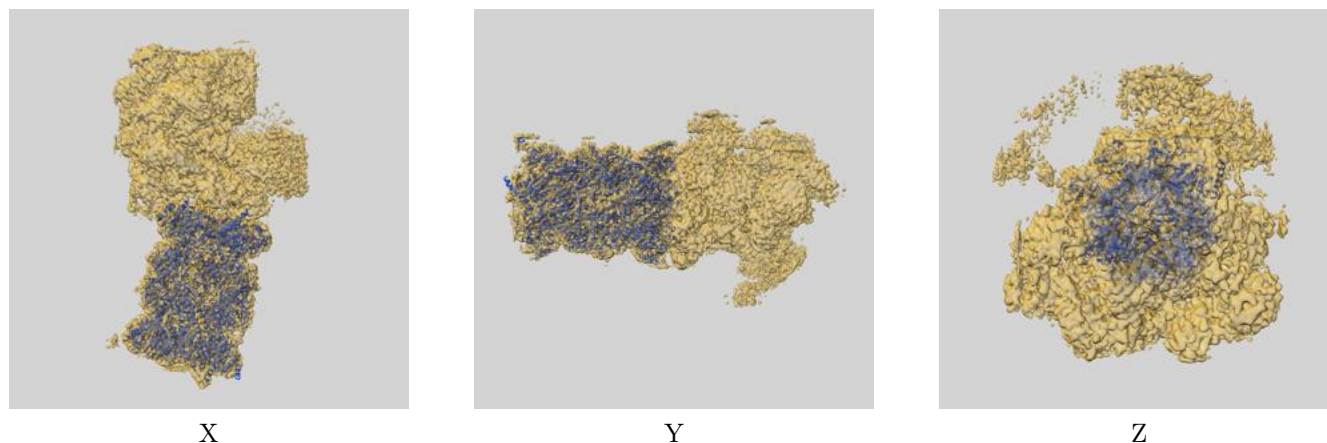
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

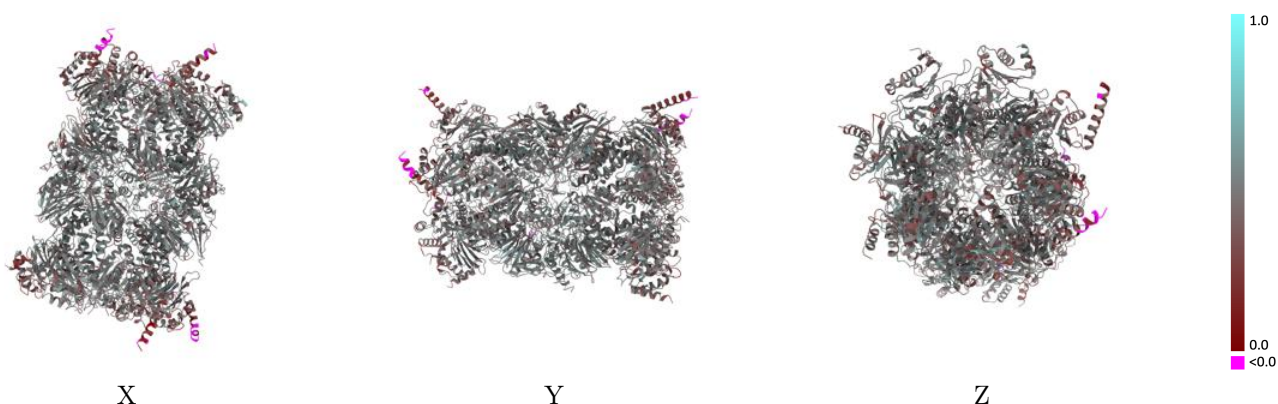
This section contains information regarding the fit between EMDB map EMD-14175 and PDB model 7QVE. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



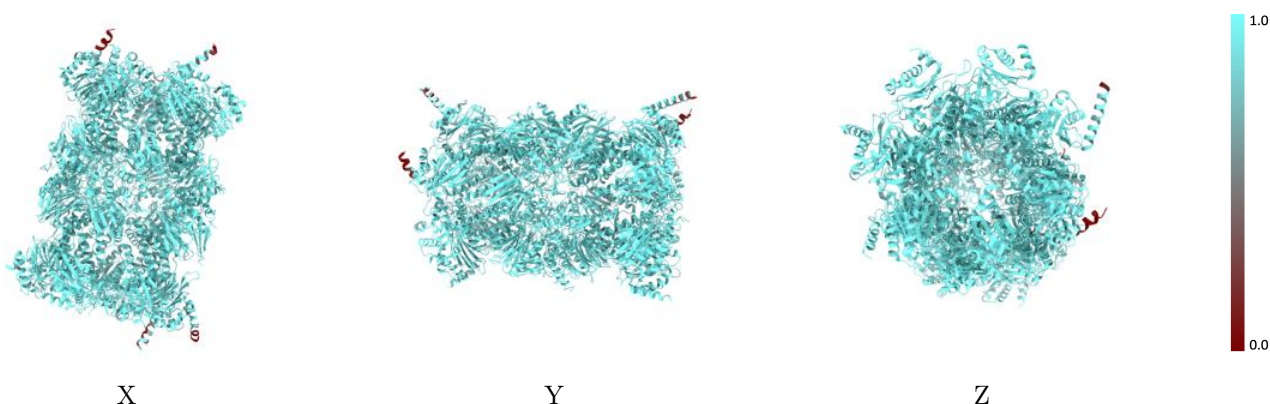
The images above show the 3D surface view of the map at the recommended contour level 0.0168 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



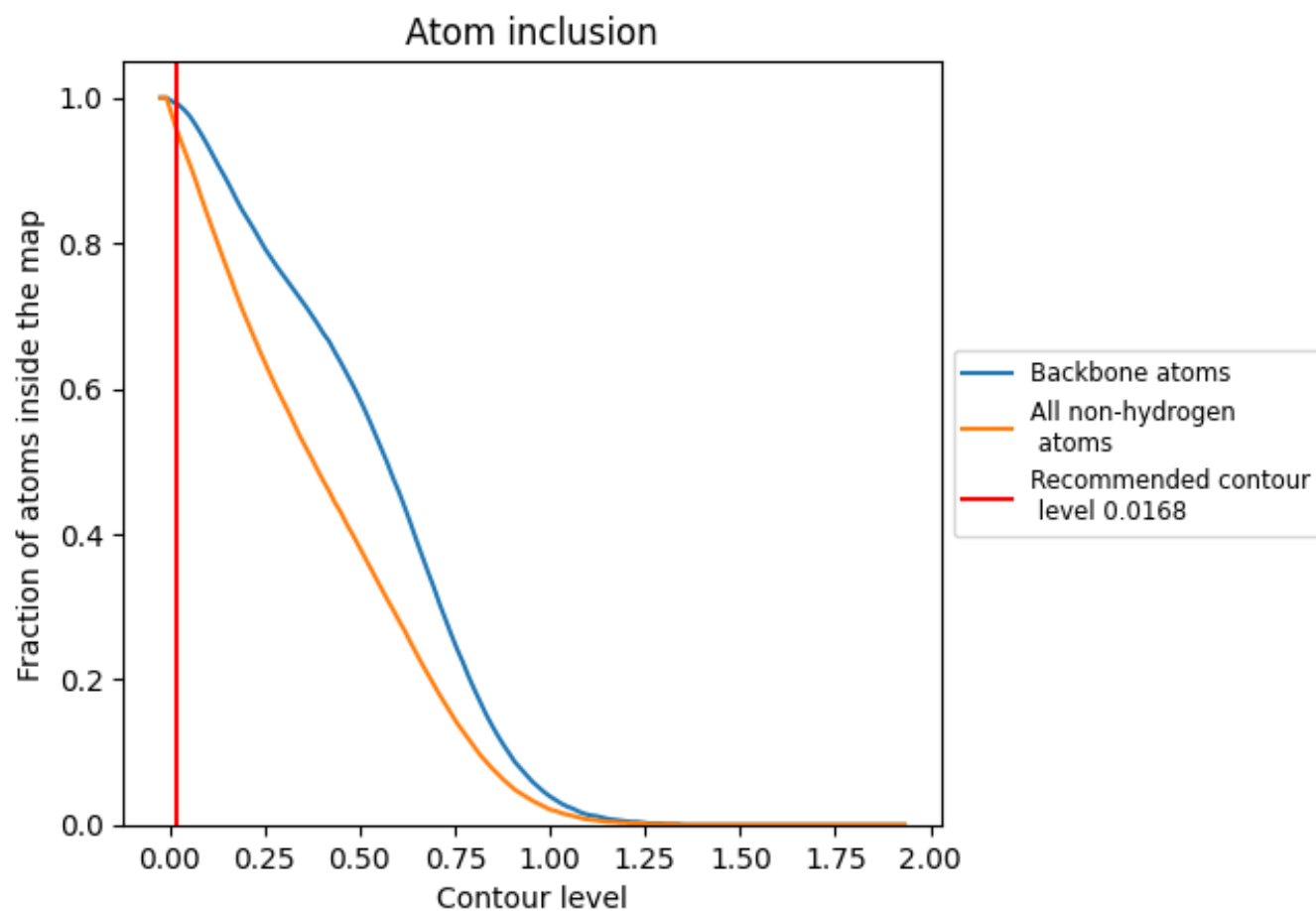
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0168).

9.4 Atom inclusion ⓘ



At the recommended contour level, 99% of all backbone atoms, 96% 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 (0.0168) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9590	 0.4500
B	 0.9570	 0.4350
C	 0.9580	 0.4350
D	 0.9230	 0.4040
E	 0.9170	 0.4070
F	 0.9570	 0.4510
G	 0.9490	 0.4270
X	 0.9440	 0.4180
a	 0.9810	 0.4990
b	 0.9620	 0.4690
c	 0.9800	 0.4730
d	 0.9670	 0.4660
e	 0.9820	 0.4710
f	 0.9770	 0.4830
g	 0.9780	 0.4930
h	 0.9570	 0.4390
i	 0.9430	 0.4100
j	 0.8980	 0.3880
k	 0.9250	 0.4070
l	 0.9620	 0.4410
m	 0.9700	 0.4550
n	 0.9560	 0.4460
o	 0.9860	 0.4890
p	 0.9640	 0.4580
q	 0.9710	 0.4670
r	 0.9740	 0.4640
s	 0.9800	 0.4690
t	 0.9840	 0.4840
u	 0.9790	 0.4860

