



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 05:10 PM UTC

PDB ID : 7D3M / pdb_00007d3m
EMDB ID : EMD-30560
Title : FOOT AND MOUTH DISEASE VIRUS O/TIBET/99-BOUND THE SINGLE CHAIN FRAGMENT ANTIBODY R50
Authors : He, Y.; Lou, Z.
Deposited on : 2020-09-19
Resolution : 3.94 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

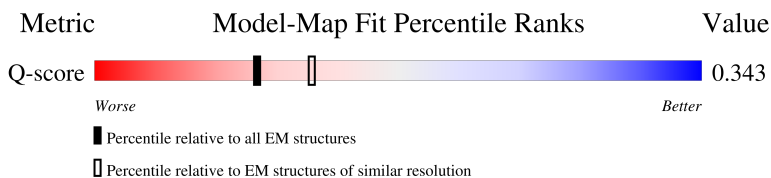
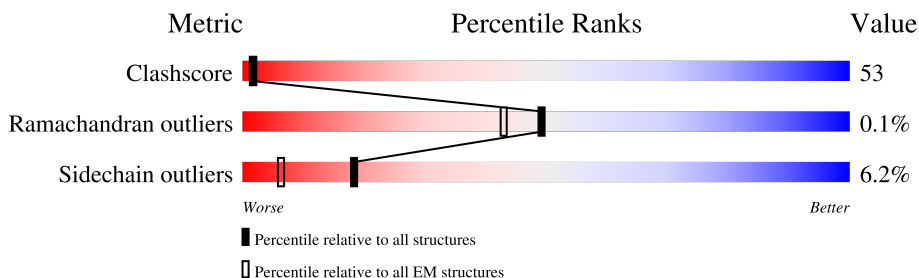
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.94 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	7757 (3.44 - 4.43)

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	213	
2	2	218	
3	3	220	
4	4	85	

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Mol	Chain	Length	Quality of chain
5	H	167	15% 40% 35% 10% • 13%
6	L	123	24% 46% 37% 5% 12%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6923 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 O/TIBET/99 VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	183	Total	C	N	O	S	0	0
			1429	901	257	267	4		

- Molecule 2 is a protein called O/TIBET/99 VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	206	Total	C	N	O	S	0	0
			1617	1031	276	303	7		

- Molecule 3 is a protein called O/TIBET/99 VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	219	Total	C	N	O	S	0	0
			1673	1073	272	319	9		

- Molecule 4 is a protein called O/TIBET/99 VP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	46	Total	C	N	O	S	0	0
			353	222	57	72	2		

- Molecule 5 is a protein called R50 VH.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	145	Total	C	N	O	S	0	0
			1074	658	195	213	8		

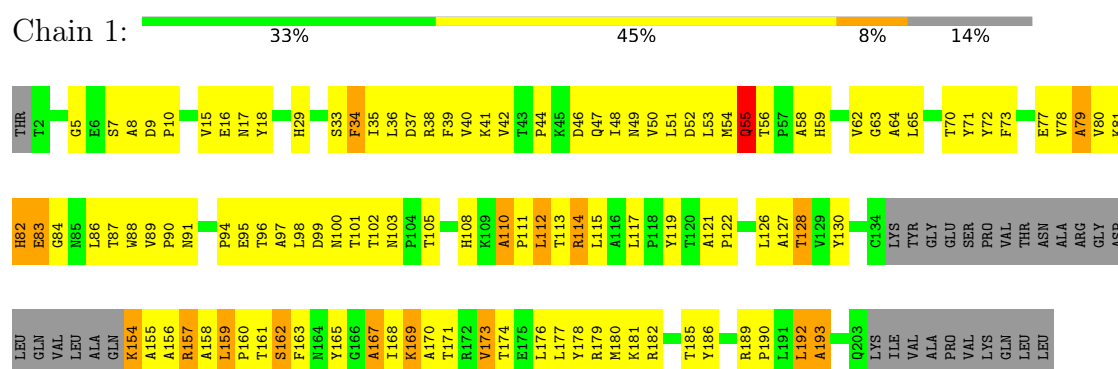
- Molecule 6 is a protein called R50 VL.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	108	Total	C	N	O	S	0	0
			777	472	134	169	2		

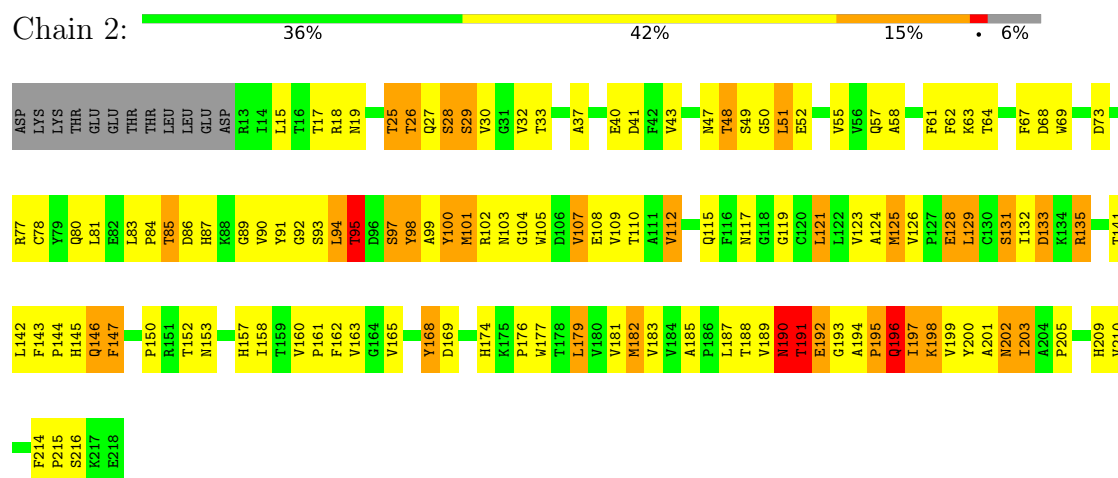
3 Residue-property plots

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.

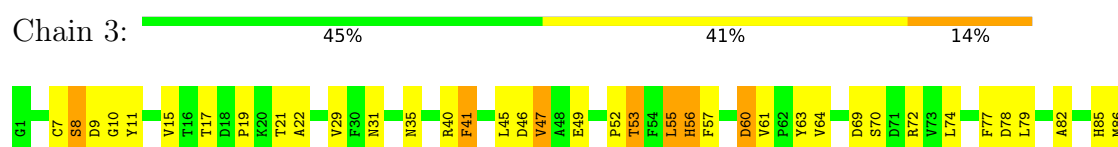
• Molecule 1: O/TIBET/99 VP1

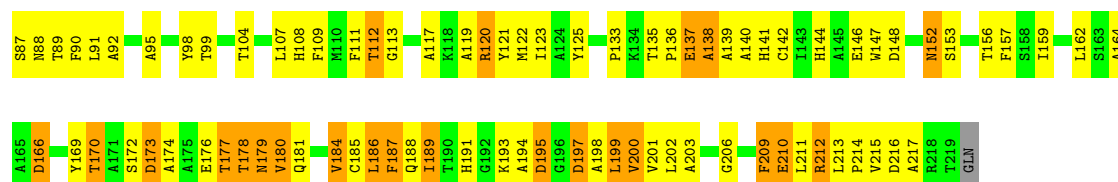


• Molecule 2: O/TIBET/99 VP2

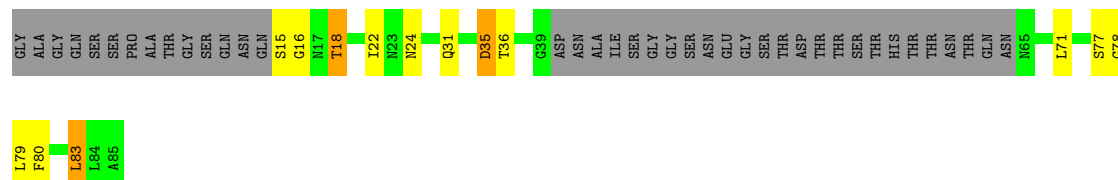
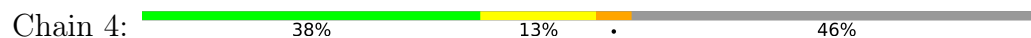


• Molecule 3: O/TIBET/99 VP3

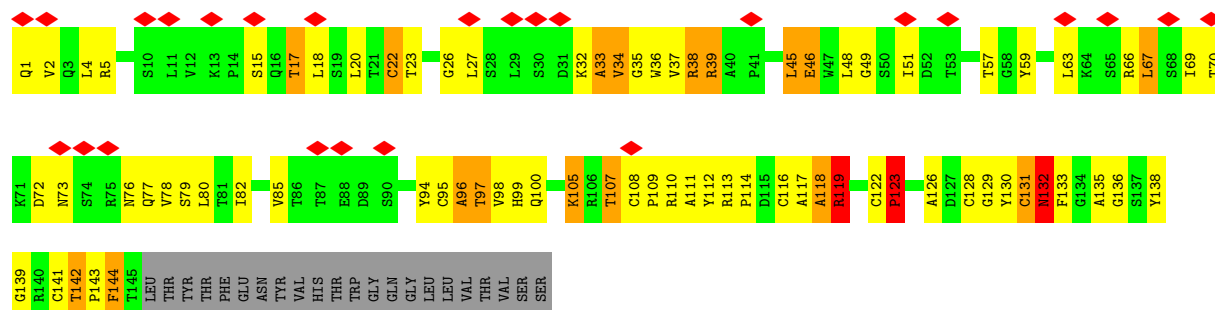




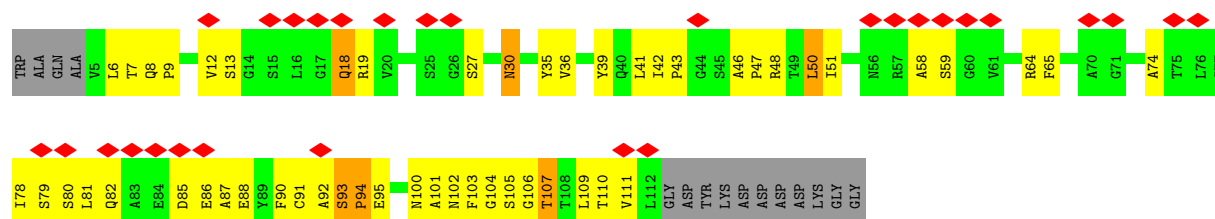
• Molecule 4: O/TIBET/99 VP4



• Molecule 5: R50 VH



• Molecule 6: R50 VL



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT	Depositor
Number of particles used	15460, 15460	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.63	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.140	Depositor
Minimum map value	-0.090	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0032	Depositor
Map size ($\text{\AA}$)	427.80002, 427.80002, 427.80002	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.93000007, 0.93000007, 0.93000007	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	0.74	1/1462 (0.1%)	1.52	34/1998 (1.7%)
2	2	0.60	2/1661 (0.1%)	1.54	46/2269 (2.0%)
3	3	0.67	1/1723 (0.1%)	1.55	49/2355 (2.1%)
4	4	0.59	0/359	1.49	3/481 (0.6%)
5	H	0.90	3/1097 (0.3%)	1.60	28/1495 (1.9%)
6	L	0.42	1/790 (0.1%)	0.98	11/1076 (1.0%)
All	All	0.69	8/7092 (0.1%)	1.49	171/9674 (1.8%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	123	PRO	N-CA	17.64	1.69	1.47
3	3	31	ASN	C-N	14.63	1.50	1.33
1	1	159	LEU	C-N	12.92	1.50	1.33
5	H	142	THR	C-N	12.89	1.50	1.33
6	L	94	PRO	N-CD	6.92	1.57	1.47
2	2	200	TYR	C-N	-6.87	1.24	1.33
2	2	195	PRO	N-CD	5.34	1.55	1.47
5	H	122	CYS	C-N	5.09	1.45	1.33

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	18	THR	CB-CA-C	-24.93	73.88	111.77
2	2	196	GLN	N-CA-C	23.70	143.28	111.28
3	3	178	THR	CB-CA-C	20.58	140.21	116.54
1	1	18	TYR	N-CA-C	19.35	137.86	111.74
5	H	142	THR	CA-C-N	17.59	137.34	119.76
5	H	142	THR	C-N-CA	17.59	137.34	119.76
1	1	159	LEU	CA-C-N	17.46	137.75	119.76
1	1	159	LEU	C-N-CA	17.46	137.75	119.76
3	3	31	ASN	CA-C-N	16.25	137.11	120.38
3	3	31	ASN	C-N-CA	16.25	137.11	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	122	CYS	CA-C-N	15.58	139.31	119.84
5	H	122	CYS	C-N-CA	15.58	139.31	119.84
2	2	190	ASN	N-CA-C	-14.49	87.04	109.07
1	1	16	GLU	N-CA-C	-13.36	96.42	113.12
3	3	179	ASN	N-CA-C	-12.88	89.96	109.14
1	1	83	GLU	N-CA-C	12.80	128.90	113.28
1	1	17	ASN	N-CA-C	-12.70	92.33	110.24
3	3	210	GLU	N-CA-CB	12.61	130.00	110.84
5	H	131	CYS	N-CA-C	12.15	124.60	111.36
2	2	195	PRO	N-CA-C	-12.14	90.59	110.74
3	3	22	ALA	N-CA-C	12.08	125.17	110.19
2	2	28	SER	N-CA-C	-11.78	90.89	109.50
2	2	152	THR	N-CA-C	11.73	135.79	110.80
2	2	195	PRO	CB-CA-C	-11.57	102.15	111.87
2	2	191	THR	N-CA-CB	-11.54	91.91	110.14
2	2	190	ASN	CB-CA-C	11.25	134.63	110.45
3	3	61	VAL	N-CA-CB	-10.78	104.39	111.83
3	3	153	SER	N-CA-C	10.78	126.76	113.50
1	1	35	ILE	N-CA-C	-10.55	100.25	113.22
3	3	179	ASN	CB-CA-C	10.27	133.56	110.67
2	2	28	SER	CB-CA-C	10.26	130.83	109.38
5	H	123	PRO	CA-N-CD	-10.15	97.79	112.00
1	1	162	SER	N-CA-C	10.04	125.33	113.18
2	2	95	THR	N-CA-C	10.01	123.45	111.33
3	3	210	GLU	N-CA-C	-9.89	90.42	108.02
2	2	131	SER	N-CA-C	9.53	124.54	111.39
3	3	21	THR	CB-CA-C	-9.40	93.61	109.50
2	2	197	ILE	N-CA-C	9.40	122.95	109.51
3	3	88	ASN	N-CA-C	9.39	122.71	111.82
2	2	199	VAL	N-CA-CB	-9.12	98.85	111.25
3	3	113	GLY	N-CA-C	-9.10	93.79	112.34
2	2	51	LEU	N-CA-C	-8.96	101.00	113.37
4	4	79	LEU	CB-CA-C	-8.96	93.26	109.38
3	3	138	ALA	N-CA-C	-8.94	102.28	113.55
2	2	94	LEU	CB-CA-C	8.88	125.77	110.68
5	H	45	LEU	N-CA-C	8.70	121.83	110.43
3	3	153	SER	N-CA-CB	-8.61	97.87	110.53
5	H	131	CYS	CB-CA-C	-8.49	96.42	110.85
5	H	119	ARG	N-CA-C	-8.34	103.23	113.41
1	1	34	PHE	CB-CA-C	-8.33	95.38	109.38
3	3	209	PHE	CB-CA-C	-8.24	100.14	111.51
1	1	173	VAL	N-CA-C	-8.23	96.65	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	199	VAL	N-CA-C	8.19	119.63	108.17
6	L	94	PRO	N-CA-C	-8.18	95.61	112.47
3	3	197	ASP	CB-CA-C	-8.14	97.63	109.84
6	L	93	SER	CB-CA-C	7.94	120.45	110.76
1	1	17	ASN	CB-CA-C	-7.94	96.92	109.70
2	2	198	LYS	CB-CA-C	-7.93	96.45	109.53
1	1	55	GLN	N-CA-C	-7.90	102.28	112.23
3	3	60	ASP	N-CA-C	7.89	122.31	111.90
2	2	202	ASN	N-CA-C	-7.85	93.15	107.75
5	H	38	ARG	CB-CA-C	-7.71	96.28	110.62
1	1	192	LEU	CB-CA-C	-7.62	93.70	109.94
2	2	200	TYR	O-C-N	-7.59	114.01	123.27
3	3	197	ASP	CA-C-N	-7.54	109.66	122.33
3	3	197	ASP	C-N-CA	-7.54	109.66	122.33
1	1	193	ALA	N-CA-CB	-7.54	99.24	110.85
5	H	33	ALA	CB-CA-C	-7.51	97.41	109.80
3	3	178	THR	CA-C-O	-7.49	107.31	119.21
2	2	201	ALA	N-CA-CB	-7.48	98.82	110.57
2	2	200	TYR	CB-CA-C	-7.45	94.61	109.35
3	3	187	PHE	CB-CA-C	-7.43	98.70	109.84
5	H	118	ALA	N-CA-C	-7.38	104.23	113.23
5	H	34	VAL	N-CA-C	7.35	119.06	109.58
3	3	111	PHE	CB-CA-C	-7.29	98.33	110.29
2	2	146	GLN	N-CA-C	-7.28	96.30	108.75
1	1	110	ALA	C-N-CD	7.23	136.51	120.60
2	2	29	SER	N-CA-CB	7.23	127.27	111.87
3	3	120	ARG	N-CA-CB	-7.19	98.71	110.43
1	1	83	GLU	CB-CA-C	-7.09	96.11	109.72
1	1	79	ALA	N-CA-C	-7.04	95.81	108.48
3	3	82	ALA	N-CA-C	7.04	121.58	112.92
2	2	27	GLN	N-CA-C	-6.97	104.93	113.50
2	2	147	PHE	N-CA-C	-6.84	98.25	109.40
2	2	203	ILE	N-CA-C	-6.79	98.65	108.36
3	3	177	THR	CA-C-N	6.71	134.43	122.89
3	3	177	THR	C-N-CA	6.71	134.43	122.89
5	H	96	ALA	CB-CA-C	6.68	123.00	110.63
3	3	40	ARG	CB-CA-C	-6.65	97.20	109.37
3	3	200	VAL	N-CA-CB	6.55	122.18	111.44
3	3	41	PHE	N-CA-CB	-6.51	100.36	110.65
3	3	119	ALA	CB-CA-C	-6.51	96.07	109.94
2	2	135	ARG	N-CA-C	-6.50	105.36	113.55
5	H	97	THR	N-CA-C	6.49	120.08	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	22	ALA	N-CA-CB	-6.48	101.44	110.25
3	3	55	LEU	CB-CA-C	-6.46	97.54	109.37
5	H	132	ASN	N-CA-C	-6.46	97.89	108.41
2	2	196	GLN	N-CA-CB	-6.43	101.58	111.74
6	L	18	GLN	CB-CA-C	-6.42	95.96	109.38
6	L	19	ARG	N-CA-C	6.40	119.94	109.76
1	1	82	HIS	CB-CA-C	-6.37	97.30	109.66
3	3	112	THR	N-CA-CB	-6.30	100.29	110.69
6	L	30	ASN	N-CA-C	6.25	122.50	114.56
5	H	33	ALA	N-CA-C	6.23	120.08	110.42
5	H	67	LEU	N-CA-C	6.18	119.32	109.24
3	3	120	ARG	CB-CA-C	6.18	119.94	109.75
2	2	124	ALA	CB-CA-C	6.16	125.08	111.09
2	2	147	PHE	N-CA-CB	6.15	121.53	110.83
3	3	180	VAL	N-CA-C	-6.15	106.23	113.42
1	1	34	PHE	N-CA-C	6.13	122.64	114.12
2	2	129	LEU	N-CA-C	6.11	118.66	110.35
5	H	39	ARG	N-CA-C	6.08	119.55	109.46
3	3	197	ASP	CA-C-O	-6.04	114.38	120.96
6	L	30	ASN	CB-CA-C	-6.02	99.74	109.13
1	1	173	VAL	N-CA-CB	6.01	119.43	111.25
5	H	27	LEU	N-CA-C	6.01	119.71	112.38
3	3	212	ARG	N-CA-CB	-5.98	101.33	111.31
5	H	33	ALA	N-CA-CB	-5.98	101.24	110.56
1	1	185	THR	CB-CA-C	-5.96	99.41	109.83
2	2	128	GLU	N-CA-C	5.95	119.78	111.74
1	1	108	HIS	N-CA-C	5.94	118.34	109.25
1	1	79	ALA	CB-CA-C	5.90	119.83	109.80
1	1	167	ALA	CB-CA-C	5.82	121.20	109.68
3	3	166	ASP	N-CA-C	5.79	119.96	113.01
1	1	162	SER	N-CA-CB	-5.75	100.75	110.41
3	3	56	HIS	N-CA-CB	-5.74	100.92	110.39
1	1	114	ARG	N-CA-CB	-5.72	101.30	110.63
2	2	169	ASP	N-CA-CB	-5.67	102.54	111.05
2	2	185	ALA	CA-C-N	-5.66	114.11	119.89
2	2	185	ALA	C-N-CA	-5.66	114.11	119.89
5	H	22	CYS	CB-CA-C	-5.59	98.42	110.45
1	1	84	GLY	N-CA-C	-5.55	102.84	111.12
3	3	41	PHE	N-CA-C	5.55	117.73	108.02
1	1	193	ALA	N-CA-C	5.53	118.70	110.14
6	L	107	THR	N-CA-C	5.51	118.91	110.20
2	2	25	THR	CB-CA-C	-5.51	98.80	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	56	THR	CA-C-N	-5.49	114.12	119.78
1	1	56	THR	C-N-CA	-5.49	114.12	119.78
1	1	186	TYR	N-CA-CB	-5.49	101.38	111.37
3	3	209	PHE	N-CA-C	-5.48	97.70	107.28
2	2	125	MET	N-CA-CB	5.47	119.59	111.23
3	3	87	SER	CB-CA-C	5.46	119.96	110.68
3	3	61	VAL	N-CA-C	5.45	113.89	107.84
2	2	125	MET	N-CA-C	-5.43	99.53	108.49
5	H	66	ARG	CB-CA-C	5.37	118.57	109.55
3	3	111	PHE	N-CA-C	5.35	117.44	109.25
5	H	17	THR	N-CA-C	-5.31	99.10	108.23
5	H	132	ASN	N-CA-CB	5.28	118.89	110.65
2	2	124	ALA	N-CA-C	-5.27	101.11	108.96
3	3	35	ASN	N-CA-C	5.23	116.84	110.41
4	4	35	ASP	N-CA-CB	-5.22	102.74	111.20
3	3	187	PHE	N-CA-C	5.22	117.91	110.24
2	2	192	GLU	N-CA-C	5.21	119.49	113.18
2	2	200	TYR	N-CA-C	5.19	117.91	109.24
3	3	200	VAL	N-CA-C	-5.19	100.73	108.46
5	H	32	LYS	CB-CA-C	-5.19	101.48	110.45
5	H	46	GLU	N-CA-CB	-5.19	102.97	110.70
2	2	146	GLN	CB-CA-C	5.17	119.92	109.68
5	H	105	LYS	N-CA-C	5.16	117.71	110.23
6	L	50	LEU	CB-CA-C	-5.15	101.10	109.13
2	2	168	TYR	CB-CA-C	-5.14	99.69	109.66
2	2	192	GLU	CB-CA-C	5.13	120.16	109.95
2	2	26	THR	CB-CA-C	5.12	120.09	109.38
1	1	59	HIS	N-CA-C	5.12	116.86	111.28
3	3	152	ASN	CB-CA-C	-5.12	99.60	109.37
6	L	93	SER	N-CA-C	-5.09	103.54	108.07
2	2	104	GLY	N-CA-C	-5.06	102.34	111.19
6	L	19	ARG	N-CA-CB	-5.02	102.17	109.95
1	1	16	GLU	CA-C-N	5.02	127.98	120.90
1	1	16	GLU	C-N-CA	5.02	127.98	120.90
6	L	58	ALA	N-CA-C	5.02	117.62	109.79

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	1429	0	1425	214	0
2	2	1617	0	1572	202	0
3	3	1673	0	1599	164	0
4	4	353	0	324	13	0
5	H	1074	0	1021	154	0
6	L	777	0	734	88	0
All	All	6923	0	6675	724	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 53.

All (724) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:99:HIS:CE1	6:L:92:ALA:HB3	1.25	1.66
2:2:69:TRP:CH2	2:2:121:LEU:CD1	1.77	1.65
2:2:69:TRP:CD2	2:2:121:LEU:HD11	1.32	1.62
2:2:69:TRP:CZ3	2:2:121:LEU:CD1	1.79	1.61
2:2:69:TRP:CZ3	2:2:121:LEU:HD13	1.10	1.57
2:2:69:TRP:CZ2	2:2:121:LEU:HD12	1.37	1.55
2:2:69:TRP:CH2	2:2:121:LEU:HD12	1.29	1.54
2:2:69:TRP:CE2	2:2:121:LEU:HD11	1.48	1.46
1:1:51:LEU:HD12	1:1:168:ILE:CD1	1.43	1.45
5:H:123:PRO:CA	5:H:123:PRO:N	1.69	1.44
1:1:51:LEU:CD1	1:1:168:ILE:HD11	1.47	1.42
2:2:69:TRP:CE3	2:2:121:LEU:CD1	2.02	1.42
5:H:94:TYR:OH	6:L:43:PRO:CA	1.68	1.41
1:1:82:HIS:HE1	1:1:113:THR:CG2	1.37	1.37
2:2:69:TRP:CZ2	2:2:121:LEU:CD1	1.99	1.36
5:H:99:HIS:HE1	6:L:92:ALA:CB	1.38	1.36
5:H:100:GLN:NE2	6:L:35:TYR:HB2	1.40	1.34
5:H:100:GLN:HE22	6:L:35:TYR:CB	1.39	1.33
2:2:69:TRP:CE3	2:2:121:LEU:HD13	1.65	1.30
2:2:98:TYR:CE2	2:2:210:VAL:HG21	1.66	1.30
3:3:109:PHE:CE2	3:3:186:LEU:HD21	1.68	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:69:TRP:CD2	2:2:121:LEU:CD1	2.19	1.24
1:1:82:HIS:CE1	1:1:113:THR:CG2	2.23	1.22
2:2:40:GLU:OE1	2:2:102:ARG:NH1	1.69	1.21
2:2:26:THR:HG22	2:2:28:SER:O	1.42	1.19
2:2:69:TRP:CE2	2:2:121:LEU:CD1	2.16	1.19
2:2:196:GLN:O	2:2:196:GLN:NE2	1.77	1.18
3:3:99:THR:C	3:3:170:THR:OG1	1.87	1.18
2:2:98:TYR:HD2	2:2:210:VAL:CB	1.57	1.17
3:3:109:PHE:CE2	3:3:186:LEU:CD2	2.26	1.17
2:2:26:THR:CG2	2:2:28:SER:O	1.93	1.16
1:1:159:LEU:HD21	1:1:163:PHE:HD2	1.05	1.16
3:3:99:THR:O	3:3:170:THR:OG1	1.62	1.16
2:2:69:TRP:CE3	2:2:121:LEU:HD11	1.68	1.15
2:2:195:PRO:O	2:2:195:PRO:HG2	1.46	1.15
5:H:99:HIS:CE1	6:L:92:ALA:CB	2.21	1.14
2:2:112:VAL:O	2:2:197:ILE:HG21	1.45	1.14
6:L:30:ASN:O	6:L:93:SER:HB2	1.47	1.12
1:1:82:HIS:CE1	1:1:113:THR:HG21	1.82	1.12
3:3:112:THR:HG22	3:3:198:ALA:O	1.48	1.12
5:H:38:ARG:O	5:H:46:GLU:HB3	1.48	1.12
1:1:98:LEU:HD12	1:1:169:LYS:HG2	1.33	1.11
1:1:159:LEU:HD21	1:1:163:PHE:CD2	1.85	1.11
2:2:216:SER:HB3	3:3:141:HIS:NE2	1.66	1.11
3:3:176:GLU:HB2	5:H:110:ARG:CD	1.80	1.11
2:2:98:TYR:CD2	2:2:210:VAL:HB	1.87	1.10
1:1:119:TYR:HE1	1:1:126:LEU:CD1	1.66	1.09
3:3:112:THR:HG23	3:3:112:THR:O	1.29	1.09
3:3:135:THR:OG1	3:3:136:PRO:HD2	1.53	1.09
3:3:176:GLU:HB2	5:H:110:ARG:HD3	1.13	1.08
2:2:103:ASN:O	2:2:162:PHE:HB2	1.52	1.08
3:3:112:THR:O	3:3:112:THR:CG2	1.97	1.08
1:1:77:GLU:OE2	1:1:179:ARG:HD3	1.54	1.08
3:3:52:PRO:HB2	3:3:202:LEU:HD23	1.34	1.07
1:1:39:PHE:CE1	1:1:179:ARG:HB2	1.90	1.07
3:3:117:ALA:HB1	3:3:194:ALA:HB2	1.37	1.06
1:1:82:HIS:HE1	1:1:113:THR:HG21	0.93	1.06
1:1:82:HIS:CE1	1:1:113:THR:HG22	1.90	1.05
1:1:126:LEU:HD23	1:1:163:PHE:HB3	1.36	1.05
2:2:107:VAL:HG21	2:2:179:LEU:CD1	1.86	1.05
2:2:98:TYR:HD2	2:2:210:VAL:HB	0.96	1.05
3:3:99:THR:C	3:3:170:THR:HG1	1.61	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:100:GLN:HE22	6:L:35:TYR:HB2	0.87	1.04
1:1:156:ALA:HB3	5:H:123:PRO:HG3	1.40	1.03
1:1:53:LEU:HD23	1:1:165:TYR:HE1	1.26	1.01
3:3:109:PHE:HE2	3:3:186:LEU:CD2	1.64	1.01
2:2:117:ASN:O	2:2:150:PRO:HB2	1.62	1.00
5:H:112:TYR:HB3	5:H:128:CYS:SG	2.01	1.00
3:3:112:THR:CG2	3:3:198:ALA:O	2.09	0.99
1:1:193:ALA:O	2:2:135:ARG:NH2	1.96	0.98
5:H:4:LEU:CD2	5:H:97:THR:HB	1.93	0.98
1:1:39:PHE:CE1	1:1:179:ARG:HD2	1.98	0.98
2:2:98:TYR:CE2	2:2:210:VAL:CG2	2.46	0.97
5:H:126:ALA:HB2	5:H:143:PRO:HB3	1.44	0.97
2:2:99:ALA:HB2	2:2:214:PHE:HE1	1.26	0.97
5:H:100:GLN:NE2	6:L:35:TYR:CB	2.12	0.96
2:2:195:PRO:O	2:2:195:PRO:CG	2.09	0.95
1:1:98:LEU:CD1	1:1:169:LYS:HG2	1.95	0.95
5:H:110:ARG:HG3	5:H:138:TYR:CE1	2.03	0.94
2:2:98:TYR:CD2	2:2:210:VAL:CB	2.46	0.94
3:3:140:ALA:HA	3:3:144:HIS:CD2	2.03	0.94
5:H:4:LEU:HD22	5:H:97:THR:HB	1.50	0.93
2:2:69:TRP:CE3	2:2:197:ILE:HD11	2.04	0.93
2:2:98:TYR:CD2	2:2:210:VAL:CG2	2.51	0.93
3:3:172:SER:OG	5:H:135:ALA:HB3	1.69	0.93
1:1:54:MET:HE2	1:1:155:ALA:CA	2.00	0.92
2:2:174:HIS:O	2:2:176:PRO:HD3	1.70	0.92
5:H:95:CYS:SG	6:L:103:PHE:CD2	2.63	0.92
1:1:89:VAL:HG11	1:1:98:LEU:HD21	1.52	0.91
1:1:53:LEU:HD23	1:1:165:TYR:CE1	2.06	0.91
2:2:112:VAL:O	2:2:197:ILE:CG2	2.19	0.90
1:1:98:LEU:HD12	1:1:169:LYS:CG	2.00	0.90
1:1:154:LYS:HE2	1:1:154:LYS:HA	1.52	0.90
1:1:39:PHE:HE1	1:1:179:ARG:HB2	1.37	0.90
5:H:94:TYR:OH	6:L:43:PRO:HA	0.72	0.90
1:1:192:LEU:HD22	2:2:135:ARG:HG2	1.52	0.89
1:1:159:LEU:HD23	1:1:160:PRO:HD2	1.55	0.89
1:1:119:TYR:CE1	1:1:126:LEU:CD1	2.55	0.89
5:H:33:ALA:O	5:H:98:VAL:HB	1.73	0.89
1:1:102:THR:CG2	3:3:216:ASP:HB2	2.03	0.88
2:2:83:LEU:HD22	2:2:203:ILE:HD13	1.54	0.88
2:2:98:TYR:CD2	2:2:210:VAL:HG21	2.07	0.88
3:3:177:THR:O	3:3:177:THR:HG22	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:154:LYS:O	1:1:157:ARG:O	1.93	0.87
5:H:107:THR:CG2	5:H:144:PHE:CE2	2.57	0.87
1:1:176:LEU:HD12	1:1:177:LEU:H	1.40	0.87
6:L:30:ASN:HA	6:L:94:PRO:O	1.75	0.87
1:1:39:PHE:CD1	1:1:179:ARG:HB2	2.09	0.86
2:2:216:SER:CB	3:3:141:HIS:NE2	2.39	0.86
1:1:167:ALA:HB3	5:H:133:PHE:CZ	2.11	0.86
2:2:98:TYR:HE2	2:2:210:VAL:HG21	1.04	0.85
5:H:94:TYR:CZ	6:L:43:PRO:HA	2.08	0.85
5:H:100:GLN:NE2	6:L:35:TYR:CA	2.40	0.85
5:H:107:THR:HG23	5:H:144:PHE:CE2	2.11	0.85
1:1:102:THR:HG21	3:3:216:ASP:HB2	1.59	0.85
1:1:83:GLU:OE2	1:1:171:THR:HB	1.75	0.85
2:2:83:LEU:CD2	2:2:203:ILE:HD13	2.07	0.85
3:3:121:TYR:CE2	3:3:199:LEU:HD22	2.12	0.85
5:H:35:GLY:CA	5:H:98:VAL:HG23	2.07	0.84
2:2:107:VAL:HG21	2:2:179:LEU:HD11	1.57	0.84
5:H:110:ARG:HG3	5:H:138:TYR:HE1	1.42	0.84
1:1:95:GLU:HB2	5:H:131:CYS:O	1.78	0.83
1:1:34:PHE:CG	1:1:34:PHE:O	2.31	0.83
2:2:69:TRP:CH2	2:2:119:GLY:HA3	2.14	0.83
1:1:42:VAL:HG21	1:1:178:TYR:CE2	2.14	0.83
5:H:126:ALA:HB2	5:H:143:PRO:CB	2.08	0.83
2:2:191:THR:HB	2:2:192:GLU:OE2	1.79	0.83
3:3:117:ALA:CB	3:3:194:ALA:HB2	2.09	0.83
1:1:40:VAL:HG11	1:1:62:VAL:HB	1.59	0.82
6:L:12:VAL:HG21	6:L:109:LEU:HD22	1.59	0.82
5:H:94:TYR:HH	6:L:43:PRO:CA	1.72	0.82
1:1:98:LEU:CD1	1:1:169:LYS:CG	2.57	0.82
1:1:167:ALA:CB	5:H:133:PHE:CZ	2.63	0.82
2:2:109:VAL:HG21	2:2:123:VAL:HG11	1.61	0.82
1:1:126:LEU:HD23	1:1:163:PHE:CB	2.10	0.81
5:H:35:GLY:N	5:H:98:VAL:HG23	1.95	0.81
1:1:159:LEU:CD2	1:1:163:PHE:CD2	2.63	0.81
2:2:57:GLN:O	2:2:90:VAL:HG11	1.80	0.81
2:2:94:LEU:HB3	2:2:101:MET:HE1	1.63	0.81
5:H:39:ARG:NH1	5:H:94:TYR:CD2	2.49	0.80
5:H:113:ARG:CG	5:H:116:CYS:HB2	2.10	0.80
1:1:154:LYS:HA	1:1:154:LYS:CE	2.11	0.80
4:4:24:ASN:ND2	4:4:31:GLN:OE1	2.14	0.80
5:H:100:GLN:CD	6:L:35:TYR:H	1.89	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:112:TYR:CB	5:H:128:CYS:SG	2.71	0.79
6:L:12:VAL:HG21	6:L:109:LEU:CD2	2.11	0.79
5:H:38:ARG:O	5:H:46:GLU:CB	2.29	0.79
1:1:39:PHE:HE1	1:1:179:ARG:CB	1.96	0.79
3:3:140:ALA:HA	3:3:144:HIS:HD2	1.43	0.78
5:H:95:CYS:HB2	6:L:90:PHE:CD2	2.18	0.78
1:1:46:ASP:O	1:1:173:VAL:HG22	1.83	0.78
2:2:99:ALA:HB2	2:2:214:PHE:CE1	2.17	0.78
1:1:176:LEU:O	1:1:177:LEU:HD23	1.83	0.78
1:1:102:THR:HG21	3:3:216:ASP:CB	2.14	0.77
2:2:195:PRO:O	2:2:196:GLN:HG3	1.85	0.77
1:1:119:TYR:HE1	1:1:126:LEU:HD11	1.48	0.77
3:3:176:GLU:CB	5:H:110:ARG:CD	2.61	0.77
6:L:12:VAL:HG13	6:L:107:THR:HG21	1.64	0.77
2:2:30:VAL:HB	2:2:153:ASN:HD22	1.49	0.77
1:1:49:ASN:HD21	1:1:176:LEU:HD22	1.47	0.77
5:H:34:VAL:C	5:H:98:VAL:HG23	2.10	0.77
1:1:39:PHE:CE1	1:1:179:ARG:CB	2.67	0.76
1:1:156:ALA:CB	5:H:123:PRO:HG3	2.15	0.76
2:2:69:TRP:CH2	2:2:121:LEU:HD13	1.72	0.76
4:4:83:LEU:HD23	4:4:83:LEU:O	1.86	0.76
5:H:126:ALA:CB	5:H:143:PRO:HB3	2.15	0.76
3:3:121:TYR:CE2	3:3:199:LEU:CD2	2.70	0.75
5:H:99:HIS:HD2	5:H:100:GLN:HE21	1.33	0.75
5:H:37:VAL:HG11	6:L:103:PHE:HB2	1.66	0.75
2:2:216:SER:HB3	3:3:141:HIS:CD2	2.20	0.75
1:1:51:LEU:HD12	1:1:168:ILE:HD12	1.66	0.75
2:2:117:ASN:OD1	2:2:193:GLY:HA3	1.87	0.75
5:H:108:CYS:O	5:H:108:CYS:SG	2.45	0.75
1:1:50:VAL:HG23	5:H:119:ARG:HD3	1.69	0.74
5:H:100:GLN:CD	6:L:35:TYR:N	2.45	0.74
1:1:58:ALA:O	1:1:64:ALA:HB2	1.87	0.74
5:H:100:GLN:HE22	6:L:35:TYR:CA	2.00	0.74
1:1:181:LYS:O	1:1:182:ARG:HG2	1.87	0.74
3:3:135:THR:C	3:3:187:PHE:HE2	1.96	0.74
5:H:94:TYR:HH	6:L:43:PRO:HA	0.93	0.74
5:H:98:VAL:HA	6:L:103:PHE:HZ	1.52	0.74
1:1:39:PHE:CE1	1:1:179:ARG:CD	2.70	0.74
1:1:112:LEU:HD23	1:1:112:LEU:N	2.02	0.74
1:1:159:LEU:HD23	1:1:160:PRO:CD	2.17	0.74
2:2:216:SER:N	3:3:141:HIS:HD2	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:119:TYR:CE1	1:1:126:LEU:HD11	2.23	0.73
5:H:113:ARG:CZ	5:H:131:CYS:SG	2.77	0.73
1:1:94:PRO:O	1:1:97:ALA:CB	2.38	0.72
1:1:176:LEU:HD12	1:1:177:LEU:N	2.03	0.72
2:2:197:ILE:HD12	2:2:197:ILE:O	1.90	0.72
1:1:119:TYR:CE1	1:1:126:LEU:HD12	2.22	0.72
2:2:92:GLY:O	2:2:95:THR:HG22	1.89	0.72
3:3:177:THR:O	3:3:177:THR:CG2	2.38	0.72
1:1:54:MET:HE2	1:1:155:ALA:HB2	1.71	0.71
3:3:8:SER:HB3	3:3:11:TYR:HB2	1.72	0.71
2:2:117:ASN:HD21	2:2:194:ALA:N	1.89	0.71
3:3:195:ASP:OD1	3:3:195:ASP:N	2.22	0.71
1:1:42:VAL:HG21	1:1:178:TYR:CD2	2.25	0.71
1:1:192:LEU:HD22	2:2:135:ARG:CG	2.20	0.71
5:H:100:GLN:NE2	6:L:35:TYR:N	2.38	0.71
1:1:54:MET:HE2	1:1:155:ALA:CB	2.20	0.71
1:1:89:VAL:CG1	1:1:98:LEU:HD21	2.20	0.70
2:2:69:TRP:CZ2	2:2:119:GLY:HA3	2.26	0.70
5:H:99:HIS:CD2	5:H:100:GLN:HG2	2.26	0.70
6:L:12:VAL:HG22	6:L:107:THR:HG22	1.74	0.69
5:H:113:ARG:NH1	5:H:131:CYS:SG	2.66	0.69
1:1:52:ASP:OD1	1:1:55:GLN:HG3	1.92	0.69
5:H:98:VAL:HA	6:L:103:PHE:CZ	2.27	0.69
1:1:119:TYR:HE1	1:1:126:LEU:HD12	1.52	0.69
1:1:154:LYS:HE2	1:1:154:LYS:CA	2.19	0.69
2:2:99:ALA:CB	2:2:214:PHE:HE1	2.02	0.69
3:3:109:PHE:HE2	3:3:186:LEU:HD23	1.58	0.69
1:1:51:LEU:C	1:1:51:LEU:HD23	2.16	0.69
1:1:94:PRO:HD2	1:1:97:ALA:HB2	1.73	0.69
5:H:70:THR:HG1	5:H:79:SER:HG	1.36	0.69
1:1:48:ILE:HB	1:1:169:LYS:HD3	1.76	0.68
2:2:55:VAL:HG11	2:2:94:LEU:HD21	1.76	0.68
3:3:199:LEU:HD12	3:3:200:VAL:H	1.59	0.68
3:3:173:ASP:O	3:3:179:ASN:OD1	2.12	0.68
6:L:86:GLU:OE1	6:L:111:VAL:N	2.26	0.68
5:H:35:GLY:CA	5:H:98:VAL:CG2	2.72	0.68
1:1:54:MET:HE2	1:1:155:ALA:N	2.08	0.67
2:2:69:TRP:HE3	2:2:197:ILE:HD11	1.56	0.67
2:2:107:VAL:HG11	2:2:125:MET:SD	2.34	0.67
1:1:10:PRO:HG2	4:4:71:LEU:HG	1.76	0.67
2:2:48:THR:HG22	3:3:162:LEU:HB2	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:69:TRP:HE3	2:2:197:ILE:CD1	2.07	0.67
3:3:185:CYS:HB3	3:3:187:PHE:CE1	2.30	0.67
5:H:95:CYS:SG	6:L:103:PHE:CE2	2.87	0.66
1:1:70:THR:O	1:1:128:THR:OG1	2.12	0.66
2:2:126:VAL:HG11	2:2:129:LEU:HD23	1.77	0.66
5:H:39:ARG:NH1	5:H:94:TYR:CE2	2.62	0.66
5:H:35:GLY:HA2	5:H:98:VAL:CG2	2.25	0.66
2:2:69:TRP:CE3	2:2:197:ILE:CD1	2.79	0.66
1:1:54:MET:HE2	1:1:155:ALA:HA	1.76	0.65
1:1:54:MET:HG2	1:1:155:ALA:HB2	1.77	0.65
1:1:51:LEU:HD12	1:1:168:ILE:HD11	0.70	0.65
5:H:15:SER:H	5:H:85:VAL:HB	1.60	0.65
5:H:109:PRO:HG3	5:H:144:PHE:HB3	1.76	0.65
3:3:78:ASP:OD1	3:3:79:LEU:N	2.29	0.65
1:1:83:GLU:OE2	1:1:171:THR:CB	2.43	0.65
5:H:114:PRO:HA	5:H:128:CYS:HA	1.78	0.65
6:L:78:ILE:CG2	6:L:85:ASP:OD2	2.45	0.65
2:2:115:GLN:HG2	2:2:115:GLN:O	1.96	0.65
1:1:95:GLU:CG	5:H:131:CYS:O	2.45	0.64
2:2:62:PHE:HB3	2:2:87:HIS:HE1	1.62	0.64
1:1:160:PRO:HD2	1:1:163:PHE:CE2	2.33	0.64
2:2:50:GLY:C	2:2:52:GLU:H	2.04	0.63
2:2:97:SER:C	2:2:98:TYR:HD1	2.06	0.63
1:1:49:ASN:HD21	1:1:176:LEU:CD2	2.11	0.63
2:2:133:ASP:OD1	2:2:133:ASP:N	2.28	0.63
1:1:53:LEU:CD2	1:1:165:TYR:CE1	2.78	0.63
5:H:34:VAL:O	5:H:98:VAL:HG21	1.98	0.63
1:1:54:MET:HG2	1:1:155:ALA:CB	2.29	0.63
2:2:55:VAL:HG11	2:2:94:LEU:CD2	2.28	0.63
5:H:45:LEU:HG	6:L:105:SER:H	1.63	0.63
2:2:26:THR:HG21	2:2:28:SER:O	1.98	0.62
3:3:181:GLN:OE1	3:3:181:GLN:HA	1.98	0.62
5:H:100:GLN:OE1	6:L:35:TYR:N	2.30	0.62
6:L:8:GLN:HE21	6:L:106:GLY:HA2	1.63	0.62
1:1:37:ASP:OD1	1:1:180:MET:O	2.17	0.62
1:1:83:GLU:O	1:1:83:GLU:CD	2.42	0.62
2:2:215:PRO:N	3:3:142:CYS:SG	2.72	0.62
2:2:216:SER:CB	3:3:141:HIS:CD2	2.81	0.62
6:L:46:ALA:O	6:L:48:ARG:NH1	2.33	0.62
2:2:80:GLN:NE2	2:2:129:LEU:HD11	2.15	0.62
2:2:215:PRO:CA	3:3:142:CYS:SG	2.87	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:135:THR:C	3:3:187:PHE:CE2	2.77	0.62
5:H:112:TYR:HE2	5:H:141:CYS:H	1.48	0.62
1:1:95:GLU:CB	5:H:131:CYS:O	2.45	0.62
3:3:122:MET:HG3	3:3:146:GLU:HG2	1.82	0.61
3:3:104:THR:OG1	3:3:206:GLY:HA3	2.00	0.61
3:3:194:ALA:HB1	3:3:197:ASP:CG	2.25	0.61
5:H:95:CYS:SG	6:L:103:PHE:HD2	2.17	0.61
6:L:95:GLU:N	6:L:100:ASN:O	2.30	0.61
1:1:8:ALA:HB1	2:2:145:HIS:CE1	2.35	0.61
5:H:113:ARG:CD	5:H:116:CYS:HB2	2.30	0.61
1:1:161:THR:HB	5:H:139:GLY:O	2.01	0.61
5:H:99:HIS:CD2	5:H:100:GLN:HE21	2.16	0.61
6:L:78:ILE:HG21	6:L:85:ASP:OD2	2.01	0.61
1:1:112:LEU:HD23	1:1:112:LEU:H	1.64	0.61
1:1:156:ALA:HB3	5:H:123:PRO:CG	2.25	0.61
1:1:15:VAL:HG12	1:1:15:VAL:O	2.01	0.61
1:1:111:PRO:HD2	3:3:9:ASP:HB3	1.81	0.61
3:3:174:ALA:HB2	3:3:179:ASN:ND2	2.15	0.61
5:H:142:THR:HG23	5:H:143:PRO:HD2	1.83	0.61
5:H:100:GLN:NE2	6:L:35:TYR:H	1.97	0.61
1:1:77:GLU:OE2	1:1:179:ARG:CD	2.42	0.60
3:3:188:GLN:O	3:3:188:GLN:HG2	1.99	0.60
5:H:1:GLN:N	6:L:59:SER:O	2.27	0.60
2:2:30:VAL:HB	2:2:153:ASN:ND2	2.16	0.60
1:1:167:ALA:HB2	5:H:133:PHE:CZ	2.35	0.60
1:1:94:PRO:O	1:1:97:ALA:HB3	2.01	0.60
3:3:186:LEU:HD12	3:3:186:LEU:O	2.01	0.60
5:H:112:TYR:HB3	5:H:128:CYS:HG	1.65	0.60
2:2:87:HIS:CD2	2:2:90:VAL:O	2.55	0.60
3:3:52:PRO:HB2	3:3:202:LEU:CD2	2.20	0.60
3:3:107:LEU:HD13	3:3:159:ILE:HD12	1.84	0.60
5:H:99:HIS:HE1	6:L:92:ALA:CA	2.11	0.60
6:L:41:LEU:HG	6:L:47:PRO:HB3	1.82	0.60
2:2:183:VAL:O	2:2:183:VAL:HG23	2.00	0.59
3:3:108:HIS:HB2	3:3:202:LEU:HB2	1.83	0.59
5:H:34:VAL:C	5:H:98:VAL:CG2	2.74	0.59
1:1:101:THR:HA	1:1:105:THR:HG21	1.82	0.59
1:1:48:ILE:HB	1:1:169:LYS:CD	2.32	0.59
1:1:83:GLU:O	1:1:83:GLU:CG	2.50	0.59
3:3:159:ILE:HD11	3:3:184:VAL:HG11	1.84	0.59
6:L:81:LEU:HD21	6:L:111:VAL:HG22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:98:TYR:HE2	2:2:210:VAL:CG2	1.92	0.59
2:2:189:VAL:HG21	2:2:195:PRO:HA	1.83	0.59
3:3:63:TYR:HA	3:3:199:LEU:O	2.02	0.59
3:3:159:ILE:CD1	3:3:184:VAL:HG11	2.33	0.59
1:1:42:VAL:HG21	1:1:178:TYR:HE2	1.67	0.59
1:1:157:ARG:NH2	5:H:142:THR:OG1	2.36	0.59
2:2:55:VAL:HG21	2:2:94:LEU:HD21	1.85	0.59
2:2:110:THR:HG22	2:2:110:THR:O	2.02	0.58
5:H:5:ARG:HB3	5:H:23:THR:HB	1.85	0.58
1:1:36:LEU:HD12	1:1:62:VAL:HG22	1.84	0.58
5:H:100:GLN:HE21	6:L:35:TYR:HB2	1.57	0.58
2:2:85:THR:O	2:2:85:THR:HG23	2.04	0.58
3:3:152:ASN:OD1	3:3:152:ASN:O	2.21	0.58
1:1:80:VAL:O	1:1:112:LEU:HB2	2.03	0.58
2:2:29:SER:OG	2:2:30:VAL:N	2.35	0.58
3:3:89:THR:HG23	3:3:92:ALA:H	1.69	0.58
5:H:18:LEU:HD22	5:H:82:ILE:HD12	1.86	0.58
1:1:91:ASN:HD22	1:1:121:ALA:HA	1.69	0.58
1:1:98:LEU:HD13	1:1:169:LYS:CG	2.34	0.58
3:3:109:PHE:CD2	3:3:186:LEU:HD21	2.31	0.58
2:2:189:VAL:HG13	2:2:193:GLY:O	2.04	0.58
5:H:113:ARG:HG3	5:H:116:CYS:HB2	1.86	0.58
1:1:39:PHE:CZ	1:1:179:ARG:HD2	2.37	0.58
3:3:77:PHE:CE1	3:3:184:VAL:HG21	2.38	0.58
4:4:83:LEU:HD23	4:4:83:LEU:C	2.29	0.58
1:1:98:LEU:HD13	1:1:169:LYS:HB2	1.85	0.58
1:1:111:PRO:HB2	1:1:112:LEU:CD2	2.34	0.58
2:2:195:PRO:O	2:2:195:PRO:CD	2.51	0.57
6:L:65:PHE:HE1	6:L:79:SER:O	1.87	0.57
2:2:216:SER:H	3:3:141:HIS:HD2	1.52	0.57
6:L:8:GLN:HG3	6:L:9:PRO:HD2	1.86	0.57
6:L:27:SER:H	6:L:30:ASN:HD21	1.52	0.57
3:3:176:GLU:HG3	5:H:110:ARG:NE	2.19	0.57
2:2:216:SER:N	3:3:141:HIS:CD2	2.72	0.57
3:3:125:TYR:O	3:3:142:CYS:HB3	2.05	0.57
5:H:129:GLY:HA2	5:H:141:CYS:HB3	1.87	0.57
3:3:123:ILE:HG13	3:3:185:CYS:O	2.05	0.57
3:3:212:ARG:HE	3:3:213:LEU:HD23	1.70	0.57
5:H:110:ARG:HE	5:H:110:ARG:HA	1.70	0.57
1:1:179:ARG:HH12	1:1:181:LYS:HG2	1.70	0.57
3:3:64:VAL:HG21	3:3:74:LEU:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:88:GLU:OE1	6:L:106:GLY:C	2.48	0.57
1:1:41:LYS:HA	1:1:177:LEU:CD2	2.35	0.56
1:1:182:ARG:HG3	1:1:182:ARG:O	2.05	0.56
4:4:22:ILE:HG22	4:4:22:ILE:O	2.05	0.56
6:L:86:GLU:HG2	6:L:111:VAL:CG2	2.35	0.56
1:1:111:PRO:HB2	1:1:112:LEU:HD23	1.87	0.56
2:2:37:ALA:HB3	2:2:161:PRO:HG2	1.87	0.56
5:H:39:ARG:NH1	5:H:94:TYR:HD2	2.02	0.56
6:L:88:GLU:OE1	6:L:106:GLY:O	2.23	0.56
1:1:49:ASN:ND2	1:1:176:LEU:CD2	2.69	0.56
3:3:95:ALA:HB1	3:3:170:THR:CG2	2.36	0.56
3:3:193:LYS:HG3	3:3:193:LYS:O	2.06	0.56
1:1:9:ASP:OD1	1:1:10:PRO:HD2	2.06	0.56
4:4:77:SER:OG	4:4:78:GLY:N	2.38	0.56
2:2:135:ARG:HG3	2:2:135:ARG:HH11	1.71	0.56
1:1:96:THR:HG22	1:1:96:THR:O	2.06	0.56
2:2:93:SER:O	2:2:94:LEU:C	2.49	0.56
3:3:57:PHE:HD1	3:3:85:HIS:HD2	1.52	0.56
2:2:98:TYR:CD1	2:2:98:TYR:N	2.73	0.55
5:H:95:CYS:HG	6:L:103:PHE:HD2	1.43	0.55
2:2:73:ASP:OD1	2:2:77:ARG:NH1	2.39	0.55
2:2:107:VAL:CG2	2:2:179:LEU:HD11	2.34	0.55
3:3:95:ALA:HB1	3:3:170:THR:HG21	1.88	0.55
3:3:185:CYS:HB3	3:3:187:PHE:CD1	2.41	0.55
1:1:53:LEU:O	1:1:54:MET:HB3	2.06	0.55
1:1:86:LEU:HD12	1:1:168:ILE:CG2	2.37	0.55
3:3:109:PHE:HE2	3:3:186:LEU:HD21	1.22	0.55
5:H:107:THR:HG22	5:H:144:PHE:CE2	2.42	0.55
1:1:102:THR:HG21	3:3:216:ASP:CG	2.32	0.55
3:3:99:THR:CA	3:3:170:THR:OG1	2.54	0.55
1:1:83:GLU:CD	1:1:83:GLU:C	2.75	0.55
2:2:99:ALA:C	2:2:100:TYR:CD1	2.85	0.55
2:2:80:GLN:HE22	2:2:129:LEU:HD11	1.72	0.55
1:1:40:VAL:HG23	1:1:40:VAL:O	2.07	0.54
2:2:189:VAL:HG22	2:2:194:ALA:O	2.07	0.54
3:3:135:THR:CA	3:3:187:PHE:HE2	2.20	0.54
6:L:50:LEU:HB3	6:L:51:ILE:HD12	1.88	0.54
2:2:100:TYR:CD1	2:2:100:TYR:N	2.73	0.54
5:H:22:CYS:O	5:H:77:GLN:HA	2.08	0.54
6:L:12:VAL:HG23	6:L:109:LEU:HA	1.90	0.54
2:2:112:VAL:CG2	2:2:197:ILE:HG22	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:64:ARG:NH1	6:L:82:GLN:OE1	2.40	0.54
1:1:170:ALA:HB3	1:1:173:VAL:HG13	1.89	0.54
1:1:42:VAL:HG11	1:1:178:TYR:HE2	1.72	0.54
2:2:30:VAL:CB	2:2:153:ASN:HD22	2.19	0.54
5:H:126:ALA:CB	5:H:143:PRO:CB	2.82	0.54
6:L:86:GLU:HG2	6:L:111:VAL:HG23	1.89	0.54
1:1:36:LEU:HG	1:1:180:MET:HE2	1.90	0.54
1:1:44:PRO:HG3	1:1:174:THR:O	2.08	0.54
3:3:199:LEU:HD12	3:3:200:VAL:N	2.21	0.54
5:H:5:ARG:O	5:H:23:THR:N	2.31	0.54
6:L:18:GLN:CD	6:L:18:GLN:O	2.50	0.54
2:2:102:ARG:HD2	2:2:168:TYR:CE1	2.43	0.54
1:1:86:LEU:HD12	1:1:168:ILE:HG23	1.90	0.53
2:2:49:SER:C	2:2:51:LEU:H	2.16	0.53
2:2:99:ALA:C	2:2:100:TYR:HD1	2.16	0.53
1:1:98:LEU:HD13	1:1:169:LYS:CB	2.37	0.53
3:3:135:THR:OG1	3:3:136:PRO:CD	2.43	0.53
4:4:15:SER:OG	4:4:16:GLY:N	2.41	0.53
5:H:49:GLY:HA3	5:H:59:TYR:HD1	1.72	0.53
3:3:176:GLU:HG3	5:H:110:ARG:CZ	2.38	0.53
6:L:86:GLU:OE1	6:L:111:VAL:HB	2.08	0.53
1:1:192:LEU:HD22	2:2:135:ARG:CB	2.38	0.53
5:H:34:VAL:O	5:H:98:VAL:CG2	2.57	0.53
5:H:126:ALA:CB	5:H:143:PRO:CA	2.86	0.53
5:H:144:PHE:CD1	5:H:144:PHE:C	2.87	0.53
3:3:144:HIS:C	3:3:144:HIS:HD1	2.16	0.53
3:3:174:ALA:HB2	3:3:179:ASN:HD21	1.72	0.53
1:1:110:ALA:HB1	1:1:111:PRO:HA	1.91	0.53
6:L:13:SER:HA	6:L:110:THR:HG22	1.90	0.53
2:2:50:GLY:C	2:2:52:GLU:N	2.61	0.53
2:2:109:VAL:HG11	2:2:123:VAL:HG11	1.91	0.53
3:3:112:THR:HG21	3:3:198:ALA:O	2.03	0.53
3:3:123:ILE:O	3:3:144:HIS:HB2	2.08	0.53
1:1:34:PHE:O	1:1:34:PHE:CD2	2.62	0.53
1:1:54:MET:HG2	1:1:54:MET:O	2.09	0.53
5:H:126:ALA:HB2	5:H:143:PRO:CD	2.38	0.53
3:3:45:LEU:HD21	3:3:211:LEU:CD1	2.39	0.53
5:H:49:GLY:HA3	5:H:59:TYR:CD1	2.43	0.52
1:1:54:MET:CE	1:1:155:ALA:HB2	2.40	0.52
1:1:41:LYS:HA	1:1:177:LEU:HD23	1.91	0.52
1:1:130:TYR:HB2	1:1:159:LEU:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:179:ARG:NH1	1:1:181:LYS:CG	2.73	0.52
2:2:86:ASP:OD1	2:2:86:ASP:O	2.28	0.52
6:L:12:VAL:CG1	6:L:107:THR:HG21	2.35	0.52
1:1:100:ASN:ND2	3:3:217:ALA:HA	2.24	0.52
1:1:192:LEU:HD22	2:2:135:ARG:HB3	1.90	0.52
3:3:121:TYR:CD2	3:3:199:LEU:CD2	2.93	0.52
1:1:94:PRO:O	1:1:97:ALA:HB2	2.10	0.52
5:H:113:ARG:HD2	5:H:116:CYS:HB2	1.91	0.52
3:3:17:THR:O	3:3:19:PRO:HD3	2.10	0.51
5:H:48:LEU:HD23	5:H:49:GLY:H	1.74	0.51
5:H:142:THR:CG2	5:H:143:PRO:HD2	2.39	0.51
3:3:120:ARG:HG2	3:3:189:ILE:HD11	1.91	0.51
2:2:102:ARG:O	2:2:102:ARG:HG3	2.08	0.51
2:2:192:GLU:CD	2:2:192:GLU:N	2.69	0.51
1:1:71:TYR:OH	2:2:128:GLU:OE1	2.26	0.51
2:2:216:SER:H	3:3:141:HIS:CD2	2.28	0.51
2:2:102:ARG:HG2	2:2:209:HIS:HB2	1.91	0.50
3:3:185:CYS:HB3	3:3:187:PHE:HE1	1.74	0.50
1:1:54:MET:O	1:1:54:MET:CG	2.59	0.50
3:3:60:ASP:O	3:3:60:ASP:OD1	2.29	0.50
3:3:184:VAL:C	3:3:185:CYS:SG	2.94	0.50
5:H:97:THR:HG21	6:L:39:TYR:CE2	2.47	0.50
5:H:110:ARG:NE	5:H:110:ARG:HA	2.26	0.50
1:1:88:TRP:CE2	1:1:117:LEU:HD22	2.46	0.50
2:2:58:ALA:HA	2:2:90:VAL:CG1	2.41	0.50
2:2:49:SER:C	2:2:51:LEU:N	2.69	0.50
2:2:97:SER:HB3	2:2:98:TYR:CD1	2.46	0.50
5:H:34:VAL:HG11	5:H:78:VAL:HG11	1.92	0.50
5:H:116:CYS:SG	5:H:119:ARG:NH2	2.85	0.50
2:2:47:ASN:ND2	3:3:164:ALA:O	2.45	0.50
4:4:24:ASN:HD22	4:4:31:GLN:HG2	1.77	0.50
5:H:112:TYR:HE2	5:H:141:CYS:N	2.08	0.50
5:H:113:ARG:HG3	5:H:116:CYS:H	1.76	0.49
3:3:57:PHE:CD1	3:3:85:HIS:HD2	2.29	0.49
2:2:107:VAL:HG21	2:2:179:LEU:HD13	1.87	0.49
3:3:86:MET:O	3:3:89:THR:HG22	2.11	0.49
5:H:144:PHE:C	5:H:144:PHE:HD1	2.20	0.49
2:2:117:ASN:HD21	2:2:193:GLY:C	2.19	0.49
1:1:48:ILE:HG23	1:1:48:ILE:O	2.12	0.49
1:1:179:ARG:HH12	1:1:181:LYS:CG	2.24	0.49
1:1:193:ALA:O	2:2:135:ARG:CZ	2.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:83:LEU:HB3	2:2:105:TRP:CH2	2.47	0.49
2:2:94:LEU:HB3	2:2:101:MET:CE	2.40	0.49
2:2:83:LEU:HD21	2:2:203:ILE:HD13	1.90	0.49
2:2:215:PRO:HB3	3:3:142:CYS:SG	2.52	0.49
6:L:18:GLN:CD	6:L:18:GLN:C	2.81	0.49
6:L:30:ASN:C	6:L:93:SER:HB2	2.31	0.49
2:2:33:THR:HB	2:2:146:GLN:HE21	1.77	0.49
2:2:68:ASP:OD1	2:2:198:LYS:HG2	2.13	0.49
2:2:123:VAL:HG23	2:2:158:ILE:HD11	1.95	0.49
3:3:53:THR:HG21	3:3:90:PHE:H	1.78	0.49
2:2:160:VAL:HB	2:2:177:TRP:CH2	2.48	0.49
2:2:135:ARG:HG3	2:2:135:ARG:NH1	2.28	0.48
5:H:100:GLN:NE2	6:L:35:TYR:C	2.70	0.48
1:1:102:THR:HG21	3:3:216:ASP:OD2	2.14	0.48
3:3:173:ASP:CG	5:H:111:ALA:CB	2.85	0.48
1:1:65:LEU:O	1:1:65:LEU:HD23	2.13	0.48
1:1:9:ASP:OD1	1:1:10:PRO:CD	2.61	0.48
1:1:94:PRO:CD	1:1:97:ALA:HB2	2.41	0.48
2:2:196:GLN:O	2:2:196:GLN:CD	2.52	0.48
3:3:64:VAL:CG1	3:3:199:LEU:HB3	2.43	0.48
3:3:98:TYR:HD2	3:3:211:LEU:HD22	1.78	0.48
6:L:30:ASN:CA	6:L:94:PRO:O	2.57	0.48
6:L:91:CYS:SG	6:L:92:ALA:N	2.87	0.48
1:1:105:THR:O	3:3:15:VAL:HA	2.14	0.48
2:2:125:MET:SD	2:2:179:LEU:HD12	2.54	0.48
2:2:43:VAL:HG21	2:2:209:HIS:CE1	2.48	0.48
3:3:135:THR:O	3:3:138:ALA:HB3	2.13	0.48
5:H:20:LEU:H	5:H:80:LEU:HD22	1.79	0.48
5:H:126:ALA:CA	5:H:143:PRO:HB3	2.44	0.48
2:2:83:LEU:HD13	2:2:105:TRP:CE3	2.49	0.48
4:4:18:THR:CG2	4:4:18:THR:O	2.30	0.48
5:H:110:ARG:NE	5:H:110:ARG:CA	2.77	0.48
1:1:34:PHE:CD2	1:1:34:PHE:C	2.86	0.47
1:1:89:VAL:HG11	1:1:98:LEU:CD2	2.36	0.47
2:2:131:SER:O	2:2:132:ILE:C	2.57	0.47
2:2:78:CYS:HA	2:2:181:VAL:O	2.13	0.47
3:3:41:PHE:HB2	3:3:47:VAL:HG23	1.97	0.47
3:3:173:ASP:OD2	5:H:111:ALA:HB3	2.15	0.47
1:1:130:TYR:HB3	1:1:158:ALA:O	2.15	0.47
3:3:77:PHE:O	3:3:184:VAL:HG22	2.15	0.47
5:H:36:TRP:O	5:H:48:LEU:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:51:ILE:HD11	5:H:69:ILE:HB	1.95	0.47
1:1:51:LEU:C	1:1:51:LEU:CD2	2.85	0.47
1:1:77:GLU:HG2	1:1:181:LYS:HD3	1.97	0.47
1:1:89:VAL:HG22	1:1:90:PRO:HD2	1.95	0.47
2:2:123:VAL:HG12	2:2:181:VAL:HG22	1.97	0.47
2:2:126:VAL:CG1	2:2:129:LEU:HD23	2.45	0.47
3:3:45:LEU:HD13	3:3:210:GLU:HA	1.96	0.47
6:L:12:VAL:CG2	6:L:109:LEU:CD2	2.89	0.47
1:1:111:PRO:CD	3:3:9:ASP:HB3	2.45	0.47
3:3:194:ALA:HB1	3:3:197:ASP:OD2	2.15	0.47
2:2:69:TRP:HB3	2:2:197:ILE:HD12	1.97	0.46
3:3:176:GLU:CB	5:H:110:ARG:HD2	2.44	0.46
5:H:72:ASP:OD1	5:H:73:ASN:N	2.48	0.46
5:H:117:ALA:O	5:H:118:ALA:HB3	2.15	0.46
1:1:70:THR:HA	1:1:128:THR:OG1	2.16	0.46
2:2:48:THR:HG21	2:2:168:TYR:CE2	2.50	0.46
1:1:110:ALA:HA	1:1:111:PRO:C	2.40	0.46
3:3:147:TRP:HD1	3:3:148:ASP:O	1.98	0.46
1:1:53:LEU:HB2	1:1:72:TYR:OH	2.15	0.46
1:1:81:LYS:O	1:1:174:THR:OG1	2.30	0.46
2:2:81:LEU:O	2:2:179:LEU:N	2.47	0.46
2:2:97:SER:C	2:2:98:TYR:CD1	2.91	0.46
6:L:86:GLU:OE1	6:L:111:VAL:CB	2.63	0.46
1:1:101:THR:HA	1:1:105:THR:CG2	2.46	0.46
2:2:123:VAL:HG22	2:2:146:GLN:O	2.16	0.46
6:L:41:LEU:C	6:L:87:ALA:HB1	2.40	0.46
2:2:112:VAL:HG22	2:2:197:ILE:HG22	1.97	0.46
3:3:144:HIS:C	3:3:144:HIS:ND1	2.73	0.46
5:H:126:ALA:HB2	5:H:143:PRO:HD3	1.98	0.46
1:1:51:LEU:CD1	1:1:168:ILE:CD1	2.35	0.45
2:2:19:ASN:HB2	2:2:61:PHE:HE1	1.80	0.45
4:4:18:THR:O	4:4:18:THR:HG22	2.15	0.45
5:H:51:ILE:HD13	5:H:57:THR:HG22	1.98	0.45
5:H:94:TYR:OH	6:L:43:PRO:C	2.54	0.45
6:L:50:LEU:C	6:L:51:ILE:HD12	2.41	0.45
1:1:10:PRO:CG	4:4:71:LEU:HG	2.46	0.45
1:1:130:TYR:CG	1:1:160:PRO:HD3	2.51	0.45
2:2:216:SER:OG	3:3:141:HIS:NE2	2.50	0.45
3:3:72:ARG:HD2	3:3:136:PRO:HG3	1.97	0.45
5:H:4:LEU:CD2	5:H:97:THR:CB	2.82	0.45
3:3:174:ALA:CB	3:3:179:ASN:ND2	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:191:HIS:O	3:3:191:HIS:CG	2.70	0.45
1:1:71:TYR:HE2	2:2:163:VAL:HG22	1.82	0.45
3:3:187:PHE:HD1	3:3:187:PHE:H	1.65	0.45
3:3:197:ASP:OD1	3:3:197:ASP:N	2.48	0.45
6:L:78:ILE:HG23	6:L:85:ASP:OD2	2.17	0.45
2:2:41:ASP:OD1	2:2:41:ASP:N	2.50	0.45
1:1:161:THR:HG22	5:H:136:GLY:HA2	1.98	0.45
5:H:107:THR:HG23	5:H:144:PHE:CZ	2.52	0.45
1:1:103:ASN:OD1	3:3:215:VAL:HG23	2.17	0.44
2:2:143:PHE:HB3	2:2:144:PRO:HD2	1.98	0.44
2:2:187:LEU:HG	2:2:188:THR:N	2.32	0.44
2:2:215:PRO:CB	3:3:142:CYS:SG	3.06	0.44
3:3:55:LEU:HD11	3:3:203:ALA:HB2	1.99	0.44
5:H:107:THR:CG2	5:H:144:PHE:CD2	2.99	0.44
6:L:6:LEU:HD12	6:L:7:THR:H	1.82	0.44
1:1:38:ARG:O	1:1:40:VAL:HG13	2.16	0.44
2:2:80:GLN:CD	2:2:129:LEU:HD11	2.42	0.44
3:3:176:GLU:OE2	3:3:176:GLU:HA	2.17	0.44
1:1:46:ASP:HB3	1:1:47:GLN:H	1.65	0.44
4:4:80:PHE:O	4:4:80:PHE:CD1	2.70	0.44
5:H:113:ARG:NE	5:H:131:CYS:SG	2.91	0.44
1:1:122:PRO:HG3	3:3:169:TYR:CE1	2.53	0.44
1:1:167:ALA:HB3	5:H:133:PHE:HZ	1.74	0.44
2:2:86:ASP:OD1	2:2:86:ASP:C	2.61	0.44
2:2:91:TYR:O	2:2:91:TYR:CD1	2.70	0.44
3:3:123:ILE:HD13	3:3:157:PHE:CD2	2.52	0.44
6:L:95:GLU:OE2	6:L:102:ASN:HB2	2.17	0.44
1:1:82:HIS:CE1	1:1:86:LEU:HD22	2.52	0.44
1:1:89:VAL:HB	1:1:98:LEU:CD2	2.47	0.44
1:1:95:GLU:C	1:1:95:GLU:CD	2.85	0.44
2:2:69:TRP:HH2	2:2:119:GLY:HA3	1.74	0.44
3:3:108:HIS:CG	3:3:156:THR:HG22	2.53	0.44
6:L:30:ASN:O	6:L:93:SER:CB	2.41	0.44
1:1:42:VAL:HG11	1:1:178:TYR:CE2	2.53	0.44
2:2:61:PHE:HD2	2:2:202:ASN:HB3	1.83	0.44
2:2:189:VAL:C	2:2:190:ASN:CG	2.85	0.44
1:1:87:THR:O	1:1:87:THR:OG1	2.33	0.44
1:1:130:TYR:CB	1:1:158:ALA:O	2.66	0.44
1:1:193:ALA:O	2:2:135:ARG:NE	2.51	0.44
2:2:67:PHE:CE1	2:2:181:VAL:HG11	2.53	0.44
2:2:83:LEU:HD21	2:2:203:ILE:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:22:CYS:HB2	5:H:96:ALA:HB1	2.00	0.44
6:L:93:SER:O	6:L:101:ALA:HA	2.18	0.44
1:1:53:LEU:N	1:1:53:LEU:HD22	2.33	0.44
3:3:49:GLU:OE1	3:3:49:GLU:HA	2.18	0.44
3:3:122:MET:HE2	3:3:187:PHE:HB2	2.00	0.44
3:3:212:ARG:HE	3:3:213:LEU:CD2	2.30	0.44
5:H:99:HIS:CE1	6:L:92:ALA:CA	2.95	0.44
3:3:109:PHE:CD2	3:3:201:VAL:HG12	2.53	0.43
5:H:35:GLY:N	5:H:96:ALA:O	2.44	0.43
6:L:12:VAL:HG21	6:L:109:LEU:HD23	1.94	0.43
2:2:62:PHE:HB3	2:2:87:HIS:CE1	2.49	0.43
5:H:2:VAL:HB	5:H:26:GLY:HA3	2.01	0.43
5:H:48:LEU:HD23	5:H:49:GLY:N	2.32	0.43
1:1:83:GLU:O	1:1:83:GLU:HG2	2.18	0.43
2:2:107:VAL:CG1	2:2:125:MET:HE2	2.48	0.43
3:3:55:LEU:HD13	3:3:201:VAL:HG23	2.00	0.43
1:1:73:PHE:O	1:1:73:PHE:CG	2.71	0.43
1:1:78:VAL:CG2	1:1:176:LEU:HD11	2.49	0.43
2:2:57:GLN:OE1	2:2:57:GLN:N	2.51	0.43
2:2:103:ASN:HD22	2:2:205:PRO:HB3	1.82	0.43
3:3:98:TYR:HE1	3:3:214:PRO:HB3	1.82	0.43
3:3:133:PRO:HG3	3:3:139:ALA:HB2	2.01	0.43
4:4:35:ASP:OD1	4:4:36:THR:N	2.51	0.43
2:2:58:ALA:HA	2:2:90:VAL:HG12	2.00	0.43
1:1:8:ALA:HB3	2:2:145:HIS:O	2.19	0.43
5:H:131:CYS:O	5:H:131:CYS:SG	2.76	0.43
1:1:95:GLU:HG3	5:H:131:CYS:O	2.19	0.43
2:2:87:HIS:CD2	2:2:89:GLY:H	2.37	0.43
2:2:102:ARG:HH21	2:2:162:PHE:HD2	1.66	0.43
1:1:70:THR:HG22	1:1:189:ARG:CD	2.48	0.43
1:1:88:TRP:CG	1:1:89:VAL:N	2.87	0.43
2:2:63:LYS:O	2:2:64:THR:OG1	2.36	0.43
2:2:83:LEU:CD2	2:2:203:ILE:CD1	2.89	0.43
3:3:91:LEU:HA	3:3:91:LEU:HD12	1.74	0.43
6:L:80:SER:O	6:L:82:GLN:HG3	2.19	0.43
1:1:102:THR:CB	3:3:216:ASP:HB2	2.49	0.43
1:1:114:ARG:C	1:1:115:LEU:HD12	2.44	0.43
1:1:157:ARG:HA	1:1:157:ARG:HD2	1.59	0.43
2:2:78:CYS:HB3	2:2:182:MET:HG3	2.00	0.43
2:2:142:LEU:HA	2:2:142:LEU:HD23	1.77	0.43
1:1:112:LEU:N	1:1:112:LEU:CD2	2.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:17:THR:OG1	2:2:18:ARG:N	2.52	0.43
5:H:107:THR:HG22	5:H:144:PHE:CD2	2.53	0.43
5:H:113:ARG:HD2	5:H:116:CYS:SG	2.59	0.43
6:L:27:SER:H	6:L:30:ASN:ND2	2.13	0.43
3:3:120:ARG:CG	3:3:189:ILE:HD11	2.48	0.42
3:3:140:ALA:O	3:3:144:HIS:CD2	2.72	0.42
5:H:45:LEU:HD23	6:L:104:GLY:HA2	2.01	0.42
1:1:162:SER:OG	3:3:169:TYR:OH	2.35	0.42
1:1:89:VAL:CG1	1:1:98:LEU:CD2	2.96	0.42
1:1:190:PRO:HD3	2:2:143:PHE:CZ	2.54	0.42
2:2:55:VAL:HG21	2:2:94:LEU:CD2	2.48	0.42
2:2:102:ARG:CG	2:2:209:HIS:HB2	2.48	0.42
3:3:53:THR:O	3:3:202:LEU:HA	2.19	0.42
3:3:166:ASP:OD1	3:3:166:ASP:N	2.50	0.42
3:3:180:VAL:O	3:3:180:VAL:HG12	2.19	0.42
6:L:12:VAL:CG2	6:L:109:LEU:HD23	2.48	0.42
2:2:15:LEU:HD11	2:2:32:VAL:HG23	2.02	0.42
2:2:33:THR:HB	2:2:146:GLN:NE2	2.33	0.42
3:3:74:LEU:HD11	3:3:188:GLN:HB3	2.01	0.42
3:3:99:THR:O	3:3:170:THR:N	2.33	0.42
5:H:63:LEU:O	5:H:67:LEU:HG	2.20	0.42
6:L:41:LEU:HB2	6:L:88:GLU:HB2	2.00	0.42
1:1:100:ASN:ND2	3:3:216:ASP:O	2.29	0.42
5:H:126:ALA:HB1	5:H:143:PRO:CA	2.49	0.42
6:L:36:VAL:HG13	6:L:91:CYS:SG	2.59	0.42
3:3:72:ARG:CD	3:3:136:PRO:HG3	2.50	0.42
6:L:42:ILE:HA	6:L:87:ALA:CB	2.49	0.42
1:1:34:PHE:O	1:1:34:PHE:CD1	2.71	0.42
2:2:215:PRO:HA	3:3:142:CYS:SG	2.59	0.42
1:1:126:LEU:CD2	1:1:163:PHE:HB3	2.27	0.42
1:1:127:ALA:HB2	2:2:165:VAL:CG1	2.49	0.42
3:3:109:PHE:CZ	3:3:186:LEU:CD2	2.93	0.42
3:3:189:ILE:H	3:3:189:ILE:HG13	1.54	0.42
5:H:23:THR:HA	5:H:76:ASN:O	2.20	0.42
1:1:78:VAL:HG22	1:1:79:ALA:N	2.35	0.42
1:1:95:GLU:HB2	5:H:132:ASN:HA	2.02	0.42
2:2:25:THR:O	2:2:25:THR:HG23	2.17	0.42
1:1:78:VAL:HG21	1:1:168:ILE:CD1	2.50	0.42
1:1:130:TYR:CB	1:1:159:LEU:HA	2.50	0.42
2:2:43:VAL:HG23	2:2:102:ARG:HD3	2.01	0.42
3:3:69:ASP:OD1	3:3:70:SER:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:33:SER:O	1:1:37:ASP:OD2	2.38	0.41
1:1:90:PRO:HB3	3:3:213:LEU:HD12	2.02	0.41
2:2:107:VAL:HG11	2:2:125:MET:CE	2.49	0.41
2:2:189:VAL:HG12	2:2:190:ASN:N	2.35	0.41
3:3:45:LEU:CD1	3:3:210:GLU:HA	2.49	0.41
3:3:109:PHE:CE2	3:3:186:LEU:HD22	2.38	0.41
5:H:72:ASP:HB3	5:H:77:GLN:O	2.19	0.41
2:2:43:VAL:HG21	2:2:209:HIS:CD2	2.55	0.41
6:L:50:LEU:O	6:L:51:ILE:HG13	2.20	0.41
2:2:84:PRO:HA	2:2:105:TRP:CH2	2.55	0.41
2:2:86:ASP:O	2:2:86:ASP:CG	2.63	0.41
2:2:128:GLU:OE2	2:2:174:HIS:HE1	2.03	0.41
6:L:64:ARG:HD2	6:L:82:GLN:HE22	1.85	0.41
3:3:56:HIS:CE1	3:3:60:ASP:HA	2.56	0.41
3:3:60:ASP:O	3:3:60:ASP:CG	2.64	0.41
5:H:110:ARG:HG3	5:H:138:TYR:CZ	2.54	0.41
1:1:112:LEU:O	3:3:10:GLY:HA3	2.19	0.41
1:1:126:LEU:HD23	1:1:163:PHE:CA	2.50	0.41
1:1:161:THR:HG21	5:H:130:TYR:CE2	2.56	0.41
2:2:67:PHE:HE1	2:2:181:VAL:HG11	1.85	0.41
1:1:29:HIS:HA	1:1:34:PHE:CE2	2.55	0.41
3:3:69:ASP:CG	3:3:70:SER:H	2.28	0.41
1:1:70:THR:HG22	1:1:189:ARG:HD2	2.03	0.41
2:2:73:ASP:OD1	2:2:77:ARG:HD3	2.21	0.41
2:2:141:THR:OG1	2:2:145:HIS:NE2	2.54	0.41
3:3:45:LEU:CD1	3:3:210:GLU:HG3	2.51	0.41
3:3:63:TYR:CA	3:3:199:LEU:O	2.68	0.41
3:3:91:LEU:HD11	3:3:209:PHE:CE2	2.56	0.41
3:3:135:THR:CA	3:3:187:PHE:CE2	3.02	0.41
3:3:136:PRO:O	3:3:137:GLU:HG2	2.21	0.41
5:H:17:THR:O	5:H:17:THR:HG23	2.21	0.41
1:1:100:ASN:C	1:1:102:THR:H	2.29	0.41
1:1:100:ASN:HD21	3:3:217:ALA:C	2.29	0.41
2:2:99:ALA:CB	2:2:214:PHE:CE1	2.93	0.41
3:3:185:CYS:CB	3:3:187:PHE:CE1	3.02	0.41
2:2:58:ALA:HA	2:2:90:VAL:HG11	2.03	0.40
2:2:103:ASN:OD1	2:2:103:ASN:N	2.54	0.40
5:H:113:ARG:HD2	5:H:116:CYS:CB	2.51	0.40
2:2:163:VAL:HG12	2:2:177:TRP:CZ2	2.55	0.40
1:1:5:GLY:C	1:1:7:SER:N	2.79	0.40
1:1:167:ALA:CB	5:H:133:PHE:CE1	3.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:189:VAL:CG2	2:2:194:ALA:O	2.69	0.40
6:L:92:ALA:HB2	6:L:103:PHE:CD2	2.56	0.40
1:1:58:ALA:HA	1:1:63:GLY:O	2.21	0.40
2:2:32:VAL:HG22	2:2:157:HIS:ND1	2.37	0.40
2:2:107:VAL:HG11	2:2:125:MET:HE2	2.03	0.40
6:L:36:VAL:HG11	6:L:74:ALA:HB1	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	1	179/213 (84%)	161 (90%)	18 (10%)	0	100	100
2	2	204/218 (94%)	181 (89%)	23 (11%)	0	100	100
3	3	217/220 (99%)	201 (93%)	16 (7%)	0	100	100
4	4	42/85 (49%)	36 (86%)	6 (14%)	0	100	100
5	H	143/167 (86%)	136 (95%)	6 (4%)	1 (1%)	18	53
6	L	106/123 (86%)	101 (95%)	5 (5%)	0	100	100
All	All	891/1026 (87%)	816 (92%)	74 (8%)	1 (0%)	49	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	H	123	PRO

5.3.2 Protein sidechains [i](#)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	153/178 (86%)	146 (95%)	7 (5%)	24	48
2	2	178/190 (94%)	160 (90%)	18 (10%)	7	26
3	3	174/175 (99%)	159 (91%)	15 (9%)	10	33
4	4	37/67 (55%)	36 (97%)	1 (3%)	39	60
5	H	115/141 (82%)	110 (96%)	5 (4%)	26	49
6	L	88/98 (90%)	88 (100%)	0	100	100
All	All	745/849 (88%)	699 (94%)	46 (6%)	18	42

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	55	GLN
1	1	99	ASP
1	1	112	LEU
1	1	128	THR
1	1	154	LYS
1	1	157	ARG
1	1	169	LYS
2	2	48	THR
2	2	85	THR
2	2	95	THR
2	2	97	SER
2	2	98	TYR
2	2	100	TYR
2	2	101	MET
2	2	107	VAL
2	2	108	GLU
2	2	112	VAL
2	2	121	LEU
2	2	133	ASP
2	2	147	PHE
2	2	179	LEU
2	2	182	MET
2	2	190	ASN
2	2	191	THR
2	2	196	GLN
3	3	7	CYS

Continued on next page...

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Mol	Chain	Res	Type
3	3	8	SER
3	3	29	VAL
3	3	46	ASP
3	3	47	VAL
3	3	53	THR
3	3	137	GLU
3	3	170	THR
3	3	173	ASP
3	3	178	THR
3	3	184	VAL
3	3	186	LEU
3	3	189	ILE
3	3	195	ASP
3	3	199	LEU
4	4	83	LEU
5	H	105	LYS
5	H	107	THR
5	H	119	ARG
5	H	132	ASN
5	H	144	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	47	GLN
1	1	82	HIS
1	1	108	HIS
2	2	47	ASN
2	2	65	HIS
2	2	87	HIS
2	2	103	ASN
2	2	117	ASN
2	2	146	GLN
2	2	174	HIS
3	3	85	HIS
3	3	179	ASN
5	H	99	HIS
5	H	100	GLN
6	L	8	GLN
6	L	18	GLN
6	L	30	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 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.

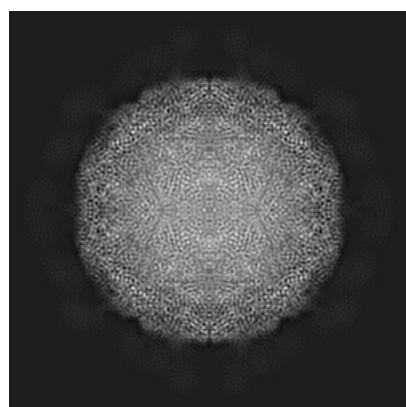
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30560. These allow visual inspection of the internal detail of the map and identification of artifacts.

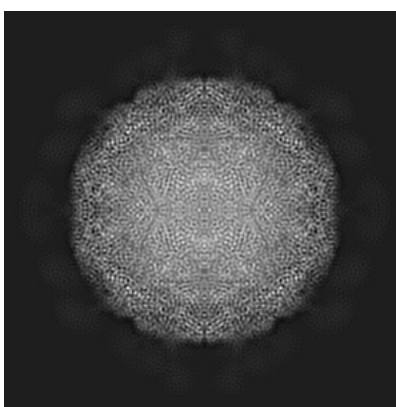
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

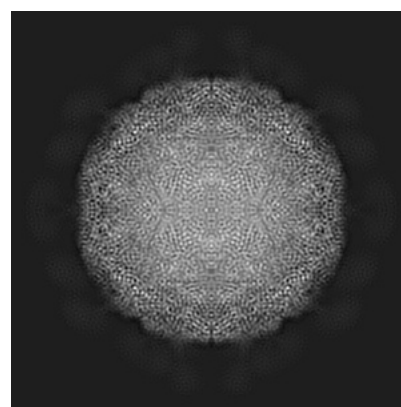
6.1.1 Primary map



X



Y

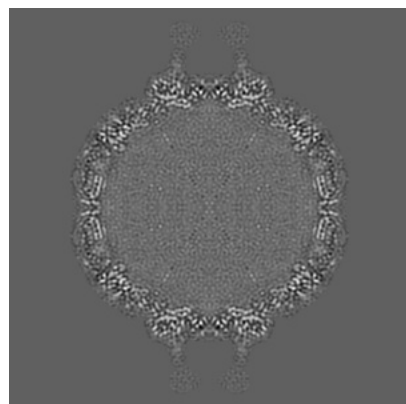


Z

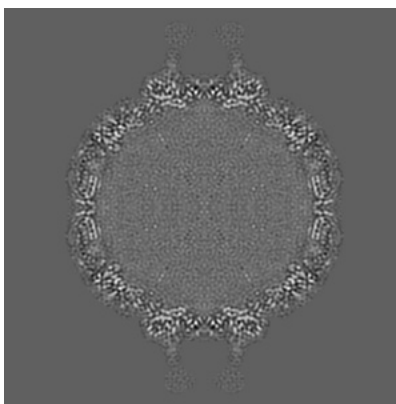
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

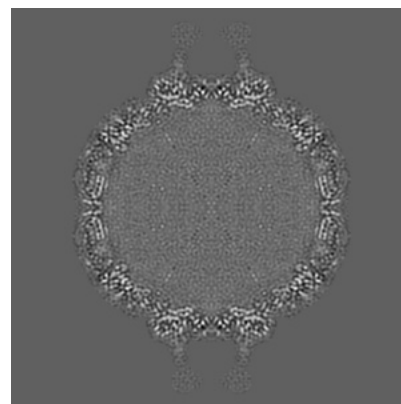
6.2.1 Primary map



X Index: 230



Y Index: 230

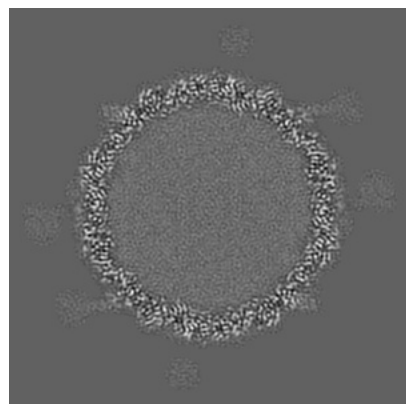


Z Index: 230

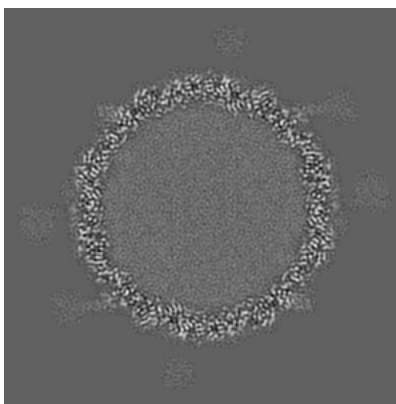
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

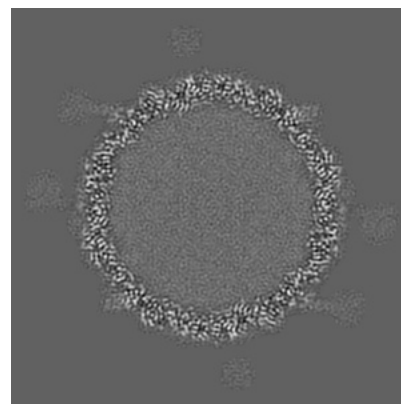
6.3.1 Primary map



X Index: 261



Y Index: 261

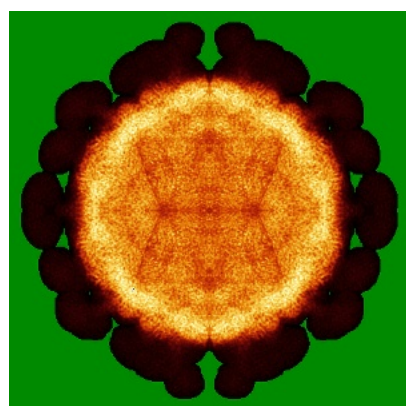


Z Index: 199

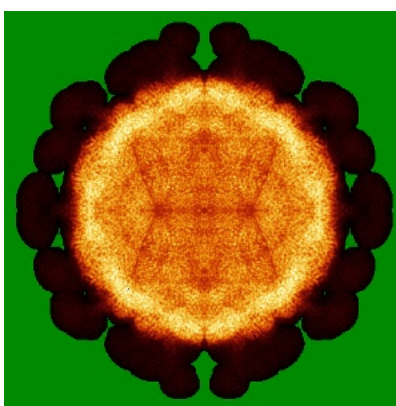
The images above show the largest variance slices of the map in three orthogonal directions.

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

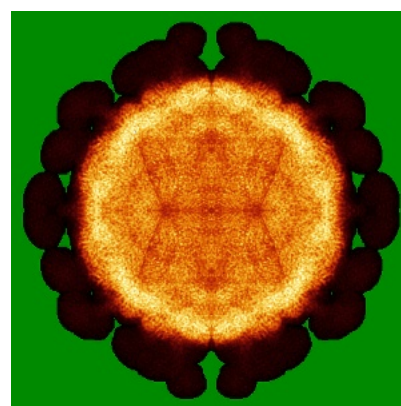
6.4.1 Primary map



X



Y

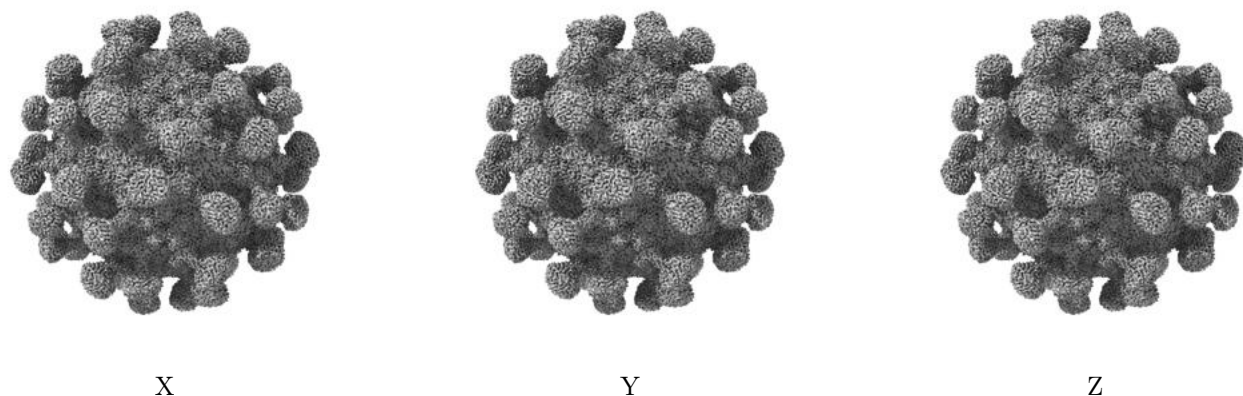


Z

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 0.0032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

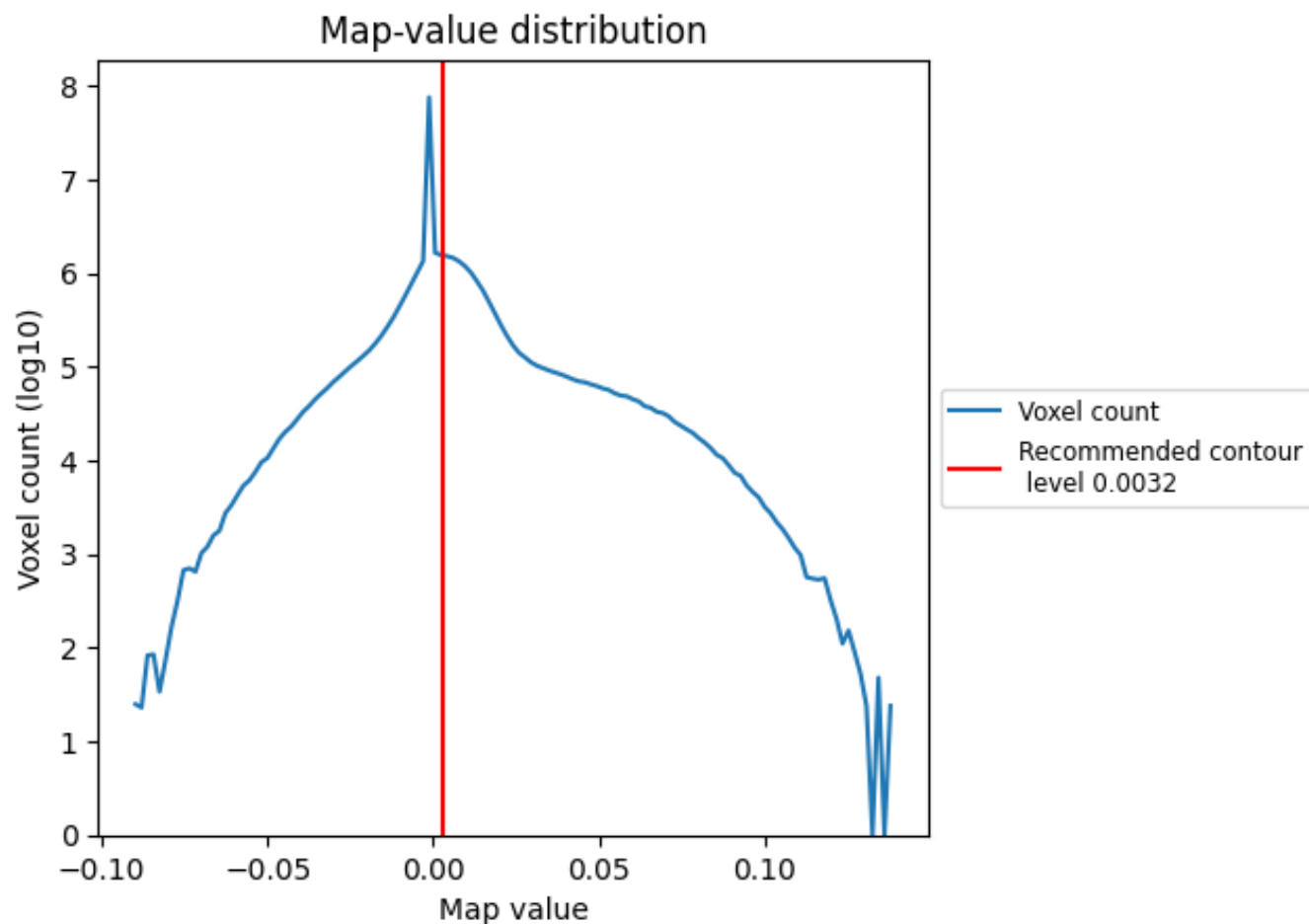
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

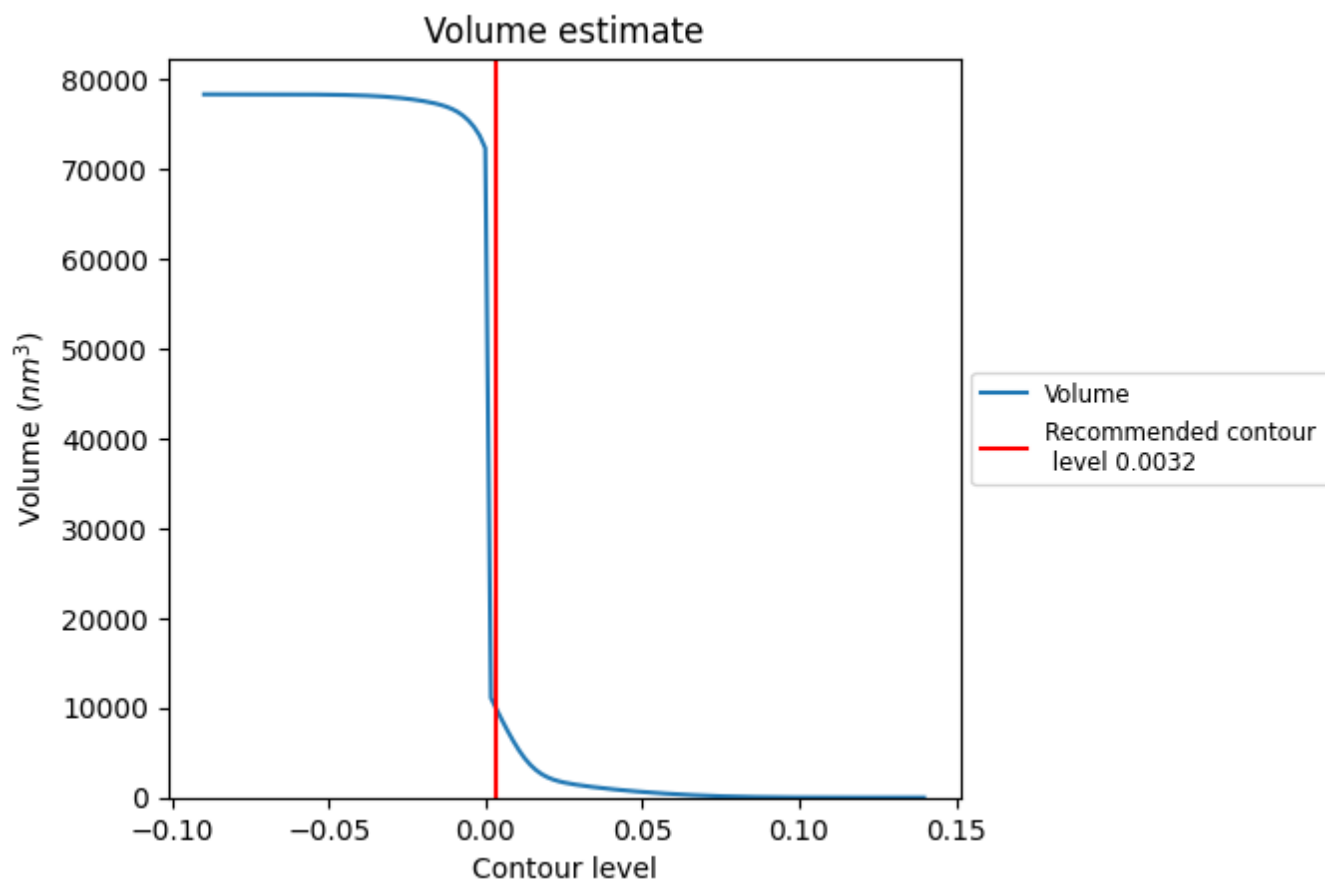
This section contains the results of statistical analysis of the map.

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.

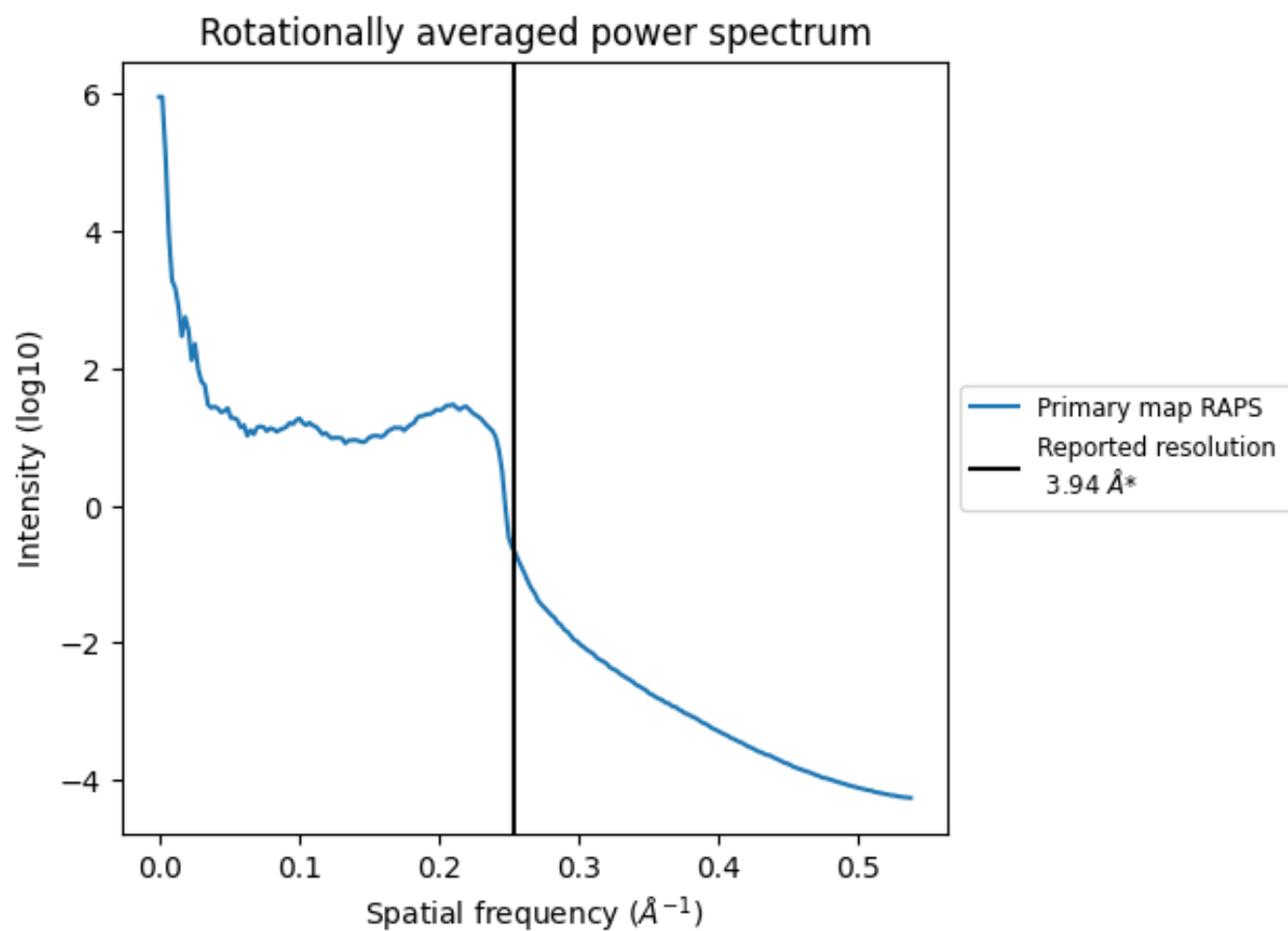
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 10018 nm^3 ; this corresponds to an approximate mass of 9050 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 0.254 Å⁻¹

8 Fourier-Shell correlation ⓘ

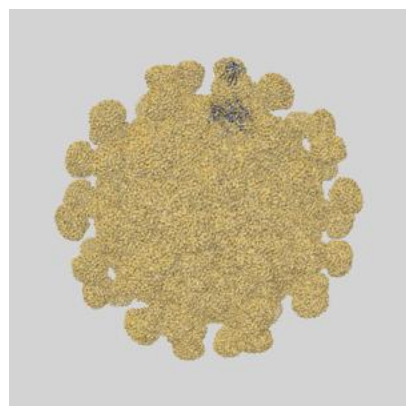
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

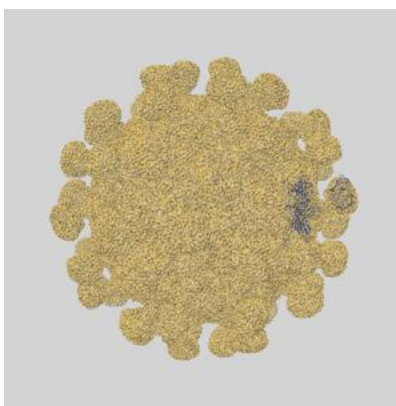
This section contains information regarding the fit between EMDB map EMD-30560 and PDB model 7D3M. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

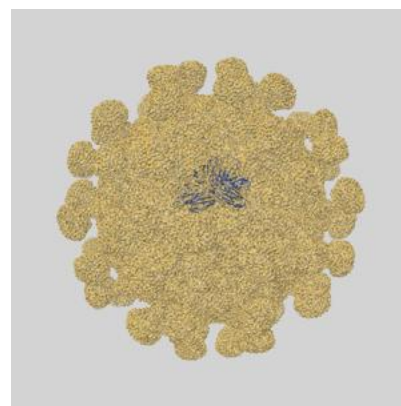
9.1.1 Map-model overlay [i](#)



X

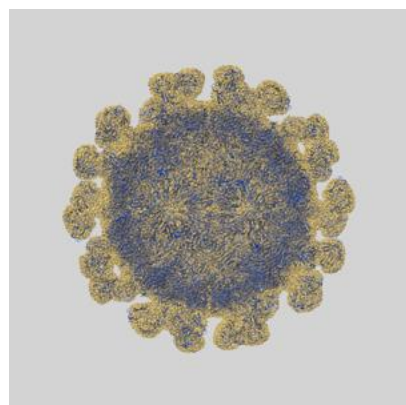


Y

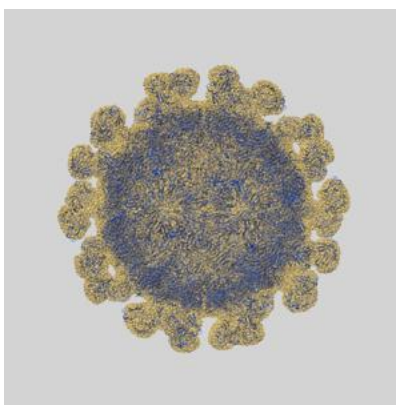


Z

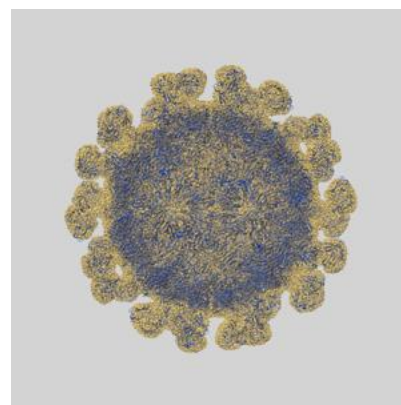
9.1.2 Map-model assembly overlay [i](#)



X



Y



Z

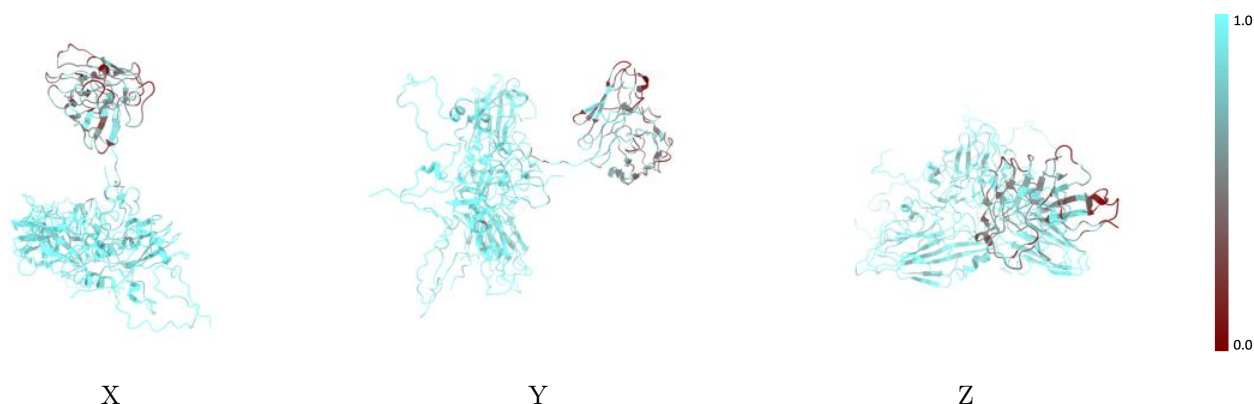
The images above show the 3D surface view of the map at the recommended contour level 0.0032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



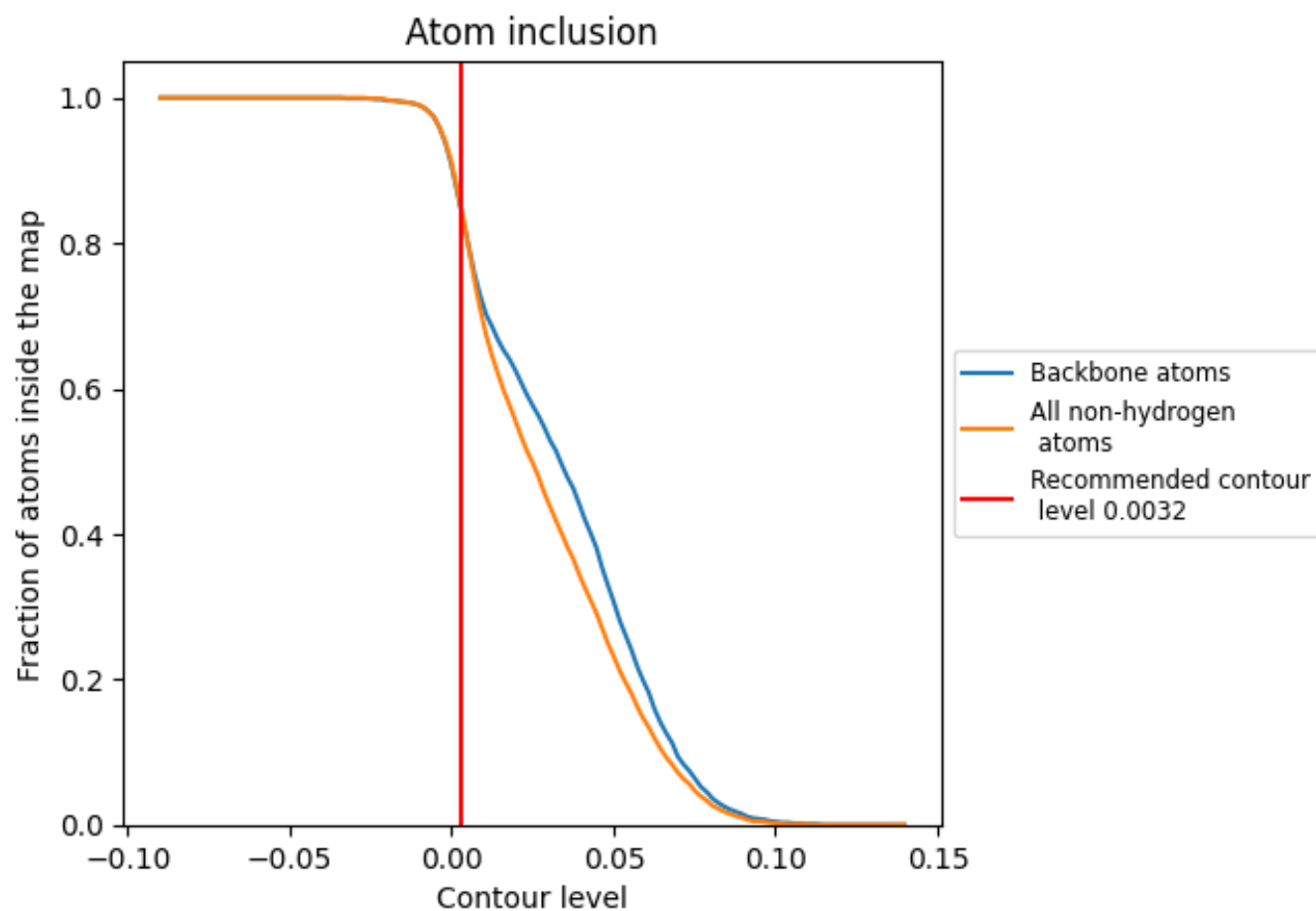
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0032).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (0.0032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8430	0.3430
1	0.9230	0.4070
2	0.9240	0.4040
3	0.9310	0.3980
4	0.9230	0.3940
H	0.6490	0.2020
L	0.5680	0.1540

1.0

0.0

<0.0