



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 9, 2019 – 02:00 AM EST

PDB ID : 6QT9
EMDB ID: : EMD-4633
Title : Cryo-EM structure of SH1 full particle.
Authors : De Colibus, L.; Roine, E.; Walter, T.S.; Ilca, S.L.; Wang, X.; Wang, N.;
Roseman, A.M.; Bamford, D.; Huiskonen, J.T.; Stuart, D.I.
Deposited on : 2019-02-22
Resolution : 3.80 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB 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.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

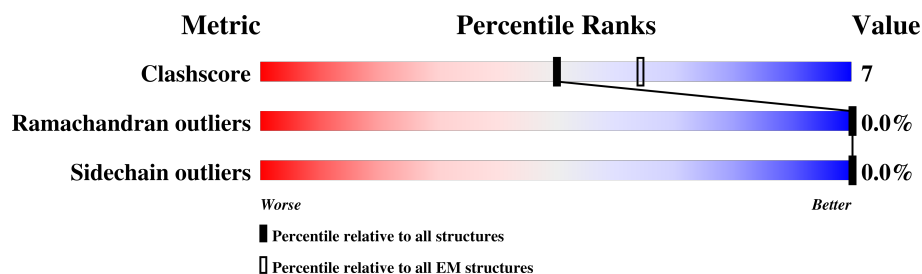
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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.






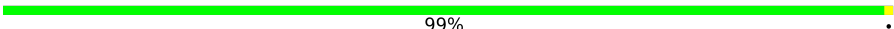
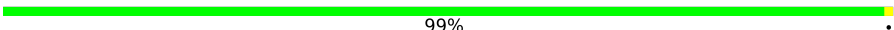
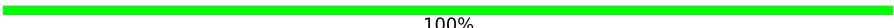
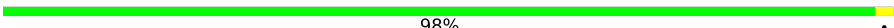
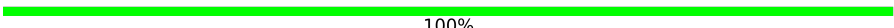
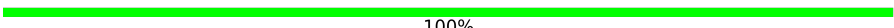
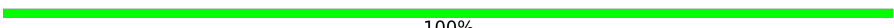
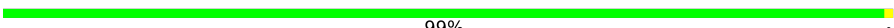
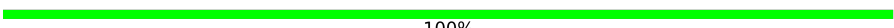
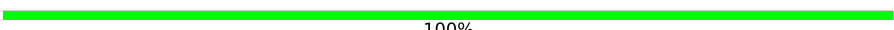
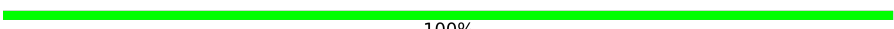
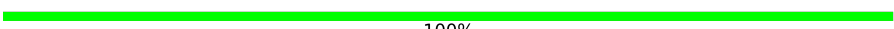
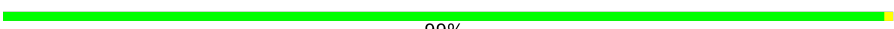
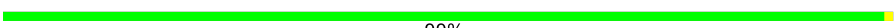
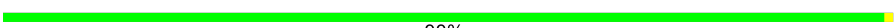

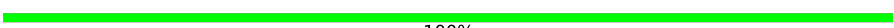

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	A	226	
1	D	226	
2	C	225	
2	E	225	
2	F	225	
2	G	225	
2	H	225	
2	I	225	
2	J	225	

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Mol	Chain	Length	Quality of chain
2	K	225	 81% 19%
2	L	225	 86% 14%
2	M	225	 87% 13%
3	a	173	 99% .
3	b	173	 99% .
3	c	173	 100%
3	d	173	 98% .
3	e	173	 100%
3	f	173	 100%
3	i	173	 100%
3	j	173	 99% .
3	k	173	 100%
3	m	173	 100%
3	o	173	 100%
4	g	167	 100%
4	l	167	 99% .
4	n	167	 99% .
5	h	175	 99% .
6	Y	135	 85% 15%
7	X	24	 100%
8	W	80	 86% 14%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 82012 atoms, of which 39642 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 ORF 25.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	226	Total	C	H	N	O	S	0	0
			3422	1105	1654	292	369	2		
1	D	226	Total	C	H	N	O	S	0	0
			3422	1105	1654	292	369	2		

- Molecule 2 is a protein called ORF 25.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	225	Total	C	H	N	O	S	0	0
			3407	1100	1648	291	366	2		
2	E	225	Total	C	H	N	O	S	0	0
			3407	1100	1648	291	366	2		
2	F	225	Total	C	H	N	O	S	0	0
			3406	1100	1647	291	366	2		
2	G	225	Total	C	H	N	O	S	0	0
			3405	1100	1646	291	366	2		
2	H	225	Total	C	H	N	O	S	0	0
			3407	1100	1648	291	366	2		
2	I	225	Total	C	H	N	O	S	0	0
			3407	1100	1648	291	366	2		
2	J	225	Total	C	H	N	O	S	0	0
			3407	1100	1648	291	366	2		
2	K	225	Total	C	H	N	O	S	0	0
			3407	1100	1648	291	366	2		
2	L	225	Total	C	H	N	O	S	0	0
			3407	1100	1648	291	366	2		
2	M	225	Total	C	H	N	O	S	0	0
			3407	1100	1648	291	366	2		

- Molecule 3 is a protein called ORF 24.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	a	173	Total	C	H	N	O	S	0	0
			2578	815	1256	224	279	4		

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Mol	Chain	Residues	Atoms						AltConf	Trace
3	b	173	Total	C	H	N	O	S	0	0
			2579	815	1257	224	279	4		
3	c	173	Total	C	H	N	O	S	0	0
			2579	815	1257	224	279	4		
3	d	173	Total	C	H	N	O	S	0	0
			2579	815	1257	224	279	4		
3	e	173	Total	C	H	N	O	S	0	0
			2579	815	1257	224	279	4		
3	f	173	Total	C	H	N	O	S	0	0
			2579	815	1257	224	279	4		
3	i	173	Total	C	H	N	O	S	0	0
			2578	815	1256	224	279	4		
3	j	173	Total	C	H	N	O	S	0	0
			2579	815	1257	224	279	4		
3	k	173	Total	C	H	N	O	S	0	0
			2579	815	1257	224	279	4		
3	m	173	Total	C	H	N	O	S	0	0
			2579	815	1257	224	279	4		
3	o	173	Total	C	H	N	O	S	0	0
			2579	815	1257	224	279	4		

- Molecule 4 is a protein called ORF 24.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	g	167	Total	C	H	N	O	S	0	0
			2499	791	1217	216	271	4		
4	l	167	Total	C	H	N	O	S	0	0
			2499	791	1217	216	271	4		
4	n	167	Total	C	H	N	O	S	0	0
			2499	791	1217	216	271	4		

- Molecule 5 is a protein called ORF 24.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	h	175	Total	C	H	N	O	S	0	0
			2611	824	1275	227	281	4		

- Molecule 6 is a protein called ORF 31.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	Y	135	Total	C	H	N	O		0	0
			1927	617	928	175	207			

- Molecule 7 is a protein called VP12.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	X	24	Total	C	H	N	O	0	0
			218	72	98	24	24		

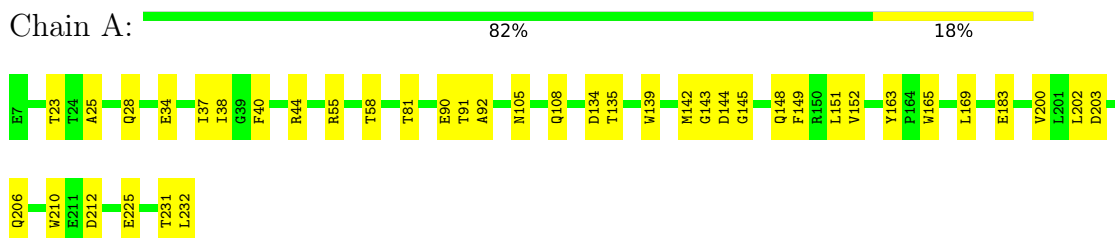
- Molecule 8 is a protein called VP13.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	W	80	Total	C	H	N	O	0	0
			481	240	80	80	81		

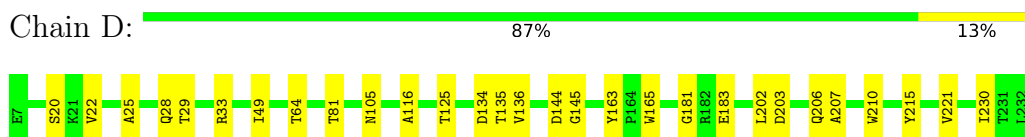
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

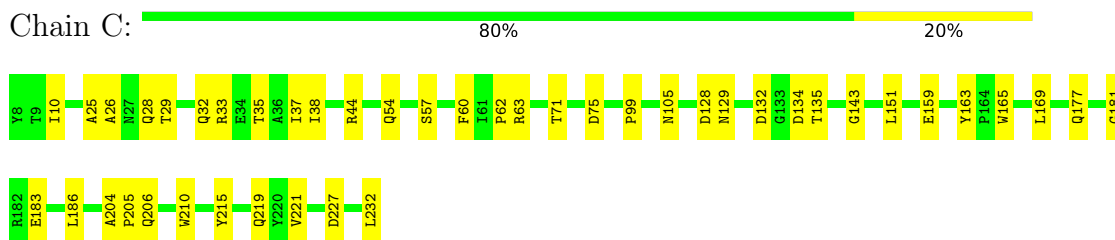
- Molecule 1: ORF 25



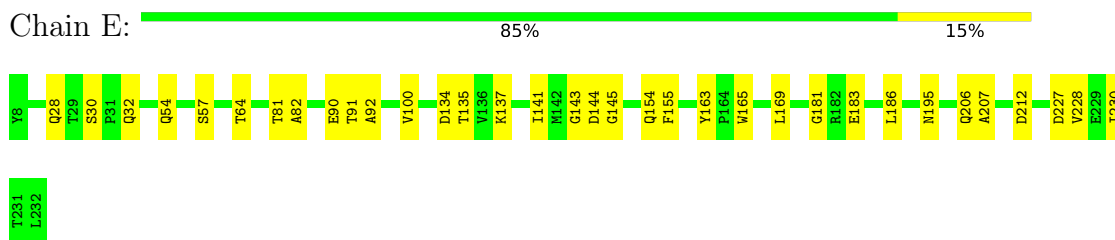
- Molecule 1: ORF 25



- Molecule 2: ORF 25



- Molecule 2: ORF 25



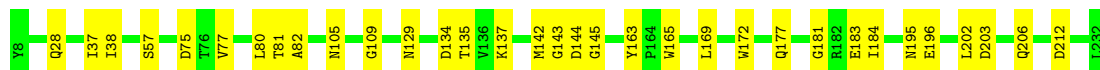
- Molecule 2: ORF 25





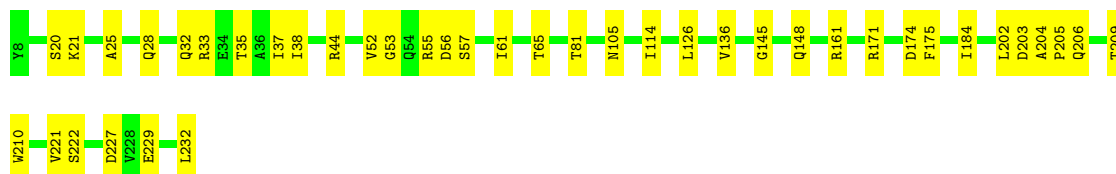
- Molecule 2: ORF 25

Chain G: 85% 15%



- Molecule 2: ORF 25

Chain H: 82% 18%



- Molecule 2: ORF 25

Chain I: 85% 14%



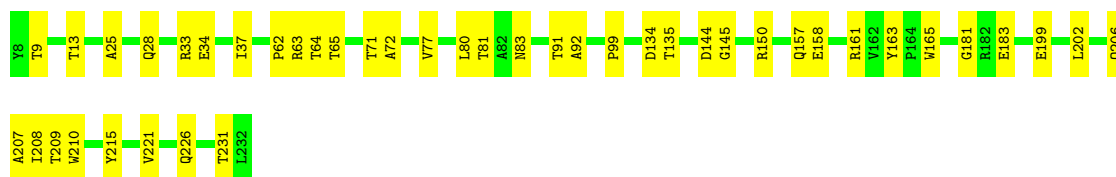
- Molecule 2: ORF 25

Chain J: 84% 16%



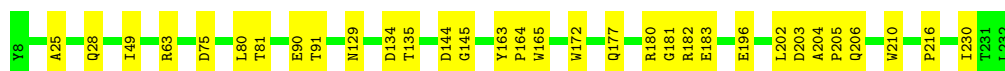
- Molecule 2: ORF 25

Chain K: 81% 19%

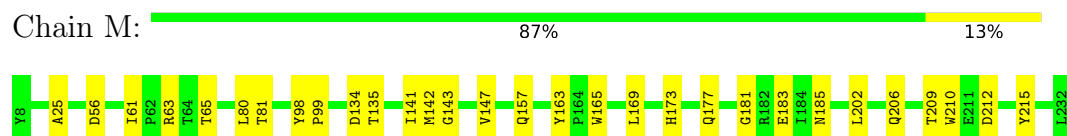


- Molecule 2: ORF 25

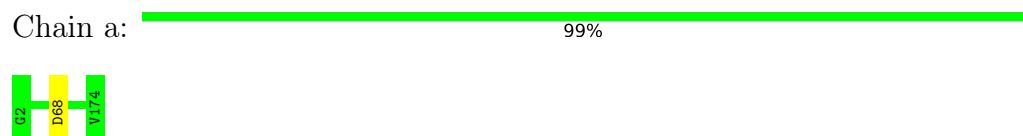
Chain L: 86% 14%



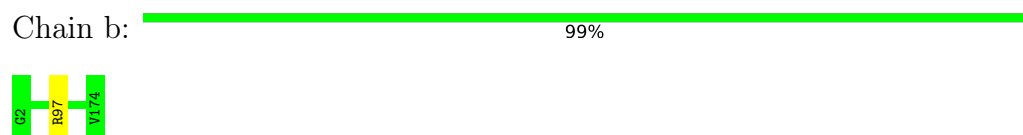
- Molecule 2: ORF 25



- Molecule 3: ORF 24



- Molecule 3: ORF 24

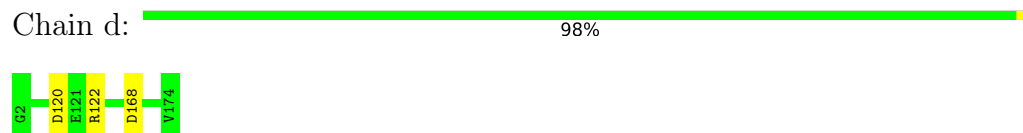


- Molecule 3: ORF 24



There are no outlier residues recorded for this chain.

- Molecule 3: ORF 24



- Molecule 3: ORF 24



There are no outlier residues recorded for this chain.

- Molecule 3: ORF 24



There are no outlier residues recorded for this chain.

- Molecule 3: ORF 24



There are no outlier residues recorded for this chain.

- Molecule 3: ORF 24





- Molecule 3: ORF 24

Chain k: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: ORF 24

Chain m: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: ORF 24

Chain o: 100%

There are no outlier residues recorded for this chain.

- Molecule 4: ORF 24

Chain g: 100%

There are no outlier residues recorded for this chain.

- Molecule 4: ORF 24

Chain l: 99%



- Molecule 4: ORF 24

Chain n: 99%



- Molecule 5: ORF 24

Chain h: 99%



- Molecule 6: ORF 31

Chain Y: 85% 15%




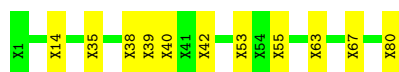
- Molecule 7: VP12

Chain X:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: VP13

Chain W:  86% 14%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C532	Depositor
Number of particles used	16185	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	37037	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.49	0/1808	0.69	2/2475 (0.1%)
1	D	0.49	0/1808	0.65	0/2475
2	C	0.43	0/1799	0.63	0/2463
2	E	0.46	0/1799	0.65	0/2463
2	F	0.48	0/1799	0.65	0/2463
2	G	0.48	0/1799	0.65	0/2463
2	H	0.61	0/1799	0.70	0/2463
2	I	0.45	0/1799	0.65	1/2463 (0.0%)
2	J	0.48	0/1799	0.65	0/2463
2	K	0.51	0/1799	0.66	0/2463
2	L	0.49	0/1799	0.64	0/2463
2	M	0.45	0/1799	0.63	0/2463
3	a	0.40	0/1344	0.71	1/1825 (0.1%)
3	b	0.44	0/1344	0.70	2/1825 (0.1%)
3	c	0.45	0/1344	0.66	0/1825
3	d	0.45	0/1344	0.75	3/1825 (0.2%)
3	e	0.46	0/1344	0.66	0/1825
3	f	0.43	0/1344	0.66	0/1825
3	i	0.41	0/1344	0.64	0/1825
3	j	0.40	0/1344	0.67	1/1825 (0.1%)
3	k	0.47	0/1344	0.68	0/1825
3	m	0.43	0/1344	0.66	0/1825
3	o	0.44	0/1344	0.64	0/1825
4	g	0.45	0/1304	0.65	0/1771
4	l	0.47	0/1304	0.71	2/1771 (0.1%)
4	n	0.45	0/1304	0.67	1/1771 (0.1%)
5	h	0.61	0/1358	0.74	0/1843
6	Y	0.66	0/1016	0.71	0/1389
All	All	0.48	0/42676	0.67	13/58200 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	j	0	1
5	h	0	1
6	Y	0	1
8	W	0	4
All	All	0	7

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	d	168	ASP	CB-CG-OD1	8.80	126.22	118.30
3	a	68	ASP	CB-CG-OD1	6.93	124.54	118.30
3	b	97	ARG	NE-CZ-NH1	6.76	123.68	120.30
3	d	120	ASP	CB-CG-OD1	6.70	124.33	118.30
4	l	120	ASP	CB-CG-OD1	6.04	123.74	118.30
3	b	97	ARG	NE-CZ-NH2	-5.89	117.35	120.30
4	n	172	ARG	NE-CZ-NH1	5.47	123.04	120.30
4	l	172	ARG	NE-CZ-NH1	5.42	123.01	120.30
3	j	120	ASP	CB-CG-OD1	5.29	123.06	118.30
2	I	180	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	44	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	55	ARG	NE-CZ-NH1	5.08	122.84	120.30
3	d	122	ARG	NE-CZ-NH1	5.05	122.82	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	W	38	UNK	Peptide
8	W	40	UNK	Peptide
8	W	53	UNK	Peptide
8	W	55	UNK	Peptide
6	Y	80	ILE	Peptide
5	h	164	ASP	Peptide
3	j	164	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1768	1654	1654	24	0
1	D	1768	1654	1654	16	0
2	C	1759	1648	1648	33	0
2	E	1759	1648	1648	21	0
2	F	1759	1647	1648	14	0
2	G	1759	1646	1648	22	0
2	H	1759	1648	1648	25	0
2	I	1759	1648	1648	21	0
2	J	1759	1648	1648	21	0
2	K	1759	1648	1648	28	0
2	L	1759	1648	1648	20	0
2	M	1759	1648	1648	20	0
3	a	1322	1256	1257	0	0
3	b	1322	1257	1257	0	0
3	c	1322	1257	1257	0	0
3	d	1322	1257	1257	0	0
3	e	1322	1257	1257	0	0
3	f	1322	1257	1257	0	0
3	i	1322	1256	1257	0	0
3	j	1322	1257	1257	0	0
3	k	1322	1257	1257	0	0
3	m	1322	1257	1257	0	0
3	o	1322	1257	1257	0	0
4	g	1282	1217	1217	0	0
4	l	1282	1217	1217	0	0
4	n	1282	1217	1217	0	0
5	h	1336	1275	1275	0	0
6	Y	999	928	903	12	0
7	X	120	98	26	0	0
8	W	401	80	89	4	0
All	All	42370	39642	39559	271	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 7.

All (271) 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)
2:F:81:THR:O	2:F:206:GLN:NE2	2.16	0.79
2:F:28:GLN:NE2	2:F:206:GLN:O	2.17	0.78
2:C:63:ARG:HD2	2:C:221:VAL:O	1.84	0.77
2:M:81:THR:OG1	2:M:206:GLN:OE1	2.04	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:33:ARG:NH1	2:J:34:GLU:O	2.20	0.75
2:K:81:THR:OG1	2:K:206:GLN:OE1	2.04	0.75
2:K:33:ARG:NH1	2:K:34:GLU:O	2.20	0.75
2:G:28:GLN:NE2	2:G:206:GLN:O	2.20	0.74
2:L:180:ARG:O	2:L:182:ARG:NH1	2.21	0.72
2:J:28:GLN:NE2	2:J:206:GLN:O	2.23	0.71
2:J:180:ARG:O	2:J:182:ARG:NH1	2.24	0.71
1:A:81:THR:OG1	1:A:206:GLN:OE1	2.09	0.71
2:L:28:GLN:NE2	2:L:206:GLN:O	2.24	0.70
2:F:79:SER:OG	2:F:121:ALA:O	2.06	0.70
2:L:164:PRO:O	2:M:157:GLN:NE2	2.24	0.70
2:E:81:THR:OG1	2:E:206:GLN:OE1	2.09	0.70
2:M:181:GLY:N	2:M:183:GLU:OE1	2.25	0.69
2:J:164:PRO:O	2:K:157:GLN:NE2	2.25	0.69
2:K:64:THR:OG1	2:K:207:ALA:O	2.10	0.69
2:E:28:GLN:NE2	2:E:206:GLN:O	2.25	0.69
2:G:75:ASP:OD1	2:G:129:ASN:ND2	2.26	0.68
2:G:181:GLY:N	2:G:183:GLU:OE1	2.27	0.68
2:H:81:THR:O	2:H:206:GLN:NE2	2.27	0.68
1:A:105:ASN:ND2	1:A:108:GLN:OE1	2.27	0.67
2:H:55:ARG:NH2	2:H:229:GLU:OE1	2.28	0.66
2:C:44:ARG:O	2:E:195:ASN:ND2	2.28	0.66
2:H:37:ILE:HD11	2:H:202:LEU:HD23	1.78	0.66
2:E:57:SER:OG	2:E:227:ASP:OD2	2.12	0.66
1:D:81:THR:OG1	1:D:206:GLN:OE1	2.14	0.66
2:I:81:THR:OG1	2:I:206:GLN:OE1	2.08	0.66
2:H:20:SER:OG	2:H:21:LYS:N	2.29	0.65
2:J:137:LYS:NZ	2:J:214:ASP:OD2	2.29	0.65
2:K:63:ARG:NH2	2:K:99:PRO:O	2.29	0.65
2:E:137:LYS:NZ	2:E:212:ASP:OD2	2.22	0.64
6:Y:48:SER:O	6:Y:53:ASN:ND2	2.30	0.64
1:A:34:GLU:OE2	1:A:148:GLN:NE2	2.30	0.64
1:D:28:GLN:NE2	1:D:206:GLN:O	2.31	0.64
2:J:84:ILE:O	2:J:85:GLN:NE2	2.31	0.63
1:A:183:GLU:OE1	1:A:183:GLU:N	2.31	0.63
2:G:81:THR:OG1	2:G:206:GLN:OE1	2.15	0.63
2:E:30:SER:O	2:E:32:GLN:NE2	2.33	0.62
2:K:37:ILE:HD11	2:K:202:LEU:HD23	1.81	0.62
2:I:52:VAL:N	2:I:56:ASP:OD2	2.32	0.62
2:C:54:GLN:NE2	2:C:186:LEU:O	2.33	0.61
2:C:183:GLU:OE1	2:C:183:GLU:N	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:163:TYR:O	2:K:165:TRP:N	2.33	0.60
2:I:181:GLY:N	2:I:183:GLU:OE1	2.35	0.60
2:C:75:ASP:OD1	2:C:129:ASN:ND2	2.34	0.60
2:K:63:ARG:HD2	2:K:221:VAL:O	2.02	0.59
2:L:196:GLU:N	2:L:196:GLU:OE2	2.34	0.59
2:E:64:THR:OG1	2:E:207:ALA:O	2.08	0.59
1:A:38:ILE:HD11	1:A:210:TRP:CZ2	2.37	0.59
1:D:163:TYR:O	1:D:165:TRP:N	2.35	0.59
2:L:75:ASP:OD1	2:L:129:ASN:ND2	2.36	0.59
2:I:28:GLN:NE2	2:I:206:GLN:O	2.36	0.59
1:D:183:GLU:N	1:D:183:GLU:OE1	2.35	0.58
2:F:181:GLY:N	2:F:183:GLU:OE1	2.36	0.58
2:G:143:GLY:O	2:G:169:LEU:HD23	2.04	0.58
2:E:163:TYR:O	2:E:165:TRP:N	2.35	0.58
2:M:163:TYR:O	2:M:165:TRP:N	2.36	0.58
6:Y:59:SER:OG	6:Y:60:THR:N	2.37	0.58
2:I:33:ARG:O	2:I:35:THR:HG23	2.02	0.58
2:H:33:ARG:O	2:H:35:THR:HG23	2.04	0.57
2:J:183:GLU:OE1	2:J:183:GLU:N	2.35	0.57
2:G:195:ASN:N	2:G:196:GLU:OE1	2.37	0.57
1:A:163:TYR:O	1:A:165:TRP:N	2.37	0.57
6:Y:144:GLN:O	6:Y:145:ILE:HD13	2.04	0.57
2:C:163:TYR:O	2:C:165:TRP:N	2.36	0.57
2:L:172:TRP:O	2:L:177:GLN:NE2	2.38	0.57
2:L:49:ILE:HG23	2:L:230:ILE:HD13	1.87	0.56
2:L:204:ALA:HB1	2:L:205:PRO:HD2	1.88	0.56
2:G:196:GLU:OE1	2:G:196:GLU:N	2.39	0.56
2:M:56:ASP:O	2:M:185:ASN:ND2	2.38	0.56
1:D:29:THR:HG21	1:D:33:ARG:NH2	2.22	0.55
2:C:63:ARG:HH22	2:C:99:PRO:HD2	1.71	0.55
2:K:181:GLY:N	2:K:183:GLU:OE1	2.39	0.55
2:K:9:THR:HG22	2:K:231:THR:HA	1.88	0.55
2:M:25:ALA:HB1	2:M:210:TRP:CZ3	2.41	0.55
2:C:63:ARG:NH1	2:C:215:TYR:OH	2.40	0.55
2:H:32:GLN:NE2	2:H:204:ALA:O	2.39	0.55
2:H:25:ALA:HB1	2:H:210:TRP:CZ3	2.41	0.55
2:E:183:GLU:N	2:E:183:GLU:OE1	2.39	0.55
2:G:57:SER:OG	2:G:184:ILE:O	2.16	0.55
2:H:55:ARG:NE	2:H:56:ASP:OD1	2.39	0.55
2:C:62:PRO:O	2:C:63:ARG:HG3	2.07	0.55
2:K:62:PRO:O	2:K:63:ARG:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:161:ARG:NH1	2:K:83:ASN:OD1	33.51	0.54
2:C:38:ILE:HD11	2:C:210:TRP:CZ2	2.43	0.54
2:C:33:ARG:O	2:C:35:THR:HG23	2.07	0.54
2:E:134:ASP:OD1	2:E:135:THR:N	2.40	0.54
2:J:134:ASP:OD1	2:J:135:THR:N	2.39	0.54
2:K:25:ALA:HB1	2:K:210:TRP:CE3	2.43	0.54
2:C:151:LEU:O	2:C:159:GLU:N	2.39	0.54
2:C:60:PHE:O	2:C:177:GLN:NE2	2.41	0.54
2:H:57:SER:OG	2:H:227:ASP:OD2	2.25	0.54
2:C:26:ALA:O	2:C:37:ILE:HG23	2.08	0.54
2:J:163:TYR:O	2:J:165:TRP:N	2.41	0.53
2:F:134:ASP:OD1	2:F:135:THR:N	2.41	0.53
2:M:143:GLY:O	2:M:169:LEU:HD23	2.08	0.53
2:E:90:GLU:OE2	2:E:91:THR:N	2.41	0.53
2:L:49:ILE:HG23	2:L:230:ILE:CD1	2.39	0.53
2:F:163:TYR:O	2:F:165:TRP:N	2.41	0.53
2:I:29:THR:HG23	2:I:35:THR:HG21	1.90	0.53
2:F:146:ASP:OD1	2:F:146:ASP:N	2.42	0.52
2:I:163:TYR:O	2:I:165:TRP:N	2.39	0.52
2:G:134:ASP:OD1	2:G:135:THR:N	2.43	0.52
2:G:172:TRP:O	2:G:177:GLN:NE2	2.41	0.52
2:I:146:ASP:O	2:I:202:LEU:HD12	2.09	0.52
2:K:144:ASP:OD1	2:K:145:GLY:N	2.43	0.52
1:A:90:GLU:N	1:A:90:GLU:OE1	2.43	0.52
1:D:64:THR:OG1	1:D:207:ALA:O	2.25	0.52
2:M:134:ASP:OD1	2:M:135:THR:N	2.43	0.52
2:M:65:THR:CB	2:M:209:THR:HG21	2.40	0.52
8:W:35:UNK:O	8:W:39:UNK:HA	2.10	0.52
1:A:28:GLN:HB3	1:A:37:ILE:HD11	1.92	0.51
2:L:163:TYR:O	2:L:165:TRP:N	2.43	0.51
2:H:204:ALA:HB1	2:H:205:PRO:HD2	1.92	0.51
2:J:172:TRP:O	2:J:177:GLN:NE2	2.43	0.51
1:A:23:THR:HG22	1:A:40:PHE:HA	1.93	0.51
2:E:181:GLY:N	2:E:183:GLU:OE1	2.44	0.51
2:G:37:ILE:HG22	2:G:38:ILE:HG13	1.93	0.51
1:A:149:PHE:CE1	1:A:200:VAL:HG22	2.46	0.51
2:H:65:THR:OG1	2:H:209:THR:HG21	2.10	0.51
2:F:28:GLN:N	2:F:28:GLN:OE1	2.42	0.51
2:G:82:ALA:HB1	2:G:143:GLY:HA3	1.93	0.51
2:M:65:THR:OG1	2:M:209:THR:HG21	2.09	0.51
2:M:61:ILE:HD12	2:M:98:TYR:CZ	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ALA:HB1	1:A:210:TRP:CZ3	2.46	0.51
2:G:144:ASP:OD1	2:G:145:GLY:N	2.43	0.51
2:M:147:VAL:HG12	2:M:202:LEU:HB2	1.93	0.51
2:K:25:ALA:HB1	2:K:210:TRP:CZ3	2.45	0.50
2:H:174:ASP:OD1	2:H:175:PHE:N	2.44	0.50
2:I:34:GLU:OE2	2:I:161:ARG:NH2	2.44	0.50
2:M:212:ASP:OD1	2:M:215:TYR:N	2.44	0.50
2:G:142:MET:HB3	2:G:169:LEU:HD21	1.93	0.50
2:L:145:GLY:HA3	2:L:204:ALA:HB2	1.94	0.50
2:C:134:ASP:OD1	2:C:135:THR:N	2.45	0.50
2:L:25:ALA:HB1	2:L:210:TRP:CZ3	2.47	0.50
2:H:44:ARG:NH1	6:Y:74:GLU:OE1	2.45	0.50
2:J:34:GLU:N	2:J:203:ASP:OD1	2.45	0.49
2:H:61:ILE:O	2:H:222:SER:OG	2.10	0.49
2:I:93:ILE:HD11	2:I:100:VAL:HG12	1.93	0.49
2:K:134:ASP:OD1	2:K:135:THR:N	2.44	0.49
2:K:65:THR:OG1	2:K:209:THR:HG21	2.12	0.49
8:W:63:UNK:O	8:W:67:UNK:N	2.46	0.49
2:C:38:ILE:HD11	2:C:210:TRP:CH2	2.47	0.48
2:E:143:GLY:O	2:E:169:LEU:HD23	2.13	0.48
2:F:49:ILE:HG23	2:F:230:ILE:HD13	1.95	0.48
2:G:202:LEU:HD12	2:G:203:ASP:N	2.28	0.48
2:C:181:GLY:N	2:C:183:GLU:OE1	2.47	0.48
2:H:28:GLN:N	2:H:28:GLN:OE1	2.46	0.48
2:I:183:GLU:OE1	2:I:183:GLU:N	2.44	0.48
2:I:32:GLN:NE2	2:I:204:ALA:O	2.46	0.48
6:Y:93:ILE:HD12	6:Y:95:ILE:HD11	1.95	0.48
6:Y:138:SER:O	6:Y:140:THR:OG1	2.16	0.48
2:C:128:ASP:OD1	2:C:129:ASN:N	2.47	0.48
2:M:142:MET:HB3	2:M:169:LEU:HD21	1.95	0.48
1:A:143:GLY:O	1:A:169:LEU:HD23	2.13	0.47
2:C:57:SER:OG	2:C:227:ASP:OD2	2.19	0.47
2:G:105:ASN:O	2:G:109:GLY:N	2.45	0.47
2:C:143:GLY:O	2:C:169:LEU:HD23	2.14	0.47
2:H:171:ARG:O	2:H:184:ILE:HD11	2.13	0.47
6:Y:50:ASN:OD1	6:Y:53:ASN:N	2.47	0.47
2:E:228:VAL:HG23	2:E:230:ILE:HD11	1.95	0.47
2:I:25:ALA:HB1	2:I:210:TRP:CZ3	2.49	0.47
2:I:37:ILE:HD11	2:I:202:LEU:HD23	1.96	0.47
2:L:144:ASP:OD1	2:L:145:GLY:N	2.47	0.47
2:G:77:VAL:CG1	2:G:80:LEU:HD21	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Y:88:ARG:HH12	6:Y:143:ILE:HG21	1.80	0.47
2:C:105:ASN:ND2	2:C:134:ASP:OD2	2.47	0.47
2:K:150:ARG:NH2	2:K:199:GLU:OE1	2.48	0.47
2:H:33:ARG:N	2:H:203:ASP:OD1	2.48	0.47
1:A:231:THR:HG22	1:A:232:LEU:HG	1.97	0.46
2:C:10:ILE:HD11	2:E:155:PHE:CE2	2.50	0.46
1:D:25:ALA:HB1	1:D:210:TRP:CZ3	2.51	0.46
2:E:144:ASP:OD1	2:E:145:GLY:N	2.48	0.46
2:C:25:ALA:HB1	2:C:210:TRP:CZ3	2.50	0.46
2:J:181:GLY:N	2:J:183:GLU:OE1	2.49	0.46
2:L:134:ASP:OD1	2:L:135:THR:N	2.46	0.46
1:D:215:TYR:CD2	1:D:221:VAL:HG12	2.51	0.46
2:M:25:ALA:HB1	2:M:210:TRP:CE3	2.51	0.46
8:W:42:UNK:CB	8:W:80:UNK:OXT	2.64	0.46
1:D:144:ASP:OD1	1:D:145:GLY:N	2.49	0.45
2:M:65:THR:HB	2:M:209:THR:HG21	1.97	0.45
2:J:142:MET:HB3	2:J:169:LEU:HD21	1.98	0.45
2:L:145:GLY:CA	2:L:204:ALA:HB2	2.46	0.45
1:A:38:ILE:HD11	1:A:210:TRP:HZ2	1.80	0.45
2:C:219:GLN:N	2:C:219:GLN:OE1	2.49	0.45
2:K:183:GLU:OE1	2:K:183:GLU:N	2.46	0.45
1:A:151:LEU:HD12	1:A:152:VAL:H	1.80	0.45
2:I:142:MET:O	2:I:173:HIS:NE2	2.49	0.45
2:C:32:GLN:NE2	2:C:204:ALA:O	2.46	0.45
1:A:139:TRP:NE1	1:A:212:ASP:OD2	2.50	0.45
2:E:100:VAL:O	2:E:141:ILE:HG23	2.17	0.45
2:I:134:ASP:OD1	2:I:135:THR:N	2.45	0.45
2:I:144:ASP:OD1	2:I:145:GLY:N	2.48	0.45
2:E:54:GLN:N	2:E:186:LEU:O	2.50	0.45
2:G:80:LEU:O	2:G:81:THR:OG1	2.33	0.45
1:D:202:LEU:HD12	1:D:203:ASP:N	2.32	0.44
2:I:128:ASP:OD1	2:I:129:ASN:N	2.50	0.44
2:J:144:ASP:OD1	2:J:145:GLY:N	2.51	0.44
2:C:232:LEU:OXT	2:E:154:GLN:NE2	2.49	0.44
2:H:114:ILE:HG23	2:H:126:LEU:HD23	2.00	0.44
2:J:31:PRO:O	2:J:33:ARG:N	2.51	0.44
2:L:90:GLU:OE2	2:L:91:THR:N	2.51	0.44
2:E:90:GLU:OE2	2:E:92:ALA:N	2.47	0.44
2:F:142:MET:O	2:F:173:HIS:NE2	2.51	0.44
1:A:142:MET:HB3	1:A:169:LEU:HD21	1.99	0.44
2:C:204:ALA:HB1	2:C:205:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:80:LEU:O	2:I:81:THR:OG1	2.36	0.43
6:Y:43:ARG:HG2	6:Y:44:THR:HG23	2.00	0.43
1:A:134:ASP:OD1	1:A:135:THR:N	2.47	0.43
2:C:29:THR:HG21	2:C:33:ARG:NH2	2.34	0.43
2:I:180:ARG:NE	8:W:14:UNK:CB	2.81	0.43
1:A:202:LEU:HD12	1:A:203:ASP:H	1.82	0.43
2:M:61:ILE:HD11	2:M:177:GLN:OE1	2.17	0.43
2:G:77:VAL:HG12	2:G:80:LEU:HD21	2.01	0.43
2:H:105:ASN:HA	2:H:136:VAL:HG22	2.00	0.43
2:K:91:THR:OG1	2:K:92:ALA:N	2.52	0.43
6:Y:101:ASN:OD1	6:Y:101:ASN:N	2.52	0.43
6:Y:75:ARG:NE	6:Y:77:ASP:OD2	2.51	0.43
2:K:71:THR:OG1	2:K:72:ALA:N	2.51	0.43
1:A:58:THR:HG23	1:A:225:GLU:O	2.19	0.43
1:D:20:SER:OG	1:D:22:VAL:HG22	2.19	0.42
2:J:147:VAL:HG12	2:J:202:LEU:HD13	2.01	0.42
2:J:161:ARG:NH2	2:K:158:GLU:OE1	2.50	0.42
2:K:77:VAL:HG12	2:K:80:LEU:HD21	2.01	0.42
2:H:232:LEU:HB3	6:Y:101:ASN:HB2	2.01	0.42
1:D:134:ASP:OD1	1:D:135:THR:N	2.49	0.42
2:G:28:GLN:OE1	2:G:28:GLN:N	2.49	0.42
2:M:63:ARG:NH2	2:M:99:PRO:O	2.48	0.42
2:C:63:ARG:NH2	2:C:99:PRO:HD2	2.35	0.42
1:D:105:ASN:HA	1:D:136:VAL:HG22	2.01	0.42
2:J:71:THR:OG1	2:J:72:ALA:N	2.52	0.42
2:K:34:GLU:OE1	2:K:161:ARG:NH2	2.53	0.42
2:L:202:LEU:HD12	2:L:203:ASP:H	1.84	0.42
2:L:202:LEU:HD12	2:L:203:ASP:N	2.35	0.42
2:C:210:TRP:HA	2:C:221:VAL:HG22	2.01	0.42
2:K:215:TYR:CD1	2:K:221:VAL:HG12	2.54	0.42
1:D:49:ILE:HG23	1:D:230:ILE:HD13	2.01	0.42
2:G:137:LYS:NZ	2:G:212:ASP:OD2	2.34	0.42
2:H:148:GLN:OE1	2:H:161:ARG:NH1	2.53	0.42
2:C:28:GLN:NE2	2:C:206:GLN:O	2.53	0.42
2:F:183:GLU:N	2:F:183:GLU:OE1	2.46	0.42
2:J:143:GLY:O	2:J:169:LEU:HD23	2.20	0.42
1:A:37:ILE:HG22	1:A:38:ILE:HG13	2.02	0.42
2:K:28:GLN:OE1	2:K:208:ILE:HG22	2.20	0.42
2:M:141:ILE:HD12	2:M:173:HIS:CD2	2.55	0.42
2:J:80:LEU:O	2:J:81:THR:OG1	2.38	0.41
1:A:151:LEU:HD12	1:A:152:VAL:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:37:ILE:HG22	2:C:38:ILE:HG13	2.02	0.41
2:F:215:TYR:CD2	2:F:221:VAL:HG12	2.55	0.41
2:H:145:GLY:CA	2:H:204:ALA:HB2	2.50	0.41
2:E:82:ALA:HB2	2:E:206:GLN:HE22	1.85	0.41
1:A:144:ASP:OD1	1:A:145:GLY:N	2.50	0.41
1:D:181:GLY:N	1:D:183:GLU:OE1	2.53	0.41
2:L:181:GLY:N	2:L:183:GLU:OE1	2.53	0.41
2:L:80:LEU:O	2:L:81:THR:OG1	2.38	0.41
1:A:91:THR:OG1	1:A:92:ALA:N	2.53	0.41
2:C:71:THR:OG1	2:C:132:ASP:OD2	2.33	0.41
2:G:163:TYR:O	2:G:165:TRP:N	2.50	0.41
2:H:37:ILE:HG22	2:H:38:ILE:HG13	2.02	0.41
2:J:221:VAL:HG23	2:J:222:SER:CB	2.51	0.41
2:H:52:VAL:HG12	2:H:53:GLY:O	2.21	0.41
1:D:116:ALA:HB3	1:D:125:THR:HB	2.02	0.41
2:F:210:TRP:HA	2:F:221:VAL:HG22	2.03	0.41
2:F:141:ILE:HD12	2:F:173:HIS:CD2	2.56	0.41
2:K:13:THR:OG1	2:K:226:GLN:O	2.20	0.41
2:K:63:ARG:NH2	2:K:99:PRO:HD2	2.37	0.40
2:M:80:LEU:O	2:M:81:THR:OG1	2.39	0.40
2:H:221:VAL:HG23	2:H:222:SER:HB3	2.03	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	A	224/226 (99%)	195 (87%)	29 (13%)	0	100	100
1	D	224/226 (99%)	196 (88%)	28 (12%)	0	100	100
2	C	223/225 (99%)	196 (88%)	27 (12%)	0	100	100
2	E	223/225 (99%)	197 (88%)	26 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	223/225 (99%)	200 (90%)	23 (10%)	0	100	100
2	G	223/225 (99%)	196 (88%)	27 (12%)	0	100	100
2	H	223/225 (99%)	196 (88%)	27 (12%)	0	100	100
2	I	223/225 (99%)	200 (90%)	23 (10%)	0	100	100
2	J	223/225 (99%)	199 (89%)	24 (11%)	0	100	100
2	K	223/225 (99%)	195 (87%)	28 (13%)	0	100	100
2	L	223/225 (99%)	201 (90%)	21 (9%)	1 (0%)	36	75
2	M	223/225 (99%)	195 (87%)	28 (13%)	0	100	100
3	a	171/173 (99%)	149 (87%)	22 (13%)	0	100	100
3	b	171/173 (99%)	154 (90%)	17 (10%)	0	100	100
3	c	171/173 (99%)	153 (90%)	18 (10%)	0	100	100
3	d	171/173 (99%)	154 (90%)	17 (10%)	0	100	100
3	e	171/173 (99%)	151 (88%)	20 (12%)	0	100	100
3	f	171/173 (99%)	150 (88%)	21 (12%)	0	100	100
3	i	171/173 (99%)	154 (90%)	17 (10%)	0	100	100
3	j	171/173 (99%)	153 (90%)	18 (10%)	0	100	100
3	k	171/173 (99%)	156 (91%)	15 (9%)	0	100	100
3	m	171/173 (99%)	141 (82%)	30 (18%)	0	100	100
3	o	171/173 (99%)	150 (88%)	21 (12%)	0	100	100
4	g	165/167 (99%)	146 (88%)	19 (12%)	0	100	100
4	l	165/167 (99%)	146 (88%)	19 (12%)	0	100	100
4	n	165/167 (99%)	145 (88%)	20 (12%)	0	100	100
5	h	173/175 (99%)	148 (86%)	24 (14%)	1 (1%)	27	67
6	Y	133/135 (98%)	107 (80%)	26 (20%)	0	100	100
All	All	5360/5416 (99%)	4723 (88%)	635 (12%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	h	29	ALA
2	L	216	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	191/191 (100%)	191 (100%)	0	100	100
1	D	191/191 (100%)	191 (100%)	0	100	100
2	C	190/190 (100%)	190 (100%)	0	100	100
2	E	190/190 (100%)	190 (100%)	0	100	100
2	F	190/190 (100%)	190 (100%)	0	100	100
2	G	190/190 (100%)	190 (100%)	0	100	100
2	H	190/190 (100%)	190 (100%)	0	100	100
2	I	190/190 (100%)	190 (100%)	0	100	100
2	J	190/190 (100%)	190 (100%)	0	100	100
2	K	190/190 (100%)	190 (100%)	0	100	100
2	L	190/190 (100%)	189 (100%)	1 (0%)	90	96
2	M	190/190 (100%)	190 (100%)	0	100	100
3	a	145/145 (100%)	145 (100%)	0	100	100
3	b	145/145 (100%)	145 (100%)	0	100	100
3	c	145/145 (100%)	145 (100%)	0	100	100
3	d	145/145 (100%)	145 (100%)	0	100	100
3	e	145/145 (100%)	145 (100%)	0	100	100
3	f	145/145 (100%)	145 (100%)	0	100	100
3	i	145/145 (100%)	145 (100%)	0	100	100
3	j	145/145 (100%)	145 (100%)	0	100	100
3	k	145/145 (100%)	145 (100%)	0	100	100
3	m	145/145 (100%)	145 (100%)	0	100	100
3	o	145/145 (100%)	145 (100%)	0	100	100
4	g	141/141 (100%)	141 (100%)	0	100	100
4	l	141/141 (100%)	141 (100%)	0	100	100
4	n	141/141 (100%)	141 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	h	146/146 (100%)	146 (100%)	0	100	100
6	Y	99/115 (86%)	99 (100%)	0	100	100
All	All	4545/4561 (100%)	4544 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	63	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	129	ASN
2	E	219	GLN
2	H	206	GLN
2	H	226	GLN
3	e	83	ASN
4	g	65	ASN
5	h	102	GLN
3	j	83	ASN
3	o	6	ASN
3	o	83	ASN

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 carbohydrates 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.