



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:27 AM UTC

PDB ID : 9BRA / pdb_00009bra
EMDB ID : EMD-44839
Title : Intact V-ATPase State 2 and synaptophysin complex in mouse brain isolated synaptic vesicles
Authors : Wang, C.; Jiang, W.; Yang, K.; Wang, X.; Guo, Q.; Brunger, A.T.
Deposited on : 2024-05-11
Resolution : 4.30 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 : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

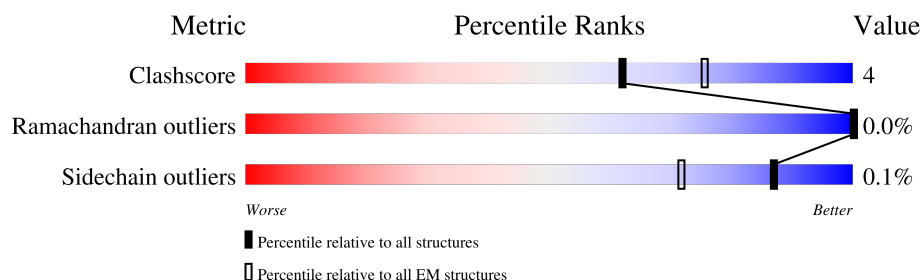
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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.



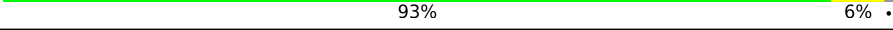
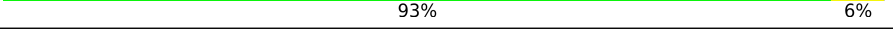
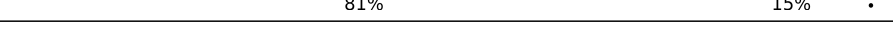
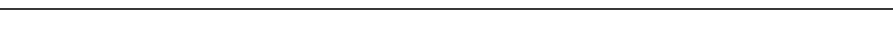
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	8	226	93% 7%
1	9	226	92% 8%
1	Q	226	93% 7%
2	R	118	90% 7% .
2	T	118	91% 6% .
2	V	118	84% 13% .
3	0	617	92% 5% .
3	1	617	93% . .
3	2	617	90% 5% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	3	511	 84% 6% 10%
4	4	511	 86% • 11%
4	5	511	 85% 5% 10%
5	6	382	 83% 10% • 6%
6	7	247	 76% 8% 16%
7	U	483	 81% 7% 12%
8	X	119	 90% • 8%
9	a	838	 82% 7% 12%
10	b	205	 93% 6% •
11	d	351	 93% 6%
12	g	155	 75% 22% •
12	h	155	 79% 18% •
12	i	155	 78% 19% •
12	j	155	 81% 15% •
12	k	155	 72% 23% • •
12	l	155	 74% 22% • •
12	m	155	 77% 19% •
12	n	155	 79% 17% •
12	o	155	 80% 17% •
13	p	350	 13% • 85%
14	c	463	 41% • 56%
15	f	98	 78% 10% 12%
16	s	314	 63% • 33%
17	e	81	 88% 10% •

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 66852 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 V-type proton ATPase subunit E 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	225	Total	C	N	O	S	0	0
			1823	1146	322	345	10		
1	9	225	Total	C	N	O	S	0	0
			1823	1146	322	345	10		
1	Q	225	Total	C	N	O	S	0	0
			1823	1146	322	345	10		

- Molecule 2 is a protein called V-type proton ATPase subunit G 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	114	Total	C	N	O	S	0	0
			925	552	192	176	5		
2	T	114	Total	C	N	O	S	0	0
			925	552	192	176	5		
2	V	114	Total	C	N	O	S	0	0
			925	552	192	176	5		

- Molecule 3 is a protein called V-type proton ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	0	596	Total	C	N	O	S	0	0
			4627	2937	782	881	27		
3	1	599	Total	C	N	O	S	0	0
			4647	2948	786	886	27		
3	2	585	Total	C	N	O	S	0	0
			4551	2891	768	866	26		

- Molecule 4 is a protein called V-type proton ATPase subunit B, brain isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	462	Total	C	N	O	S	0	0
			3617	2296	613	688	20		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	457	Total	C	N	O	S	0	0
			3575	2270	607	678	20		
4	5	458	Total	C	N	O	S	0	0
			3584	2275	608	681	20		

- Molecule 5 is a protein called V-type proton ATPase subunit C 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	360	Total	C	N	O	S	0	0
			2925	1874	494	548	9		

- Molecule 6 is a protein called V-type proton ATPase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	208	Total	C	N	O	S	0	0
			1676	1064	303	304	5		

- Molecule 7 is a protein called V-type proton ATPase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	427	Total	C	N	O	S	0	0
			3507	2227	605	650	25		

- Molecule 8 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	X	110	Total	C	N	O	S	0	0
			875	553	157	163	2		

- Molecule 9 is a protein called V-type proton ATPase 116 kDa subunit a 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	741	Total	C	N	O	S	0	0
			6027	3938	1009	1040	40		

- Molecule 10 is a protein called V-type proton ATPase 21 kDa proteolipid subunit c”.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	203	Total	C	N	O	S	0	0
			1503	996	237	259	11		

- Molecule 11 is a protein called V-type proton ATPase subunit d 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	d	350	Total	C	N	O	S	0	0
			2833	1829	460	530	14		

- Molecule 12 is a protein called V-type proton ATPase 16 kDa proteolipid subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	g	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
12	h	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
12	i	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
12	j	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
12	k	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
12	l	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
12	m	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
12	n	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
12	o	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		

- Molecule 13 is a protein called Renin receptor cytoplasmic fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	p	52	Total	C	N	O	S	0	0
			433	292	63	75	3		

- Molecule 14 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	c	203	Total	C	N	O	S	0	0
			1642	1079	259	295	9		

- Molecule 15 is a protein called Ribonuclease kappa.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	f	86	Total 666	C 440	N 103	O 116	S 7	0	0

- Molecule 16 is a protein called Synaptophysin.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	s	211	Total 1671	C 1097	N 263	O 299	S 12	0	0

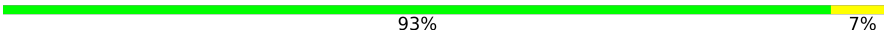
- Molecule 17 is a protein called V-type proton ATPase subunit e 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	e	79	Total 637	C 439	N 99	O 96	S 3	0	0

3 Residue-property plots [i](#)

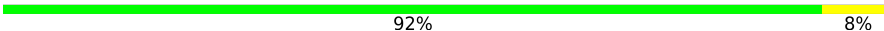
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

- Molecule 1: V-type proton ATPase subunit E 1

Chain 8:  93% 7%

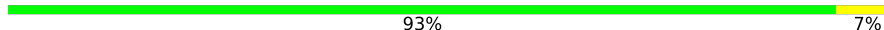


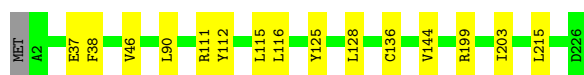
- Molecule 1: V-type proton ATPase subunit E 1

Chain 9:  92% 8%



- Molecule 1: V-type proton ATPase subunit E 1

Chain Q:  93% 7%



- Molecule 2: V-type proton ATPase subunit G 2

Chain R:  90% 7% .



- Molecule 2: V-type proton ATPase subunit G 2

Chain T:  91% 6% .



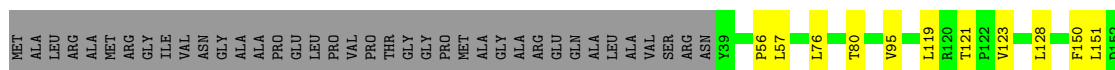
- Molecule 2: V-type proton ATPase subunit G 2

Chain V:  84% 13% .



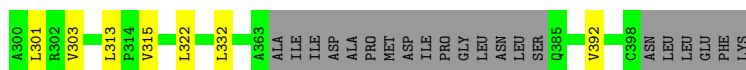
- Molecule 4: V-type proton ATPase subunit B, brain isoform

Chain 5: 85% 5% 10%



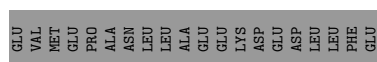
- Molecule 5: V-type proton ATPase subunit C 1

Chain 6: 83% 10% 6%



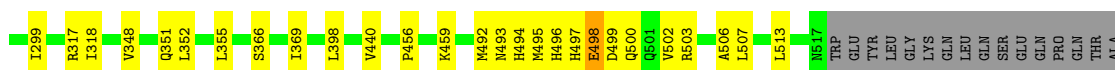
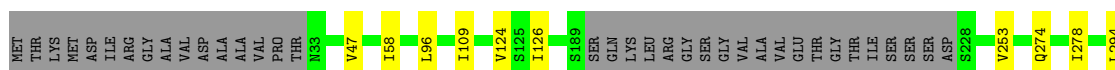
- Molecule 6: V-type proton ATPase subunit D

Chain 7: 76% 8% 16%



- Molecule 7: V-type proton ATPase subunit H

Chain U: 81% 7% 12%



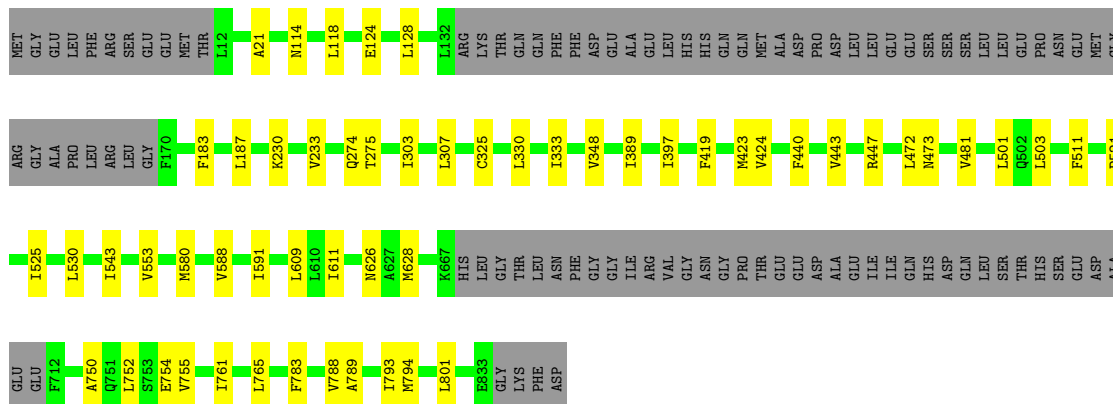
- Molecule 8: V-type proton ATPase subunit F

Chain X: 90% 8%



- Molecule 9: V-type proton ATPase 116 kDa subunit a 1

Chain a: 82% 7% 12%



- Molecule 10: V-type proton ATPase 21 kDa proteolipid subunit c''

Chain b: 93% 6%



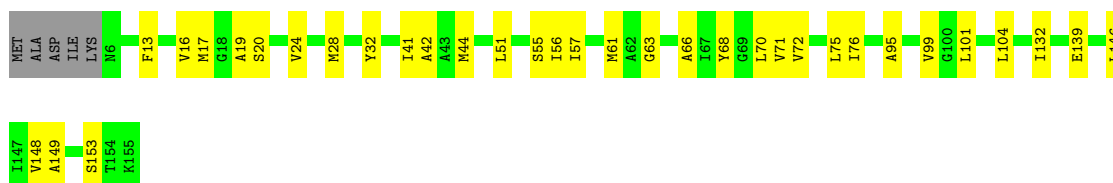
- Molecule 11: V-type proton ATPase subunit d 1

Chain d: 93% 6%



- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit c

Chain g: 75% 22%



- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit c

Chain h: 79% 18%



K155

- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit c

Chain i: 78% 19%

MET ALA ASP ASP ILE ILE LYS H6 M17 S20 M23 M24 M28 M29 G29 A30 A31 S45 S46 V57 P58 V59 V60 V61 L70 L71 V72 V73 V74 L91 A95 G96 L97 V99 G100 L101 L104 A105 I112 T121 L127 L133 L134 L135 K155

- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit c

Chain j: 81% 15%

MET ALA ASP ASP ILE ILE LYS H6 S20 V24 A31 T34 A35 S45 A66 A67 V68 V72 I84 T85 L86 S89 F90 V99 G100 L101 A105 A109 V113 Q123 L127 T134 L143 Y144 V148 K155

- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit c

Chain k: 72% 23%

MET ALA ASP ASP ILE ILE LYS H6 G15 V16 M23 V24 G33 T34 A35 K36 M44 M47 M53 I56 I57 M61 A62 G63 I64 I65 A66 I67 Y68 G69 L70 L71 V72 V74 L75 I76 A77 L80 V99 G100 L101 A109 I112 V113 G114 V118 A122

L127 L141 A149 K155

- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit c

Chain l: 74% 22%

MET ALA ASP ASP ILE ILE LYS H6 S12 V16 M17 A22 M28 M44 M47 R48 P49 I52 I64 I65 A66 I67 Y68 V72 L75 A95 G96 V99 G100 L101 F108 A109 I110 G111 I112 V118 A122 F137 A138 E139 L143 Y144 G145 L146 I147

V148 A149 L152 S153 T154 K155

- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit c

Chain m: 77% 19%

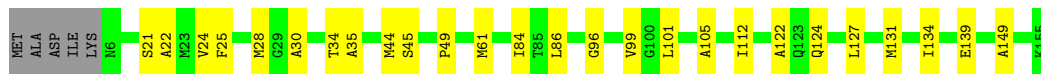
MET ALA ASP ASP ILE ILE LYS H6 F13 V16 S20 S21 A22 M23 V24 M28 G40 M44 S45 S46 V46 M47 I57 P58 V59 V60 A66 L70 N78 S79 L80 T85 L86 Y87 G96 A105 V113 G114 V118 A122 Q123 Q124 L127 I134

Y144 I147 K155

- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit c



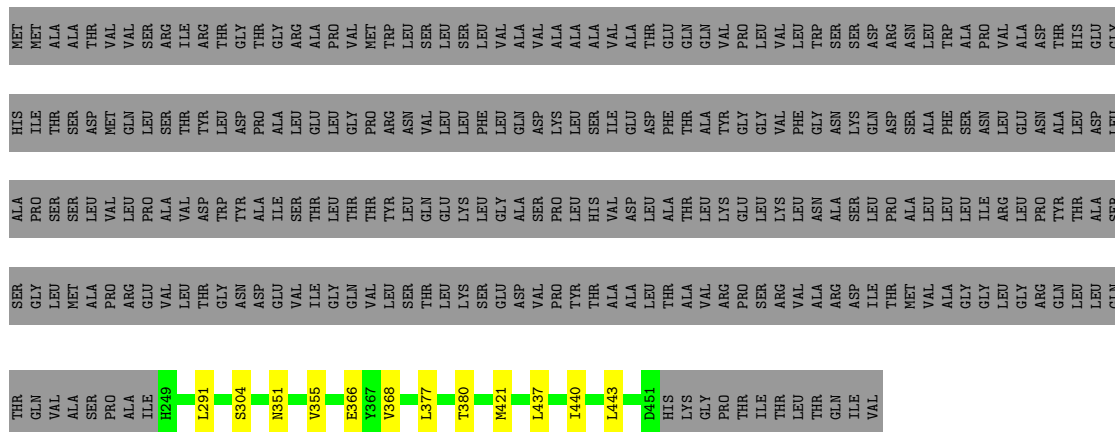
- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit c



- Molecule 13: Renin receptor cytoplasmic fragment



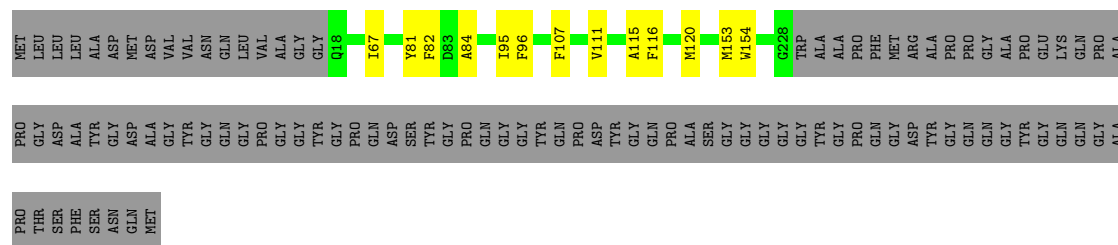
- Molecule 14: V-type proton ATPase subunit S1



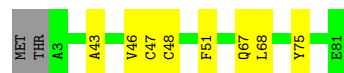
- Molecule 15: Ribonuclease kappa

MET
ALA
SER
LEU
L5
I16
I41
P45
E48
F51
N57
I58
L61
L75
V87
R90
LYS
ARG
LYS
GLU
TYR
MET
VAL

Chain s: 63% 3% 33%



Chain e: 88% 10%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25667	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	8	0.22	0/1840	0.46	0/2462
1	9	0.20	0/1840	0.44	0/2462
1	Q	0.21	0/1840	0.44	0/2462
2	R	0.25	0/930	0.51	0/1237
2	T	0.25	0/930	0.56	0/1237
2	V	0.23	0/930	0.56	0/1237
3	0	0.24	0/4722	0.44	0/6391
3	1	0.25	0/4743	0.43	0/6421
3	2	0.23	0/4643	0.42	0/6284
4	3	0.26	0/3689	0.41	0/4999
4	4	0.26	0/3646	0.42	0/4942
4	5	0.25	0/3655	0.43	0/4954
5	6	0.28	0/2979	0.53	0/4024
6	7	0.26	0/1694	0.52	0/2267
7	U	0.25	0/3574	0.52	0/4814
8	X	0.20	0/889	0.41	0/1199
9	a	0.21	0/6184	0.47	0/8368
10	b	0.24	0/1537	0.50	0/2088
11	d	0.22	0/2899	0.49	0/3927
12	g	0.29	0/1083	0.56	0/1466
12	h	0.27	0/1083	0.54	0/1466
12	i	0.25	0/1083	0.51	0/1466
12	j	0.24	0/1083	0.51	0/1466
12	k	0.41	0/1083	0.64	1/1466 (0.1%)
12	l	0.42	0/1083	0.67	0/1466
12	m	0.29	0/1083	0.56	0/1466
12	n	0.27	0/1083	0.55	0/1466
12	o	0.29	0/1083	0.56	0/1466
13	p	0.19	0/446	0.46	0/610
14	c	0.20	0/1697	0.48	0/2311
15	f	0.22	0/682	0.56	0/926
16	s	0.16	0/1716	0.40	0/2327
17	e	0.22	0/662	0.55	0/910
All	All	0.25	0/68114	0.48	1/92053 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	k	71	VAL	N-CA-C	-5.88	103.92	110.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	8	1823	0	1895	10	0
1	9	1823	0	1895	18	0
1	Q	1823	0	1895	12	0
2	R	925	0	935	6	0
2	T	925	0	935	8	0
2	V	925	0	935	12	0
3	0	4627	0	4618	21	0
3	1	4647	0	4637	16	0
3	2	4551	0	4543	22	0
4	3	3617	0	3614	23	0
4	4	3575	0	3576	14	0
4	5	3584	0	3582	18	0
5	6	2925	0	2964	54	0
6	7	1676	0	1781	27	0
7	U	3507	0	3486	31	0
8	X	875	0	883	5	0
9	a	6027	0	6059	38	0
10	b	1503	0	1551	16	0
11	d	2833	0	2770	15	0
12	g	1068	0	1136	29	0
12	h	1068	0	1136	32	0
12	i	1068	0	1136	35	0
12	j	1068	0	1136	28	0
12	k	1068	0	1136	46	0
12	l	1068	0	1136	43	0
12	m	1068	0	1136	29	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	n	1068	0	1136	30	0
12	o	1068	0	1136	28	0
13	p	433	0	432	4	0
14	c	1642	0	1568	10	0
15	f	666	0	663	10	0
16	s	1671	0	1649	7	0
17	e	637	0	652	9	0
All	All	66852	0	67742	572	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 4.

All (572) 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)
6:7:58:MET:HE1	6:7:145:LEU:HD23	1.22	1.11
10:b:150:PHE:CZ	12:o:28:MET:SD	2.52	1.02
6:7:58:MET:CE	6:7:145:LEU:HD23	1.92	0.99
5:6:58:GLU:O	5:6:62:LEU:HG	1.67	0.95
12:l:139:GLU:CD	12:l:143:LEU:HD11	1.93	0.93
5:6:70:VAL:HB	5:6:295:TRP:CZ2	2.04	0.93
1:9:16:MET:HE3	2:T:11:LEU:HD23	1.49	0.91
12:l:139:GLU:OE2	12:l:143:LEU:HD11	1.69	0.91
12:k:70:LEU:CD1	12:k:73:ALA:HB3	2.04	0.87
10:b:150:PHE:CE2	12:o:28:MET:SD	2.71	0.84
12:l:139:GLU:OE1	12:l:143:LEU:HD11	1.78	0.82
5:6:62:LEU:HD23	5:6:65:PHE:CE1	2.15	0.80
5:6:67:GLU:HA	5:6:295:TRP:CH2	2.16	0.80
5:6:208:MET:SD	5:6:233:LYS:NZ	2.52	0.80
12:i:28:MET:HE2	12:j:105:ALA:HB2	1.61	0.80
12:h:61:MET:HE2	12:h:139:GLU:HG3	1.65	0.79
12:l:139:GLU:OE1	12:l:143:LEU:CD1	2.30	0.79
12:k:70:LEU:HD12	12:k:70:LEU:O	1.83	0.79
6:7:46:GLN:NE2	6:7:50:LYS:HE3	1.97	0.78
12:h:35:ALA:HB1	12:i:112:ILE:HD11	1.64	0.78
5:6:208:MET:HE1	5:6:233:LYS:NZ	1.99	0.78
6:7:46:GLN:NE2	6:7:50:LYS:CE	2.48	0.77
12:k:70:LEU:HD13	12:k:73:ALA:HB3	1.65	0.76
12:m:20:SER:O	12:m:24:VAL:HG23	1.85	0.76
12:l:139:GLU:CD	12:l:143:LEU:CD1	2.59	0.76
6:7:58:MET:HE1	6:7:145:LEU:CD2	2.10	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:70:VAL:HB	5:6:295:TRP:CH2	2.21	0.75
12:l:139:GLU:OE2	12:l:143:LEU:CD1	2.35	0.75
3:0:39:MET:HE2	4:4:53:VAL:HG11	1.68	0.74
12:o:61:MET:HE2	12:o:139:GLU:HG3	1.71	0.72
7:U:492:MET:HE1	7:U:495:MET:HE2	1.70	0.72
16:s:111:VAL:HG13	16:s:153:MET:HE1	1.72	0.72
12:j:20:SER:O	12:j:24:VAL:HG23	1.91	0.70
12:l:139:GLU:OE2	12:l:143:LEU:CG	2.39	0.70
5:6:208:MET:CE	5:6:233:LYS:HZ3	2.03	0.70
5:6:62:LEU:HD23	5:6:65:PHE:CZ	2.27	0.69
5:6:208:MET:HE2	5:6:231:PHE:CG	2.28	0.69
6:7:46:GLN:HE21	6:7:50:LYS:HE3	1.55	0.69
12:h:80:LEU:HD12	12:h:84:ILE:HD11	1.73	0.69
12:k:70:LEU:HD12	12:k:73:ALA:HB3	1.75	0.69
6:7:46:GLN:HE21	6:7:50:LYS:CE	2.05	0.68
10:b:59:SER:OG	12:g:101:LEU:HD11	1.92	0.68
9:a:521:PRO:O	15:f:41:ILE:HD11	1.94	0.68
5:6:208:MET:CE	5:6:233:LYS:NZ	2.56	0.68
12:l:139:GLU:OE2	12:l:143:LEU:HD21	1.94	0.68
4:3:180:MET:N	4:3:180:MET:HE2	2.09	0.67
12:m:70:LEU:HD11	12:n:144:TYR:CD1	2.28	0.67
5:6:208:MET:CE	5:6:231:PHE:CD2	2.77	0.67
4:4:327:MET:HE3	4:4:368:LEU:HD12	1.77	0.67
12:h:24:VAL:HG13	12:i:101:LEU:HD11	1.77	0.66
12:i:20:SER:O	12:i:24:VAL:HG23	1.95	0.66
12:m:114:GLY:O	12:m:118:VAL:HG23	1.94	0.66
12:i:57:ILE:HG22	12:i:61:MET:CE	2.25	0.66
12:n:44:MET:SD	12:n:118:VAL:HG22	2.35	0.66
5:6:208:MET:HE1	5:6:233:LYS:HZ2	1.59	0.66
12:h:110:ILE:HD11	12:h:138:ALA:HB3	1.77	0.66
1:8:124:LEU:HD13	1:8:132:MET:HE1	1.77	0.65
10:b:150:PHE:CE1	12:o:28:MET:SD	2.89	0.65
5:6:62:LEU:HA	5:6:65:PHE:CE1	2.32	0.65
12:m:57:ILE:O	12:m:60:VAL:HG12	1.96	0.65
12:n:68:TYR:CE1	12:n:146:LEU:HD11	2.32	0.65
6:7:46:GLN:HE21	6:7:50:LYS:NZ	1.94	0.64
1:9:17:ALA:CB	5:6:313:LEU:HD22	2.28	0.64
1:8:90:LEU:HD21	2:R:84:MET:HE2	1.79	0.64
12:g:28:MET:CE	12:h:105:ALA:HB2	2.28	0.63
12:n:20:SER:O	12:n:24:VAL:HG23	1.99	0.63
12:h:24:VAL:HG13	12:i:101:LEU:CD1	2.27	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:i:70:LEU:HD11	12:j:144:TYR:CD1	2.33	0.63
12:l:16:VAL:HG23	12:l:17:MET:HE2	1.81	0.63
5:6:62:LEU:CD2	5:6:65:PHE:CZ	2.82	0.63
5:6:208:MET:HE1	5:6:231:PHE:CE2	2.34	0.63
1:9:16:MET:HE1	2:T:11:LEU:HA	1.82	0.62
11:d:106:MET:HE1	11:d:133:LEU:O	1.99	0.62
12:h:80:LEU:HD23	12:i:91:LEU:HD21	1.81	0.62
12:g:16:VAL:HG22	12:h:91:LEU:HD23	1.80	0.62
12:n:68:TYR:CD1	12:n:146:LEU:HD11	2.34	0.62
15:f:75:LEU:HD23	15:f:75:LEU:O	1.98	0.62
5:6:208:MET:HE2	5:6:231:PHE:CD2	2.35	0.61
12:g:42:ALA:HB1	12:h:117:GLY:HA2	1.82	0.61
12:i:70:LEU:HD11	12:j:144:TYR:CG	2.36	0.61
6:7:46:GLN:NE2	6:7:50:LYS:NZ	2.48	0.61
12:k:47:MET:HE3	12:k:122:ALA:HB1	1.82	0.61
12:l:47:MET:HE2	12:l:122:ALA:HA	1.82	0.61
5:6:66:VAL:HG13	5:6:295:TRP:CE2	2.36	0.61
12:o:61:MET:HE2	12:o:139:GLU:CG	2.31	0.60
12:g:99:VAL:HB	12:g:149:ALA:HB2	1.83	0.60
12:j:35:ALA:HB1	12:k:112:ILE:HG21	1.83	0.60
12:g:63:GLY:O	12:g:66:ALA:HB3	2.01	0.60
10:b:157:ILE:HD11	12:o:35:ALA:HB1	1.83	0.60
3:2:291:PHE:CE2	3:2:309:THR:HG21	2.37	0.60
12:g:70:LEU:HD23	12:h:144:TYR:CE1	2.37	0.60
12:k:44:MET:HE1	12:k:122:ALA:HA	1.82	0.60
3:1:442:ARG:NH1	4:4:427:ALA:HB1	2.16	0.60
7:U:352:LEU:HB3	7:U:369:ILE:HD11	1.83	0.59
6:7:138:TYR:O	6:7:142:VAL:HG23	2.02	0.59
12:m:47:MET:HE1	12:m:122:ALA:O	2.01	0.59
9:a:591:ILE:HG22	9:a:609:LEU:HD22	1.85	0.59
3:1:233:VAL:HG22	3:1:520:LEU:HD23	1.85	0.59
5:6:208:MET:HE1	5:6:231:PHE:CD2	2.38	0.59
1:Q:46:VAL:HG11	2:V:40:ALA:HB1	1.85	0.58
12:j:84:ILE:HG22	12:j:86:LEU:H	1.68	0.58
4:5:121:THR:HG21	4:5:277:LEU:HD11	1.85	0.58
12:l:16:VAL:HG23	12:l:17:MET:CE	2.34	0.58
12:n:57:ILE:HG21	12:n:132:ILE:HD12	1.85	0.58
12:j:34:THR:HG22	12:k:113:VAL:HG11	1.86	0.58
12:k:70:LEU:HD12	12:k:74:VAL:H	1.67	0.58
15:f:51:PHE:HB2	15:f:58:ILE:HD11	1.85	0.58
1:9:127:LEU:HD23	1:9:132:MET:HG3	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:525:ILE:HG12	15:f:41:ILE:HD12	1.85	0.57
3:1:471:GLU:O	3:1:475:LEU:HD23	2.04	0.57
12:l:144:TYR:HA	12:l:147:ILE:HD12	1.86	0.57
3:0:550:MET:HE2	3:0:574:MET:HE1	1.84	0.57
12:h:56:ILE:HD12	12:i:133:LEU:HD22	1.86	0.57
5:6:66:VAL:O	5:6:295:TRP:CZ2	2.58	0.57
14:c:291:LEU:HD13	14:c:304:SER:O	2.05	0.57
5:6:322:LEU:HD21	5:6:332:LEU:HD21	1.87	0.57
12:h:61:MET:HE1	12:h:136:ILE:HA	1.87	0.57
12:k:70:LEU:HB2	12:l:144:TYR:CE1	2.40	0.57
12:m:44:MET:SD	12:m:118:VAL:HG13	2.44	0.57
1:Q:136:CYS:SG	1:Q:144:VAL:HG21	2.45	0.56
10:b:154:CYS:SG	12:o:34:THR:HG23	2.44	0.56
12:m:124:GLN:HB2	12:m:127:LEU:HD13	1.86	0.56
7:U:503:ARG:O	7:U:507:LEU:HD23	2.05	0.56
12:n:59:VAL:HG21	12:o:134:ILE:HD12	1.87	0.56
2:T:63:MET:HE3	2:T:63:MET:O	2.05	0.56
12:i:45:SER:OG	12:j:127:LEU:HD22	2.05	0.56
12:l:139:GLU:OE2	12:l:143:LEU:CD2	2.53	0.56
12:k:70:LEU:HD22	12:l:148:VAL:HG12	1.86	0.56
9:a:114:ASN:O	9:a:118:LEU:HD23	2.06	0.56
12:l:75:LEU:HD13	12:l:153:SER:HB2	1.88	0.56
4:3:328:TYR:HE1	4:3:372:ILE:HD11	1.70	0.56
9:a:419:PHE:CD2	9:a:423:MET:HE1	2.41	0.56
12:k:57:ILE:HG22	12:k:61:MET:SD	2.46	0.56
12:g:28:MET:HB2	12:g:104:LEU:HD13	1.87	0.56
12:j:31:ALA:HB1	12:k:109:ALA:HB2	1.88	0.56
4:5:180:MET:N	4:5:180:MET:HE2	2.21	0.56
7:U:492:MET:CE	7:U:495:MET:HE2	2.35	0.56
1:8:215:LEU:HD21	2:R:88:GLN:OE1	2.05	0.55
12:n:35:ALA:HB1	12:o:112:ILE:HG21	1.88	0.55
12:g:68:TYR:CD1	12:g:146:LEU:HD22	2.42	0.55
12:g:57:ILE:HG21	12:g:132:ILE:HD12	1.86	0.55
4:4:194:ALA:HB3	4:4:197:LEU:HD13	1.87	0.55
12:j:45:SER:OG	12:k:127:LEU:HD11	2.07	0.55
12:m:13:PHE:CE1	12:n:90:PHE:HB2	2.42	0.55
1:9:146:ALA:HB1	1:9:150:LYS:NZ	2.22	0.55
3:2:426:LEU:HD21	4:3:195:ALA:HB2	1.88	0.55
15:f:57:ASN:OD1	15:f:58:ILE:HD12	2.07	0.55
4:3:164:ILE:HD11	4:3:342:GLU:OE2	2.07	0.54
4:4:180:MET:SD	4:4:394:VAL:HG21	2.46	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:69:VAL:HA	5:6:72:LYS:HD2	1.89	0.54
9:a:397:ILE:HD13	17:e:43:ALA:HB3	1.89	0.54
12:i:72:VAL:HG21	12:i:99:VAL:HG11	1.88	0.54
12:k:23:MET:HG2	12:l:148:VAL:HG11	1.90	0.54
1:8:49:GLN:HB3	2:R:44:VAL:HG21	1.89	0.54
7:U:253:VAL:HG22	7:U:294:LEU:HD11	1.90	0.54
6:7:104:VAL:HG11	6:7:161:ALA:HB1	1.90	0.54
12:i:121:THR:HG22	12:i:127:LEU:HB2	1.89	0.54
16:s:115:ALA:HB1	16:s:154:TRP:HZ2	1.73	0.54
12:g:61:MET:HE3	12:g:139:GLU:HG2	1.87	0.54
12:h:61:MET:HE2	12:h:139:GLU:CG	2.37	0.54
1:Q:112:TYR:O	1:Q:116:LEU:HD23	2.08	0.54
7:U:274:GLN:O	7:U:278:ILE:HG22	2.08	0.54
1:9:146:ALA:HB1	1:9:150:LYS:HZ3	1.73	0.53
5:6:62:LEU:HD22	5:6:65:PHE:HZ	1.73	0.53
5:6:62:LEU:CD2	5:6:65:PHE:HZ	2.21	0.53
9:a:789:ALA:O	9:a:793:ILE:HD11	2.09	0.53
12:l:12:SER:O	12:l:16:VAL:HG22	2.08	0.53
12:o:84:ILE:HG22	12:o:86:LEU:H	1.73	0.53
9:a:325:CYS:SG	9:a:333:ILE:HD11	2.47	0.53
12:m:40:GLY:HA3	12:m:118:VAL:HG21	1.91	0.53
7:U:499:ASP:HB3	7:U:502:VAL:HG23	1.91	0.53
12:g:28:MET:HE2	12:h:105:ALA:HB2	1.90	0.53
1:9:16:MET:HA	1:9:16:MET:HE2	1.89	0.53
3:0:39:MET:CE	4:4:53:VAL:HG11	2.37	0.53
11:d:37:LEU:HD23	11:d:49:HIS:HE1	1.74	0.53
4:3:410:MET:HG3	4:3:411:THR:H	1.74	0.53
4:5:229:ILE:HB	4:5:257:VAL:HG22	1.91	0.52
6:7:62:MET:HE1	8:X:95:PRO:HG2	1.91	0.52
11:d:209:MET:O	11:d:213:LEU:HD13	2.09	0.52
12:j:24:VAL:HG22	12:k:101:LEU:HD21	1.91	0.52
1:9:17:ALA:HB2	5:6:313:LEU:HD22	1.91	0.52
3:0:287:VAL:HG23	3:0:291:PHE:CD2	2.44	0.52
11:d:37:LEU:HD23	11:d:49:HIS:CE1	2.44	0.52
12:l:139:GLU:OE1	12:l:143:LEU:HD12	2.08	0.52
7:U:58:ILE:HG23	7:U:96:LEU:HD11	1.92	0.52
12:g:57:ILE:O	12:g:61:MET:HG2	2.09	0.52
12:h:28:MET:HB2	12:h:104:LEU:HD21	1.91	0.52
12:n:84:ILE:HD13	12:n:89:SER:HB3	1.92	0.52
12:h:16:VAL:HG21	12:i:91:LEU:HA	1.91	0.52
12:h:110:ILE:CD1	12:h:138:ALA:HB3	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:28:MET:SD	12:m:105:ALA:HB2	2.50	0.52
9:a:801:LEU:CD1	12:m:60:VAL:HG11	2.40	0.52
10:b:58:ILE:HG13	12:g:148:VAL:HG11	1.91	0.52
12:k:99:VAL:HG13	12:k:149:ALA:HB2	1.90	0.52
9:a:761:ILE:HD13	9:a:783:PHE:CE1	2.45	0.52
12:m:22:ALA:HB2	12:m:96:GLY:HA2	1.91	0.52
3:2:439:LEU:HD12	3:2:444:HIS:CD2	2.45	0.51
5:6:8:ILE:HD11	5:6:322:LEU:HD22	1.92	0.51
12:i:24:VAL:HG22	12:j:101:LEU:HD21	1.92	0.51
12:i:59:VAL:HG21	12:j:134:ILE:HD12	1.92	0.51
3:2:102:ILE:HD11	3:2:104:ARG:NH2	2.25	0.51
1:Q:90:LEU:HD22	2:V:84:MET:SD	2.50	0.51
10:b:107:MET:HE2	10:b:194:ALA:HB3	1.92	0.51
12:k:35:ALA:HB1	12:l:112:ILE:HG21	1.92	0.51
12:l:22:ALA:HB2	12:l:96:GLY:HA2	1.91	0.51
12:l:75:LEU:HD13	12:l:153:SER:CB	2.40	0.51
5:6:147:LEU:HD21	5:6:273:LYS:HA	1.91	0.51
12:h:20:SER:OG	12:i:97:LEU:HD11	2.10	0.51
12:k:66:ALA:O	12:k:67:ILE:C	2.53	0.51
12:k:72:VAL:O	12:k:75:LEU:HB2	2.10	0.51
3:1:174:GLY:HA3	3:1:194:LEU:HD21	1.93	0.51
3:2:426:LEU:HD21	4:3:195:ALA:CB	2.40	0.51
12:l:139:GLU:O	12:l:143:LEU:HG	2.10	0.51
2:R:42:MET:HG3	2:R:46:GLN:HE22	1.75	0.51
5:6:43:ASP:OD2	5:6:315:VAL:HG11	2.11	0.51
5:6:62:LEU:HD23	5:6:65:PHE:HE1	1.72	0.51
12:j:24:VAL:HG22	12:k:101:LEU:CD2	2.40	0.51
7:U:500:GLN:HA	7:U:503:ARG:HD3	1.91	0.51
12:k:73:ALA:O	12:k:76:ILE:N	2.44	0.51
4:4:327:MET:HE3	4:4:368:LEU:CD1	2.40	0.51
12:j:84:ILE:HG21	12:j:89:SER:HB3	1.93	0.51
5:6:77:MET:HE1	5:6:284:LEU:HD13	1.93	0.50
9:a:765:LEU:HD22	15:f:45:PRO:HB3	1.93	0.50
12:g:44:MET:HE1	12:g:51:LEU:HD12	1.93	0.50
12:h:99:VAL:HB	12:h:149:ALA:HB2	1.92	0.50
1:8:88:ASP:HA	1:8:91:ILE:HG22	1.93	0.50
3:0:306:MET:HE3	3:0:306:MET:HA	1.92	0.50
6:7:59:GLY:HA2	6:7:62:MET:HE2	1.93	0.50
11:d:72:ASP:HB2	11:d:331:VAL:HG21	1.93	0.50
7:U:348:VAL:HG22	7:U:352:LEU:HG	1.94	0.50
3:2:193:GLU:C	3:2:194:LEU:HD12	2.37	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:57:LEU:HD12	4:5:95:VAL:CG1	2.42	0.50
12:n:72:VAL:HG21	12:n:99:VAL:HG11	1.93	0.50
4:5:253:SER:O	4:5:257:VAL:HG23	2.12	0.50
9:a:397:ILE:HD13	17:e:43:ALA:CB	2.42	0.50
12:i:95:ALA:O	12:i:99:VAL:HG12	2.12	0.50
12:n:24:VAL:HG22	12:o:101:LEU:HD11	1.92	0.49
12:h:114:GLY:O	12:h:118:VAL:HG23	2.12	0.49
12:m:24:VAL:HG22	12:n:101:LEU:HD11	1.94	0.49
12:k:16:VAL:HG23	12:l:152:LEU:HD11	1.93	0.49
3:2:291:PHE:CZ	3:2:309:THR:HG21	2.47	0.49
7:U:495:MET:HE3	9:a:274:GLN:NE2	2.27	0.49
5:6:70:VAL:O	5:6:73:VAL:HB	2.12	0.49
5:6:315:VAL:HG12	5:6:315:VAL:O	2.13	0.49
6:7:141:ALA:O	6:7:145:LEU:HG	2.13	0.49
12:g:13:PHE:CE1	12:g:17:MET:HE3	2.48	0.49
1:8:38:PHE:HZ	2:R:36:ALA:HB2	1.77	0.49
3:1:296:MET:SD	3:1:298:VAL:HG23	2.53	0.49
12:m:113:VAL:HG21	12:m:134:ILE:HG22	1.94	0.49
4:5:418:VAL:O	4:5:422:LEU:HD23	2.13	0.49
12:o:22:ALA:HB2	12:o:96:GLY:HA2	1.95	0.49
3:2:450:TRP:CZ2	3:2:483:LEU:HD13	2.48	0.49
12:l:108:PHE:O	12:l:112:ILE:HG22	2.13	0.49
3:1:264:SER:HA	3:1:272:ILE:HD13	1.93	0.48
11:d:83:PHE:CZ	11:d:320:VAL:HG22	2.48	0.48
3:2:296:MET:SD	3:2:298:VAL:HG23	2.53	0.48
5:6:73:VAL:HG13	5:6:77:MET:HE3	1.94	0.48
11:d:117:THR:OG1	11:d:144:ILE:HD11	2.13	0.48
12:g:70:LEU:HD23	12:h:144:TYR:CZ	2.48	0.48
12:h:44:MET:HE3	12:h:118:VAL:O	2.14	0.48
12:m:24:VAL:HG13	12:n:101:LEU:HD13	1.94	0.48
7:U:495:MET:HA	7:U:506:ALA:HB3	1.95	0.48
10:b:58:ILE:CD1	12:g:148:VAL:HG21	2.43	0.48
12:l:68:TYR:HB3	12:l:146:LEU:HD21	1.94	0.48
12:g:95:ALA:O	12:g:99:VAL:HG12	2.13	0.48
12:h:31:ALA:CB	12:i:105:ALA:HB1	2.43	0.48
1:Q:125:TYR:O	1:Q:128:LEU:HD21	2.14	0.48
3:2:232:ARG:HG2	3:2:537:THR:HG22	1.95	0.48
12:g:32:TYR:CZ	14:c:443:LEU:HD22	2.49	0.48
3:0:577:ILE:O	3:0:581:LEU:HD23	2.13	0.48
3:1:514:LEU:HD22	3:1:544:MET:HE1	1.95	0.48
12:i:24:VAL:HG22	12:j:101:LEU:HD11	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:i:57:ILE:HG22	12:i:61:MET:HE3	1.96	0.48
3:0:581:LEU:HD13	3:0:584:MET:SD	2.54	0.48
12:k:99:VAL:CG1	12:k:149:ALA:HB2	2.44	0.48
1:9:120:VAL:O	1:9:124:LEU:HD23	2.13	0.48
13:p:596:LYS:HE2	13:p:596:LYS:HA	1.96	0.48
3:0:580:LYS:HB3	3:0:604:LEU:HD11	1.95	0.47
4:3:328:TYR:HD1	4:3:368:LEU:HD12	1.79	0.47
4:3:379:VAL:HG13	4:3:391:PRO:HG2	1.96	0.47
7:U:47:VAL:HG11	7:U:109:ILE:HD11	1.96	0.47
1:9:150:LYS:O	1:9:154:MET:HE3	2.13	0.47
6:7:46:GLN:HE21	6:7:50:LYS:HZ2	1.61	0.47
9:a:472:LEU:HD23	9:a:473:ASN:N	2.28	0.47
12:l:44:MET:CB	12:l:118:VAL:HG22	2.45	0.47
14:c:437:LEU:HA	14:c:440:ILE:HG22	1.96	0.47
5:6:67:GLU:HA	5:6:295:TRP:CZ3	2.48	0.47
9:a:801:LEU:HD13	12:m:60:VAL:HG11	1.95	0.47
17:e:48:CYS:HA	17:e:51:PHE:CE1	2.49	0.47
4:3:354:LEU:HD11	4:3:369:THR:HG21	1.97	0.47
1:9:16:MET:HE2	1:9:19:ILE:HD11	1.96	0.47
2:V:7:GLY:O	2:V:11:LEU:HD23	2.14	0.47
4:5:123:VAL:HG21	4:5:151:LEU:HD23	1.96	0.47
5:6:44:LEU:HD12	5:6:115:ILE:O	2.15	0.47
7:U:398:LEU:HD13	7:U:440:VAL:HG13	1.97	0.47
10:b:172:LEU:HD11	12:o:49:PRO:HB3	1.97	0.47
12:g:32:TYR:CE1	14:c:443:LEU:HD22	2.50	0.47
12:h:28:MET:HE3	12:i:101:LEU:CD1	2.44	0.47
12:i:28:MET:CE	12:j:105:ALA:HB2	2.37	0.47
12:i:70:LEU:O	12:i:74:VAL:HG22	2.14	0.47
12:j:72:VAL:HG11	12:j:99:VAL:HG11	1.96	0.47
12:l:47:MET:SD	12:l:48:ARG:HB2	2.54	0.47
12:m:28:MET:N	12:m:28:MET:HE2	2.29	0.47
3:1:162:ILE:HD11	3:1:342:TYR:CZ	2.50	0.47
5:6:208:MET:SD	5:6:233:LYS:CE	3.03	0.47
12:k:72:VAL:HG21	12:k:99:VAL:HG11	1.97	0.47
12:l:49:PRO:O	12:l:52:ILE:HG22	2.14	0.47
3:2:605:LEU:HA	3:2:608:MET:HE2	1.97	0.47
11:d:307:PHE:CD1	11:d:315:VAL:HG23	2.49	0.47
1:9:115:LEU:O	1:9:119:LEU:HD23	2.14	0.46
1:Q:38:PHE:CD2	2:V:36:ALA:HB2	2.50	0.46
1:Q:215:LEU:HD12	2:V:88:GLN:HA	1.96	0.46
6:7:69:LEU:HA	6:7:134:LEU:HD11	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:i:58:PRO:HG3	12:i:135:LEU:HD11	1.97	0.46
12:n:31:ALA:HB2	12:o:105:ALA:HB1	1.97	0.46
12:h:80:LEU:CD2	12:i:91:LEU:HD21	2.45	0.46
12:m:22:ALA:HB2	12:m:96:GLY:CA	2.45	0.46
4:3:169:MET:SD	4:3:410:MET:HE2	2.55	0.46
12:m:59:VAL:HG11	12:n:134:ILE:HD13	1.97	0.46
12:m:70:LEU:HD11	12:n:144:TYR:CG	2.50	0.46
3:1:422:THR:O	3:1:426:LEU:HD23	2.15	0.46
4:3:335:TYR:C	4:3:336:GLU:HG3	2.41	0.46
12:i:23:MET:HE2	12:j:148:VAL:HB	1.96	0.46
12:n:59:VAL:HG21	12:o:134:ILE:CD1	2.46	0.46
15:f:48:GLU:CD	15:f:61:LEU:HD22	2.40	0.46
1:9:12:ILE:O	1:9:16:MET:HG2	2.16	0.46
7:U:456:PRO:O	7:U:459:LYS:HB2	2.16	0.46
12:l:65:ILE:HD11	12:l:110:ILE:HD12	1.97	0.46
14:c:368:VAL:HG13	14:c:377:LEU:HD11	1.97	0.46
3:1:442:ARG:CZ	4:4:427:ALA:HB1	2.45	0.46
12:l:72:VAL:HG21	12:l:99:VAL:HG21	1.97	0.46
16:s:67:ILE:HG23	16:s:82:PHE:CE2	2.51	0.46
7:U:366:SER:O	7:U:369:ILE:HG22	2.16	0.46
12:g:68:TYR:HD1	12:g:146:LEU:HD22	1.79	0.46
12:l:95:ALA:HB2	12:l:152:LEU:HD13	1.97	0.46
3:0:291:PHE:HA	3:0:294:LEU:HD23	1.96	0.46
3:2:495:LEU:HD21	6:7:172:ILE:HD12	1.98	0.46
6:7:108:VAL:HG23	6:7:150:SER:OG	2.16	0.46
1:8:120:VAL:O	1:8:124:LEU:HD23	2.16	0.45
3:0:61:MET:HE3	3:0:61:MET:HA	1.98	0.45
3:2:485:GLU:OE2	3:2:489:LEU:HD11	2.16	0.45
5:6:66:VAL:HG13	5:6:295:TRP:NE1	2.31	0.45
7:U:498:GLU:O	7:U:499:ASP:C	2.58	0.45
9:a:501:LEU:HD21	17:e:67:GLN:OE1	2.16	0.45
12:g:19:ALA:HB2	12:g:76:ILE:HG21	1.98	0.45
7:U:317:ARG:HE	7:U:318:ILE:HG23	1.81	0.45
12:n:45:SER:OG	12:o:127:LEU:HD13	2.17	0.45
1:Q:37:GLU:OE1	2:V:33:LEU:HD22	2.17	0.45
12:j:35:ALA:HB1	12:k:112:ILE:CG2	2.45	0.45
3:2:291:PHE:HE2	3:2:309:THR:HG21	1.79	0.45
12:g:41:ILE:HD13	12:g:55:SER:CB	2.47	0.45
12:l:139:GLU:OE2	12:l:143:LEU:HG	2.14	0.45
12:n:28:MET:HE2	12:o:105:ALA:HB2	1.97	0.45
3:2:378:LEU:O	3:2:382:LEU:HD23	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:497:HIS:O	7:U:498:GLU:C	2.59	0.45
14:c:351:ASN:OD1	14:c:380:THR:HG23	2.16	0.45
15:f:58:ILE:HG21	17:e:75:TYR:CE2	2.51	0.45
9:a:628:MET:N	9:a:628:MET:HE2	2.31	0.45
12:h:20:SER:O	12:h:24:VAL:HG23	2.17	0.45
12:l:64:ILE:O	12:l:67:ILE:HG22	2.16	0.45
4:3:444:LEU:HD11	4:3:448:ASP:HB3	1.99	0.45
9:a:481:VAL:HG22	9:a:511:PHE:HZ	1.81	0.45
12:h:59:VAL:HG21	12:i:134:ILE:CD1	2.47	0.45
12:j:68:TYR:OH	12:j:143:LEU:HD22	2.16	0.45
4:5:401:LEU:HD12	4:5:401:LEU:O	2.17	0.45
7:U:494:HIS:HA	7:U:497:HIS:HB3	1.98	0.45
12:k:24:VAL:HG13	12:l:101:LEU:HD13	1.99	0.45
12:k:61:MET:HA	12:k:64:ILE:HD12	1.99	0.45
4:4:260:PHE:C	4:4:261:LEU:HD22	2.42	0.44
12:h:65:ILE:HD11	12:h:139:GLU:OE1	2.18	0.44
12:h:141:LEU:O	12:h:144:TYR:HB3	2.17	0.44
1:Q:46:VAL:HB	2:V:44:VAL:HG11	1.99	0.44
10:b:172:LEU:HD12	12:o:45:SER:HB2	1.97	0.44
12:o:30:ALA:O	12:o:34:THR:HG22	2.17	0.44
15:f:48:GLU:OE2	15:f:61:LEU:HD22	2.16	0.44
5:6:61:LYS:O	5:6:64:ALA:HB3	2.18	0.44
12:k:68:TYR:O	12:k:71:VAL:HG22	2.17	0.44
12:n:24:VAL:HG22	12:o:101:LEU:HD21	1.98	0.44
5:6:147:LEU:HD22	5:6:276:GLN:OE1	2.17	0.44
11:d:117:THR:HG21	11:d:144:ILE:HD11	1.99	0.44
14:c:368:VAL:HG13	14:c:377:LEU:CD1	2.47	0.44
11:d:251:GLU:HG3	12:m:47:MET:HE2	1.98	0.44
12:j:109:ALA:O	12:j:113:VAL:HG22	2.17	0.44
12:m:144:TYR:HA	12:m:147:ILE:HD12	1.99	0.44
5:6:208:MET:SD	5:6:233:LYS:HE2	2.58	0.44
12:m:78:ASN:HD22	12:m:78:ASN:C	2.25	0.44
12:m:85:THR:HG23	12:m:87:TYR:H	1.83	0.44
6:7:142:VAL:HA	6:7:145:LEU:HD12	2.00	0.44
10:b:58:ILE:HG13	12:g:148:VAL:HG21	2.00	0.44
12:i:29:GLY:HA3	12:i:104:LEU:HA	1.99	0.44
1:Q:111:ARG:O	1:Q:115:LEU:HD23	2.18	0.44
3:0:425:THR:O	3:0:429:VAL:HG12	2.18	0.44
12:k:114:GLY:O	12:k:118:VAL:HG23	2.18	0.44
13:p:599:LEU:HD11	14:c:366:GLU:OE1	2.17	0.44
13:p:601:TYR:HA	13:p:604:VAL:HG22	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:185:ASN:HB2	1:8:190:ILE:HG22	1.98	0.44
9:a:793:ILE:HD12	9:a:794:MET:HE3	1.99	0.44
12:g:56:ILE:HG13	12:h:133:LEU:HD21	1.99	0.44
4:5:238:MET:HE2	4:5:238:MET:HA	2.00	0.43
7:U:493:ASN:HA	7:U:496:HIS:CE1	2.53	0.43
11:d:123:ILE:HD13	11:d:143:ASN:H	1.83	0.43
12:n:46:VAL:HG23	12:o:124:GLN:NE2	2.33	0.43
16:s:84:ALA:HB3	16:s:95:ILE:HD13	1.99	0.43
5:6:119:LEU:HD22	5:6:301:LEU:HD13	1.99	0.43
9:a:543:ILE:HD12	9:a:588:VAL:HG22	2.00	0.43
9:a:611:ILE:HD12	9:a:626:ASN:HD21	1.83	0.43
10:b:43:GLU:OE1	14:c:421:MET:HE1	2.18	0.43
12:k:72:VAL:O	12:k:73:ALA:C	2.61	0.43
4:3:46:THR:HG23	4:3:113:GLU:OE2	2.17	0.43
7:U:507:LEU:HD12	9:a:275:THR:HG22	1.99	0.43
9:a:788:VAL:HG23	9:a:789:ALA:N	2.34	0.43
11:d:111:ILE:HA	11:d:114:ILE:HG22	2.00	0.43
12:g:75:LEU:HD21	12:g:153:SER:HB2	2.00	0.43
12:k:47:MET:CE	12:k:122:ALA:HB1	2.46	0.43
3:2:34:MET:HE3	3:2:34:MET:HA	2.00	0.43
4:4:417:ASP:HB3	4:4:495:ILE:HD12	2.00	0.43
6:7:134:LEU:HD13	8:X:25:LEU:HD13	2.00	0.43
6:7:134:LEU:HD13	8:X:25:LEU:CD1	2.48	0.43
17:e:67:GLN:C	17:e:68:LEU:HD22	2.44	0.43
1:8:125:TYR:O	1:8:128:LEU:HD13	2.18	0.43
1:Q:46:VAL:HG11	2:V:40:ALA:CB	2.46	0.43
5:6:44:LEU:HD23	5:6:45:LYS:O	2.17	0.43
9:a:330:LEU:HA	9:a:333:ILE:HD12	2.01	0.43
12:o:24:VAL:HG13	12:o:25:PHE:HD2	1.84	0.43
2:R:96:LEU:O	2:R:100:LEU:HD23	2.18	0.43
12:l:99:VAL:HG23	12:l:146:LEU:HD22	1.99	0.43
3:0:496:VAL:HG13	3:0:497:GLY:N	2.34	0.43
3:2:88:VAL:HG13	3:2:103:GLN:OE1	2.18	0.43
10:b:16:TRP:CZ3	10:b:19:MET:HE2	2.54	0.43
12:k:64:ILE:O	12:k:67:ILE:HB	2.18	0.43
12:l:146:LEU:O	12:l:147:ILE:C	2.61	0.43
1:9:87:ARG:NE	2:T:84:MET:HE2	2.34	0.43
2:V:41:GLN:HA	2:V:44:VAL:HG22	2.00	0.43
9:a:424:VAL:HG22	9:a:447:ARG:NE	2.33	0.43
3:0:368:MET:HE1	6:7:196:ARG:HG3	2.01	0.43
12:j:66:ALA:HB2	12:k:141:LEU:HD11	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:f:16:ILE:HD11	15:f:87:VAL:HG21	2.00	0.43
4:5:455:LEU:O	4:5:459:GLU:OE1	2.36	0.43
12:o:99:VAL:HB	12:o:149:ALA:HB2	2.01	0.43
3:2:118:ILE:HD11	4:5:159:ASN:HA	2.01	0.42
4:5:76:LEU:HD12	4:5:80:THR:HB	2.01	0.42
5:6:62:LEU:HA	5:6:65:PHE:CZ	2.53	0.42
6:7:86:ASN:OD1	6:7:86:ASN:O	2.36	0.42
7:U:499:ASP:HB3	7:U:502:VAL:CG2	2.49	0.42
3:0:479:ALA:O	3:0:483:LEU:HD23	2.19	0.42
3:2:288:LEU:HD23	3:2:288:LEU:O	2.19	0.42
5:6:127:ALA:O	5:6:131:THR:HG23	2.19	0.42
7:U:352:LEU:HD22	7:U:369:ILE:CD1	2.49	0.42
9:a:530:LEU:HD11	12:m:78:ASN:HB3	2.00	0.42
12:i:24:VAL:HA	12:j:101:LEU:HD11	2.01	0.42
6:7:97:LYS:O	6:7:108:VAL:HG12	2.19	0.42
2:V:77:THR:O	2:V:81:VAL:HG23	2.19	0.42
4:3:418:VAL:HG12	4:3:422:LEU:HD23	2.02	0.42
12:j:35:ALA:HA	12:k:113:VAL:HG13	2.02	0.42
12:k:15:GLY:HA3	12:k:80:LEU:HD13	2.01	0.42
12:o:131:MET:O	12:o:134:ILE:HG22	2.20	0.42
4:3:47:TYR:HE2	4:3:63:VAL:HG13	1.85	0.42
9:a:21:ALA:HB2	9:a:348:VAL:HG21	2.01	0.42
9:a:303:ILE:O	9:a:307:LEU:HD23	2.20	0.42
12:k:53:MET:O	12:k:56:ILE:HG22	2.18	0.42
3:1:234:LEU:HD12	3:1:433:TRP:CE2	2.54	0.42
5:6:71:LYS:HA	5:6:71:LYS:HD2	1.44	0.42
7:U:497:HIS:HB3	7:U:502:VAL:HG11	2.01	0.42
9:a:389:ILE:H	9:a:389:ILE:HD12	1.85	0.42
12:n:28:MET:CE	12:o:105:ALA:HB2	2.50	0.42
12:o:21:SER:HA	12:o:24:VAL:HG12	2.01	0.42
9:a:752:LEU:HA	9:a:755:VAL:HG22	2.02	0.42
11:d:316:PHE:O	11:d:320:VAL:HG23	2.20	0.42
1:9:16:MET:CE	2:T:11:LEU:HA	2.50	0.42
5:6:71:LYS:O	5:6:72:LYS:C	2.63	0.42
7:U:459:LYS:HE2	7:U:513:LEU:HA	2.01	0.42
12:i:121:THR:HG22	12:i:127:LEU:CB	2.50	0.42
3:0:287:VAL:HG23	3:0:291:PHE:CE2	2.55	0.42
6:7:62:MET:HE1	8:X:95:PRO:CG	2.50	0.42
4:3:238:MET:HE2	4:3:263:LEU:HD22	2.02	0.42
9:a:124:GLU:O	9:a:128:LEU:HD23	2.20	0.42
12:g:20:SER:O	12:g:24:VAL:HG12	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:16:MET:CE	2:T:11:LEU:HD23	2.36	0.41
5:6:62:LEU:HD22	5:6:65:PHE:CZ	2.52	0.41
7:U:497:HIS:C	7:U:503:ARG:NH1	2.78	0.41
11:d:307:PHE:HD1	11:d:315:VAL:HG23	1.85	0.41
12:k:70:LEU:O	12:k:74:VAL:HG12	2.20	0.41
16:s:116:PHE:CZ	16:s:120:MET:HE3	2.55	0.41
1:9:225:LEU:HD23	1:9:225:LEU:H	1.85	0.41
4:5:56:PRO:C	4:5:57:LEU:HD22	2.45	0.41
7:U:351:GLN:O	7:U:355:LEU:HD23	2.20	0.41
9:a:503:LEU:HD13	17:e:67:GLN:HB3	2.01	0.41
9:a:553:VAL:HG11	9:a:580:MET:SD	2.60	0.41
12:m:66:ALA:HB2	12:n:141:LEU:CD1	2.50	0.41
17:e:46:VAL:HG13	17:e:47:CYS:N	2.34	0.41
4:3:169:MET:CG	4:3:410:MET:HE2	2.50	0.41
7:U:299:ILE:O	7:U:299:ILE:HG22	2.20	0.41
12:i:17:MET:HE2	12:j:90:PHE:CZ	2.56	0.41
12:k:70:LEU:HB2	12:l:144:TYR:CZ	2.56	0.41
12:m:45:SER:HB3	12:n:127:LEU:HD22	2.03	0.41
13:p:623:SER:HA	13:p:626:ILE:HG22	2.02	0.41
14:c:355:VAL:O	14:c:355:VAL:HG13	2.20	0.41
1:Q:199:ARG:O	1:Q:203:ILE:HD12	2.20	0.41
3:0:246:THR:OG1	3:0:407:VAL:HG13	2.19	0.41
3:1:149:GLY:HA2	3:1:168:LEU:HD23	2.02	0.41
5:6:299:LYS:O	5:6:303:VAL:HG23	2.20	0.41
1:9:77:ASN:O	1:9:81:LEU:HD23	2.20	0.41
3:2:89:GLU:C	3:2:90:LEU:HD22	2.46	0.41
4:3:150:PHE:C	4:3:151:LEU:HD22	2.46	0.41
4:5:57:LEU:HD12	4:5:95:VAL:HG12	2.03	0.41
4:5:180:MET:HE1	4:5:419:SER:HA	2.03	0.41
9:a:440:PHE:HA	9:a:443:VAL:HG22	2.02	0.41
10:b:107:MET:CE	10:b:194:ALA:HB3	2.50	0.41
4:3:428:ILE:O	4:3:432:VAL:HG23	2.20	0.41
4:5:128:LEU:HD12	4:5:256:ASN:C	2.45	0.41
12:h:28:MET:N	12:h:28:MET:HE2	2.34	0.41
12:k:69:GLY:O	12:k:72:VAL:HB	2.20	0.41
12:k:70:LEU:O	12:k:71:VAL:C	2.63	0.41
12:k:77:ALA:HB1	12:l:155:LYS:NZ	2.36	0.41
12:n:41:ILE:HD12	12:n:55:SER:OG	2.20	0.41
12:n:45:SER:HB2	12:o:127:LEU:HD22	2.03	0.41
16:s:81:TYR:HB2	16:s:96:PHE:CD1	2.55	0.41
3:0:24:VAL:HG12	3:0:29:VAL:HG22	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:154:CYS:O	10:b:158:VAL:HG22	2.21	0.41
12:i:46:VAL:HG13	12:j:123:GLN:OE1	2.19	0.41
12:k:33:GLY:O	12:k:36:LYS:HG2	2.21	0.41
12:m:59:VAL:HG21	12:n:134:ILE:HD11	2.01	0.41
4:3:444:LEU:HD11	4:3:448:ASP:CB	2.50	0.41
4:4:379:VAL:HG13	4:4:391:PRO:HG2	2.02	0.41
6:7:58:MET:HE1	6:7:145:LEU:HA	2.02	0.41
7:U:507:LEU:HD12	9:a:275:THR:CG2	2.50	0.41
9:a:183:PHE:CE2	9:a:187:LEU:HD11	2.55	0.41
2:V:16:LYS:O	2:V:20:GLU:OE1	2.39	0.41
3:0:271:VAL:HB	3:0:344:VAL:HG12	2.03	0.41
3:1:220:LYS:C	3:1:221:LEU:HD22	2.45	0.41
4:4:138:PRO:O	4:4:139:ILE:HD13	2.21	0.41
4:5:119:LEU:HD23	4:5:153:ILE:HD13	2.02	0.41
5:6:8:ILE:HG23	5:6:392:VAL:O	2.21	0.41
5:6:183:LEU:HD22	5:6:229:THR:HG22	2.02	0.41
9:a:230:LYS:O	9:a:233:VAL:HG12	2.21	0.41
12:g:71:VAL:HG23	12:g:72:VAL:N	2.35	0.41
12:k:24:VAL:HG22	12:l:101:LEU:HD21	2.03	0.41
12:k:70:LEU:HD13	12:k:73:ALA:CB	2.45	0.41
12:o:44:MET:HG2	12:o:122:ALA:HB2	2.02	0.41
3:1:442:ARG:NH2	4:4:428:ILE:HD13	2.35	0.41
4:5:150:PHE:C	4:5:151:LEU:HD22	2.46	0.41
5:6:126:ILE:HG21	5:6:298:ILE:HD11	2.03	0.41
3:0:220:LYS:C	3:0:221:LEU:HD22	2.46	0.40
5:6:231:PHE:O	5:6:234:ALA:HB3	2.21	0.40
12:l:146:LEU:O	12:l:149:ALA:HB3	2.21	0.40
2:T:73:VAL:O	2:T:77:THR:HG23	2.22	0.40
3:2:241:VAL:HG13	3:2:457:TYR:CG	2.57	0.40
3:2:241:VAL:HG13	3:2:457:TYR:CD2	2.56	0.40
7:U:124:VAL:HG12	7:U:126:ILE:H	1.86	0.40
12:i:57:ILE:HG22	12:i:61:MET:HE1	2.03	0.40
12:n:84:ILE:HG23	12:n:88:ARG:HB2	2.02	0.40
2:T:35:GLN:O	2:T:39:GLU:OE1	2.39	0.40
3:1:485:GLU:OE1	3:1:508:THR:HG21	2.22	0.40
6:7:148:LEU:CD2	8:X:92:LEU:HD22	2.51	0.40
12:i:31:ALA:HB2	12:j:105:ALA:HB1	2.02	0.40
12:n:44:MET:CE	12:n:118:VAL:HG13	2.51	0.40
16:s:107:PHE:O	16:s:111:VAL:HG23	2.21	0.40
1:8:18:PHE:O	1:8:22:GLU:OE1	2.40	0.40
2:V:27:LYS:O	2:V:30:ALA:HB3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:169:MET:HG3	4:3:410:MET:HE2	2.02	0.40
4:3:179:GLY:C	4:3:180:MET:HE2	2.46	0.40
4:4:154:MET:HE3	4:4:154:MET:HA	2.04	0.40
11:d:303:ASN:HB3	11:d:318:ALA:HB1	2.03	0.40
3:0:246:THR:OG1	3:0:407:VAL:HG22	2.21	0.40
3:0:609:GLN:HA	3:0:612:PHE:CE1	2.56	0.40
3:1:540:MET:HG3	3:1:584:MET:HE3	2.03	0.40
4:3:127:MET:HE1	4:3:281:THR:CG2	2.52	0.40
5:6:59:LEU:HD11	5:6:298:ILE:HG23	2.03	0.40
9:a:750:ALA:O	9:a:754:GLU:OE1	2.39	0.40
12:k:62:ALA:HB3	12:l:137:PHE:CZ	2.57	0.40
12:m:16:VAL:HG23	12:m:80:LEU:HD11	2.04	0.40
17:e:43:ALA:HA	17:e:46:VAL:HG12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	8	223/226 (99%)	216 (97%)	7 (3%)	0	100	100
1	9	223/226 (99%)	218 (98%)	5 (2%)	0	100	100
1	Q	223/226 (99%)	220 (99%)	3 (1%)	0	100	100
2	R	112/118 (95%)	110 (98%)	2 (2%)	0	100	100
2	T	112/118 (95%)	111 (99%)	1 (1%)	0	100	100
2	V	112/118 (95%)	111 (99%)	1 (1%)	0	100	100
3	0	592/617 (96%)	557 (94%)	35 (6%)	0	100	100
3	1	597/617 (97%)	569 (95%)	28 (5%)	0	100	100
3	2	577/617 (94%)	527 (91%)	50 (9%)	0	100	100
4	3	458/511 (90%)	438 (96%)	20 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	4	453/511 (89%)	424 (94%)	29 (6%)	0	100	100
4	5	454/511 (89%)	424 (93%)	30 (7%)	0	100	100
5	6	356/382 (93%)	334 (94%)	22 (6%)	0	100	100
6	7	206/247 (83%)	200 (97%)	6 (3%)	0	100	100
7	U	423/483 (88%)	400 (95%)	22 (5%)	1 (0%)	43	77
8	X	108/119 (91%)	101 (94%)	7 (6%)	0	100	100
9	a	735/838 (88%)	688 (94%)	47 (6%)	0	100	100
10	b	201/205 (98%)	195 (97%)	6 (3%)	0	100	100
11	d	348/351 (99%)	331 (95%)	17 (5%)	0	100	100
12	g	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
12	h	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
12	i	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
12	j	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
12	k	148/155 (96%)	139 (94%)	8 (5%)	1 (1%)	18	55
12	l	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
12	m	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
12	n	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
12	o	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
13	p	50/350 (14%)	43 (86%)	7 (14%)	0	100	100
14	c	201/463 (43%)	168 (84%)	33 (16%)	0	100	100
15	f	84/98 (86%)	78 (93%)	6 (7%)	0	100	100
16	s	209/314 (67%)	205 (98%)	4 (2%)	0	100	100
17	e	77/81 (95%)	76 (99%)	1 (1%)	0	100	100
All	All	8466/9742 (87%)	8028 (95%)	436 (5%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	U	498	GLU
12	k	67	ILE

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	8	197/198 (100%)	197 (100%)	0	100	100
1	9	197/198 (100%)	197 (100%)	0	100	100
1	Q	197/198 (100%)	197 (100%)	0	100	100
2	R	96/99 (97%)	96 (100%)	0	100	100
2	T	96/99 (97%)	96 (100%)	0	100	100
2	V	96/99 (97%)	96 (100%)	0	100	100
3	0	504/524 (96%)	504 (100%)	0	100	100
3	1	506/524 (97%)	506 (100%)	0	100	100
3	2	496/524 (95%)	496 (100%)	0	100	100
4	3	396/431 (92%)	396 (100%)	0	100	100
4	4	391/431 (91%)	391 (100%)	0	100	100
4	5	392/431 (91%)	392 (100%)	0	100	100
5	6	325/344 (94%)	321 (99%)	4 (1%)	63	73
6	7	179/212 (84%)	179 (100%)	0	100	100
7	U	385/429 (90%)	385 (100%)	0	100	100
8	X	94/100 (94%)	94 (100%)	0	100	100
9	a	659/741 (89%)	659 (100%)	0	100	100
10	b	156/158 (99%)	156 (100%)	0	100	100
11	d	305/306 (100%)	305 (100%)	0	100	100
12	g	109/113 (96%)	109 (100%)	0	100	100
12	h	109/113 (96%)	109 (100%)	0	100	100
12	i	109/113 (96%)	109 (100%)	0	100	100
12	j	109/113 (96%)	109 (100%)	0	100	100
12	k	109/113 (96%)	108 (99%)	1 (1%)	70	76
12	l	109/113 (96%)	107 (98%)	2 (2%)	51	67
12	m	109/113 (96%)	109 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	n	109/113 (96%)	109 (100%)	0	100	100
12	o	109/113 (96%)	109 (100%)	0	100	100
13	p	47/309 (15%)	47 (100%)	0	100	100
14	c	180/395 (46%)	180 (100%)	0	100	100
15	f	72/83 (87%)	72 (100%)	0	100	100
16	s	180/246 (73%)	180 (100%)	0	100	100
17	e	66/68 (97%)	66 (100%)	0	100	100
All	All	7193/8164 (88%)	7186 (100%)	7 (0%)	87	88

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	6	66	VAL
5	6	67	GLU
5	6	70	VAL
5	6	71	LYS
12	k	70	LEU
12	l	146	LEU
12	l	148	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
2	R	46	GLN
1	9	14	HIS
1	9	21	GLN
2	T	75	GLN
1	Q	14	HIS
3	0	140	ASN
3	0	468	HIS
3	1	397	ASN
3	2	224	ASN
3	2	444	HIS
4	3	97	GLN
4	3	350	GLN
4	3	433	GLN
6	7	46	GLN
6	7	88	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	U	56	GLN
7	U	79	GLN
7	U	88	GLN
7	U	230	GLN
7	U	496	HIS
9	a	76	ASN
9	a	316	GLN
9	a	465	ASN
9	a	720	HIS
9	a	724	HIS
11	d	57	ASN
11	d	85	HIS
11	d	339	GLN
12	h	124	GLN
12	m	78	ASN
12	o	124	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 ⓘ

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44839. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

This section was not generated.