



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:30 AM UTC

PDB ID : 7FEI / pdb_00007fei
EMDB ID : EMD-31555
Title : Complex of FMDV A/WH/CHA/09 and bovine neutralizing scFv antibody R55
Authors : He, Y.; Li, K.; Lou, Z.
Deposited on : 2021-07-20
Resolution : 3.91 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

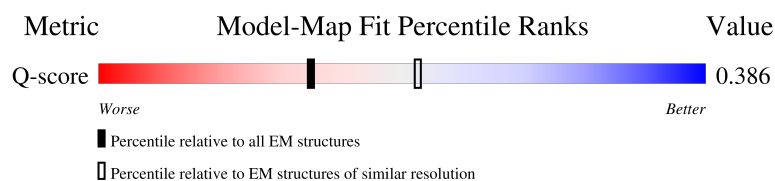
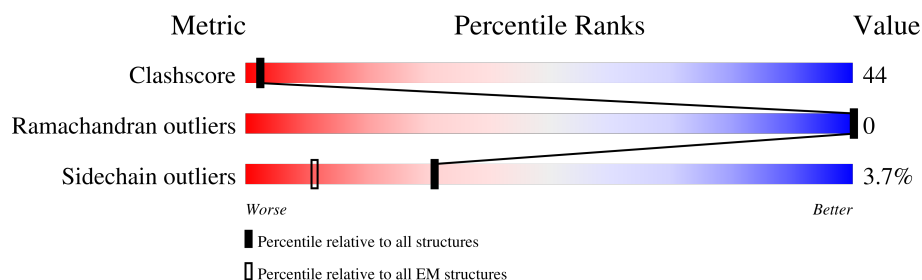
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

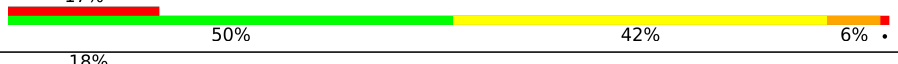
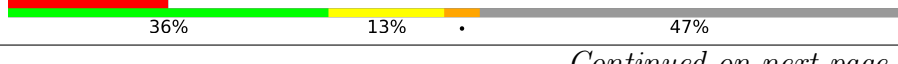
The reported resolution of this entry is 3.91 Å.

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	7920 (3.41 - 4.41)

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	1	212	
2	2	218	
3	3	221	
4	4	85	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	H	126	
6	L	123	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6684 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 Capsid protein VP0.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	189	Total	C	N	O	S	0	0
			1485	939	268	273	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	133	ASN	THR	conflict	UNP E7D639
1	193	LYS	GLU	conflict	UNP E7D639

- Molecule 2 is a protein called Capsid protein VP0.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	205	Total	C	N	O	S	0	0
			1623	1035	280	303	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	2	LYS	ASN	conflict	UNP J9PFK1
2	131	GLU	ASP	conflict	UNP J9PFK1
2	134	THR	PRO	conflict	UNP J9PFK1

- Molecule 3 is a protein called Capsid protein VP0.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	220	Total	C	N	O	S	0	0
			1691	1077	277	328	9		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	40	ARG	GLN	conflict	UNP U5JG68

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
3	59	ASP	GLY	conflict	UNP U5JG68
3	65	VAL	GLU	conflict	UNP U5JG68
3	70	GLU	ASP	conflict	UNP U5JG68
3	131	THR	GLU	conflict	UNP U5JG68
3	135	ASP	GLU	conflict	UNP U5JG68

- Molecule 4 is a protein called Capsid protein VP0.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	45	Total	C	N	O	S	0	0
			348	220	56	70	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	57	SER	THR	conflict	UNP P03309

- Molecule 5 is a protein called IG HEAVY CHAIN VARIABLE REGION.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	97	Total	C	N	O	S	0	0
			742	469	118	152	3		

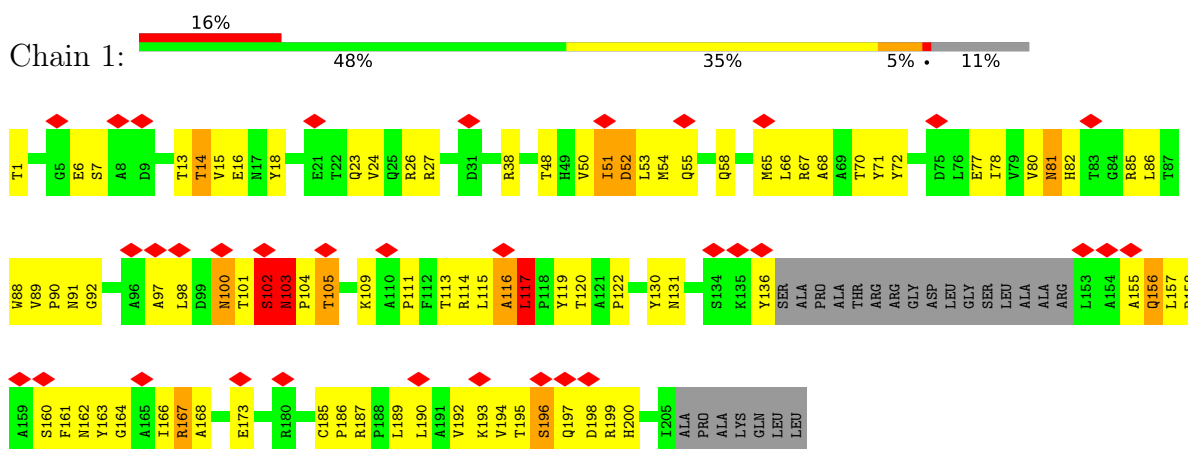
- Molecule 6 is a protein called IG LAMDA CHAIN VARIABLE REGION.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	109	Total	C	N	O	S	0	0
			795	486	138	169	2		

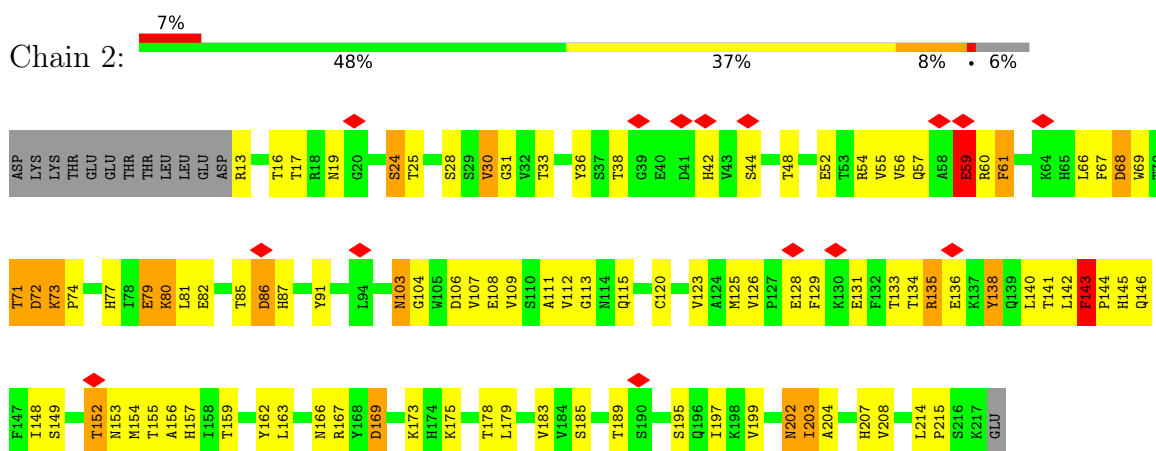
3 Residue-property plots

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.

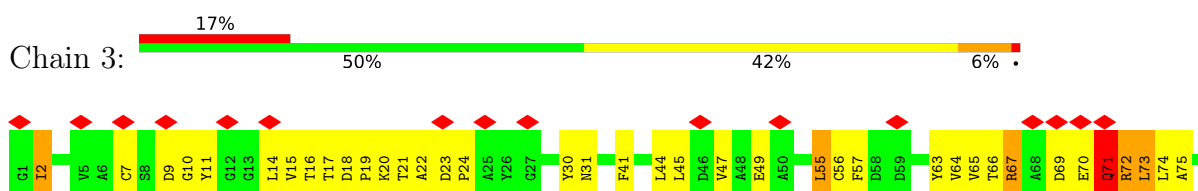
• Molecule 1: Capsid protein VP0

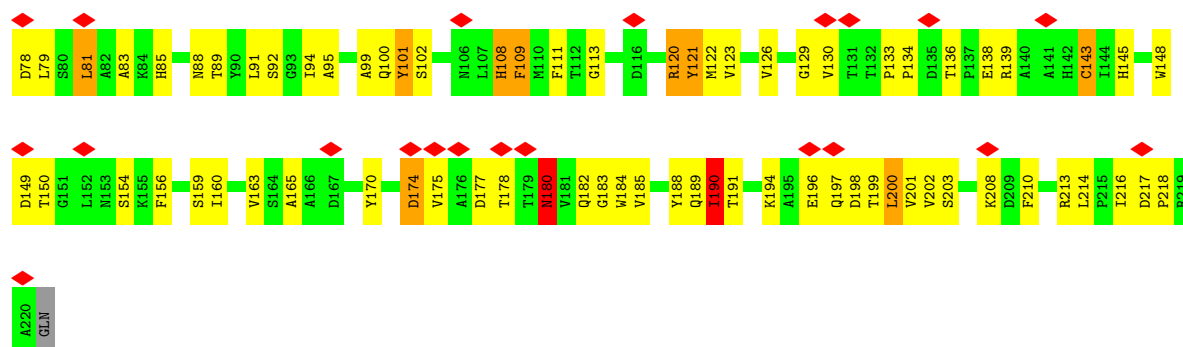


• Molecule 2: Capsid protein VP0

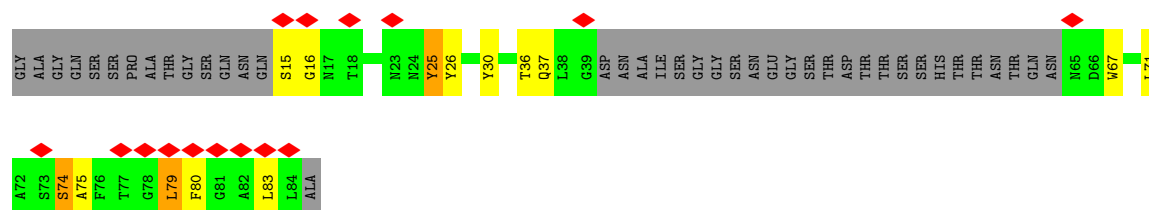
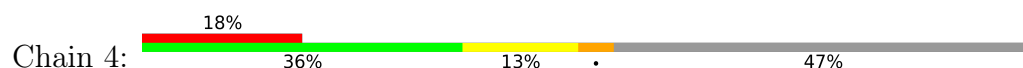


• Molecule 3: Capsid protein VP0

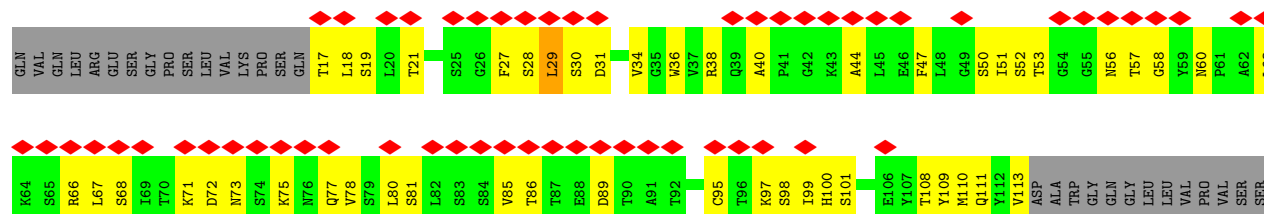




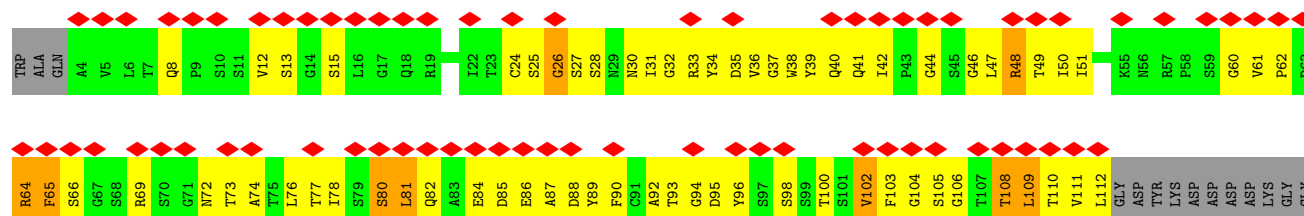
• Molecule 4: Capsid protein VP0



• Molecule 5: IG HEAVY CHAIN VARIABLE REGION



• Molecule 6: IG LAMDA CHAIN VARIABLE REGION



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14535	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-16 (4k x 4k)	Depositor
Maximum map value	0.104	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.023	Depositor
Map size ($\text{\AA}$)	446.4, 446.4, 446.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.93, 0.93, 0.93	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	1	0.55	1/1520 (0.1%)	1.43	40/2073 (1.9%)
2	2	0.75	2/1668 (0.1%)	1.41	36/2272 (1.6%)
3	3	0.74	0/1739	1.38	37/2381 (1.6%)
4	4	0.49	0/354	1.11	6/476 (1.3%)
5	H	0.50	0/757	1.05	8/1029 (0.8%)
6	L	0.61	0/808	1.48	18/1098 (1.6%)
All	All	0.66	3/6846 (0.0%)	1.37	145/9329 (1.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	143	PHE	C-N	15.23	1.50	1.33
2	2	73	LYS	C-N	7.92	1.52	1.33
1	1	103	ASN	C-N	7.24	1.50	1.33

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	60	ARG	N-CA-C	-18.90	80.80	108.96
1	1	81	ASN	N-CA-C	-17.95	82.31	110.14
1	1	51	ILE	N-CA-C	-15.52	83.30	106.88
3	3	218	PRO	CB-CA-C	15.42	137.00	111.56
2	2	60	ARG	N-CA-CB	15.31	135.75	111.56
2	2	135	ARG	N-CA-C	-14.89	93.38	113.18
6	L	102	VAL	N-CA-C	-14.68	85.81	107.98
3	3	20	LYS	N-CA-C	-14.51	87.33	109.24
1	1	81	ASN	CB-CA-C	14.24	135.35	109.71
2	2	143	PHE	CA-C-N	14.19	136.44	119.98
2	2	143	PHE	C-N-CA	14.19	136.44	119.98
6	L	103	PHE	N-CA-C	-14.07	83.92	108.13
1	1	103	ASN	CA-C-N	12.74	135.77	119.84
1	1	103	ASN	C-N-CA	12.74	135.77	119.84
1	1	155	ALA	N-CA-C	-12.51	85.97	107.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	108	THR	N-CA-C	-12.43	91.32	109.96
2	2	59	GLU	N-CA-C	-11.45	92.66	109.15
5	H	72	ASP	N-CA-C	-11.45	92.79	109.96
6	L	103	PHE	N-CA-CB	11.44	129.46	110.59
1	1	156	GLN	N-CA-C	-11.24	88.79	108.13
3	3	20	LYS	N-CA-CB	11.17	131.13	111.69
2	2	155	THR	N-CA-CB	-10.92	92.41	111.08
3	3	200	LEU	N-CA-C	-10.62	92.50	109.59
3	3	83	ALA	N-CA-C	-10.30	91.54	109.06
1	1	82	HIS	N-CA-CB	10.08	129.24	111.49
6	L	65	PHE	N-CA-C	-10.02	94.85	109.59
4	4	75	ALA	N-CA-C	-10.01	91.65	108.26
2	2	72	ASP	N-CA-C	9.96	121.72	111.07
5	H	73	ASN	N-CA-C	-9.88	101.35	113.50
1	1	26	ARG	N-CA-C	-9.87	92.82	108.90
3	3	120	ARG	N-CA-C	-9.71	93.03	109.24
6	L	108	THR	CB-CA-C	9.53	125.14	109.89
1	1	198	ASP	CB-CA-C	-9.51	94.11	110.17
2	2	125	MET	N-CA-C	-9.26	93.63	108.73
3	3	70	GLU	N-CA-C	-8.91	96.68	109.96
2	2	126	VAL	N-CA-C	-8.90	97.02	107.61
3	3	200	LEU	CB-CA-C	8.90	125.40	109.38
1	1	52	ASP	N-CA-C	-8.89	94.39	109.24
2	2	61	PHE	N-CA-C	-8.89	95.82	109.95
2	2	86	ASP	CB-CA-C	8.56	122.68	109.84
3	3	30	TYR	N-CA-C	-8.43	94.67	108.41
5	H	21	THR	N-CA-C	-8.33	95.63	109.46
6	L	65	PHE	CB-CA-C	8.32	122.74	110.26
5	H	72	ASP	CB-CA-C	8.19	123.00	109.89
1	1	14	THR	CA-C-N	8.17	134.02	120.62
1	1	14	THR	C-N-CA	8.17	134.02	120.62
6	L	48	ARG	N-CA-C	-8.11	95.51	108.73
2	2	79	GLU	N-CA-C	-8.08	95.09	108.34
1	1	156	GLN	N-CA-CB	7.96	123.72	110.59
2	2	73	LYS	CA-C-N	7.95	129.78	119.84
2	2	73	LYS	C-N-CA	7.95	129.78	119.84
3	3	190	ILE	N-CA-C	7.92	119.63	111.00
6	L	80	SER	N-CA-C	-7.86	96.66	108.99
1	1	77	GLU	N-CA-C	-7.84	95.74	108.52
5	H	85	VAL	CB-CA-C	7.78	124.00	111.32
3	3	180	ASN	N-CA-C	7.74	120.74	110.53
3	3	218	PRO	N-CA-C	-7.72	96.57	112.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	24	SER	N-CA-C	-7.69	95.73	108.34
2	2	125	MET	CB-CA-C	7.68	122.64	110.19
1	1	167	ARG	CB-CA-C	7.66	123.05	109.65
4	4	75	ALA	N-CA-CB	7.64	123.23	110.77
3	3	120	ARG	CB-CA-C	7.61	124.42	109.35
1	1	116	ALA	N-CA-C	-7.58	96.86	109.07
3	3	201	VAL	N-CA-C	-7.54	97.56	108.11
3	3	180	ASN	CB-CA-C	-7.52	94.26	109.68
6	L	81	LEU	N-CA-C	-7.51	99.11	110.14
6	L	109	LEU	N-CA-C	-7.48	98.55	110.14
3	3	31	ASN	N-CA-C	-7.45	100.70	110.39
3	3	190	ILE	CB-CA-C	-7.45	102.25	112.24
1	1	82	HIS	N-CA-C	-7.44	97.39	107.88
1	1	199	ARG	N-CA-C	-7.40	98.06	109.24
2	2	60	ARG	CB-CA-C	7.37	127.81	111.09
4	4	74	SER	N-CA-C	-7.35	94.16	107.98
2	2	155	THR	N-CA-C	7.28	121.37	109.72
6	L	66	SER	N-CA-C	-7.26	98.10	109.72
6	L	80	SER	CB-CA-C	7.25	125.39	109.94
3	3	70	GLU	CB-CA-C	7.21	120.54	110.16
2	2	86	ASP	N-CA-C	-7.15	99.73	110.24
6	L	27	SER	N-CA-C	7.15	121.17	109.94
3	3	30	TYR	CB-CA-C	7.12	121.98	110.16
3	3	178	THR	O-C-N	7.07	129.35	122.07
1	1	198	ASP	N-CA-C	7.01	122.69	113.30
3	3	108	HIS	CB-CA-C	7.00	121.91	109.65
5	H	85	VAL	N-CA-C	-6.99	99.57	109.63
1	1	26	ARG	CB-CA-C	6.94	122.41	109.71
4	4	26	TYR	N-CA-C	-6.86	99.50	110.14
6	L	26	GLY	O-C-N	-6.83	115.52	123.44
2	2	202	ASN	N-CA-C	-6.76	96.64	108.20
1	1	103	ASN	N-CA-C	-6.71	99.82	109.48
1	1	15	VAL	N-CA-C	6.67	120.37	111.17
2	2	157	HIS	N-CA-C	-6.59	97.53	108.34
6	L	27	SER	N-CA-CB	-6.58	98.16	110.07
1	1	24	VAL	N-CA-C	6.50	118.45	109.80
3	3	108	HIS	N-CA-C	-6.47	97.24	108.69
3	3	83	ALA	N-CA-CB	6.46	122.69	111.13
3	3	121	TYR	N-CA-C	-6.43	99.64	109.41
1	1	117	LEU	N-CA-C	-6.42	96.05	108.45
2	2	87	HIS	N-CA-C	-6.32	98.68	109.24
2	2	79	GLU	CB-CA-C	6.28	120.19	110.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	168	ALA	N-CA-C	-6.23	99.94	109.41
1	1	167	ARG	N-CA-C	-6.18	97.74	108.69
3	3	81	LEU	CB-CA-C	6.18	121.19	110.68
2	2	24	SER	CB-CA-C	6.16	119.99	110.14
6	L	64	ARG	N-CA-C	6.13	118.75	111.33
3	3	109	PHE	N-CA-C	-6.11	98.95	108.90
3	3	22	ALA	N-CA-C	6.09	119.36	110.17
1	1	130	TYR	N-CA-C	-6.07	98.39	108.34
1	1	116	ALA	CB-CA-C	6.06	120.20	109.72
1	1	55	GLN	N-CA-C	-5.97	105.30	113.30
1	1	38	ARG	N-CA-C	5.96	118.91	110.50
2	2	80	LYS	N-CA-C	-5.96	101.38	110.14
4	4	25	TYR	N-CA-C	5.85	119.67	112.54
6	L	46	GLY	N-CA-C	5.83	117.49	111.95
1	1	196	SER	CB-CA-C	-5.82	103.30	111.80
1	1	130	TYR	CB-CA-C	5.82	119.45	110.14
3	3	191	THR	N-CA-CB	5.80	120.16	110.59
1	1	23	GLN	CB-CA-C	-5.79	100.25	109.80
4	4	25	TYR	CB-CA-C	-5.78	98.23	110.31
3	3	21	THR	CB-CA-C	-5.71	100.37	109.80
2	2	157	HIS	CB-CA-C	5.64	119.16	110.14
5	H	86	THR	N-CA-C	-5.62	100.87	109.41
1	1	116	ALA	CA-C-N	-5.60	112.56	122.48
1	1	116	ALA	C-N-CA	-5.60	112.56	122.48
2	2	167	ARG	N-CA-C	5.58	117.04	111.07
3	3	201	VAL	N-CA-CB	5.58	119.10	111.41
3	3	71	GLN	N-CA-CB	5.56	120.18	111.56
3	3	101	TYR	CB-CA-C	-5.55	98.89	109.66
1	1	102	SER	N-CA-CB	5.54	118.36	110.16
2	2	81	LEU	CB-CA-C	5.45	119.06	109.80
5	H	29	LEU	N-CA-C	-5.44	106.48	113.01
2	2	104	GLY	N-CA-C	-5.40	102.25	112.51
1	1	27	ARG	N-CA-CB	5.38	119.86	111.64
2	2	203	ILE	N-CA-C	-5.37	100.59	108.11
2	2	81	LEU	N-CA-C	-5.33	98.88	108.48
1	1	78	ILE	N-CA-C	-5.31	100.74	108.97
2	2	38	THR	N-CA-C	-5.27	107.02	113.50
3	3	180	ASN	O-C-N	5.22	128.74	122.79
1	1	117	LEU	N-CA-CB	5.19	121.69	110.27
3	3	154	SER	N-CA-C	5.18	119.69	112.90
3	3	22	ALA	N-CA-CB	-5.12	102.26	110.51
3	3	121	TYR	N-CA-CB	5.11	119.56	111.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	71	THR	CB-CA-C	5.09	120.56	110.42
2	2	103	ASN	CB-CA-C	5.08	120.06	110.62
3	3	102	SER	N-CA-CB	-5.08	103.36	111.43
2	2	169	ASP	N-CA-CB	-5.02	103.28	111.66

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	1	1485	0	1483	182	0
2	2	1623	0	1586	155	0
3	3	1691	0	1620	169	0
4	4	348	0	321	11	0
5	H	742	0	722	59	0
6	L	795	0	761	111	0
All	All	6684	0	6493	580	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 44.

All (580) 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)
1:1:158:PRO:HD2	1:1:161:PHE:CE2	1.20	1.71
6:L:25:SER:HA	6:L:73:THR:CG2	1.38	1.50
1:1:158:PRO:CD	1:1:161:PHE:CE2	1.96	1.47
2:2:73:LYS:HE3	2:2:77:HIS:CE1	1.51	1.42
1:1:54:MET:HE1	1:1:67:ARG:NE	1.23	1.42
1:1:158:PRO:HD2	1:1:161:PHE:CD2	1.53	1.40
1:1:54:MET:CE	1:1:67:ARG:HE	1.38	1.37
1:1:54:MET:CE	1:1:67:ARG:NE	1.91	1.32
2:2:73:LYS:CE	2:2:77:HIS:CE1	2.12	1.30
1:1:158:PRO:CD	1:1:161:PHE:HE2	1.36	1.29

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:104:PRO:CG	3:3:17:THR:HG21	1.61	1.29
3:3:126:VAL:HG22	3:3:184:TRP:O	1.17	1.28
6:L:82:GLN:N	6:L:85:ASP:OD2	1.66	1.28
1:1:101:THR:CG2	1:1:105:THR:HG21	1.62	1.28
1:1:193:LYS:HB2	2:2:135:ARG:NH1	1.49	1.28
6:L:24:CYS:O	6:L:73:THR:HB	1.24	1.25
1:1:158:PRO:CG	1:1:161:PHE:HE2	1.52	1.23
6:L:92:ALA:HB1	6:L:102:VAL:HG23	1.25	1.18
1:1:91:ASN:HD21	1:1:160:SER:CA	1.58	1.17
3:3:122:MET:HE3	3:3:145:HIS:ND1	1.59	1.16
6:L:25:SER:CA	6:L:73:THR:HG22	1.76	1.15
1:1:88:TRP:NE1	1:1:117:LEU:HD22	1.62	1.15
6:L:25:SER:CA	6:L:73:THR:CG2	2.24	1.15
2:2:30:VAL:CG1	2:2:153:ASN:HD22	1.60	1.14
1:1:111:PRO:HG3	3:3:9:ASP:CG	1.74	1.12
1:1:91:ASN:HD21	1:1:160:SER:HA	1.02	1.12
1:1:50:VAL:HG11	1:1:162:ASN:HD22	1.15	1.11
1:1:104:PRO:HG3	3:3:17:THR:CG2	1.80	1.09
1:1:52:ASP:HB2	1:1:162:ASN:HB3	1.32	1.09
2:2:112:VAL:C	2:2:197:ILE:HD11	1.78	1.09
2:2:30:VAL:HG12	2:2:153:ASN:ND2	1.68	1.08
1:1:111:PRO:CG	3:3:9:ASP:OD1	2.02	1.07
1:1:54:MET:SD	1:1:67:ARG:NE	2.28	1.07
1:1:111:PRO:HG3	3:3:9:ASP:OD1	1.52	1.07
2:2:67:PHE:HB3	2:2:79:GLU:HG2	1.25	1.07
1:1:80:VAL:HG12	1:1:81:ASN:O	1.55	1.06
2:2:30:VAL:CG1	2:2:153:ASN:ND2	2.16	1.06
3:3:81:LEU:HD13	3:3:95:ALA:CB	1.87	1.04
3:3:44:LEU:HB3	3:3:94:ILE:HD11	1.38	1.03
1:1:54:MET:SD	1:1:67:ARG:CG	2.47	1.02
2:2:30:VAL:HG12	2:2:153:ASN:HD22	0.89	1.02
1:1:51:ILE:CG2	1:1:51:ILE:O	2.06	1.02
2:2:54:ARG:HH12	2:2:207:HIS:HA	1.21	1.02
1:1:101:THR:HG22	1:1:105:THR:CG2	1.91	1.01
6:L:24:CYS:O	6:L:73:THR:CB	2.08	1.00
3:3:126:VAL:CG2	3:3:184:TRP:O	2.10	1.00
1:1:51:ILE:HG22	1:1:164:GLY:O	1.62	0.99
6:L:82:GLN:HB2	6:L:84:GLU:OE2	1.63	0.98
1:1:193:LYS:CB	2:2:135:ARG:NH1	2.25	0.98
1:1:91:ASN:ND2	1:1:160:SER:HA	1.78	0.97
6:L:36:VAL:HG21	6:L:74:ALA:CB	1.92	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:73:LYS:HE2	2:2:77:HIS:CE1	2.00	0.97
1:1:101:THR:HG22	1:1:105:THR:HG21	0.99	0.97
1:1:50:VAL:HG11	1:1:162:ASN:ND2	1.80	0.97
3:3:44:LEU:HB3	3:3:94:ILE:CD1	1.93	0.97
1:1:54:MET:SD	1:1:67:ARG:HG3	2.03	0.97
1:1:158:PRO:CG	1:1:161:PHE:CE2	2.38	0.96
1:1:51:ILE:O	1:1:51:ILE:HG23	1.65	0.96
2:2:103:ASN:O	2:2:162:TYR:HB2	1.63	0.96
1:1:104:PRO:HG3	3:3:17:THR:HG21	0.97	0.96
2:2:74:PRO:HG2	5:H:100:HIS:ND1	1.81	0.94
1:1:54:MET:SD	1:1:67:ARG:CZ	2.55	0.94
1:1:104:PRO:CB	3:3:17:THR:CG2	2.46	0.94
3:3:134:PRO:HB3	3:3:139:ARG:HG2	1.50	0.94
1:1:158:PRO:CD	1:1:161:PHE:CD2	2.38	0.93
6:L:82:GLN:H	6:L:85:ASP:CG	1.74	0.93
1:1:6:GLU:OE1	2:2:152:THR:CG2	2.17	0.93
1:1:104:PRO:HB3	3:3:17:THR:CG2	1.99	0.93
6:L:25:SER:CB	6:L:73:THR:HG21	1.98	0.93
1:1:111:PRO:HG3	3:3:9:ASP:OD2	1.65	0.92
6:L:82:GLN:CB	6:L:84:GLU:OE2	2.16	0.92
1:1:158:PRO:HG2	1:1:161:PHE:HE2	1.32	0.92
6:L:25:SER:HA	6:L:73:THR:HG21	1.51	0.92
3:3:111:PHE:CZ	3:3:198:ASP:OD2	2.22	0.92
6:L:25:SER:HA	6:L:73:THR:HG22	0.94	0.91
1:1:52:ASP:HB2	1:1:162:ASN:CB	1.99	0.91
2:2:72:ASP:CG	5:H:108:THR:OG1	2.13	0.91
3:3:130:VAL:O	3:3:184:TRP:CZ3	2.24	0.91
3:3:134:PRO:CB	3:3:139:ARG:HG2	2.00	0.91
6:L:36:VAL:HA	6:L:93:THR:HB	1.53	0.90
6:L:81:LEU:C	6:L:85:ASP:OD2	2.14	0.90
1:1:101:THR:CG2	1:1:105:THR:CG2	2.48	0.90
2:2:54:ARG:NH1	2:2:207:HIS:HA	1.87	0.89
2:2:72:ASP:OD1	5:H:108:THR:OG1	1.91	0.88
1:1:122:PRO:HG3	3:3:170:TYR:HE1	1.38	0.87
1:1:104:PRO:CB	3:3:17:THR:HG21	2.03	0.87
3:3:63:TYR:HA	3:3:200:LEU:O	1.75	0.87
3:3:111:PHE:CE2	3:3:198:ASP:OD2	2.29	0.86
2:2:30:VAL:HG11	2:2:153:ASN:ND2	1.91	0.86
1:1:88:TRP:CD1	1:1:117:LEU:HD22	2.11	0.85
6:L:36:VAL:HG12	6:L:93:THR:CG2	2.05	0.85
2:2:28:SER:HB3	2:2:154:MET:HG2	1.59	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:193:LYS:HB2	2:2:135:ARG:CZ	2.06	0.85
1:1:50:VAL:CG1	1:1:162:ASN:ND2	2.40	0.84
3:3:19:PRO:HG3	4:4:30:TYR:CD2	2.12	0.84
6:L:25:SER:HB2	6:L:73:THR:HG21	1.58	0.84
1:1:6:GLU:OE1	2:2:149:SER:OG	1.94	0.84
1:1:111:PRO:HG2	3:3:9:ASP:OD1	1.76	0.84
1:1:104:PRO:CG	3:3:17:THR:CG2	2.44	0.84
1:1:160:SER:OG	3:3:170:TYR:OH	1.96	0.84
3:3:148:TRP:CE3	3:3:156:PHE:CD2	2.65	0.84
3:3:55:LEU:HD13	3:3:202:VAL:HG13	1.60	0.83
3:3:81:LEU:CD1	3:3:95:ALA:CB	2.56	0.83
2:2:72:ASP:CG	5:H:108:THR:HG1	1.87	0.83
2:2:215:PRO:HB3	3:3:143:CYS:SG	2.19	0.83
3:3:18:ASP:OD1	3:3:19:PRO:HD2	1.79	0.83
6:L:92:ALA:CB	6:L:102:VAL:HG23	2.08	0.82
6:L:41:GLN:O	6:L:87:ALA:HB1	1.80	0.82
2:2:134:THR:OG1	5:H:31:ASP:OD2	1.97	0.82
3:3:148:TRP:CE3	3:3:156:PHE:CE2	2.68	0.82
2:2:48:THR:HA	3:3:163:VAL:HB	1.61	0.82
1:1:158:PRO:HG2	1:1:161:PHE:CE2	2.09	0.82
3:3:44:LEU:CB	3:3:94:ILE:HD11	2.09	0.82
5:H:29:LEU:O	5:H:71:LYS:NZ	2.14	0.81
6:L:24:CYS:C	6:L:73:THR:HB	2.03	0.81
6:L:47:LEU:HD12	6:L:47:LEU:O	1.79	0.81
2:2:112:VAL:C	2:2:197:ILE:CD1	2.54	0.81
1:1:91:ASN:ND2	1:1:160:SER:O	2.13	0.81
3:3:71:GLN:HA	3:3:71:GLN:OE1	1.81	0.81
1:1:193:LYS:N	2:2:135:ARG:HH12	1.78	0.81
6:L:25:SER:HA	6:L:73:THR:CB	2.11	0.80
3:3:2:ILE:HD12	3:3:2:ILE:H	1.45	0.80
2:2:73:LYS:HD3	2:2:77:HIS:ND1	1.96	0.80
1:1:104:PRO:CB	3:3:17:THR:HG22	2.11	0.80
2:2:73:LYS:CE	2:2:77:HIS:ND1	2.43	0.80
1:1:160:SER:CB	3:3:170:TYR:OH	2.30	0.80
1:1:111:PRO:CG	3:3:9:ASP:CG	2.47	0.80
3:3:180:ASN:N	3:3:180:ASN:HD22	1.74	0.80
1:1:122:PRO:HG3	3:3:170:TYR:CE1	2.17	0.79
1:1:91:ASN:ND2	1:1:160:SER:CA	2.41	0.79
3:3:67:ARG:HH11	3:3:67:ARG:HB3	1.47	0.79
6:L:33:ARG:NH2	6:L:96:TYR:CD2	2.50	0.79
6:L:36:VAL:HG12	6:L:93:THR:HG21	1.64	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:29:LEU:HG	5:H:71:LYS:NZ	1.97	0.79
6:L:81:LEU:CA	6:L:85:ASP:OD2	2.31	0.78
1:1:52:ASP:CB	1:1:162:ASN:HB3	2.11	0.78
2:2:143:PHE:HB3	2:2:144:PRO:HD2	1.64	0.78
3:3:81:LEU:HD13	3:3:95:ALA:HB2	1.63	0.78
5:H:111:GLN:CD	6:L:35:ASP:O	2.26	0.78
5:H:110:MET:HE2	6:L:102:VAL:HG21	1.65	0.78
6:L:33:ARG:O	6:L:34:TYR:CD1	2.37	0.77
1:1:196:SER:O	1:1:197:GLN:HG3	1.85	0.77
2:2:195:SER:HB2	6:L:33:ARG:HD2	1.67	0.76
1:1:54:MET:HE1	1:1:67:ARG:CD	2.15	0.76
3:3:120:ARG:HG2	3:3:190:ILE:HD11	1.67	0.76
2:2:214:LEU:HD11	3:3:129:GLY:HA3	1.67	0.76
2:2:36:TYR:HA	4:4:67:TRP:CD1	2.21	0.76
6:L:69:ARG:HH11	6:L:69:ARG:HG2	1.49	0.75
2:2:73:LYS:HE2	2:2:77:HIS:HE1	1.50	0.75
3:3:182:GLN:HA	3:3:182:GLN:NE2	2.02	0.75
2:2:103:ASN:O	2:2:162:TYR:CB	2.34	0.75
6:L:36:VAL:HG12	6:L:93:THR:CB	2.16	0.75
5:H:29:LEU:HD21	5:H:71:LYS:CG	2.17	0.75
6:L:24:CYS:HB3	6:L:74:ALA:O	1.86	0.75
6:L:36:VAL:HG12	6:L:93:THR:HB	1.69	0.75
2:2:57:GLN:HA	2:2:57:GLN:NE2	2.03	0.74
5:H:40:ALA:HB3	5:H:44:ALA:HB3	1.68	0.74
1:1:104:PRO:HB3	3:3:17:THR:HG22	1.68	0.74
2:2:120:CYS:H	2:2:185:SER:HB3	1.53	0.74
1:1:54:MET:HG2	1:1:66:LEU:CD2	2.18	0.74
2:2:67:PHE:HB3	2:2:79:GLU:CG	2.14	0.74
2:2:57:GLN:HA	2:2:57:GLN:HE21	1.53	0.74
1:1:111:PRO:CG	3:3:9:ASP:OD2	2.37	0.73
5:H:29:LEU:HD11	5:H:71:LYS:HD2	1.71	0.73
1:1:97:ALA:HA	3:3:217:ASP:O	1.88	0.73
2:2:91:TYR:OH	2:2:103:ASN:ND2	2.22	0.73
2:2:143:PHE:CB	2:2:144:PRO:HD2	2.18	0.73
3:3:14:LEU:HD12	3:3:14:LEU:C	2.13	0.73
3:3:79:LEU:HB3	3:3:182:GLN:HB3	1.70	0.72
2:2:113:GLY:CA	2:2:197:ILE:HD12	2.19	0.72
2:2:55:VAL:O	2:2:208:VAL:HG13	1.87	0.72
2:2:28:SER:CB	2:2:154:MET:HG2	2.18	0.72
1:1:51:ILE:O	1:1:51:ILE:HG22	1.90	0.72
1:1:53:LEU:HD12	1:1:163:TYR:HE1	1.54	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:102:VAL:HG13	6:L:102:VAL:O	1.88	0.72
1:1:102:SER:HA	3:3:16:THR:HG21	1.72	0.72
1:1:193:LYS:CB	2:2:135:ARG:HH12	1.98	0.72
2:2:74:PRO:HG3	5:H:100:HIS:CG	2.25	0.72
3:3:56:CYS:HB2	3:3:88:ASN:OD1	1.88	0.72
3:3:72:ARG:HG3	3:3:72:ARG:NH1	2.04	0.71
1:1:54:MET:CE	1:1:67:ARG:CD	2.66	0.71
3:3:120:ARG:NH2	3:3:149:ASP:OD1	2.22	0.71
3:3:45:LEU:HD13	3:3:45:LEU:C	2.15	0.71
3:3:72:ARG:HG3	3:3:72:ARG:HH11	1.54	0.71
5:H:68:SER:O	5:H:80:LEU:HA	1.90	0.71
6:L:102:VAL:O	6:L:102:VAL:CG1	2.38	0.71
2:2:67:PHE:HD2	2:2:73:LYS:HE2	1.54	0.71
3:3:14:LEU:HD12	3:3:14:LEU:O	1.91	0.70
1:1:89:VAL:CG1	1:1:103:ASN:OD1	2.39	0.70
2:2:214:LEU:HD21	3:3:130:VAL:HG13	1.72	0.70
3:3:23:ASP:OD1	3:3:24:PRO:HD2	1.91	0.70
6:L:92:ALA:HB1	6:L:102:VAL:CG2	2.16	0.70
1:1:91:ASN:ND2	1:1:160:SER:C	2.50	0.69
5:H:34:VAL:HG21	5:H:78:VAL:HG11	1.73	0.69
6:L:69:ARG:HG3	6:L:69:ARG:O	1.92	0.69
1:1:88:TRP:HE1	1:1:117:LEU:HD22	1.52	0.69
2:2:74:PRO:CG	5:H:100:HIS:ND1	2.53	0.69
3:3:55:LEU:N	3:3:55:LEU:HD12	2.07	0.69
1:1:91:ASN:HD21	1:1:160:SER:C	2.00	0.69
2:2:107:VAL:HG23	2:2:203:ILE:HG12	1.74	0.69
6:L:86:GLU:HA	6:L:109:LEU:HD23	1.75	0.69
6:L:48:ARG:NH2	6:L:60:GLY:O	2.27	0.68
1:1:103:ASN:ND2	1:1:103:ASN:O	2.27	0.68
3:3:66:THR:OG1	3:3:189:GLN:OE1	2.07	0.68
1:1:104:PRO:CA	3:3:17:THR:HG22	2.24	0.68
2:2:113:GLY:N	2:2:197:ILE:HD11	2.09	0.68
2:2:48:THR:HA	3:3:163:VAL:CB	2.22	0.68
2:2:67:PHE:CB	2:2:79:GLU:HG2	2.13	0.68
3:3:81:LEU:CD1	3:3:95:ALA:HB1	2.21	0.68
2:2:73:LYS:CD	2:2:77:HIS:ND1	2.57	0.67
3:3:15:VAL:HB	3:3:18:ASP:HB2	1.75	0.67
6:L:84:GLU:H	6:L:84:GLU:CD	2.02	0.67
5:H:29:LEU:HG	5:H:71:LYS:HZ2	1.58	0.67
3:3:63:TYR:CA	3:3:200:LEU:O	2.42	0.67
3:3:108:HIS:HB2	3:3:203:SER:HB2	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:130:VAL:O	3:3:184:TRP:CH2	2.47	0.67
2:2:131:GLU:OE1	2:2:131:GLU:HA	1.95	0.67
2:2:74:PRO:CG	5:H:100:HIS:CG	2.78	0.66
3:3:122:MET:CE	3:3:145:HIS:ND1	2.48	0.66
6:L:36:VAL:HG21	6:L:74:ALA:HB2	1.74	0.66
3:3:81:LEU:HD12	3:3:95:ALA:HB1	1.78	0.66
6:L:81:LEU:HA	6:L:85:ASP:OD2	1.96	0.66
1:1:54:MET:SD	1:1:67:ARG:CD	2.84	0.66
2:2:148:ILE:HG13	2:2:156:ALA:HB2	1.77	0.66
2:2:166:ASN:ND2	3:3:165:ALA:HB1	2.10	0.66
2:2:189:THR:OG1	2:2:195:SER:HA	1.96	0.66
3:3:126:VAL:O	3:3:183:GLY:HA3	1.96	0.66
6:L:88:ASP:O	6:L:90:PHE:CE2	2.50	0.65
3:3:67:ARG:HH11	3:3:67:ARG:CB	2.10	0.65
5:H:47:PHE:O	5:H:60:ASN:ND2	2.30	0.65
5:H:113:VAL:HG12	6:L:49:THR:HG21	1.79	0.65
2:2:28:SER:OG	2:2:153:ASN:HA	1.97	0.65
5:H:111:GLN:CG	6:L:35:ASP:O	2.45	0.65
1:1:89:VAL:HG12	1:1:103:ASN:OD1	1.96	0.64
1:1:190:LEU:HD22	2:2:136:GLU:OE2	1.97	0.64
6:L:31:ILE:HB	6:L:72:ASN:O	1.97	0.64
6:L:37:GLY:N	6:L:92:ALA:O	2.30	0.64
6:L:38:TRP:HB2	6:L:51:ILE:HB	1.78	0.64
1:1:104:PRO:HA	3:3:17:THR:HG22	1.79	0.64
6:L:84:GLU:OE1	6:L:84:GLU:N	2.19	0.64
3:3:79:LEU:HB3	3:3:182:GLN:CB	2.27	0.64
1:1:90:PRO:HB3	3:3:214:LEU:HD13	1.79	0.64
6:L:69:ARG:HG2	6:L:69:ARG:NH1	2.12	0.64
6:L:82:GLN:N	6:L:85:ASP:CG	2.46	0.64
5:H:29:LEU:HD21	5:H:71:LYS:HG3	1.79	0.64
2:2:59:GLU:OE1	2:2:59:GLU:N	2.32	0.63
3:3:57:PHE:CD1	3:3:85:HIS:HD2	2.17	0.62
6:L:110:THR:HG22	6:L:112:LEU:H	1.63	0.62
1:1:101:THR:HG23	1:1:105:THR:CB	2.29	0.62
1:1:54:MET:SD	1:1:67:ARG:HG2	2.35	0.62
1:1:157:LEU:HD22	1:1:157:LEU:N	2.14	0.62
2:2:73:LYS:CE	2:2:77:HIS:HE1	1.95	0.62
6:L:78:ILE:HG22	6:L:80:SER:O	1.98	0.62
2:2:109:VAL:HG13	2:2:148:ILE:CD1	2.30	0.62
6:L:42:ILE:HG13	6:L:44:GLY:H	1.64	0.62
1:1:120:THR:HB	3:3:214:LEU:HD11	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:6:GLU:OE1	2:2:152:THR:HG22	1.98	0.61
2:2:113:GLY:HA2	2:2:197:ILE:HD12	1.81	0.61
6:L:26:GLY:H	6:L:73:THR:HG22	1.65	0.61
1:1:109:LYS:HG3	1:1:111:PRO:HD2	1.82	0.61
2:2:112:VAL:O	2:2:197:ILE:HG13	2.00	0.61
3:3:180:ASN:N	3:3:180:ASN:ND2	2.46	0.61
1:1:7:SER:HB2	2:2:30:VAL:CG2	2.30	0.61
1:1:52:ASP:CB	1:1:162:ASN:CB	2.76	0.61
1:1:90:PRO:CB	3:3:214:LEU:HD13	2.29	0.61
2:2:17:THR:HG22	2:2:24:SER:O	2.01	0.61
3:3:67:ARG:HH11	3:3:67:ARG:CG	2.14	0.61
3:3:56:CYS:O	3:3:85:HIS:HA	2.00	0.60
3:3:67:ARG:HG2	3:3:74:LEU:HD23	1.83	0.60
2:2:140:LEU:HD12	2:2:140:LEU:O	2.02	0.60
4:4:83:LEU:C	4:4:83:LEU:HD23	2.26	0.60
6:L:36:VAL:HG21	6:L:74:ALA:HB3	1.81	0.60
2:2:31:GLY:O	2:2:146:GLN:NE2	2.28	0.60
6:L:36:VAL:CA	6:L:93:THR:HB	2.28	0.60
1:1:103:ASN:N	1:1:103:ASN:HD22	1.99	0.60
2:2:148:ILE:HD11	2:2:156:ALA:CB	2.32	0.60
6:L:33:ARG:O	6:L:34:TYR:HD1	1.83	0.60
6:L:81:LEU:CD2	6:L:85:ASP:HB3	2.31	0.60
3:3:18:ASP:OD1	3:3:19:PRO:CD	2.49	0.59
3:3:72:ARG:HH11	3:3:72:ARG:CG	2.14	0.59
1:1:71:TYR:OH	2:2:128:GLU:OE2	2.19	0.59
1:1:120:THR:HB	3:3:214:LEU:CD1	2.32	0.59
5:H:52:SER:N	5:H:56:ASN:O	2.36	0.59
3:3:109:PHE:CD2	3:3:148:TRP:CH2	2.90	0.59
6:L:12:VAL:HG12	6:L:108:THR:O	2.03	0.59
6:L:26:GLY:N	6:L:73:THR:HG22	2.16	0.59
1:1:6:GLU:CD	2:2:152:THR:HG21	2.28	0.59
1:1:131:ASN:ND2	2:2:175:LYS:O	2.36	0.58
2:2:73:LYS:HE3	2:2:77:HIS:NE2	2.11	0.58
2:2:148:ILE:HD11	2:2:156:ALA:HB3	1.85	0.58
1:1:193:LYS:CA	2:2:135:ARG:HH12	2.16	0.58
2:2:107:VAL:HG21	2:2:179:LEU:HD13	1.85	0.58
6:L:36:VAL:CG2	6:L:74:ALA:CB	2.77	0.57
1:1:18:TYR:HD1	1:1:18:TYR:O	1.87	0.57
1:1:68:ALA:O	1:1:187:ARG:N	2.38	0.57
1:1:160:SER:HB2	3:3:170:TYR:OH	2.01	0.57
1:1:156:GLN:OE1	1:1:156:GLN:HA	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:72:ASP:OD1	5:H:108:THR:CG2	2.52	0.57
1:1:89:VAL:HG22	1:1:98:LEU:CD2	2.34	0.57
2:2:113:GLY:N	2:2:197:ILE:CD1	2.67	0.57
1:1:48:THR:OG1	1:1:167:ARG:NE	2.38	0.57
1:1:51:ILE:HG22	1:1:164:GLY:C	2.30	0.57
6:L:25:SER:CA	6:L:73:THR:HG21	2.06	0.57
6:L:33:ARG:NH2	6:L:96:TYR:CE2	2.72	0.57
3:3:122:MET:HE3	3:3:145:HIS:CG	2.37	0.56
6:L:81:LEU:HD21	6:L:109:LEU:HD21	1.86	0.56
2:2:72:ASP:OD1	5:H:108:THR:HG21	2.05	0.56
2:2:73:LYS:HE3	2:2:77:HIS:ND1	2.05	0.56
6:L:28:SER:HA	6:L:32:GLY:HA3	1.88	0.56
6:L:64:ARG:HH11	6:L:65:PHE:HE1	1.53	0.56
6:L:24:CYS:O	6:L:73:THR:CA	2.52	0.56
1:1:6:GLU:CD	2:2:152:THR:CG2	2.79	0.56
2:2:112:VAL:O	2:2:197:ILE:CD1	2.52	0.56
3:3:7:CYS:O	3:3:7:CYS:SG	2.63	0.56
3:3:100:GLN:HE21	3:3:213:ARG:HE	1.52	0.56
1:1:51:ILE:HG22	1:1:164:GLY:H	1.71	0.56
5:H:111:GLN:HG2	6:L:35:ASP:O	2.05	0.56
1:1:101:THR:HG23	1:1:105:THR:HB	1.88	0.56
1:1:113:THR:C	3:3:10:GLY:O	2.49	0.56
2:2:61:PHE:HD2	2:2:202:ASN:HB3	1.70	0.55
5:H:29:LEU:HD21	5:H:71:LYS:HG2	1.87	0.55
1:1:101:THR:HG23	1:1:105:THR:CG2	2.35	0.55
2:2:74:PRO:HG2	5:H:100:HIS:CE1	2.40	0.55
2:2:195:SER:HB2	6:L:33:ARG:CD	2.34	0.55
5:H:36:TRP:CE3	5:H:80:LEU:HD23	2.41	0.55
2:2:56:VAL:O	2:2:56:VAL:HG22	2.06	0.55
5:H:47:PHE:HB3	6:L:100:THR:HG21	1.87	0.55
2:2:82:GLU:HA	2:2:178:THR:HG22	1.88	0.55
6:L:30:ASN:OD1	6:L:31:ILE:N	2.40	0.55
1:1:53:LEU:HD12	1:1:72:TYR:CE2	2.42	0.55
2:2:61:PHE:HA	2:2:204:ALA:HB2	1.89	0.55
2:2:106:ASP:HA	2:2:159:THR:HA	1.89	0.55
6:L:25:SER:C	6:L:73:THR:HG22	2.32	0.55
6:L:95:ASP:CG	6:L:98:SER:HB2	2.31	0.55
1:1:18:TYR:O	1:1:18:TYR:CD1	2.59	0.55
6:L:13:SER:HB2	6:L:112:LEU:HD11	1.87	0.55
3:3:57:PHE:HE2	3:3:202:VAL:HG11	1.71	0.55
1:1:54:MET:HE1	1:1:67:ARG:HE	0.49	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:40:ALA:N	5:H:44:ALA:O	2.38	0.55
1:1:111:PRO:CB	3:3:9:ASP:OD2	2.55	0.54
3:3:160:ILE:HD13	3:3:185:VAL:HG21	1.88	0.54
4:4:36:THR:O	4:4:37:GLN:NE2	2.41	0.54
1:1:53:LEU:HD12	1:1:72:TYR:HE2	1.71	0.54
5:H:29:LEU:HG	5:H:71:LYS:HZ3	1.71	0.54
3:3:45:LEU:CD2	3:3:210:PHE:HD2	2.21	0.54
1:1:7:SER:HB2	2:2:30:VAL:HG21	1.89	0.54
3:3:148:TRP:CD2	3:3:156:PHE:CD2	2.96	0.54
3:3:148:TRP:CZ3	3:3:156:PHE:CD2	2.94	0.54
2:2:148:ILE:CG1	2:2:156:ALA:HB2	2.37	0.54
5:H:51:ILE:HD13	5:H:71:LYS:HB2	1.88	0.54
1:1:114:ARG:N	3:3:10:GLY:O	2.41	0.54
5:H:80:LEU:HD12	5:H:81:SER:H	1.73	0.53
3:3:45:LEU:HD13	3:3:45:LEU:O	2.08	0.53
3:3:72:ARG:O	3:3:188:TYR:HD1	1.90	0.53
3:3:194:LYS:O	3:3:194:LYS:HG3	2.07	0.53
3:3:174:ASP:OD1	3:3:174:ASP:N	2.40	0.53
3:3:57:PHE:HE1	3:3:75:ALA:HB1	1.74	0.53
2:2:68:ASP:OD1	2:2:68:ASP:N	2.41	0.53
3:3:126:VAL:HG22	3:3:184:TRP:C	2.19	0.53
1:1:89:VAL:CG2	1:1:98:LEU:CD2	2.86	0.53
3:3:109:PHE:CD2	3:3:148:TRP:HH2	2.27	0.53
6:L:40:GLN:HB2	6:L:50:ILE:HG12	1.91	0.53
3:3:81:LEU:HD13	3:3:95:ALA:HB3	1.86	0.53
1:1:54:MET:CE	1:1:67:ARG:CZ	2.80	0.52
2:2:138:TYR:HD1	2:2:138:TYR:H	1.57	0.52
2:2:109:VAL:HG11	2:2:123:VAL:HG21	1.92	0.52
2:2:129:PHE:HB2	2:2:178:THR:OG1	2.10	0.52
5:H:36:TRP:CH2	5:H:80:LEU:HB3	2.45	0.52
6:L:33:ARG:NH2	6:L:96:TYR:CG	2.62	0.52
1:1:90:PRO:HG3	3:3:214:LEU:HB3	1.91	0.52
6:L:8:GLN:NE2	6:L:104:GLY:HA2	2.25	0.52
2:2:61:PHE:CD2	2:2:202:ASN:HB3	2.45	0.52
2:2:85:THR:O	2:2:86:ASP:C	2.51	0.52
3:3:41:PHE:HE2	3:3:44:LEU:HD23	1.74	0.52
3:3:64:VAL:HG23	3:3:64:VAL:O	2.10	0.52
3:3:111:PHE:CZ	3:3:198:ASP:CG	2.88	0.52
2:2:138:TYR:HD1	2:2:138:TYR:N	2.08	0.52
3:3:108:HIS:N	3:3:203:SER:O	2.42	0.52
1:1:157:LEU:H	1:1:157:LEU:CD2	2.24	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:109:PHE:HB3	3:3:200:LEU:HD11	1.92	0.51
1:1:115:LEU:HD23	1:1:116:ALA:C	2.35	0.51
5:H:36:TRP:CD1	5:H:95:CYS:HG	2.28	0.51
6:L:82:GLN:HB2	6:L:84:GLU:CD	2.32	0.51
1:1:158:PRO:O	1:1:161:PHE:HD2	1.94	0.51
6:L:38:TRP:N	6:L:51:ILE:O	2.40	0.50
1:1:1:THR:HG21	1:1:13:THR:HB	1.93	0.50
1:1:92:GLY:O	3:3:99:ALA:HB1	2.11	0.50
2:2:115:GLN:O	2:2:115:GLN:HG3	2.12	0.50
4:4:79:LEU:N	4:4:79:LEU:CD2	2.73	0.50
3:3:67:ARG:CG	3:3:67:ARG:NH1	2.73	0.50
6:L:8:GLN:OE1	6:L:105:SER:N	2.40	0.50
1:1:54:MET:HG2	1:1:66:LEU:HD22	1.92	0.50
1:1:157:LEU:N	1:1:157:LEU:CD2	2.74	0.50
4:4:15:SER:OG	4:4:16:GLY:N	2.42	0.50
6:L:82:GLN:CB	6:L:84:GLU:CD	2.85	0.50
1:1:6:GLU:OE1	2:2:152:THR:HG21	2.04	0.50
2:2:215:PRO:CB	3:3:143:CYS:SG	2.98	0.50
1:1:114:ARG:HB3	3:3:11:TYR:HB3	1.93	0.49
1:1:190:LEU:HD13	2:2:135:ARG:HB2	1.93	0.49
2:2:67:PHE:CD2	2:2:73:LYS:HE2	2.42	0.49
6:L:81:LEU:CD2	6:L:85:ASP:CB	2.90	0.49
1:1:187:ARG:N	2:2:142:LEU:HD23	2.27	0.49
2:2:138:TYR:N	2:2:138:TYR:CD1	2.80	0.49
3:3:44:LEU:HD13	3:3:94:ILE:HD11	1.94	0.49
3:3:63:TYR:HB2	3:3:199:THR:HB	1.92	0.49
3:3:133:PRO:HG3	3:3:184:TRP:CB	2.42	0.49
1:1:104:PRO:HG3	3:3:17:THR:CB	2.42	0.49
3:3:45:LEU:C	3:3:45:LEU:CD1	2.85	0.49
1:1:53:LEU:CD1	1:1:163:TYR:HE1	2.23	0.49
1:1:50:VAL:HG13	1:1:162:ASN:ND2	2.25	0.49
6:L:81:LEU:HD22	6:L:85:ASP:CB	2.42	0.49
5:H:17:THR:OG1	5:H:18:LEU:N	2.46	0.49
5:H:50:SER:O	5:H:58:GLY:N	2.31	0.49
5:H:99:ILE:HG22	5:H:99:ILE:O	2.13	0.49
2:2:69:TRP:HE1	2:2:183:VAL:HG11	1.76	0.49
5:H:29:LEU:CD1	5:H:71:LYS:HD2	2.41	0.49
2:2:66:LEU:HB2	2:2:199:VAL:O	2.13	0.48
3:3:63:TYR:CD1	3:3:199:THR:HG22	2.47	0.48
1:1:136:TYR:CD2	3:3:177:ASP:OD2	2.66	0.48
6:L:36:VAL:CG1	6:L:93:THR:HB	2.39	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:6:GLU:CG	2:2:152:THR:HG21	2.44	0.48
1:1:48:THR:HG22	1:1:48:THR:O	2.13	0.48
1:1:115:LEU:HD23	1:1:116:ALA:O	2.14	0.48
1:1:119:TYR:HD1	1:1:163:TYR:CE2	2.32	0.48
2:2:52:GLU:CD	2:2:52:GLU:H	2.20	0.48
2:2:169:ASP:OD1	2:2:169:ASP:N	2.46	0.48
3:3:23:ASP:OD1	3:3:24:PRO:CD	2.60	0.48
3:3:57:PHE:CE2	3:3:202:VAL:HG11	2.48	0.48
1:1:7:SER:HB2	2:2:30:VAL:HG22	1.94	0.48
3:3:73:LEU:C	3:3:73:LEU:CD2	2.86	0.48
5:H:27:PHE:O	5:H:97:LYS:HE2	2.14	0.48
3:3:91:LEU:HD11	3:3:210:PHE:CE2	2.49	0.48
3:3:63:TYR:CB	3:3:199:THR:HB	2.43	0.48
2:2:148:ILE:HD11	2:2:156:ALA:N	2.29	0.48
5:H:36:TRP:CG	5:H:95:CYS:HG	2.31	0.48
6:L:61:VAL:HG22	6:L:62:PRO:HD2	1.94	0.48
1:1:187:ARG:C	2:2:142:LEU:HD22	2.39	0.47
4:4:79:LEU:N	4:4:79:LEU:HD22	2.29	0.47
1:1:52:ASP:HB2	1:1:162:ASN:HB2	1.93	0.47
1:1:186:PRO:HB2	2:2:142:LEU:HD21	1.95	0.47
6:L:36:VAL:CG2	6:L:74:ALA:HB2	2.41	0.47
3:3:159:SER:O	3:3:159:SER:OG	2.32	0.47
1:1:194:VAL:HG21	1:1:200:HIS:HA	1.95	0.47
2:2:73:LYS:NZ	6:L:35:ASP:OD2	2.47	0.47
3:3:134:PRO:CG	3:3:139:ARG:HG2	2.45	0.47
1:1:187:ARG:C	2:2:142:LEU:CD2	2.87	0.47
2:2:112:VAL:O	2:2:197:ILE:CG1	2.61	0.47
3:3:57:PHE:HE2	3:3:202:VAL:CG1	2.28	0.47
3:3:148:TRP:CZ3	3:3:156:PHE:CE2	3.03	0.47
1:1:101:THR:HG22	1:1:101:THR:O	2.14	0.47
6:L:41:GLN:C	6:L:87:ALA:HB1	2.39	0.47
2:2:113:GLY:CA	2:2:197:ILE:CD1	2.91	0.47
2:2:141:THR:OG1	2:2:145:HIS:CE1	2.68	0.47
3:3:45:LEU:HD21	3:3:210:PHE:HD2	1.79	0.47
6:L:39:TYR:HD1	6:L:49:THR:HG22	1.79	0.47
3:3:182:GLN:HA	3:3:182:GLN:HE21	1.75	0.47
3:3:196:GLU:HG3	3:3:197:GLN:NE2	2.30	0.47
1:1:85:ARG:HH12	1:1:101:THR:HG21	1.78	0.46
5:H:27:PHE:O	5:H:28:SER:C	2.58	0.46
5:H:51:ILE:HA	5:H:57:THR:HA	1.97	0.46
1:1:81:ASN:HB3	1:1:173:GLU:HG2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:89:VAL:CG2	1:1:98:LEU:HD21	2.45	0.46
3:3:133:PRO:HG3	3:3:184:TRP:HB2	1.96	0.46
6:L:48:ARG:HH21	6:L:61:VAL:HG23	1.80	0.46
6:L:81:LEU:HD23	6:L:85:ASP:HB3	1.97	0.46
1:1:70:THR:HG22	1:1:187:ARG:HE	1.80	0.46
1:1:187:ARG:CA	2:2:142:LEU:HD23	2.46	0.46
1:1:195:THR:C	1:1:196:SER:HG	2.23	0.46
3:3:67:ARG:HG2	3:3:74:LEU:CD2	2.44	0.46
4:4:25:TYR:O	4:4:25:TYR:CG	2.68	0.46
6:L:8:GLN:HE22	6:L:104:GLY:HA2	1.81	0.46
6:L:82:GLN:HB3	6:L:84:GLU:OE2	2.10	0.46
2:2:72:ASP:OD1	5:H:108:THR:CB	2.63	0.46
3:3:45:LEU:HD21	3:3:210:PHE:HB3	1.97	0.46
1:1:51:ILE:CG2	1:1:164:GLY:H	2.27	0.46
1:1:190:LEU:HD22	2:2:136:GLU:CD	2.41	0.46
5:H:53:THR:HG21	5:H:101:SER:HB3	1.97	0.46
3:3:67:ARG:NH1	3:3:67:ARG:HG3	2.31	0.46
1:1:101:THR:O	1:1:105:THR:HG22	2.16	0.46
2:2:13:ARG:O	2:2:13:ARG:HG2	2.15	0.45
6:L:92:ALA:CB	6:L:102:VAL:CG2	2.84	0.45
2:2:19:ASN:HB2	2:2:61:PHE:CE1	2.52	0.45
1:1:70:THR:HG23	1:1:185:CYS:O	2.15	0.45
6:L:50:ILE:HD12	6:L:65:PHE:CD2	2.51	0.45
5:H:19:SER:HB2	5:H:81:SER:OG	2.17	0.45
5:H:80:LEU:HD12	5:H:81:SER:N	2.31	0.45
6:L:33:ARG:C	6:L:34:TYR:HD1	2.24	0.45
2:2:109:VAL:HG13	2:2:148:ILE:HD12	1.97	0.45
2:2:166:ASN:HD22	3:3:165:ALA:HB1	1.79	0.45
3:3:120:ARG:HG2	3:3:190:ILE:CD1	2.44	0.45
3:3:148:TRP:O	3:3:148:TRP:CD1	2.70	0.45
5:H:66:ARG:NH1	5:H:89:ASP:OD2	2.50	0.45
1:1:100:ASN:N	1:1:100:ASN:HD22	2.14	0.45
2:2:72:ASP:OD2	5:H:108:THR:OG1	2.34	0.44
6:L:81:LEU:HD22	6:L:85:ASP:HB2	2.00	0.44
2:2:108:GLU:N	2:2:202:ASN:O	2.49	0.44
2:2:189:THR:HG23	2:2:189:THR:O	2.17	0.44
5:H:75:LYS:HB2	5:H:77:GLN:HG2	1.99	0.44
1:1:58:GLN:HA	1:1:67:ARG:NH1	2.32	0.44
3:3:123:VAL:O	3:3:145:HIS:HB2	2.17	0.44
3:3:63:TYR:CB	3:3:200:LEU:O	2.65	0.44
3:3:136:THR:HG22	3:3:138:GLU:HG2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:50:VAL:CG1	1:1:162:ASN:CG	2.90	0.44
3:3:180:ASN:HD22	3:3:180:ASN:H	1.60	0.44
1:1:193:LYS:CA	2:2:135:ARG:NH1	2.77	0.44
4:4:80:PHE:O	4:4:80:PHE:CD1	2.70	0.44
6:L:40:GLN:HB2	6:L:50:ILE:CG1	2.47	0.44
2:2:197:ILE:HG23	2:2:197:ILE:O	2.16	0.44
6:L:93:THR:OG1	6:L:94:GLY:N	2.50	0.44
3:3:196:GLU:HA	3:3:196:GLU:OE1	2.17	0.44
6:L:89:TYR:O	6:L:106:GLY:HA2	2.18	0.44
2:2:67:PHE:O	2:2:67:PHE:CG	2.70	0.43
2:2:111:ALA:HB2	2:2:199:VAL:HG22	2.00	0.43
5:H:50:SER:N	5:H:58:GLY:O	2.31	0.43
1:1:65:MET:HE2	1:1:65:MET:HB2	1.88	0.43
2:2:28:SER:OG	2:2:154:MET:N	2.43	0.43
3:3:44:LEU:CD1	3:3:94:ILE:HD11	2.47	0.43
3:3:63:TYR:CD1	3:3:63:TYR:O	2.71	0.43
2:2:42:HIS:CE1	2:2:44:SER:HB3	2.53	0.43
2:2:166:ASN:HB3	3:3:165:ALA:O	2.18	0.43
3:3:57:PHE:CE1	3:3:85:HIS:HD2	2.35	0.43
6:L:15:SER:HA	6:L:111:VAL:O	2.18	0.43
3:3:113:GLY:HA3	3:3:198:ASP:OD1	2.19	0.43
1:1:51:ILE:HG22	1:1:164:GLY:N	2.33	0.43
1:1:114:ARG:HD2	3:3:11:TYR:CD2	2.53	0.43
4:4:71:LEU:O	4:4:74:SER:O	2.36	0.43
1:1:86:LEU:HD11	1:1:166:ILE:HB	2.01	0.43
5:H:38:ARG:NH2	5:H:40:ALA:HB2	2.34	0.43
1:1:52:ASP:HA	1:1:162:ASN:HA	2.00	0.43
2:2:33:THR:HG21	2:2:146:GLN:HG3	2.00	0.43
1:1:88:TRP:CZ2	1:1:117:LEU:HB2	2.54	0.43
5:H:63:LEU:HG	5:H:67:LEU:HD11	2.00	0.43
6:L:25:SER:CB	6:L:73:THR:CG2	2.71	0.42
1:1:71:TYR:HE2	2:2:163:LEU:HD13	1.84	0.42
2:2:80:LYS:HD3	2:2:129:PHE:CE2	2.54	0.42
3:3:111:PHE:HD2	3:3:121:TYR:HE2	1.66	0.42
5:H:28:SER:C	5:H:30:SER:H	2.27	0.42
6:L:39:TYR:CD1	6:L:49:THR:HG22	2.54	0.42
2:2:16:THR:HG23	2:2:25:THR:HG22	2.02	0.42
6:L:82:GLN:O	6:L:85:ASP:HB2	2.19	0.42
2:2:109:VAL:HG13	2:2:148:ILE:HD11	2.01	0.42
3:3:66:THR:O	3:3:66:THR:HG23	2.19	0.42
5:H:53:THR:CG2	5:H:101:SER:HB3	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:44:LEU:CB	3:3:94:ILE:CD1	2.79	0.42
1:1:186:PRO:C	2:2:142:LEU:HD23	2.44	0.42
2:2:52:GLU:OE2	2:2:52:GLU:N	2.46	0.42
3:3:65:VAL:CG2	3:3:197:GLN:HA	2.49	0.42
6:L:33:ARG:O	6:L:33:ARG:HG3	2.20	0.42
1:1:14:THR:OG1	1:1:16:GLU:HG2	2.20	0.42
5:H:98:SER:HB2	5:H:109:TYR:CZ	2.55	0.42
1:1:158:PRO:CD	1:1:161:PHE:HD2	2.22	0.41
1:1:85:ARG:NH1	1:1:101:THR:HG21	2.36	0.41
1:1:187:ARG:N	2:2:142:LEU:CD2	2.83	0.41
4:4:71:LEU:HD12	4:4:71:LEU:HA	1.87	0.41
1:1:187:ARG:NH2	2:2:128:GLU:O	2.53	0.41
1:1:103:ASN:HB3	3:3:216:ILE:HA	2.03	0.41
1:1:136:TYR:CE1	2:2:173:LYS:HE2	2.55	0.41
2:2:141:THR:OG1	2:2:145:HIS:NE2	2.53	0.41
3:3:89:THR:HG23	3:3:92:SER:H	1.86	0.41
3:3:111:PHE:CD1	3:3:150:THR:HG21	2.55	0.41
2:2:66:LEU:HD23	2:2:66:LEU:HA	1.83	0.41
3:3:14:LEU:C	3:3:14:LEU:CD1	2.86	0.41
6:L:31:ILE:HD12	6:L:73:THR:HA	2.01	0.41
1:1:114:ARG:HD2	3:3:11:TYR:HD2	1.84	0.41
3:3:133:PRO:HG3	3:3:184:TRP:CG	2.56	0.41
1:1:53:LEU:HD12	1:1:163:TYR:CE1	2.44	0.41
1:1:70:THR:HG22	1:1:187:ARG:NE	2.35	0.41
2:2:42:HIS:HE1	2:2:44:SER:HB3	1.86	0.41
2:2:108:GLU:HB3	2:2:202:ASN:HB2	2.03	0.41
3:3:101:TYR:CD2	3:3:101:TYR:C	2.93	0.41
1:1:68:ALA:HB2	1:1:189:LEU:HD13	2.02	0.41
5:H:110:MET:O	6:L:39:TYR:OH	2.39	0.40
6:L:76:LEU:HD12	6:L:77:THR:N	2.37	0.40
1:1:192:VAL:C	2:2:135:ARG:HH22	2.30	0.40
3:3:78:ASP:OD2	3:3:180:ASN:ND2	2.53	0.40
5:H:36:TRP:CD1	5:H:36:TRP:N	2.89	0.40
1:1:50:VAL:CG1	1:1:162:ASN:CB	2.98	0.40
1:1:91:ASN:CG	1:1:160:SER:HA	2.40	0.40
3:3:49:GLU:OE2	3:3:208:LYS:HA	2.20	0.40
6:L:35:ASP:N	6:L:35:ASP:OD1	2.55	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	1	185/212 (87%)	172 (93%)	13 (7%)	0	100	100
2	2	203/218 (93%)	192 (95%)	11 (5%)	0	100	100
3	3	218/221 (99%)	213 (98%)	5 (2%)	0	100	100
4	4	41/85 (48%)	38 (93%)	3 (7%)	0	100	100
5	H	95/126 (75%)	92 (97%)	3 (3%)	0	100	100
6	L	107/123 (87%)	93 (87%)	14 (13%)	0	100	100
All	All	849/985 (86%)	800 (94%)	49 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	1	160/175 (91%)	155 (97%)	5 (3%)	35	56
2	2	181/194 (93%)	173 (96%)	8 (4%)	25	48
3	3	181/182 (100%)	168 (93%)	13 (7%)	13	38
4	4	37/67 (55%)	36 (97%)	1 (3%)	39	60
5	H	85/110 (77%)	85 (100%)	0	100	100
6	L	90/100 (90%)	90 (100%)	0	100	100
All	All	734/828 (89%)	707 (96%)	27 (4%)	31	52

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	100	ASN
1	1	102	SER
1	1	103	ASN
1	1	105	THR
1	1	117	LEU
2	2	30	VAL
2	2	59	GLU
2	2	68	ASP
2	2	71	THR
2	2	133	THR
2	2	138	TYR
2	2	143	PHE
2	2	152	THR
3	3	2	ILE
3	3	47	VAL
3	3	55	LEU
3	3	67	ARG
3	3	69	ASP
3	3	71	GLN
3	3	72	ARG
3	3	73	LEU
3	3	143	CYS
3	3	174	ASP
3	3	175	VAL
3	3	180	ASN
3	3	190	ILE
4	4	79	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	49	HIS
1	1	91	ASN
1	1	100	ASN
1	1	162	ASN
1	1	197	GLN
2	2	42	HIS
2	2	57	GLN
2	2	103	ASN
2	2	153	ASN
2	2	166	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	196	GLN
3	3	85	HIS
3	3	100	GLN
3	3	180	ASN
3	3	182	GLN
3	3	197	GLN
4	4	32	ASN
4	4	37	GLN
5	H	39	GLN
5	H	100	HIS
6	L	41	GLN
6	L	72	ASN
6	L	82	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.

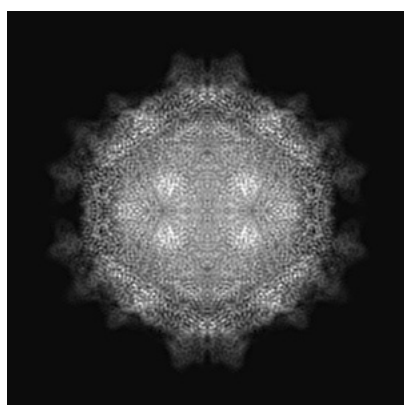
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31555. These allow visual inspection of the internal detail of the map and identification of artifacts.

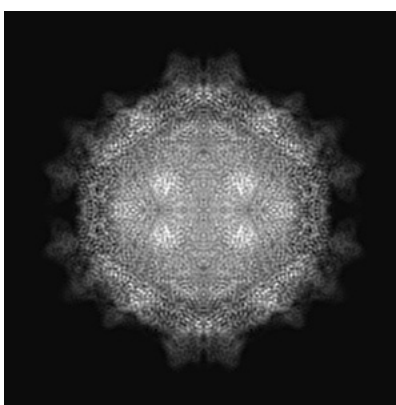
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

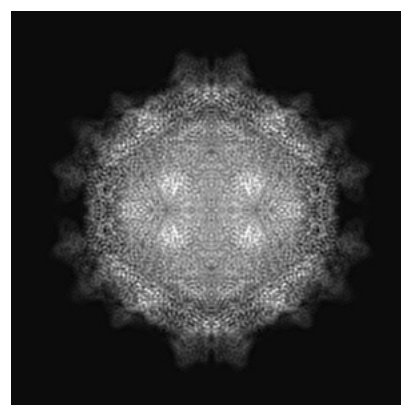
6.1.1 Primary map



X



Y

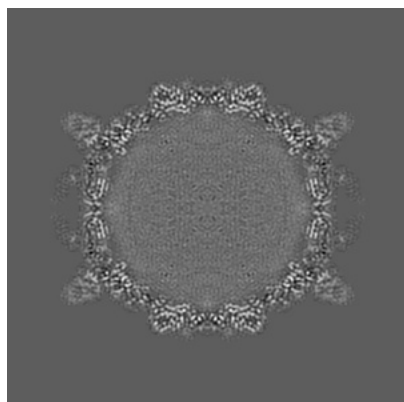


Z

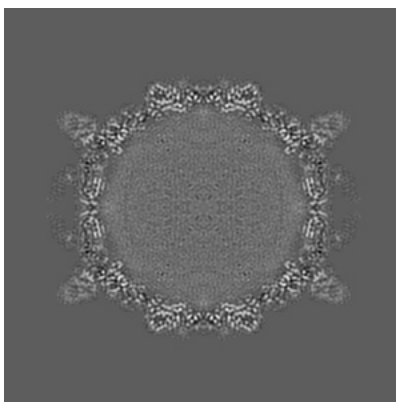
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

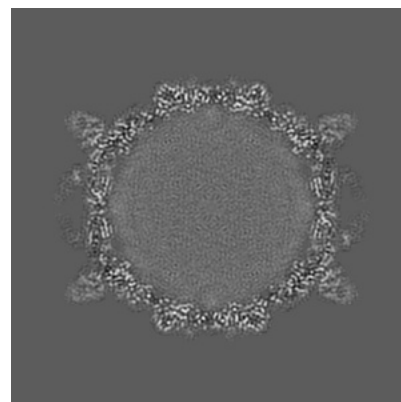
6.2.1 Primary map



X Index: 240



Y Index: 240

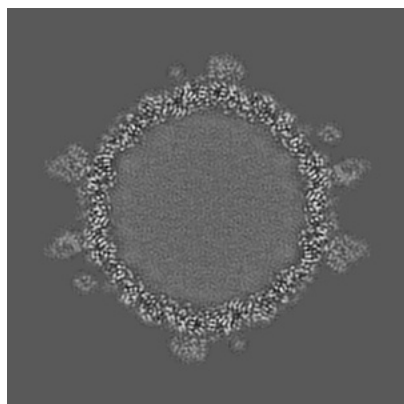


Z Index: 240

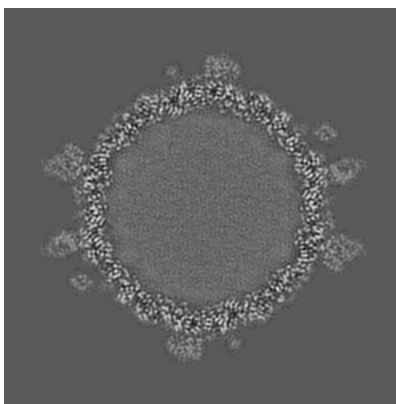
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

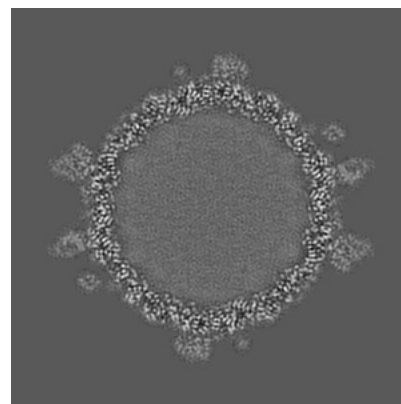
6.3.1 Primary map



X Index: 209



Y Index: 209

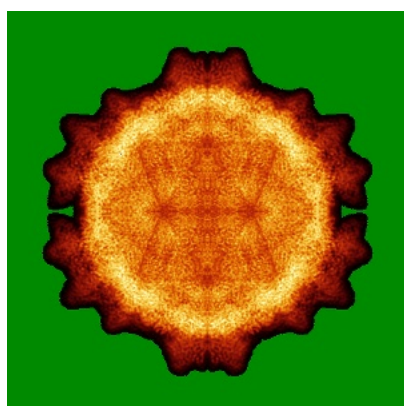


Z Index: 208

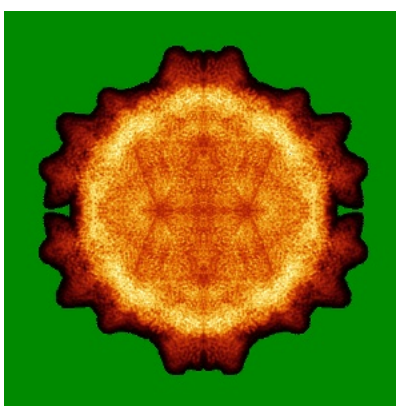
The images above show the largest variance slices of the map in three orthogonal directions.

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

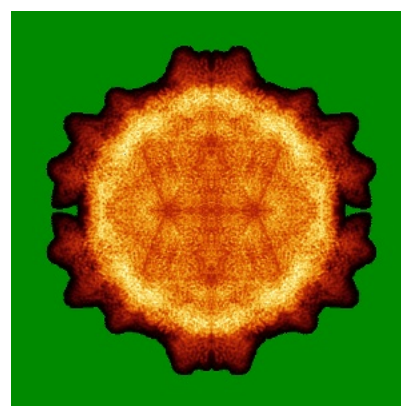
6.4.1 Primary map



X



Y

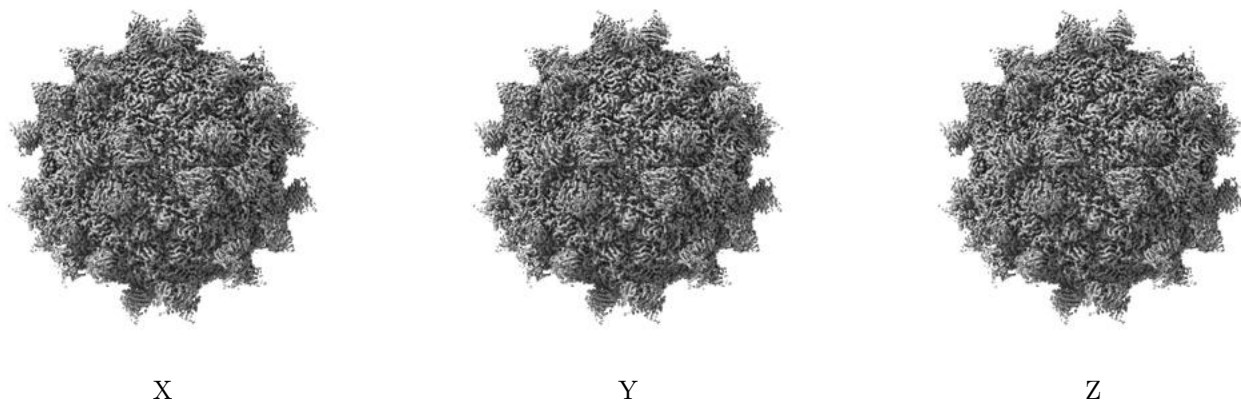


Z

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 0.023. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

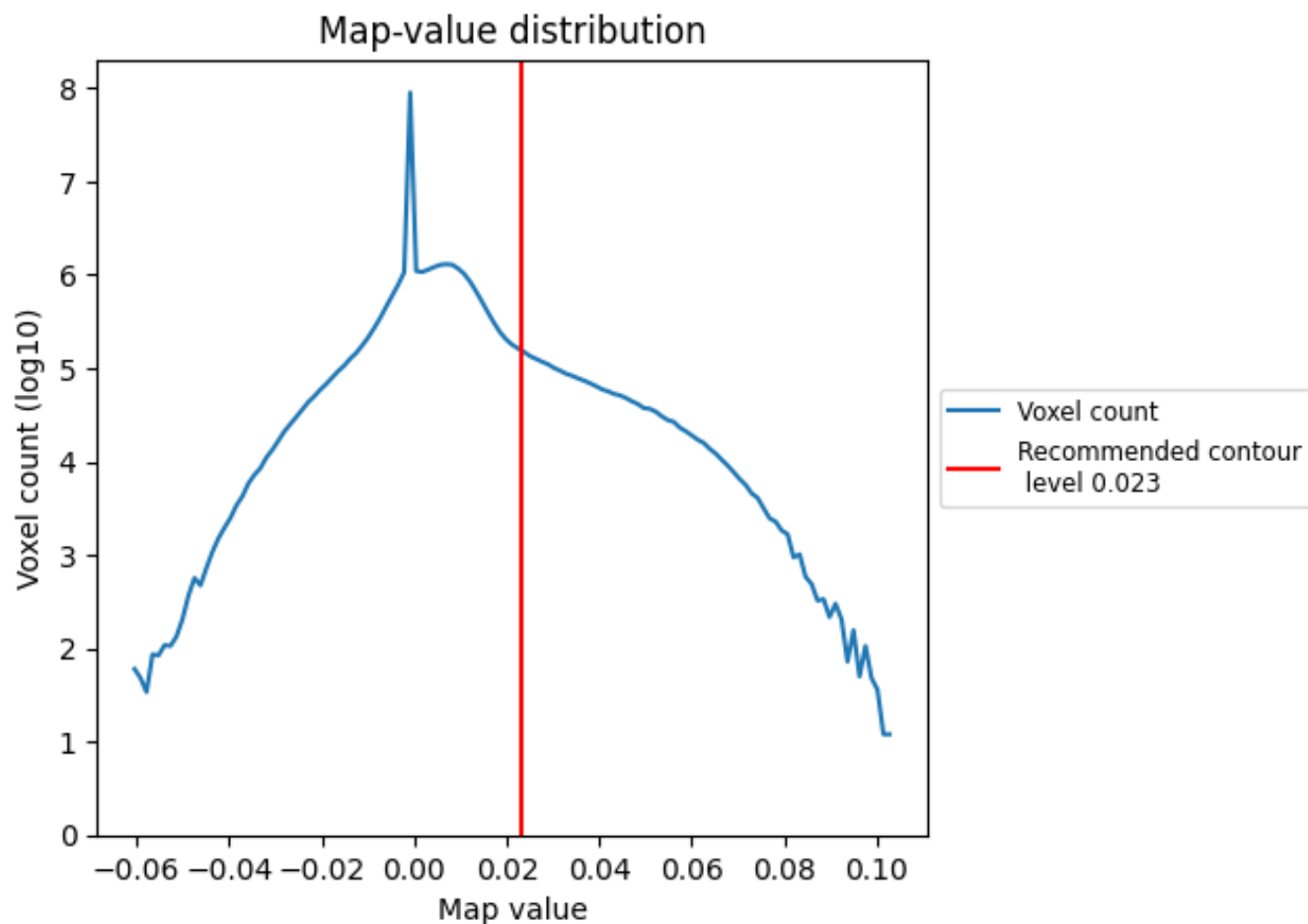
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

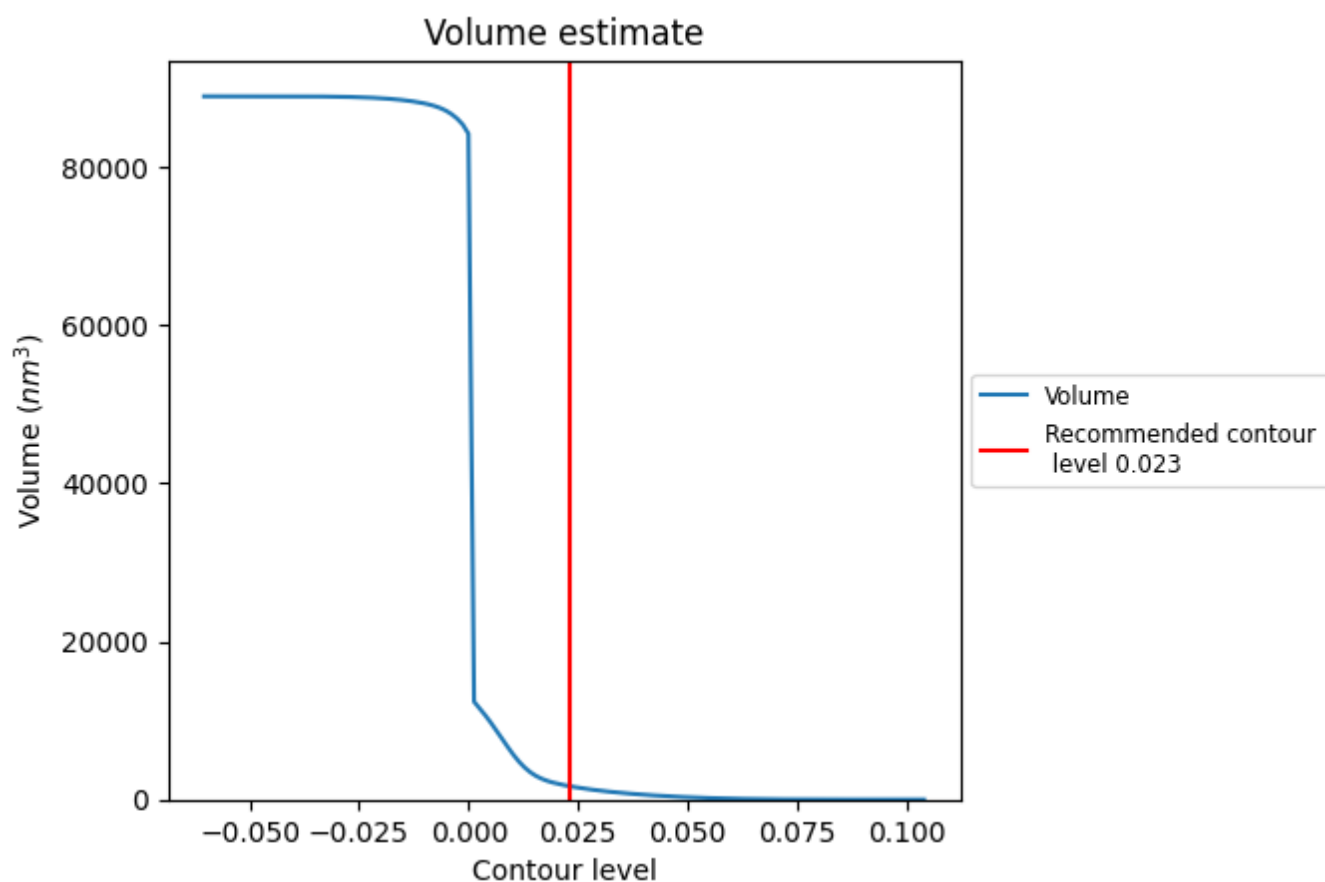
This section contains the results of statistical analysis of the map.

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.

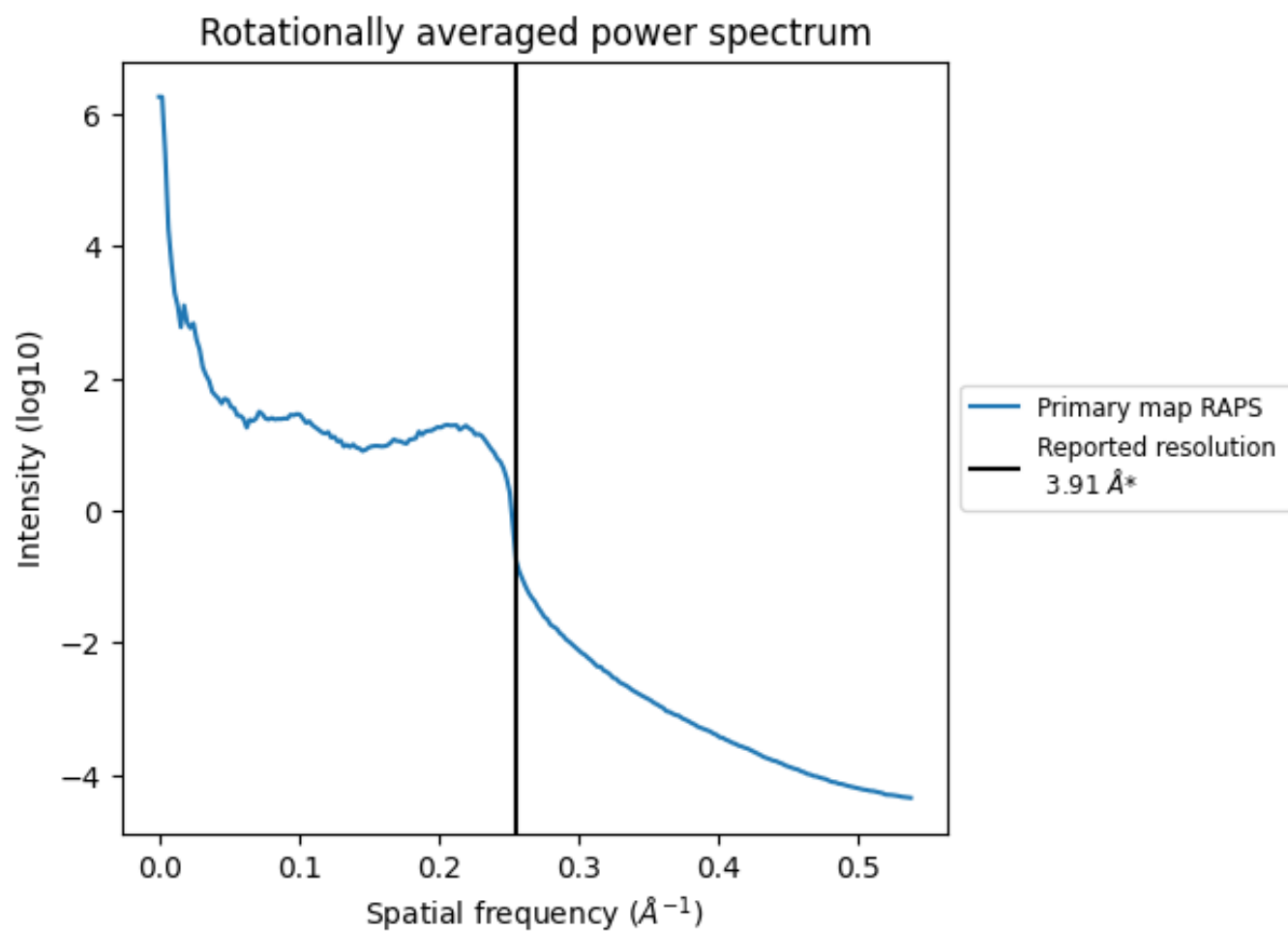
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1699 nm³; this corresponds to an approximate mass of 1535 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



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

8 Fourier-Shell correlation

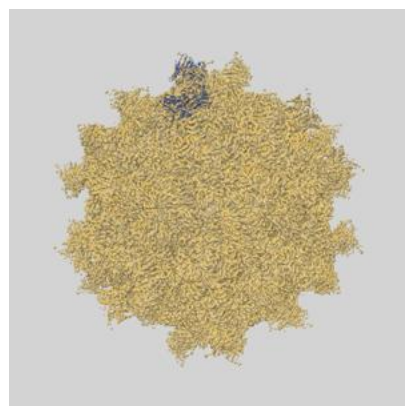
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

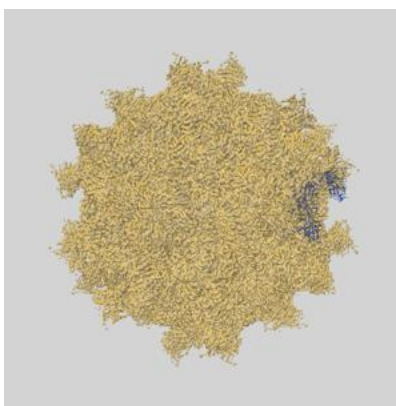
This section contains information regarding the fit between EMDB map EMD-31555 and PDB model 7FEI. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

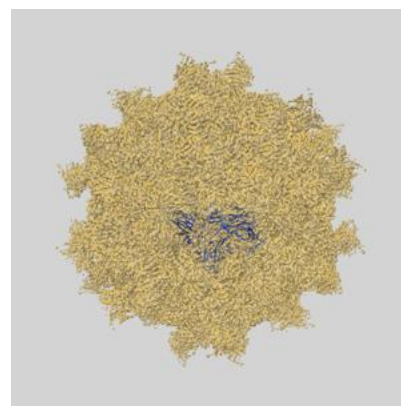
9.1.1 Map-model overlay [i](#)



X

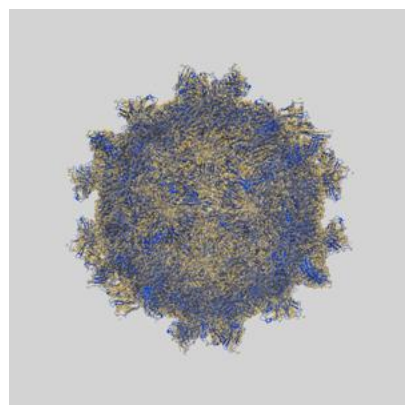


Y

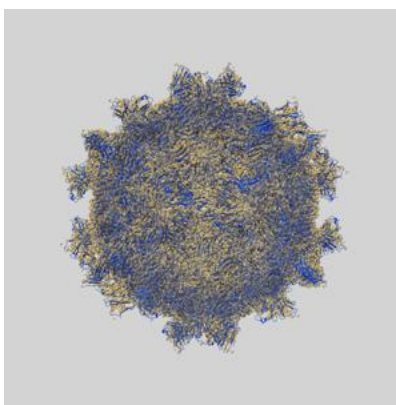


Z

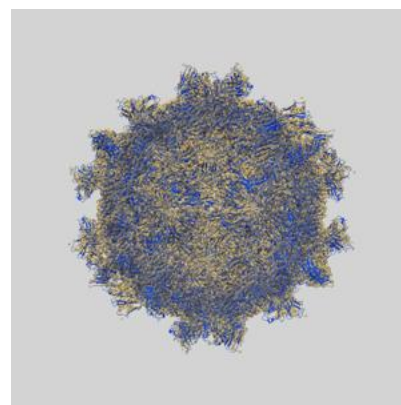
9.1.2 Map-model assembly overlay [i](#)



X



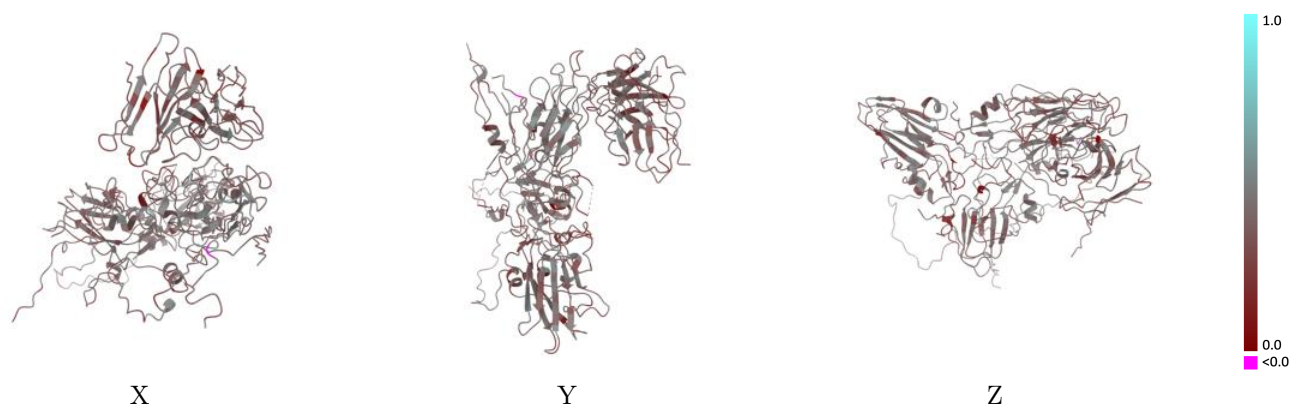
Y



Z

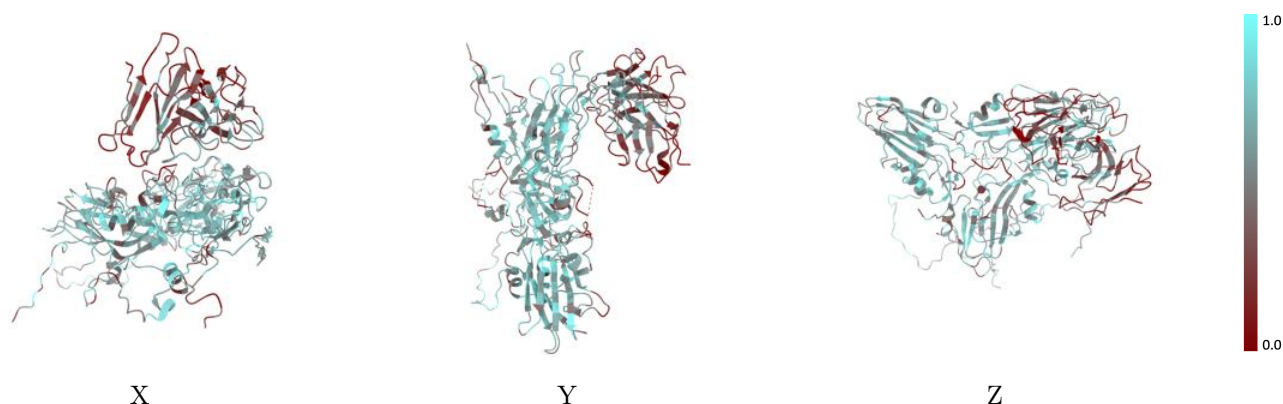
The images above show the 3D surface view of the map at the recommended contour level 0.023 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



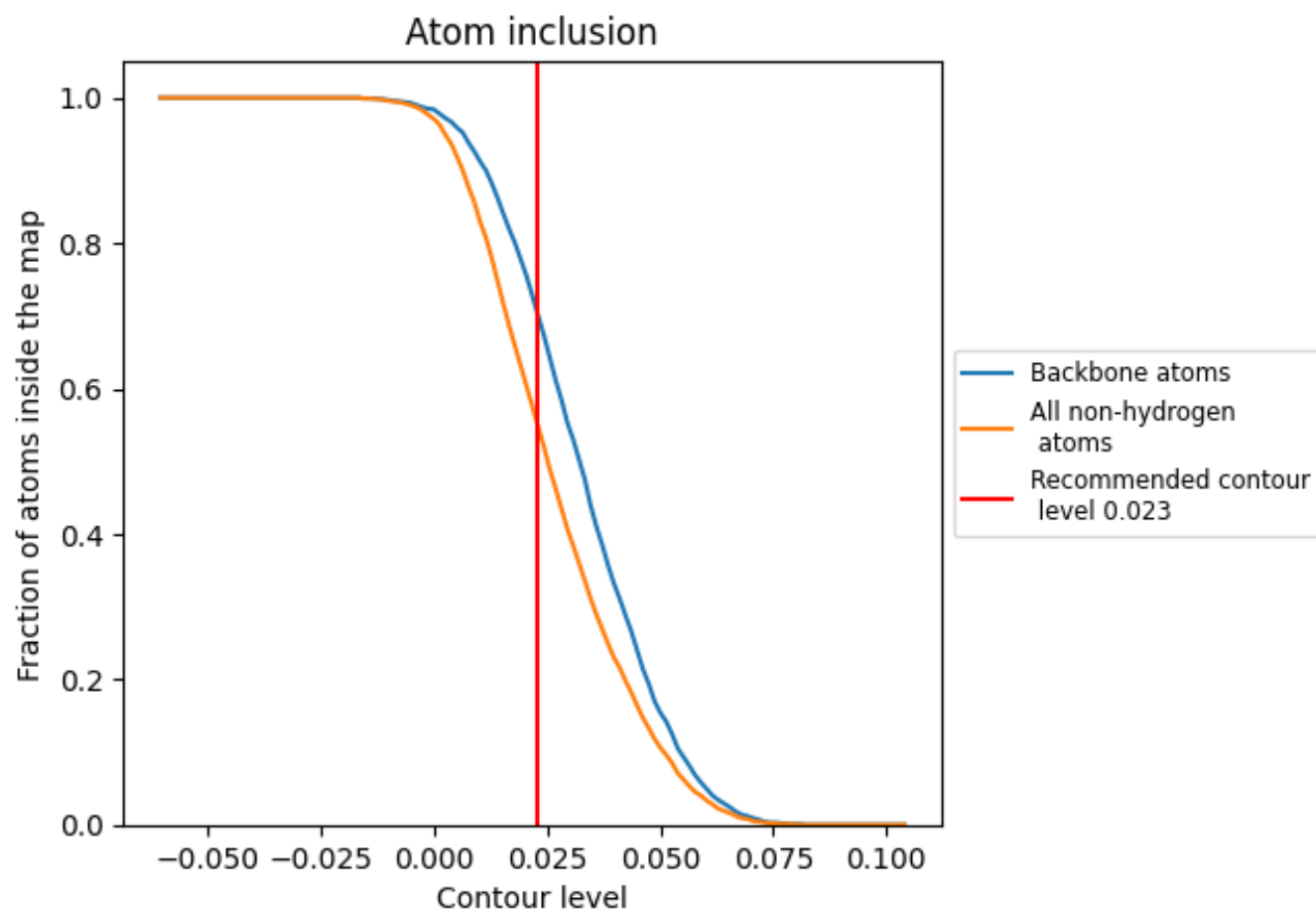
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.023).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 55% 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 (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5470	0.3860
1	0.5930	0.3890
2	0.6440	0.4080
3	0.6200	0.3860
4	0.4880	0.3870
H	0.3420	0.3650
L	0.3230	0.3510

1.0

0.0

<0.0