



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:23 PM UTC

PDB ID : 7D3R / pdb_00007d3r
EMDB ID : EMD-30565
Title : FOOT AND MOUTH DISEASE VIRUS A/WH/CHA/09-BOUND THE SINGLE CHAIN FRAGME ANTIBODY R50
Authors : He, Y.; Lou, Z.
Deposited on : 2020-09-20
Resolution : 3.49 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:

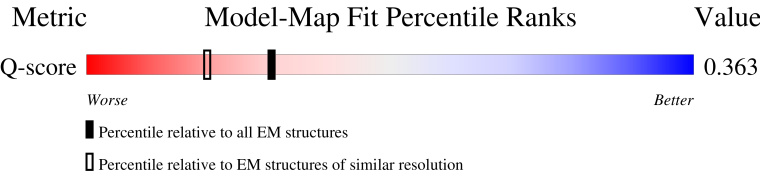
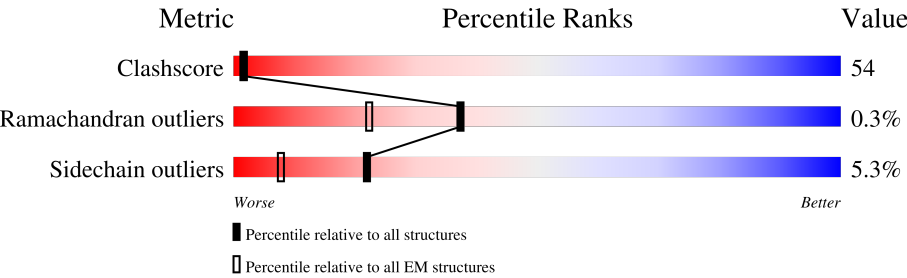
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.49 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	13600 (2.99 - 3.99)

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	36% 44% 8% 12%
2	2	218	50% 39% 6% 6%
3	3	221	53% 37% 8% .
4	4	85	40% 11% . 47%

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Mol	Chain	Length	Quality of chain
5	H	167	27% 24% 45% 17% 14%
6	L	123	49% 37% 44% 7% 12%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6976 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 A/WH/CHA/09 VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	186	Total	C	N	O	S	0	0
			1460	921	264	270	5		

- Molecule 2 is a protein called A/WH/CHA/09 VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	206	Total	C	N	O	S	0	0
			1633	1040	281	307	5		

- Molecule 3 is a protein called A/WH/CHA/09 VP3.

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

- Molecule 4 is a protein called A/WH/CHA/09 VP4.

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

- Molecule 5 is a protein called R50 VH.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	144	Total	C	N	O	S	0	0
			1067	654	194	211	8		

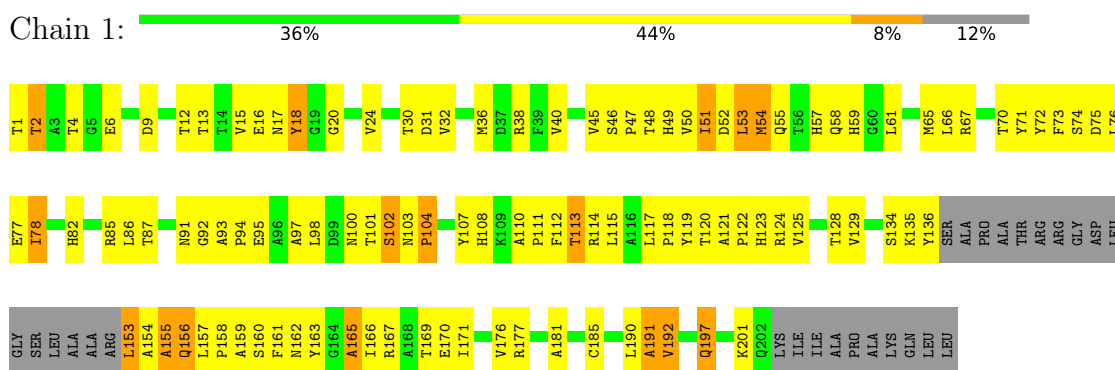
- Molecule 6 is a protein called R50 VL.

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.

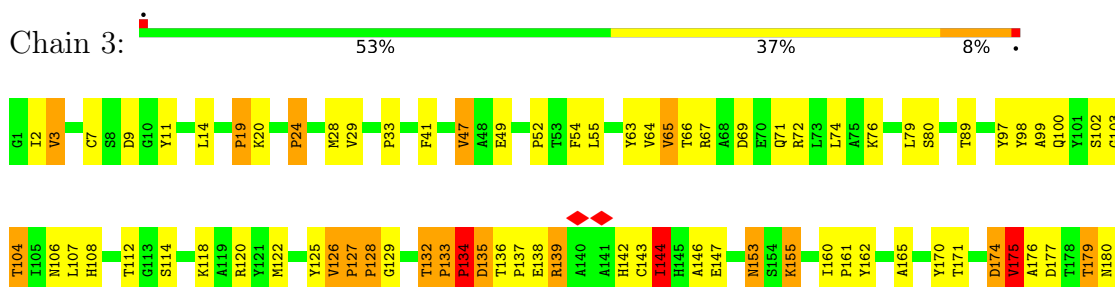
• Molecule 1: A/WH/CHA/09 VP1



• Molecule 2: A/WH/CHA/09 VP2

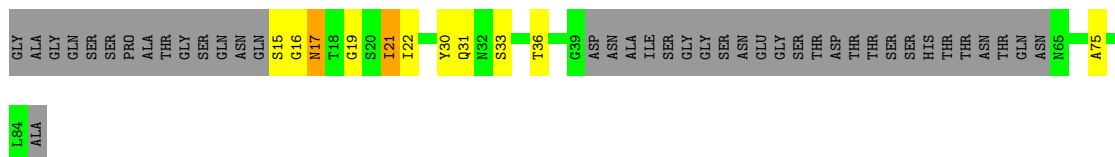
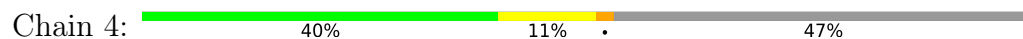


• Molecule 3: A/WH/CHA/09 VP3

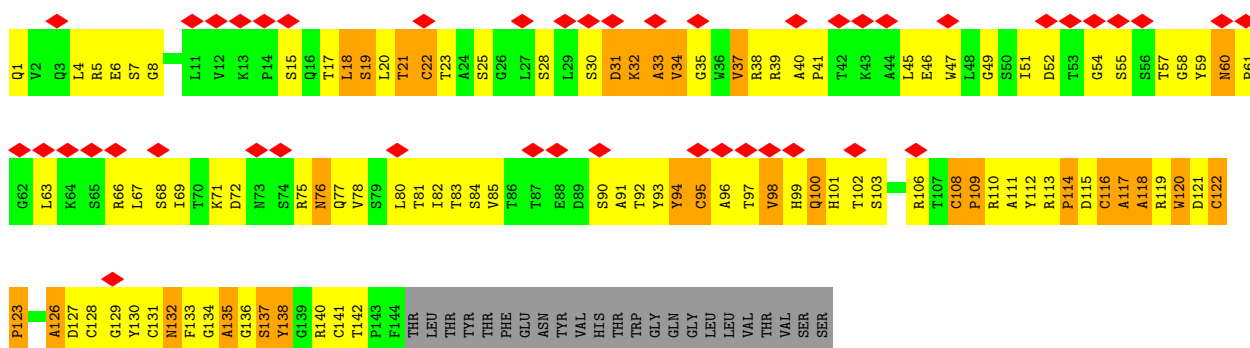
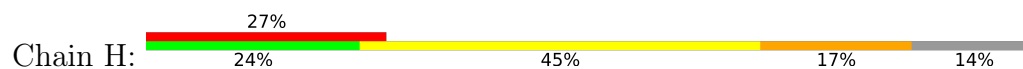




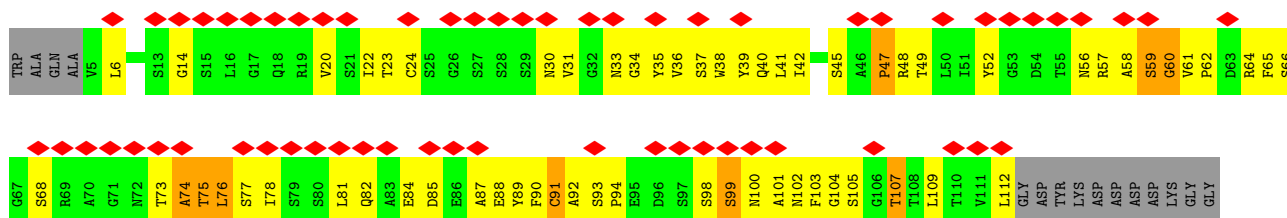
• Molecule 4: A/WH/CHA/09 VP4



• 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	0.128	Depositor
Minimum map value	-0.075	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.003	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 [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.73	0/1495	1.25	21/2040 (1.0%)
2	2	0.92	1/1678 (0.1%)	1.18	9/2284 (0.4%)
3	3	1.06	7/1739 (0.4%)	1.67	37/2381 (1.6%)
4	4	0.45	0/354	1.01	3/476 (0.6%)
5	H	1.01	5/1090 (0.5%)	2.10	49/1485 (3.3%)
6	L	0.48	0/790	1.23	15/1076 (1.4%)
All	All	0.88	13/7146 (0.2%)	1.49	134/9742 (1.4%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	128	PRO	N-CA	19.15	1.70	1.47
5	H	114	PRO	N-CA	17.64	1.70	1.47
3	3	134	PRO	N-CA	17.60	1.69	1.47
3	3	132	THR	C-N	14.58	1.50	1.33
5	H	108	CYS	C-N	13.25	1.50	1.33
3	3	127	PRO	N-CA	11.42	1.70	1.46
3	3	126	VAL	C-N	10.42	1.45	1.33
2	2	205	PRO	N-CD	9.93	1.61	1.47
3	3	127	PRO	C-N	9.01	1.45	1.33
5	H	122	CYS	C-N	7.29	1.50	1.33
5	H	123	PRO	N-CD	5.17	1.54	1.47
3	3	133	PRO	C-N	5.02	1.45	1.33
5	H	113	ARG	C-N	5.01	1.45	1.33

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	25	SER	N-CA-C	28.49	148.56	113.23
3	3	174	ASP	CB-CA-C	-18.85	78.79	111.22
3	3	126	VAL	CA-C-N	18.31	139.24	120.38
3	3	126	VAL	C-N-CA	18.31	139.24	120.38
3	3	127	PRO	CA-C-N	18.14	138.39	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	127	PRO	C-N-CA	18.14	138.39	119.89
3	3	132	THR	CA-C-N	17.93	138.85	120.38
3	3	132	THR	C-N-CA	17.93	138.85	120.38
3	3	104	THR	N-CA-C	17.91	133.63	110.53
5	H	108	CYS	CA-C-N	17.15	138.27	119.92
5	H	108	CYS	C-N-CA	17.15	138.27	119.92
6	L	59	SER	N-CA-C	-16.95	88.23	110.43
3	3	104	THR	N-CA-CB	-16.83	86.37	110.44
3	3	133	PRO	CA-C-N	16.43	140.38	119.84
3	3	133	PRO	C-N-CA	16.43	140.38	119.84
5	H	113	ARG	CA-C-N	15.72	139.49	119.84
5	H	113	ARG	C-N-CA	15.72	139.49	119.84
1	1	156	GLN	N-CA-C	12.59	128.68	108.41
5	H	34	VAL	N-CA-C	12.26	125.92	109.37
5	H	122	CYS	CA-C-N	12.09	134.95	119.84
5	H	122	CYS	C-N-CA	12.09	134.95	119.84
3	3	175	VAL	CB-CA-C	11.51	130.16	111.29
5	H	118	ALA	N-CA-C	-11.11	99.54	112.87
5	H	109	PRO	CB-CA-C	-11.04	96.88	111.12
5	H	31	ASP	N-CA-C	-10.95	99.76	113.55
5	H	95	CYS	N-CA-C	10.79	125.77	109.25
3	3	144	ILE	N-CA-C	-10.77	92.44	108.17
5	H	98	VAL	CA-C-N	10.73	135.73	120.28
5	H	98	VAL	C-N-CA	10.73	135.73	120.28
5	H	18	LEU	N-CA-C	-10.37	95.19	110.23
3	3	20	LYS	N-CA-C	10.15	122.90	110.41
1	1	156	GLN	N-CA-CB	-10.07	94.19	110.21
1	1	170	GLU	N-CA-C	-9.93	90.63	107.80
6	L	59	SER	CB-CA-C	9.88	130.11	109.65
1	1	54	MET	N-CA-CB	9.75	126.97	110.49
3	3	134	PRO	CA-N-CD	-9.59	98.57	112.00
5	H	25	SER	CB-CA-C	-9.59	90.09	109.55
5	H	114	PRO	CA-N-CD	-9.10	99.26	112.00
5	H	110	ARG	N-CA-C	9.05	123.33	111.75
1	1	155	ALA	CB-CA-C	9.01	127.94	110.46
1	1	165	ALA	N-CA-CB	-8.92	96.58	110.85
6	L	99	SER	N-CA-C	8.88	123.81	111.92
3	3	127	PRO	CA-N-CD	-8.84	99.63	112.00
5	H	33	ALA	CA-C-N	8.68	132.17	120.63
5	H	33	ALA	C-N-CA	8.68	132.17	120.63
1	1	192	VAL	N-CA-C	8.62	120.60	109.30
5	H	18	LEU	CB-CA-C	8.51	123.85	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	135	ALA	CB-CA-C	8.41	123.24	109.70
2	2	204	ALA	CB-CA-C	8.39	122.76	108.91
1	1	55	GLN	N-CA-C	-8.32	103.14	113.38
5	H	135	ALA	N-CA-C	-8.22	98.65	110.24
5	H	100	GLN	N-CA-C	8.20	122.31	110.10
1	1	171	ILE	N-CA-C	-8.19	96.65	108.36
5	H	99	HIS	CB-CA-C	8.16	125.73	110.63
5	H	30	SER	CB-CA-C	-8.11	95.75	109.38
4	4	75	ALA	N-CA-C	8.10	122.16	110.10
3	3	103	GLY	N-CA-C	-8.05	94.10	113.18
6	L	60	GLY	N-CA-C	8.03	127.45	115.08
3	3	24	PRO	CB-CA-C	7.88	120.15	111.56
3	3	128	PRO	CA-N-CD	-7.83	101.03	112.00
5	H	76	ASN	CB-CA-C	-7.54	100.80	111.80
3	3	19	PRO	N-CA-C	7.49	123.18	114.20
5	H	136	GLY	N-CA-C	-7.25	100.55	111.14
5	H	39	ARG	N-CA-C	7.25	120.71	108.90
1	1	201	LYS	N-CA-C	7.21	121.37	112.58
5	H	117	ALA	N-CA-C	-7.04	103.19	114.09
2	2	205	PRO	N-CA-C	-7.02	98.00	112.47
5	H	95	CYS	N-CA-CB	-6.80	98.79	109.87
5	H	60	ASN	N-CA-C	6.79	119.26	109.48
1	1	53	LEU	CB-CA-C	-6.77	96.89	111.78
1	1	170	GLU	CB-CA-C	6.73	120.45	110.62
1	1	54	MET	N-CA-C	-6.71	96.51	110.80
5	H	116	CYS	CA-C-N	6.71	132.10	121.44
5	H	116	CYS	C-N-CA	6.71	132.10	121.44
6	L	75	THR	CB-CA-C	-6.70	95.66	109.94
3	3	98	TYR	N-CA-C	6.69	120.95	110.32
5	H	33	ALA	CB-CA-C	-6.54	98.01	111.22
6	L	73	THR	CB-CA-C	-6.48	96.51	110.45
5	H	121	ASP	CB-CA-C	6.43	120.05	110.14
5	H	33	ALA	N-CA-C	-6.39	100.49	109.69
2	2	213	GLU	N-CA-C	6.37	120.07	110.64
5	H	116	CYS	N-CA-C	-6.37	106.22	112.97
1	1	191	ALA	N-CA-C	6.29	118.41	110.24
6	L	56	ASN	CA-C-N	6.27	132.39	122.36
6	L	56	ASN	C-N-CA	6.27	132.39	122.36
3	3	171	THR	CB-CA-C	-6.26	101.00	110.90
1	1	102	SER	N-CA-C	-6.26	106.61	114.56
3	3	146	ALA	N-CA-CB	-6.18	101.60	111.62
3	3	175	VAL	CA-C-O	-6.18	113.06	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	94	TYR	CB-CA-C	6.14	122.46	110.67
4	4	17	ASN	N-CA-C	6.14	119.61	111.75
5	H	126	ALA	N-CA-CB	-6.08	101.29	110.35
6	L	74	ALA	N-CA-CB	-6.07	101.94	111.05
1	1	169	THR	N-CA-C	6.02	118.37	111.02
6	L	76	LEU	N-CA-CB	-6.01	101.46	111.20
6	L	76	LEU	CB-CA-C	5.98	121.26	109.66
6	L	107	THR	N-CA-CB	-5.97	101.25	110.56
5	H	122	CYS	CB-CA-C	-5.86	98.63	110.17
3	3	14	LEU	N-CA-C	5.85	117.83	108.41
4	4	17	ASN	CB-CA-C	5.83	121.76	110.46
2	2	144	PRO	N-CA-C	-5.75	102.18	111.03
5	H	127	ASP	CB-CA-C	-5.73	98.16	109.67
2	2	116	PHE	N-CA-C	-5.69	105.67	113.30
5	H	39	ARG	N-CA-CB	-5.68	101.14	110.68
1	1	155	ALA	N-CA-C	-5.67	104.50	111.75
3	3	134	PRO	CB-CA-C	-5.67	102.21	111.56
3	3	219	ARG	N-CA-C	-5.67	101.52	109.96
3	3	174	ASP	CA-C-N	5.66	132.16	121.97
3	3	174	ASP	C-N-CA	5.66	132.16	121.97
5	H	22	CYS	N-CA-CB	-5.65	101.72	111.55
6	L	91	CYS	CB-CA-C	-5.65	98.30	110.45
2	2	205	PRO	CA-N-CD	-5.59	104.17	112.00
6	L	31	VAL	N-CA-C	-5.54	106.40	111.67
1	1	165	ALA	N-CA-C	5.50	118.70	109.95
1	1	104	PRO	CB-CA-C	5.48	118.60	111.64
5	H	37	VAL	CB-CA-C	-5.48	102.31	111.29
1	1	38	ARG	N-CA-C	5.45	117.90	110.55
3	3	139	ARG	N-CA-C	5.44	120.02	113.17
5	H	32	LYS	O-C-N	-5.43	115.98	122.65
5	H	19	SER	N-CA-CB	5.39	119.89	111.64
3	3	98	TYR	N-CA-CB	-5.37	101.66	110.41
5	H	127	ASP	N-CA-C	5.29	119.83	112.90
3	3	135	ASP	N-CA-C	-5.29	101.54	109.95
3	3	47	VAL	N-CA-C	-5.28	107.27	111.81
2	2	38	THR	N-CA-C	-5.26	106.88	113.72
6	L	56	ASN	N-CA-C	5.25	115.32	108.07
2	2	204	ALA	N-CA-C	-5.24	99.97	108.82
5	H	21	THR	CB-CA-C	-5.20	98.64	110.07
3	3	139	ARG	N-CA-CB	-5.17	102.84	110.49
3	3	171	THR	N-CA-C	5.14	116.69	111.14
3	3	144	ILE	N-CA-CB	5.12	119.87	111.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	192	VAL	CB-CA-C	-5.03	103.76	111.71
2	2	205	PRO	N-CA-CB	5.02	108.52	103.25
3	3	20	LYS	N-CA-CB	-5.01	103.52	110.38

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	1460	0	1448	221	0
2	2	1633	0	1593	139	0
3	3	1691	0	1620	166	0
4	4	348	0	321	13	0
5	H	1067	0	1016	254	0
6	L	777	0	734	130	0
All	All	6976	0	6732	744	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 54.

All (744) 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:100:GLN:HB2	6:L:101:ALA:CB	1.25	1.67
1:1:158:PRO:HD2	1:1:161:PHE:CE2	1.17	1.66
5:H:98:VAL:HG22	6:L:103:PHE:CE1	1.14	1.62
6:L:34:GLY:HA3	6:L:94:PRO:CD	1.22	1.58
1:1:158:PRO:CG	1:1:161:PHE:HE2	1.15	1.57
5:H:35:GLY:CA	5:H:98:VAL:HG23	1.33	1.56
1:1:158:PRO:CD	1:1:161:PHE:CE2	1.81	1.53
5:H:98:VAL:HG22	6:L:103:PHE:CZ	1.43	1.51
3:3:128:PRO:N	3:3:128:PRO:CA	1.70	1.49
3:3:134:PRO:N	3:3:134:PRO:CA	1.69	1.45
3:3:80:SER:CB	3:3:180:ASN:HD22	1.28	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:114:PRO:N	5:H:114:PRO:CA	1.69	1.40
5:H:100:GLN:CB	6:L:101:ALA:HB1	1.53	1.38
3:3:127:PRO:N	3:3:127:PRO:CA	1.70	1.37
5:H:95:CYS:SG	6:L:41:LEU:HD13	1.64	1.37
1:1:82:HIS:CE1	1:1:113:THR:HG21	1.58	1.36
6:L:34:GLY:CA	6:L:94:PRO:CD	2.01	1.36
1:1:82:HIS:CE1	1:1:113:THR:CG2	2.08	1.36
5:H:98:VAL:CG2	6:L:103:PHE:CE1	2.09	1.34
1:1:158:PRO:CG	1:1:161:PHE:CE2	2.06	1.31
5:H:100:GLN:NE2	6:L:35:TYR:O	1.61	1.31
1:1:158:PRO:CD	1:1:161:PHE:HE2	1.24	1.30
6:L:36:VAL:HG13	6:L:91:CYS:SG	1.71	1.29
1:1:135:LYS:NZ	1:1:158:PRO:HB3	1.48	1.27
5:H:35:GLY:HA2	5:H:98:VAL:CG2	1.65	1.26
5:H:41:PRO:HD3	5:H:90:SER:O	1.11	1.26
5:H:98:VAL:CG2	6:L:103:PHE:CZ	2.18	1.25
2:2:37:SER:OG	2:2:161:PRO:HG3	1.38	1.23
2:2:105:TRP:CD1	2:2:177:TRP:HB2	1.74	1.23
5:H:95:CYS:SG	6:L:41:LEU:CD1	2.26	1.22
5:H:35:GLY:CA	5:H:98:VAL:CG2	2.19	1.20
3:3:80:SER:HB3	3:3:180:ASN:ND2	1.56	1.18
1:1:158:PRO:HD2	1:1:161:PHE:CD2	1.77	1.18
5:H:117:ALA:HB2	5:H:129:GLY:HA3	1.25	1.18
6:L:34:GLY:CA	6:L:94:PRO:HD2	1.70	1.16
5:H:35:GLY:O	5:H:96:ALA:HA	1.47	1.15
5:H:34:VAL:HG11	5:H:78:VAL:HG21	1.29	1.13
5:H:100:GLN:CB	6:L:101:ALA:CB	2.16	1.13
1:1:134:SER:HA	1:1:156:GLN:NE2	1.63	1.13
2:2:214:LEU:HD23	3:3:127:PRO:HG2	1.29	1.13
5:H:103:SER:OG	6:L:33:ASN:ND2	1.83	1.12
5:H:117:ALA:CB	5:H:129:GLY:HA3	1.79	1.11
2:2:34:TYR:CD1	2:2:159:THR:CG2	2.34	1.10
1:1:76:LEU:HD11	1:1:176:VAL:HG13	1.21	1.10
1:1:76:LEU:HD11	1:1:176:VAL:CG1	1.81	1.10
2:2:34:TYR:CD1	2:2:159:THR:HG21	1.85	1.10
3:3:80:SER:CB	3:3:180:ASN:ND2	2.10	1.10
2:2:18:ARG:HG3	2:2:23:THR:HG22	1.12	1.08
3:3:174:ASP:OD1	5:H:111:ALA:CB	2.00	1.08
1:1:82:HIS:HE1	1:1:113:THR:CG2	1.56	1.08
1:1:158:PRO:HG2	1:1:161:PHE:CE2	1.87	1.08
5:H:75:ARG:NH1	5:H:77:GLN:OE1	1.86	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:80:SER:HB2	3:3:180:ASN:HD22	1.17	1.07
1:1:82:HIS:CE1	1:1:113:THR:HG23	1.86	1.06
1:1:51:ILE:CD1	1:1:117:LEU:HD21	1.86	1.06
1:1:197:GLN:HE21	1:1:197:GLN:HA	1.20	1.06
2:2:47:ASN:O	3:3:162:TYR:O	1.74	1.05
3:3:80:SER:HB3	3:3:180:ASN:HD22	0.95	1.05
2:2:107:VAL:HG11	2:2:179:LEU:HD13	1.32	1.05
5:H:35:GLY:HA3	5:H:98:VAL:HG23	1.07	1.05
1:1:97:ALA:HB2	3:3:218:PRO:HB3	1.39	1.05
5:H:41:PRO:CD	5:H:90:SER:O	2.04	1.05
1:1:93:ALA:HB1	3:3:216:ILE:CD1	1.86	1.05
5:H:98:VAL:CG1	6:L:101:ALA:HB3	1.89	1.03
5:H:122:CYS:HB2	5:H:123:PRO:HD3	1.40	1.01
1:1:82:HIS:HE1	1:1:113:THR:HG21	0.88	1.01
5:H:35:GLY:HA2	5:H:98:VAL:HG23	1.18	1.01
5:H:112:TYR:CD2	5:H:129:GLY:O	2.12	1.01
2:2:18:ARG:CG	2:2:23:THR:HG22	1.90	1.01
2:2:34:TYR:HD1	2:2:159:THR:CG2	1.73	1.00
3:3:174:ASP:OD1	5:H:111:ALA:HB2	1.61	1.00
2:2:103:ASN:HD22	2:2:205:PRO:HB3	1.22	0.99
1:1:158:PRO:HG2	1:1:161:PHE:HE2	1.16	0.99
6:L:34:GLY:HA3	6:L:94:PRO:HD3	1.40	0.99
1:1:159:ALA:HB3	5:H:135:ALA:HA	1.42	0.99
1:1:158:PRO:CD	1:1:161:PHE:CD2	2.40	0.98
6:L:65:PHE:HE1	6:L:85:ASP:OD2	1.43	0.98
3:3:19:PRO:HB2	4:4:19:GLY:H	1.26	0.98
2:2:214:LEU:HD23	3:3:127:PRO:CG	1.94	0.98
3:3:24:PRO:HB2	4:4:30:TYR:O	1.64	0.98
1:1:93:ALA:CB	3:3:216:ILE:CD1	2.43	0.97
1:1:134:SER:HA	1:1:156:GLN:HE22	1.20	0.97
1:1:97:ALA:HB2	3:3:218:PRO:CB	1.96	0.96
1:1:135:LYS:HZ2	1:1:158:PRO:HB3	1.17	0.96
2:2:105:TRP:HD1	2:2:177:TRP:HB2	1.25	0.96
3:3:139:ARG:NH2	3:3:186:CYS:SG	2.40	0.95
1:1:159:ALA:HB3	5:H:135:ALA:CA	1.96	0.95
2:2:107:VAL:HG21	2:2:179:LEU:HD22	1.49	0.95
5:H:112:TYR:HH	5:H:138:TYR:C	1.74	0.95
6:L:34:GLY:CA	6:L:94:PRO:HD3	1.89	0.94
3:3:192:HIS:HB2	3:3:195:ALA:HB3	1.48	0.94
3:3:139:ARG:HH12	3:3:186:CYS:HB2	1.31	0.94
3:3:132:THR:HG21	3:3:184:TRP:CG	2.02	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:135:LYS:HZ1	1:1:158:PRO:HB3	1.26	0.94
1:1:48:THR:HG22	5:H:119:ARG:NH2	1.81	0.93
2:2:18:ARG:HG3	2:2:23:THR:CG2	1.99	0.93
5:H:35:GLY:O	5:H:96:ALA:CA	2.17	0.93
5:H:112:TYR:OH	5:H:138:TYR:O	1.87	0.93
5:H:138:TYR:CD2	5:H:142:THR:HG21	2.02	0.93
1:1:136:TYR:CZ	2:2:173:LYS:HE2	2.02	0.93
1:1:134:SER:CA	1:1:156:GLN:HE22	1.81	0.92
2:2:214:LEU:CD2	3:3:127:PRO:HG2	1.99	0.92
1:1:48:THR:O	5:H:119:ARG:HG2	1.69	0.92
2:2:37:SER:OG	2:2:161:PRO:CG	2.17	0.92
5:H:102:THR:HG21	6:L:99:SER:HA	1.50	0.92
1:1:13:THR:CG2	1:1:17:ASN:HD21	1.82	0.92
6:L:65:PHE:CE1	6:L:85:ASP:CG	2.47	0.92
5:H:33:ALA:HB1	5:H:51:ILE:O	1.70	0.91
3:3:33:PRO:HB3	4:4:36:THR:OG1	1.70	0.91
1:1:153:LEU:HG	1:1:155:ALA:H	1.35	0.91
6:L:34:GLY:CA	6:L:94:PRO:CG	2.49	0.91
1:1:165:ALA:HB1	5:H:133:PHE:CZ	2.05	0.91
1:1:76:LEU:CD1	1:1:176:VAL:HG13	2.02	0.90
2:2:22:THR:HG21	2:2:60:ARG:HG2	1.54	0.90
5:H:98:VAL:CG2	6:L:103:PHE:HE1	1.67	0.90
6:L:65:PHE:HE1	6:L:85:ASP:CG	1.80	0.90
1:1:165:ALA:CB	5:H:133:PHE:CZ	2.56	0.89
5:H:100:GLN:HB2	6:L:101:ALA:HB2	1.51	0.89
2:2:107:VAL:CG2	2:2:179:LEU:HD22	2.03	0.88
5:H:35:GLY:HA3	5:H:98:VAL:CG2	1.97	0.88
1:1:136:TYR:CE2	2:2:173:LYS:HE2	2.08	0.88
3:3:24:PRO:CB	4:4:30:TYR:O	2.22	0.88
1:1:13:THR:CG2	1:1:17:ASN:ND2	2.38	0.87
1:1:159:ALA:HB1	5:H:134:GLY:O	1.73	0.87
2:2:48:THR:HG21	2:2:168:TYR:CE1	2.09	0.87
5:H:98:VAL:CG2	6:L:103:PHE:HZ	1.84	0.87
1:1:71:TYR:OH	2:2:128:GLU:OE1	1.91	0.87
1:1:158:PRO:CB	1:1:161:PHE:CE2	2.56	0.87
1:1:153:LEU:HD11	1:1:155:ALA:HB3	1.57	0.86
5:H:122:CYS:HB2	5:H:123:PRO:CD	2.04	0.86
3:3:54:PHE:O	3:3:89:THR:HG22	1.75	0.85
1:1:111:PRO:CB	3:3:9:ASP:OD1	2.24	0.85
6:L:94:PRO:HA	6:L:101:ALA:HA	1.58	0.85
1:1:153:LEU:CD1	1:1:155:ALA:HB3	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:123:HIS:HB3	2:2:165:VAL:HG12	1.58	0.84
1:1:45:VAL:HG23	1:1:49:HIS:CD2	2.12	0.84
1:1:100:ASN:ND2	3:3:217:ASP:O	2.10	0.84
2:2:35:GLY:HA3	2:2:144:PRO:HB3	1.59	0.84
1:1:93:ALA:HB2	3:3:216:ILE:HD12	1.59	0.84
5:H:95:CYS:SG	6:L:41:LEU:HD11	2.18	0.84
2:2:35:GLY:O	2:2:161:PRO:HD2	1.78	0.83
2:2:105:TRP:HD1	2:2:177:TRP:CB	1.90	0.83
5:H:34:VAL:HG11	5:H:78:VAL:CG2	2.08	0.83
5:H:117:ALA:HB2	5:H:129:GLY:CA	2.09	0.83
1:1:53:LEU:CD2	1:1:176:VAL:HG11	2.08	0.83
2:2:103:ASN:O	2:2:162:TYR:HB2	1.78	0.82
1:1:134:SER:CB	1:1:156:GLN:HE22	1.93	0.82
1:1:53:LEU:HD21	1:1:176:VAL:HG11	1.62	0.81
5:H:33:ALA:HB2	5:H:52:ASP:HA	1.63	0.81
1:1:97:ALA:HB2	3:3:218:PRO:CA	2.10	0.81
5:H:59:TYR:HE1	5:H:69:ILE:HG12	1.44	0.81
5:H:112:TYR:CE2	5:H:129:GLY:O	2.34	0.81
5:H:98:VAL:HG22	6:L:103:PHE:HE1	0.98	0.81
1:1:122:PRO:HD2	1:1:160:SER:OG	1.81	0.80
6:L:64:ARG:NH2	6:L:84:GLU:OE1	2.13	0.80
2:2:163:LEU:HD12	2:2:163:LEU:O	1.82	0.80
5:H:68:SER:O	5:H:81:THR:OG1	2.00	0.80
2:2:105:TRP:CD1	2:2:177:TRP:CB	2.59	0.80
1:1:13:THR:HG23	1:1:17:ASN:HD21	1.46	0.79
1:1:46:SER:HB2	1:1:47:PRO:HD2	1.63	0.79
5:H:120:TRP:H	5:H:120:TRP:CD1	1.95	0.79
1:1:91:ASN:ND2	1:1:121:ALA:HA	1.96	0.79
1:1:165:ALA:CB	5:H:133:PHE:CE1	2.65	0.79
2:2:123:VAL:HG12	2:2:181:VAL:HG22	1.64	0.79
6:L:34:GLY:HA2	6:L:94:PRO:HG3	1.64	0.79
1:1:91:ASN:OD1	1:1:162:ASN:OD1	2.01	0.78
2:2:105:TRP:HA	2:2:105:TRP:CE3	2.18	0.78
5:H:40:ALA:HA	5:H:91:ALA:HB2	1.65	0.78
6:L:34:GLY:HA2	6:L:94:PRO:CD	2.09	0.78
1:1:159:ALA:CB	5:H:134:GLY:O	2.32	0.78
2:2:34:TYR:CE1	2:2:159:THR:HG21	2.17	0.78
2:2:83:LEU:HB2	2:2:177:TRP:O	1.84	0.78
5:H:100:GLN:CD	6:L:93:SER:HA	2.09	0.78
5:H:32:LYS:HA	5:H:101:HIS:CE1	2.19	0.78
1:1:30:THR:O	1:1:30:THR:HG22	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:134:SER:CA	1:1:156:GLN:NE2	2.42	0.77
1:1:111:PRO:HB3	3:3:9:ASP:OD1	1.82	0.77
5:H:112:TYR:OH	5:H:138:TYR:C	2.27	0.77
5:H:138:TYR:CD2	5:H:142:THR:CG2	2.67	0.77
5:H:38:ARG:HA	5:H:92:THR:O	1.85	0.77
5:H:49:GLY:HA3	5:H:59:TYR:HA	1.65	0.77
5:H:98:VAL:HG13	6:L:101:ALA:HB3	1.66	0.77
1:1:86:LEU:HD11	1:1:166:ILE:HB	1.65	0.76
3:3:41:PHE:HB2	3:3:47:VAL:CG2	2.15	0.76
5:H:59:TYR:CE1	5:H:69:ILE:HG12	2.21	0.76
1:1:48:THR:CG2	5:H:119:ARG:NH2	2.49	0.75
2:2:216:SER:HB3	3:3:142:HIS:CE1	2.22	0.75
5:H:6:GLU:HB3	5:H:94:TYR:O	1.86	0.75
1:1:91:ASN:HD22	1:1:121:ALA:HA	1.50	0.75
1:1:93:ALA:HB1	3:3:216:ILE:HD11	1.69	0.75
2:2:34:TYR:HD1	2:2:159:THR:HG23	1.52	0.74
2:2:55:VAL:HG11	2:2:94:LEU:HD11	1.68	0.74
5:H:120:TRP:CZ2	5:H:130:TYR:HD2	2.05	0.74
1:1:197:GLN:HA	1:1:197:GLN:NE2	2.00	0.74
1:1:72:TYR:HE2	1:1:163:TYR:HH	1.33	0.74
5:H:108:CYS:HB2	5:H:109:PRO:HD2	1.68	0.74
2:2:213:GLU:O	3:3:143:CYS:HA	1.88	0.74
5:H:37:VAL:HG12	5:H:47:TRP:HA	1.70	0.74
6:L:24:CYS:HB2	6:L:38:TRP:HZ2	1.52	0.74
1:1:51:ILE:HD13	1:1:117:LEU:HD21	1.70	0.74
2:2:107:VAL:CG1	2:2:179:LEU:HD13	2.17	0.74
6:L:34:GLY:HA3	6:L:94:PRO:HD2	0.74	0.73
6:L:34:GLY:HA2	6:L:94:PRO:CG	2.15	0.73
2:2:22:THR:CG2	2:2:60:ARG:HG2	2.17	0.73
5:H:120:TRP:CZ2	5:H:130:TYR:CD2	2.76	0.73
1:1:92:GLY:HA3	3:3:170:TYR:CE1	2.23	0.73
5:H:32:LYS:NZ	6:L:52:TYR:HD2	1.88	0.72
1:1:95:GLU:CB	5:H:132:ASN:HA	2.19	0.72
1:1:95:GLU:H	5:H:132:ASN:HA	1.54	0.72
6:L:24:CYS:HB3	6:L:74:ALA:HB3	1.72	0.72
1:1:165:ALA:HB2	5:H:133:PHE:CE1	2.25	0.72
2:2:122:LEU:HD23	2:2:122:LEU:C	2.14	0.72
5:H:35:GLY:HA2	5:H:98:VAL:CB	2.19	0.72
3:3:174:ASP:OD1	5:H:111:ALA:HB1	1.89	0.72
6:L:65:PHE:CZ	6:L:85:ASP:HB2	2.25	0.72
1:1:93:ALA:HB1	3:3:216:ILE:HD13	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:103:ASN:ND2	2:2:205:PRO:HB3	2.00	0.72
5:H:98:VAL:HG23	6:L:103:PHE:CZ	2.21	0.72
1:1:93:ALA:CB	3:3:216:ILE:HD12	2.15	0.72
2:2:192:ILE:HD12	2:2:192:ILE:N	2.05	0.71
5:H:23:THR:HA	5:H:76:ASN:O	1.89	0.71
6:L:34:GLY:HA3	6:L:94:PRO:CG	2.13	0.71
2:2:122:LEU:HD23	2:2:122:LEU:O	1.91	0.71
3:3:80:SER:HB2	3:3:180:ASN:ND2	1.94	0.71
1:1:51:ILE:CD1	1:1:117:LEU:CD2	2.67	0.71
5:H:112:TYR:HD2	5:H:129:GLY:O	1.72	0.71
5:H:45:LEU:HD23	6:L:104:GLY:HA2	1.73	0.70
1:1:95:GLU:HB2	5:H:132:ASN:HA	1.74	0.70
1:1:97:ALA:CB	3:3:218:PRO:HA	2.19	0.70
3:3:132:THR:HG21	3:3:184:TRP:CB	2.22	0.70
3:3:139:ARG:HH12	3:3:186:CYS:CB	2.04	0.70
5:H:100:GLN:NE2	6:L:93:SER:HA	2.07	0.70
1:1:48:THR:HG22	5:H:119:ARG:HH21	1.56	0.69
6:L:36:VAL:CG1	6:L:91:CYS:SG	2.66	0.69
6:L:82:GLN:HG2	6:L:84:GLU:H	1.56	0.69
3:3:132:THR:CG2	3:3:184:TRP:CG	2.75	0.69
5:H:40:ALA:CA	5:H:91:ALA:HB2	2.20	0.69
2:2:48:THR:CG2	2:2:168:TYR:CE1	2.76	0.69
1:1:153:LEU:HG	1:1:155:ALA:N	2.07	0.69
1:1:13:THR:HG21	1:1:17:ASN:ND2	2.07	0.68
1:1:97:ALA:HB2	3:3:218:PRO:HA	1.74	0.68
3:3:126:VAL:HG11	3:3:132:THR:HG22	1.76	0.68
5:H:1:GLN:CB	6:L:60:GLY:O	2.42	0.68
5:H:102:THR:HG21	6:L:99:SER:CA	2.24	0.68
3:3:132:THR:CG2	3:3:184:TRP:CD2	2.76	0.68
2:2:101:MET:HB3	2:2:210:VAL:HG12	1.76	0.68
5:H:117:ALA:C	5:H:119:ARG:H	2.00	0.68
2:2:105:TRP:HD1	2:2:177:TRP:CG	2.11	0.67
3:3:126:VAL:CG1	3:3:184:TRP:HB2	2.25	0.67
5:H:103:SER:HG	6:L:33:ASN:ND2	1.93	0.67
1:1:50:VAL:HG12	1:1:52:ASP:H	1.60	0.66
1:1:157:LEU:HB2	5:H:140:ARG:HH11	1.60	0.66
6:L:92:ALA:HA	6:L:103:PHE:HA	1.76	0.66
1:1:158:PRO:N	1:1:161:PHE:CD2	2.62	0.66
5:H:117:ALA:C	5:H:119:ARG:N	2.52	0.66
5:H:35:GLY:N	5:H:98:VAL:H	1.93	0.66
5:H:129:GLY:HA2	5:H:141:CYS:CB	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:65:PHE:HZ	6:L:85:ASP:HB2	1.58	0.66
1:1:97:ALA:CB	3:3:218:PRO:CA	2.74	0.66
1:1:158:PRO:HB2	1:1:161:PHE:CE2	2.28	0.66
5:H:51:ILE:HD12	5:H:57:THR:HG22	1.78	0.66
3:3:41:PHE:CD2	3:3:47:VAL:HG21	2.31	0.66
3:3:216:ILE:HG23	3:3:218:PRO:HD3	1.78	0.66
1:1:82:HIS:NE2	1:1:113:THR:CG2	2.59	0.65
1:1:93:ALA:CB	3:3:216:ILE:HD11	2.26	0.65
2:2:43:VAL:HG21	2:2:209:HIS:NE2	2.11	0.65
3:3:136:THR:HG22	3:3:188:TYR:CD1	2.31	0.65
6:L:41:LEU:HB2	6:L:88:GLU:O	1.96	0.65
6:L:65:PHE:CZ	6:L:85:ASP:CG	2.73	0.65
1:1:54:MET:O	1:1:67:ARG:NH2	2.29	0.65
3:3:33:PRO:CB	4:4:36:THR:OG1	2.45	0.65
1:1:97:ALA:CB	3:3:218:PRO:HB3	2.22	0.65
2:2:18:ARG:CB	2:2:23:THR:HG22	2.27	0.65
6:L:14:GLY:O	6:L:112:LEU:HB3	1.97	0.65
6:L:91:CYS:SG	6:L:92:ALA:N	2.70	0.65
2:2:100:TYR:OH	3:3:128:PRO:HG2	1.96	0.65
5:H:18:LEU:HD21	5:H:93:TYR:CE1	2.31	0.65
6:L:65:PHE:HD1	6:L:78:ILE:HD12	1.61	0.65
2:2:62:PHE:CE1	2:2:203:ILE:HB	2.32	0.65
5:H:8:GLY:HA3	5:H:20:LEU:HD13	1.79	0.65
1:1:95:GLU:N	5:H:132:ASN:HA	2.12	0.64
2:2:192:ILE:HD12	2:2:192:ILE:H	1.60	0.64
2:2:112:VAL:O	2:2:197:ILE:HG23	1.98	0.64
5:H:18:LEU:O	5:H:81:THR:HA	1.98	0.64
5:H:116:CYS:O	5:H:130:TYR:O	2.15	0.64
1:1:102:SER:HB2	3:3:217:ASP:CB	2.27	0.64
4:4:21:ILE:O	4:4:22:ILE:HG23	1.97	0.64
5:H:34:VAL:HG21	5:H:78:VAL:HG11	1.80	0.64
5:H:129:GLY:HA2	5:H:141:CYS:HB2	1.79	0.64
5:H:32:LYS:NZ	6:L:52:TYR:CD2	2.65	0.64
1:1:72:TYR:HE2	1:1:163:TYR:OH	1.80	0.64
4:4:21:ILE:O	4:4:21:ILE:HG23	1.97	0.64
6:L:65:PHE:CE1	6:L:85:ASP:OD2	2.35	0.64
1:1:51:ILE:HD12	1:1:117:LEU:HD21	1.77	0.64
2:2:22:THR:CG2	2:2:60:ARG:CG	2.76	0.64
1:1:158:PRO:HB2	1:1:161:PHE:CD2	2.33	0.63
3:3:19:PRO:HB2	4:4:19:GLY:N	2.07	0.63
1:1:134:SER:OG	1:1:156:GLN:NE2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:72:ARG:HE	3:3:190:ILE:HA	1.63	0.63
1:1:190:LEU:HD11	2:2:135:ARG:HB3	1.80	0.63
5:H:35:GLY:HA3	5:H:98:VAL:N	2.14	0.63
6:L:38:TRP:HB3	6:L:89:TYR:HD2	1.64	0.63
1:1:158:PRO:CB	1:1:161:PHE:CD2	2.82	0.62
5:H:138:TYR:CG	5:H:142:THR:CG2	2.81	0.62
5:H:119:ARG:H	5:H:119:ARG:HD3	1.65	0.62
6:L:41:LEU:C	6:L:87:ALA:HB1	2.24	0.62
5:H:51:ILE:HD13	5:H:71:LYS:HB2	1.81	0.62
1:1:153:LEU:HG	1:1:154:ALA:N	2.15	0.62
2:2:75:PHE:HA	2:2:183:VAL:O	2.00	0.62
2:2:107:VAL:HG23	2:2:203:ILE:HG12	1.80	0.62
5:H:100:GLN:HB2	6:L:101:ALA:CA	2.20	0.62
5:H:100:GLN:CD	6:L:93:SER:CA	2.72	0.62
1:1:125:VAL:O	2:2:165:VAL:HG13	2.00	0.62
1:1:135:LYS:NZ	1:1:158:PRO:CB	2.42	0.62
3:3:136:THR:HG22	3:3:188:TYR:HB3	1.82	0.61
5:H:100:GLN:CB	6:L:101:ALA:HB2	2.18	0.61
2:2:107:VAL:HG11	2:2:179:LEU:CD1	2.19	0.61
5:H:23:THR:HG23	5:H:76:ASN:HB3	1.82	0.61
6:L:65:PHE:HZ	6:L:85:ASP:CB	2.12	0.61
3:3:41:PHE:CB	3:3:47:VAL:CG2	2.79	0.61
1:1:100:ASN:HD22	3:3:217:ASP:C	2.08	0.61
1:1:111:PRO:CG	3:3:9:ASP:OD1	2.49	0.61
5:H:115:ASP:O	5:H:118:ALA:HB2	2.01	0.61
1:1:111:PRO:HG3	3:3:9:ASP:OD1	2.01	0.61
1:1:51:ILE:HD13	1:1:117:LEU:CD2	2.30	0.61
2:2:67:PHE:HD2	2:2:73:LYS:HE2	1.66	0.61
5:H:47:TRP:CZ2	6:L:100:ASN:HB3	2.36	0.61
2:2:100:TYR:HB3	2:2:168:TYR:HB3	1.83	0.60
5:H:98:VAL:HG23	6:L:103:PHE:HZ	1.60	0.60
6:L:42:ILE:HB	6:L:45:SER:HB3	1.83	0.60
6:L:65:PHE:CZ	6:L:85:ASP:CB	2.84	0.60
3:3:144:ILE:HG21	3:3:161:PRO:HG3	1.82	0.60
1:1:75:ASP:OD1	1:1:118:PRO:HA	2.02	0.60
2:2:216:SER:CB	3:3:142:HIS:CE1	2.84	0.59
4:4:15:SER:OG	4:4:16:GLY:N	2.29	0.59
2:2:105:TRP:HD1	2:2:177:TRP:CD1	2.21	0.59
5:H:130:TYR:CE2	5:H:132:ASN:O	2.55	0.59
6:L:24:CYS:HB2	6:L:38:TRP:CZ2	2.37	0.59
1:1:158:PRO:HD2	1:1:161:PHE:CZ	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:158:PRO:O	1:1:161:PHE:HD2	1.85	0.59
3:3:41:PHE:CG	3:3:47:VAL:HG21	2.38	0.59
5:H:71:LYS:HA	5:H:78:VAL:HG13	1.85	0.59
3:3:2:ILE:HG22	3:3:3:VAL:N	2.16	0.59
1:1:15:VAL:HG12	1:1:15:VAL:O	2.03	0.59
3:3:176:ALA:O	3:3:179:THR:O	2.20	0.59
5:H:122:CYS:CB	5:H:123:PRO:CD	2.77	0.59
5:H:97:THR:HG23	5:H:97:THR:O	2.02	0.59
1:1:51:ILE:CD1	1:1:76:LEU:HD23	2.33	0.59
5:H:100:GLN:HB2	6:L:101:ALA:HB1	0.61	0.58
5:H:98:VAL:HG12	6:L:101:ALA:HB3	1.78	0.58
5:H:128:CYS:SG	5:H:128:CYS:O	2.60	0.58
1:1:94:PRO:HA	5:H:132:ASN:HB3	1.85	0.58
2:2:67:PHE:HB3	2:2:79:GLU:HG2	1.84	0.58
3:3:24:PRO:HB3	4:4:30:TYR:O	2.01	0.58
1:1:135:LYS:HZ1	1:1:158:PRO:CB	2.09	0.58
3:3:127:PRO:N	3:3:127:PRO:C	2.60	0.58
3:3:132:THR:HG23	3:3:184:TRP:CD2	2.38	0.58
5:H:100:GLN:HE22	6:L:35:TYR:C	2.07	0.58
5:H:120:TRP:H	5:H:120:TRP:HD1	1.48	0.58
1:1:51:ILE:HD12	1:1:76:LEU:HD23	1.86	0.57
1:1:165:ALA:HB1	5:H:133:PHE:CE1	2.38	0.57
5:H:120:TRP:CH2	5:H:130:TYR:CE2	2.92	0.57
1:1:2:THR:HG23	1:1:2:THR:O	2.03	0.57
3:3:29:VAL:HG23	4:4:33:SER:HB2	1.87	0.57
3:3:197:GLN:HG3	3:3:197:GLN:O	2.05	0.57
5:H:32:LYS:HA	5:H:101:HIS:HE1	1.69	0.57
6:L:66:SER:O	6:L:77:SER:N	2.35	0.57
2:2:107:VAL:HG21	2:2:179:LEU:CD2	2.31	0.57
3:3:135:ASP:HB2	3:3:137:PRO:HD2	1.87	0.57
5:H:138:TYR:CG	5:H:142:THR:HG21	2.38	0.57
5:H:34:VAL:CG1	5:H:78:VAL:HG21	2.18	0.57
6:L:23:THR:HA	6:L:75:THR:HA	1.85	0.57
1:1:6:GLU:OE1	1:1:6:GLU:N	2.38	0.57
3:3:55:LEU:HD23	3:3:89:THR:HG21	1.87	0.57
5:H:130:TYR:CZ	5:H:132:ASN:O	2.58	0.57
3:3:97:TYR:O	3:3:216:ILE:HG22	2.04	0.56
5:H:69:ILE:HG22	5:H:80:LEU:HA	1.86	0.56
1:1:117:LEU:O	1:1:117:LEU:HD12	2.05	0.56
2:2:192:ILE:H	2:2:192:ILE:CD1	2.18	0.56
3:3:174:ASP:CG	5:H:111:ALA:CB	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:6:GLU:HG3	5:H:94:TYR:CB	2.34	0.56
5:H:35:GLY:CA	5:H:98:VAL:N	2.69	0.56
5:H:35:GLY:HA3	6:L:103:PHE:HZ	1.71	0.56
6:L:6:LEU:N	6:L:102:ASN:OD1	2.39	0.56
5:H:98:VAL:HG12	5:H:98:VAL:O	2.05	0.56
5:H:100:GLN:CB	6:L:101:ALA:CA	2.81	0.56
5:H:100:GLN:CG	6:L:101:ALA:HB1	2.30	0.56
6:L:99:SER:O	6:L:99:SER:OG	2.19	0.56
1:1:13:THR:HG21	1:1:17:ASN:HD21	1.65	0.56
1:1:72:TYR:CE2	1:1:163:TYR:OH	2.57	0.56
3:3:136:THR:CG2	3:3:188:TYR:HB3	2.36	0.56
5:H:6:GLU:HG3	5:H:94:TYR:CD1	2.40	0.56
1:1:135:LYS:HZ2	1:1:158:PRO:CB	2.05	0.56
3:3:69:ASP:OD1	3:3:69:ASP:N	2.38	0.56
3:3:132:THR:HG23	3:3:184:TRP:CE3	2.40	0.56
3:3:132:THR:HB	3:3:139:ARG:NH2	2.20	0.56
6:L:39:TYR:O	6:L:89:TYR:HA	2.06	0.56
2:2:81:LEU:N	2:2:179:LEU:O	2.35	0.55
2:2:114:ASN:HB3	2:2:193:GLY:HA2	1.87	0.55
6:L:22:ILE:HD11	6:L:109:LEU:HD21	1.87	0.55
2:2:83:LEU:O	2:2:175:LYS:HB3	2.07	0.55
3:3:24:PRO:HB3	4:4:31:GLN:HA	1.89	0.55
5:H:114:PRO:N	5:H:114:PRO:C	2.60	0.55
1:1:16:GLU:HA	1:1:20:GLY:O	2.06	0.55
3:3:132:THR:CG2	3:3:184:TRP:HB2	2.37	0.55
2:2:109:VAL:CG2	2:2:179:LEU:HD21	2.36	0.55
5:H:6:GLU:HG3	5:H:94:TYR:HB3	1.88	0.55
5:H:33:ALA:CB	5:H:52:ASP:HA	2.35	0.55
1:1:6:GLU:HG2	2:2:152:THR:OG1	2.07	0.54
1:1:135:LYS:O	5:H:137:SER:O	2.24	0.54
2:2:162:TYR:CD1	2:2:162:TYR:C	2.85	0.54
5:H:38:ARG:HE	5:H:46:GLU:HG2	1.72	0.54
1:1:192:VAL:HG13	1:1:192:VAL:O	2.07	0.54
5:H:32:LYS:HG2	5:H:101:HIS:NE2	2.22	0.54
1:1:100:ASN:HD21	3:3:219:ARG:N	2.05	0.54
3:3:79:LEU:HD11	3:3:160:ILE:HG21	1.89	0.54
3:3:120:ARG:HB3	3:3:191:THR:HG22	1.90	0.54
2:2:35:GLY:O	2:2:161:PRO:CD	2.54	0.54
6:L:58:ALA:C	6:L:59:SER:O	2.39	0.54
1:1:73:PHE:CD1	1:1:73:PHE:C	2.85	0.54
2:2:22:THR:HG23	2:2:60:ARG:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:132:THR:HB	3:3:139:ARG:HH21	1.73	0.54
5:H:130:TYR:OH	5:H:134:GLY:O	2.25	0.54
5:H:6:GLU:CB	5:H:94:TYR:O	2.54	0.54
1:1:31:ASP:OD1	1:1:32:VAL:N	2.38	0.54
1:1:51:ILE:O	1:1:51:ILE:HG13	2.07	0.54
2:2:80:LYS:HA	2:2:180:VAL:HA	1.90	0.54
5:H:100:GLN:HG3	6:L:93:SER:C	2.33	0.54
3:3:139:ARG:NH1	3:3:186:CYS:HB2	2.11	0.54
5:H:52:ASP:C	5:H:71:LYS:HZ2	2.16	0.54
5:H:120:TRP:CD1	5:H:120:TRP:N	2.73	0.54
1:1:103:ASN:O	1:1:104:PRO:C	2.51	0.53
3:3:189:GLN:NE2	3:3:192:HIS:HB3	2.23	0.53
5:H:35:GLY:CA	5:H:98:VAL:CB	2.80	0.53
1:1:12:THR:HG23	1:1:12:THR:O	2.07	0.53
2:2:52:GLU:HG3	2:2:168:TYR:OH	2.08	0.53
1:1:92:GLY:O	3:3:99:ALA:HB1	2.07	0.53
3:3:133:PRO:HB3	3:3:138:GLU:HB3	1.89	0.53
1:1:51:ILE:CG2	1:1:166:ILE:HG23	2.38	0.53
2:2:22:THR:HG23	2:2:60:ARG:CG	2.39	0.53
2:2:34:TYR:HD1	2:2:159:THR:HG21	1.41	0.53
3:3:126:VAL:O	3:3:126:VAL:HG13	2.08	0.53
5:H:18:LEU:N	5:H:82:ILE:O	2.33	0.53
1:1:158:PRO:N	1:1:161:PHE:HD2	2.07	0.53
1:1:136:TYR:CZ	2:2:173:LYS:CE	2.84	0.53
3:3:100:GLN:HE21	3:3:213:ARG:HE	1.57	0.53
1:1:76:LEU:HD11	1:1:176:VAL:HG11	1.82	0.53
2:2:151:ARG:HG2	2:2:152:THR:HG23	1.90	0.53
5:H:115:ASP:C	5:H:117:ALA:H	2.17	0.53
3:3:132:THR:CG2	3:3:184:TRP:CB	2.87	0.53
5:H:47:TRP:HZ2	6:L:100:ASN:HB3	1.73	0.53
1:1:48:THR:CG2	5:H:119:ARG:HH22	2.22	0.52
1:1:117:LEU:HD12	1:1:117:LEU:C	2.34	0.52
1:1:153:LEU:HD12	1:1:155:ALA:HB3	1.90	0.52
2:2:83:LEU:CB	2:2:177:TRP:O	2.57	0.52
3:3:191:THR:HG23	3:3:191:THR:O	2.09	0.52
4:4:17:ASN:OD1	4:4:17:ASN:O	2.26	0.52
2:2:19:ASN:HB2	2:2:61:PHE:CE2	2.45	0.52
3:3:79:LEU:HB2	3:3:183:GLY:O	2.09	0.52
5:H:120:TRP:CH2	5:H:130:TYR:HE2	2.27	0.52
5:H:45:LEU:HG	6:L:105:SER:HB2	1.90	0.52
5:H:112:TYR:CZ	5:H:138:TYR:CD2	2.98	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:84:PRO:HG3	2:2:171:TYR:CG	2.45	0.52
1:1:165:ALA:HB2	5:H:133:PHE:CD1	2.44	0.52
1:1:159:ALA:CB	5:H:134:GLY:C	2.82	0.52
3:3:54:PHE:O	3:3:89:THR:CG2	2.55	0.52
5:H:35:GLY:HA2	5:H:98:VAL:HB	1.92	0.52
5:H:37:VAL:HG11	6:L:103:PHE:HB2	1.92	0.52
2:2:75:PHE:HD2	2:2:184:VAL:O	1.93	0.51
3:3:122:MET:HB2	3:3:147:GLU:HG2	1.91	0.51
6:L:91:CYS:O	6:L:104:GLY:N	2.41	0.51
5:H:4:LEU:HD21	5:H:97:THR:HB	1.93	0.51
5:H:112:TYR:CZ	5:H:138:TYR:HD2	2.29	0.51
1:1:156:GLN:O	1:1:156:GLN:HG3	2.11	0.51
2:2:192:ILE:N	2:2:192:ILE:CD1	2.73	0.51
5:H:37:VAL:HG23	5:H:95:CYS:HB2	1.92	0.51
5:H:67:LEU:HG	5:H:82:ILE:HG12	1.91	0.51
2:2:62:PHE:CZ	2:2:203:ILE:HB	2.45	0.51
5:H:54:GLY:O	5:H:55:SER:OG	2.23	0.51
5:H:130:TYR:CZ	5:H:134:GLY:O	2.64	0.51
1:1:157:LEU:HD22	1:1:157:LEU:N	2.26	0.51
1:1:165:ALA:HB3	5:H:133:PHE:CE2	2.46	0.51
5:H:138:TYR:HB2	5:H:142:THR:HG23	1.92	0.51
5:H:112:TYR:CE2	5:H:138:TYR:HD2	2.28	0.51
1:1:85:ARG:NH1	1:1:101:THR:HG22	2.25	0.51
1:1:77:GLU:HB3	1:1:177:ARG:HB3	1.92	0.50
3:3:104:THR:HB	3:3:207:GLY:HA3	1.93	0.50
1:1:136:TYR:HE1	3:3:129:GLY:HA2	1.75	0.50
2:2:52:GLU:O	2:2:52:GLU:HG2	2.11	0.50
2:2:35:GLY:CA	2:2:144:PRO:HB3	2.36	0.50
1:1:98:LEU:HD13	5:H:133:PHE:HE2	1.75	0.50
1:1:100:ASN:HD21	3:3:218:PRO:C	2.19	0.50
1:1:110:ALA:HB3	1:1:111:PRO:HD3	1.93	0.50
5:H:126:ALA:HB1	5:H:142:THR:C	2.37	0.50
1:1:159:ALA:HB1	5:H:134:GLY:C	2.37	0.50
3:3:136:THR:HG22	3:3:188:TYR:CG	2.47	0.50
5:H:115:ASP:O	5:H:118:ALA:CB	2.59	0.50
3:3:153:ASN:OD1	3:3:153:ASN:N	2.43	0.50
6:L:98:SER:OG	6:L:100:ASN:OD1	2.28	0.50
5:H:35:GLY:C	5:H:98:VAL:HG23	2.26	0.50
1:1:165:ALA:CB	5:H:133:PHE:CE2	2.94	0.50
3:3:2:ILE:CG2	3:3:3:VAL:N	2.74	0.50
3:3:76:LYS:HB2	3:3:186:CYS:SG	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:40:VAL:O	1:1:40:VAL:HG13	2.11	0.50
5:H:66:ARG:HB2	5:H:83:THR:O	2.11	0.50
6:L:93:SER:N	6:L:102:ASN:O	2.33	0.50
1:1:159:ALA:HB3	5:H:135:ALA:N	2.26	0.49
3:3:112:THR:OG1	3:3:199:THR:OG1	2.30	0.49
1:1:52:ASP:HB2	1:1:162:ASN:HB3	1.93	0.49
1:1:91:ASN:HB2	1:1:120:THR:OG1	2.11	0.49
2:2:37:SER:OG	2:2:161:PRO:CB	2.60	0.49
5:H:35:GLY:O	5:H:96:ALA:CB	2.60	0.49
5:H:45:LEU:CD2	6:L:105:SER:H	2.25	0.49
5:H:119:ARG:N	5:H:119:ARG:HD3	2.26	0.49
1:1:52:ASP:HB2	1:1:162:ASN:CB	2.42	0.49
2:2:213:GLU:HB2	3:3:143:CYS:N	2.28	0.49
3:3:65:VAL:HG23	3:3:199:THR:HG22	1.95	0.49
3:3:132:THR:HG22	3:3:184:TRP:HB2	1.94	0.49
5:H:28:SER:HA	5:H:32:LYS:HE3	1.95	0.49
6:L:22:ILE:HB	6:L:76:LEU:HD23	1.95	0.49
6:L:40:GLN:O	6:L:47:PRO:HA	2.13	0.49
3:3:108:HIS:HB2	3:3:203:SER:HB2	1.94	0.49
2:2:143:PHE:HB3	2:2:144:PRO:HD2	1.95	0.49
2:2:146:GLN:HB3	2:2:156:ALA:HB1	1.94	0.49
3:3:106:ASN:HB2	3:3:205:SER:OG	2.12	0.49
5:H:35:GLY:N	5:H:98:VAL:N	2.60	0.49
1:1:85:ARG:HD3	1:1:107:TYR:CE2	2.47	0.49
2:2:34:TYR:HA	2:2:159:THR:O	2.13	0.49
5:H:17:THR:HA	5:H:83:THR:HA	1.95	0.49
6:L:65:PHE:CD1	6:L:78:ILE:HD12	2.45	0.49
3:3:125:TYR:O	3:3:143:CYS:HB3	2.11	0.49
3:3:160:ILE:HD13	3:3:185:VAL:HG21	1.95	0.49
3:3:97:TYR:O	3:3:216:ILE:N	2.42	0.48
5:H:1:GLN:H3	6:L:58:ALA:HB3	1.78	0.48
1:1:123:HIS:CB	2:2:165:VAL:HG12	2.35	0.48
2:2:148:ILE:HG12	2:2:156:ALA:HB2	1.96	0.48
6:L:93:SER:O	6:L:102:ASN:N	2.46	0.48
1:1:129:VAL:HG11	2:2:130:LYS:HB2	1.94	0.48
2:2:123:VAL:HG23	2:2:123:VAL:O	2.13	0.48
3:3:7:CYS:O	3:3:7:CYS:SG	2.70	0.48
1:1:122:PRO:HD2	1:1:160:SER:HG	1.75	0.48
2:2:79:GLU:HG3	2:2:79:GLU:O	2.12	0.48
3:3:132:THR:HG21	3:3:184:TRP:CD2	2.45	0.47
2:2:105:TRP:HA	2:2:105:TRP:HE3	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:144:ILE:HD13	3:3:161:PRO:HG3	1.95	0.47
6:L:37:SER:HB3	6:L:39:TYR:HE1	1.79	0.47
1:1:157:LEU:N	1:1:157:LEU:CD2	2.77	0.47
1:1:51:ILE:HD11	1:1:117:LEU:HD21	1.88	0.47
2:2:32:VAL:HG13	2:2:157:HIS:ND1	2.29	0.47
5:H:31:ASP:OD1	5:H:32:LYS:N	2.48	0.47
5:H:112:TYR:CZ	5:H:138:TYR:O	2.67	0.47
6:L:34:GLY:CA	6:L:94:PRO:HG3	2.27	0.47
5:H:35:GLY:HA2	5:H:98:VAL:HG21	1.80	0.47
2:2:18:ARG:HB2	2:2:23:THR:HG22	1.97	0.47
2:2:213:GLU:HB2	3:3:143:CYS:H	1.79	0.47
3:3:107:LEU:HD12	3:3:204:VAL:HG23	1.97	0.47
3:3:132:THR:CG2	3:3:184:TRP:CE3	2.97	0.47
5:H:4:LEU:C	5:H:5:ARG:HD2	2.39	0.47
5:H:106:ARG:NH1	5:H:106:ARG:HB2	2.29	0.47
5:H:95:CYS:SG	6:L:90:PHE:CG	3.06	0.47
1:1:78:ILE:HG22	1:1:115:LEU:HB2	1.97	0.46
1:1:85:ARG:HH12	1:1:101:THR:HG22	1.79	0.46
3:3:120:ARG:HB3	3:3:191:THR:CG2	2.45	0.46
2:2:100:TYR:OH	3:3:128:PRO:CG	2.63	0.46
5:H:116:CYS:CB	5:H:131:CYS:SG	3.03	0.46
5:H:4:LEU:C	6:L:47:PRO:HD2	2.41	0.46
6:L:30:ASN:O	6:L:93:SER:HB2	2.15	0.46
2:2:61:PHE:CD1	2:2:204:ALA:HB2	2.51	0.46
3:3:41:PHE:CB	3:3:47:VAL:HG21	2.46	0.46
5:H:66:ARG:NH2	5:H:84:SER:O	2.48	0.46
2:2:216:SER:OG	3:3:142:HIS:CE1	2.69	0.46
3:3:52:PRO:HB3	3:3:205:SER:HB3	1.98	0.46
1:1:98:LEU:HD23	1:1:167:ARG:NE	2.31	0.46
1:1:95:GLU:HB2	5:H:132:ASN:CA	2.45	0.46
5:H:66:ARG:HD3	5:H:84:SER:HB3	1.97	0.46
5:H:100:GLN:NE2	6:L:92:ALA:O	2.49	0.46
1:1:190:LEU:HD12	1:1:190:LEU:HA	1.76	0.46
5:H:4:LEU:O	6:L:47:PRO:HD2	2.15	0.46
1:1:15:VAL:HG13	1:1:18:TYR:CE1	2.51	0.46
1:1:54:MET:SD	1:1:128:THR:HG22	2.56	0.46
3:3:99:ALA:HB3	3:3:214:LEU:HB2	1.97	0.46
6:L:22:ILE:O	6:L:76:LEU:N	2.26	0.46
6:L:30:ASN:HA	6:L:94:PRO:O	2.15	0.46
1:1:114:ARG:HD2	3:3:11:TYR:HD2	1.81	0.45
1:1:136:TYR:CE2	2:2:173:LYS:CE	2.92	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:191:ALA:O	2:2:135:ARG:NH2	2.49	0.45
2:2:216:SER:HB3	3:3:142:HIS:NE2	2.31	0.45
1:1:100:ASN:ND2	3:3:218:PRO:HA	2.31	0.45
3:3:49:GLU:HB3	3:3:206:ALA:HB3	1.99	0.45
5:H:7:SER:O	5:H:21:THR:O	2.34	0.45
6:L:57:ARG:NE	6:L:61:VAL:HB	2.31	0.45
1:1:48:THR:HG22	1:1:48:THR:O	2.17	0.45
5:H:6:GLU:CD	5:H:94:TYR:HB3	2.41	0.45
5:H:51:ILE:HD11	5:H:55:SER:HA	1.98	0.45
1:1:102:SER:HB2	3:3:217:ASP:HB3	1.98	0.45
5:H:63:LEU:HB2	5:H:67:LEU:HD13	1.98	0.45
6:L:39:TYR:CE2	6:L:49:THR:HB	2.51	0.45
1:1:70:THR:HB	1:1:185:CYS:HB2	1.98	0.45
5:H:1:GLN:N	6:L:58:ALA:HB3	2.31	0.45
2:2:63:LYS:HE3	2:2:202:ASN:ND2	2.31	0.45
2:2:80:LYS:HD3	2:2:129:PHE:CE1	2.50	0.45
6:L:68:SER:O	6:L:75:THR:O	2.33	0.45
1:1:73:PHE:CE2	1:1:119:TYR:CD2	3.05	0.45
2:2:140:LEU:O	2:2:140:LEU:HG	2.17	0.45
5:H:98:VAL:CB	6:L:103:PHE:HE1	2.28	0.45
1:1:72:TYR:CD2	1:1:72:TYR:O	2.70	0.45
3:3:136:THR:N	3:3:137:PRO:CD	2.80	0.45
5:H:4:LEU:CB	6:L:47:PRO:HG2	2.47	0.45
6:L:38:TRP:CD1	6:L:76:LEU:HD13	2.52	0.45
1:1:72:TYR:O	1:1:72:TYR:CG	2.70	0.44
1:1:95:GLU:H	5:H:132:ASN:CA	2.27	0.44
1:1:158:PRO:HG2	1:1:161:PHE:CZ	2.45	0.44
5:H:22:CYS:O	5:H:77:GLN:HA	2.17	0.44
2:2:87:HIS:CD2	2:2:91:TYR:HB3	2.52	0.44
2:2:107:VAL:HG22	2:2:179:LEU:HD22	1.92	0.44
5:H:100:GLN:HG3	6:L:93:SER:N	2.32	0.44
1:1:82:HIS:HE2	1:1:108:HIS:HA	1.82	0.44
5:H:120:TRP:CH2	5:H:130:TYR:CD2	3.05	0.44
1:1:160:SER:CB	3:3:170:TYR:HH	2.31	0.44
2:2:18:ARG:HB2	2:2:23:THR:CG2	2.47	0.44
2:2:67:PHE:O	2:2:67:PHE:CD1	2.70	0.44
2:2:166:ASN:CB	3:3:165:ALA:HB1	2.48	0.44
5:H:15:SER:HA	5:H:84:SER:HA	2.00	0.44
5:H:19:SER:O	5:H:19:SER:OG	2.32	0.44
5:H:132:ASN:N	5:H:132:ASN:OD1	2.51	0.44
1:1:98:LEU:HD13	5:H:133:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:112:PHE:O	1:1:112:PHE:CD1	2.70	0.44
2:2:67:PHE:O	2:2:67:PHE:CG	2.70	0.44
2:2:213:GLU:O	3:3:143:CYS:CA	2.61	0.44
1:1:100:ASN:ND2	3:3:218:PRO:C	2.75	0.44
1:1:100:ASN:ND2	3:3:218:PRO:CA	2.81	0.44
5:H:28:SER:O	5:H:32:LYS:HD2	2.17	0.44
5:H:45:LEU:HD22	6:L:6:LEU:O	2.18	0.44
5:H:98:VAL:HG13	6:L:101:ALA:CB	2.44	0.44
5:H:103:SER:O	6:L:33:ASN:ND2	2.50	0.44
5:H:138:TYR:CD2	5:H:142:THR:HG23	2.51	0.44
5:H:6:GLU:OE2	5:H:94:TYR:HB3	2.18	0.44
6:L:40:GLN:HE21	6:L:48:ARG:HB3	1.83	0.44
3:3:63:TYR:HB2	3:3:199:THR:HB	2.00	0.44
3:3:174:ASP:O	3:3:174:ASP:OD2	2.35	0.44
1:1:159:ALA:HB3	5:H:134:GLY:C	2.43	0.43
2:2:214:LEU:HD23	3:3:127:PRO:HG3	1.91	0.43
5:H:108:CYS:HB2	5:H:109:PRO:CD	2.44	0.43
5:H:119:ARG:HH11	5:H:120:TRP:HE1	1.66	0.43
1:1:57:HIS:CD2	1:1:59:HIS:HB2	2.53	0.43
2:2:166:ASN:HB3	3:3:165:ALA:C	2.43	0.43
3:3:136:THR:HG22	3:3:188:TYR:CB	2.48	0.43
5:H:122:CYS:H	5:H:123:PRO:HD2	1.82	0.43
6:L:20:VAL:HG11	6:L:81:LEU:HD13	1.99	0.43
1:1:110:ALA:N	1:1:111:PRO:CD	2.81	0.43
2:2:100:TYR:HH	3:3:128:PRO:HG2	1.82	0.43
3:3:64:VAL:HG21	3:3:74:LEU:HB3	1.99	0.43
5:H:17:THR:O	5:H:18:LEU:C	2.61	0.43
1:1:57:HIS:CD2	1:1:59:HIS:H	2.36	0.43
5:H:63:LEU:CB	5:H:67:LEU:HD13	2.48	0.43
1:1:15:VAL:O	1:1:15:VAL:CG1	2.64	0.43
1:1:51:ILE:HG21	1:1:166:ILE:HG23	2.01	0.43
2:2:126:VAL:HG13	2:2:143:PHE:CZ	2.53	0.43
5:H:120:TRP:HB3	5:H:140:ARG:HH21	1.83	0.43
1:1:135:LYS:HE3	1:1:158:PRO:HG3	1.99	0.43
3:3:41:PHE:HB2	3:3:47:VAL:HG23	1.95	0.43
1:1:160:SER:CB	3:3:170:TYR:OH	2.66	0.43
3:3:107:LEU:HD22	3:3:160:ILE:HD11	2.00	0.43
3:3:182:GLN:N	3:3:182:GLN:CD	2.76	0.43
5:H:75:ARG:O	5:H:77:GLN:HG3	2.18	0.43
5:H:117:ALA:HB1	5:H:129:GLY:HA3	1.86	0.43
6:L:62:PRO:HG3	6:L:64:ARG:HH21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:93:ALA:O	5:H:133:PHE:O	2.36	0.43
2:2:182:MET:HE3	2:2:184:VAL:HG22	1.99	0.43
5:H:49:GLY:HA3	5:H:58:GLY:O	2.18	0.43
6:L:38:TRP:CG	6:L:76:LEU:HD22	2.54	0.43
2:2:80:LYS:HA	2:2:179:LEU:O	2.19	0.42
2:2:114:ASN:CB	2:2:193:GLY:HA2	2.49	0.42
5:H:47:TRP:CZ2	5:H:49:GLY:HA2	2.54	0.42
3:3:64:VAL:CG2	3:3:74:LEU:HB3	2.50	0.42
3:3:66:THR:OG1	3:3:189:GLN:NE2	2.50	0.42
3:3:125:TYR:HB3	3:3:144:ILE:HG23	2.00	0.42
5:H:102:THR:HG21	6:L:99:SER:C	2.43	0.42
5:H:116:CYS:HG	5:H:131:CYS:HG	0.48	0.42
5:H:129:GLY:HA2	5:H:141:CYS:HA	2.00	0.42
2:2:22:THR:HG21	2:2:60:ARG:CG	2.32	0.42
3:3:189:GLN:CD	3:3:192:HIS:HB3	2.44	0.42
5:H:72:ASP:HB3	5:H:77:GLN:O	2.18	0.42
3:3:118:LYS:O	3:3:193:GLY:N	2.53	0.42
5:H:37:VAL:HG11	6:L:103:PHE:CB	2.49	0.42
5:H:60:ASN:HA	5:H:61:PRO:HD3	1.83	0.42
1:1:124:ARG:HB2	2:2:165:VAL:O	2.19	0.42
1:1:158:PRO:CA	1:1:161:PHE:HD2	2.33	0.42
3:3:54:PHE:HA	3:3:203:SER:HA	2.02	0.42
5:H:4:LEU:HA	5:H:23:THR:O	2.20	0.42
6:L:78:ILE:HG21	6:L:85:ASP:OD2	2.20	0.42
1:1:50:VAL:HG22	5:H:133:PHE:CE1	2.55	0.42
1:1:30:THR:O	1:1:30:THR:CG2	2.56	0.42
1:1:91:ASN:ND2	1:1:121:ALA:CA	2.76	0.42
2:2:217:LYS:HB3	2:2:217:LYS:HE3	1.90	0.42
5:H:92:THR:HG22	5:H:94:TYR:H	1.83	0.42
1:1:74:SER:HB3	1:1:181:ALA:HA	2.02	0.42
1:1:98:LEU:HD21	1:1:167:ARG:HB2	2.01	0.42
2:2:43:VAL:HG21	2:2:209:HIS:HE2	1.84	0.42
1:1:48:THR:OG1	1:1:167:ARG:HG3	2.20	0.41
1:1:153:LEU:CG	1:1:154:ALA:N	2.80	0.41
2:2:174:HIS:ND1	2:2:174:HIS:C	2.77	0.41
1:1:76:LEU:CD1	1:1:176:VAL:CG1	2.71	0.41
1:1:1:THR:HG23	1:1:13:THR:OG1	2.20	0.41
2:2:16:THR:HG23	2:2:25:THR:OG1	2.20	0.41
2:2:62:PHE:CE2	2:2:203:ILE:HD12	2.55	0.41
3:3:67:ARG:HE	3:3:71:GLN:HG2	1.86	0.41
3:3:133:PRO:HA	3:3:134:PRO:HD3	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:132:THR:HA	3:3:133:PRO:HD3	1.82	0.41
5:H:37:VAL:HG11	6:L:103:PHE:CG	2.55	0.41
1:1:87:THR:O	1:1:166:ILE:HA	2.21	0.41
1:1:95:GLU:HB2	5:H:131:CYS:O	2.21	0.41
3:3:193:GLY:C	3:3:195:ALA:N	2.78	0.41
1:1:50:VAL:HG22	5:H:133:PHE:HE1	1.84	0.41
5:H:4:LEU:HB2	6:L:47:PRO:HG2	2.03	0.41
2:2:28:SER:O	2:2:153:ASN:HB2	2.20	0.41
2:2:41:ASP:OD1	2:2:41:ASP:N	2.50	0.41
5:H:100:GLN:O	6:L:101:ALA:HB2	2.20	0.41
3:3:79:LEU:HD22	3:3:125:TYR:CE1	2.56	0.41
3:3:80:SER:HB2	3:3:180:ASN:CB	2.51	0.41
3:3:133:PRO:HD2	3:3:139:ARG:HE	1.86	0.41
5:H:130:TYR:CE2	5:H:134:GLY:O	2.73	0.41
1:1:36:MET:HE1	1:1:66:LEU:HB2	2.03	0.41
2:2:213:GLU:HB2	3:3:143:CYS:CA	2.51	0.41
5:H:38:ARG:O	5:H:38:ARG:HG3	2.17	0.41
5:H:45:LEU:HD23	6:L:105:SER:H	1.86	0.41
6:L:34:GLY:HA2	6:L:94:PRO:HD3	1.80	0.41
2:2:75:PHE:CD1	2:2:75:PHE:C	2.99	0.40
5:H:98:VAL:CG1	6:L:103:PHE:HE1	2.34	0.40
1:1:9:ASP:OD1	1:1:9:ASP:N	2.53	0.40
1:1:48:THR:CG2	5:H:119:ARG:HH21	2.25	0.40
1:1:53:LEU:HD21	1:1:76:LEU:HD11	2.02	0.40
1:1:61:LEU:O	1:1:65:MET:HB2	2.21	0.40
1:1:158:PRO:CA	1:1:161:PHE:CD2	3.04	0.40
3:3:128:PRO:N	3:3:128:PRO:C	2.66	0.40
5:H:100:GLN:CB	6:L:101:ALA:HA	2.52	0.40
6:L:57:ARG:HB2	6:L:61:VAL:HG21	2.02	0.40
1:1:52:ASP:OD1	1:1:52:ASP:C	2.65	0.40
2:2:78:ILE:HD11	2:2:137:LYS:HG2	2.04	0.40
3:3:108:HIS:HB3	3:3:155:LYS:HE2	2.03	0.40
1:1:197:GLN:HE21	1:1:197:GLN:CA	2.00	0.40
2:2:159:THR:HG23	2:2:159:THR:O	2.21	0.40
2:2:189:THR:HG21	2:2:195:SER:HA	2.03	0.40
5:H:138:TYR:CE2	5:H:142:THR:HG21	2.52	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	182/212 (86%)	169 (93%)	13 (7%)	0	100	100
2	2	204/218 (94%)	195 (96%)	9 (4%)	0	100	100
3	3	218/221 (99%)	196 (90%)	20 (9%)	2 (1%)	14	47
4	4	41/85 (48%)	36 (88%)	5 (12%)	0	100	100
5	H	142/167 (85%)	118 (83%)	24 (17%)	0	100	100
6	L	106/123 (86%)	97 (92%)	8 (8%)	1 (1%)	14	47
All	All	893/1026 (87%)	811 (91%)	79 (9%)	3 (0%)	37	67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	3	175	VAL
3	3	134	PRO
6	L	47	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	157/175 (90%)	147 (94%)	10 (6%)	16	42
2	2	182/194 (94%)	170 (93%)	12 (7%)	15	41
3	3	181/182 (100%)	170 (94%)	11 (6%)	17	43
4	4	37/67 (55%)	36 (97%)	1 (3%)	39	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	H	114/141 (81%)	109 (96%)	5 (4%)	25	51
6	L	88/98 (90%)	87 (99%)	1 (1%)	65	74
All	All	759/857 (89%)	719 (95%)	40 (5%)	22	47

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	2	THR
1	1	4	THR
1	1	18	TYR
1	1	24	VAL
1	1	51	ILE
1	1	58	GLN
1	1	78	ILE
1	1	113	THR
1	1	153	LEU
1	1	197	GLN
2	2	13	ARG
2	2	75	PHE
2	2	83	LEU
2	2	107	VAL
2	2	115	GLN
2	2	122	LEU
2	2	162	TYR
2	2	166	ASN
2	2	174	HIS
2	2	178	THR
2	2	180	VAL
2	2	192	ILE
3	3	3	VAL
3	3	28	MET
3	3	65	VAL
3	3	102	SER
3	3	114	SER
3	3	144	ILE
3	3	153	ASN
3	3	155	LYS
3	3	175	VAL
3	3	177	ASP
3	3	179	THR
4	4	21	ILE

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Mol	Chain	Res	Type
5	H	85	VAL
5	H	120	TRP
5	H	132	ASN
5	H	137	SER
5	H	138	TYR
6	L	107	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	17	ASN
1	1	49	HIS
1	1	57	HIS
1	1	59	HIS
1	1	91	ASN
1	1	100	ASN
1	1	123	HIS
1	1	156	GLN
1	1	197	GLN
2	2	87	HIS
2	2	145	HIS
3	3	100	GLN
3	3	142	HIS
3	3	180	ASN
6	L	33	ASN
6	L	40	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.

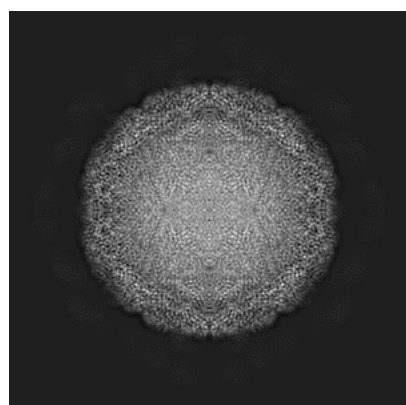
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30565. These allow visual inspection of the internal detail of the map and identification of artifacts.

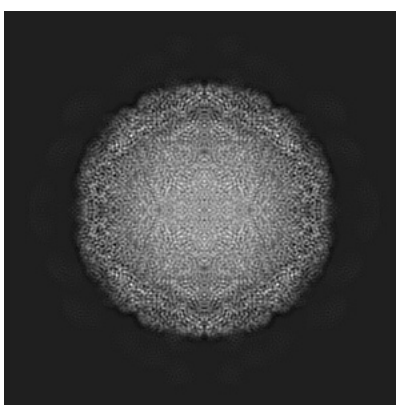
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

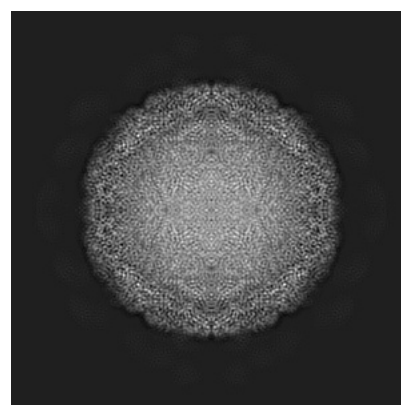
6.1.1 Primary map



X



Y

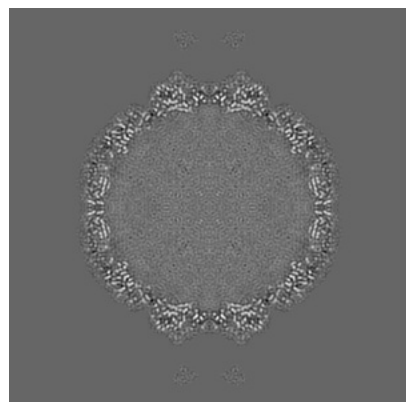


Z

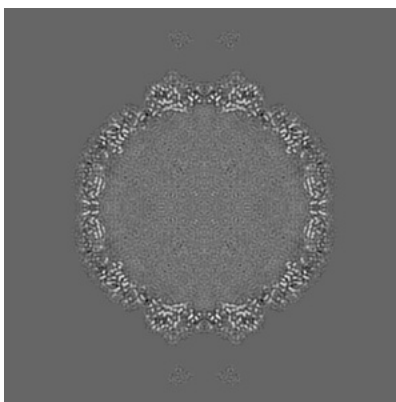
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

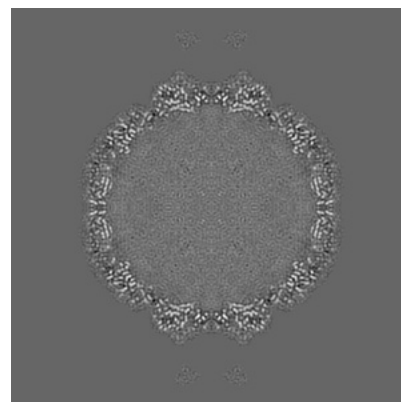
6.2.1 Primary map



X Index: 240



Y Index: 240

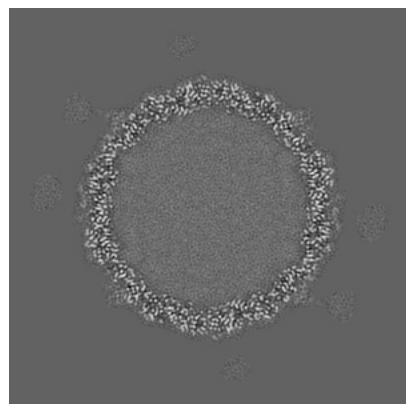


Z Index: 240

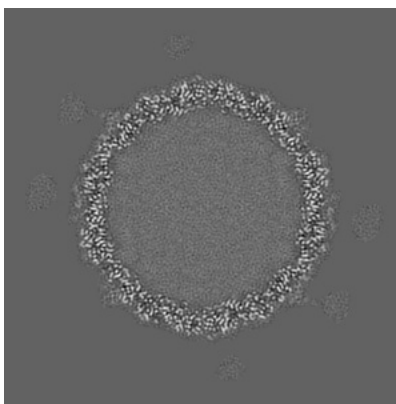
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

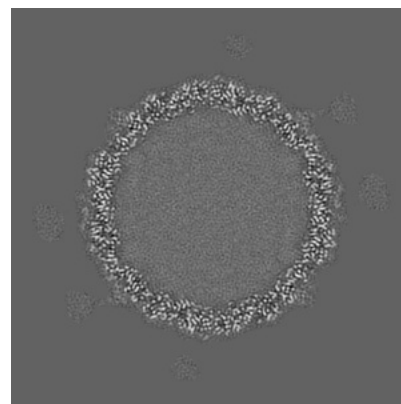
6.3.1 Primary map



X Index: 209



Y Index: 209

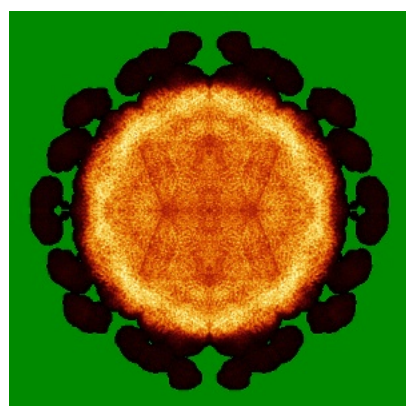


Z Index: 271

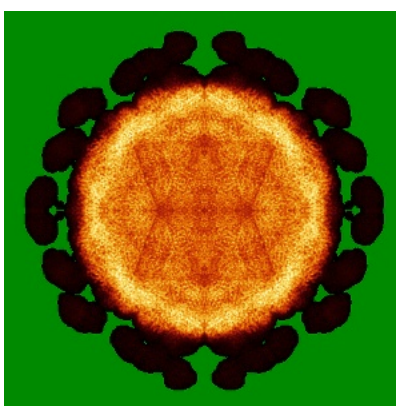
The images above show the largest variance slices of the map in three orthogonal directions.

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

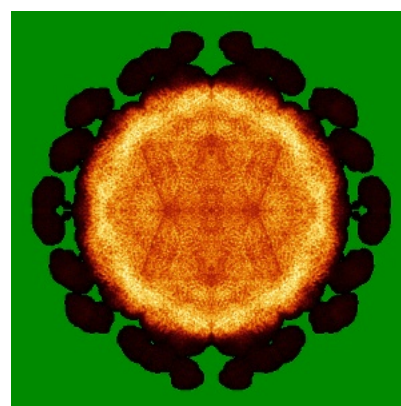
6.4.1 Primary map



X



Y

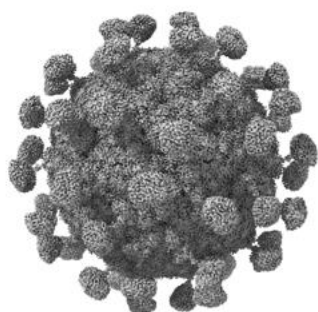


Z

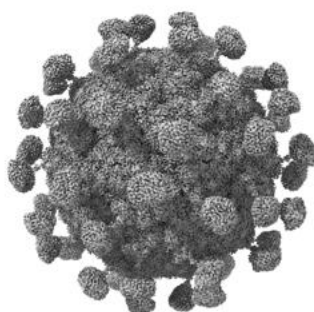
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

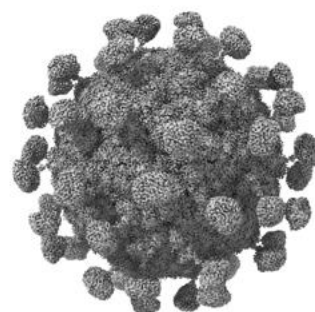
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.003. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

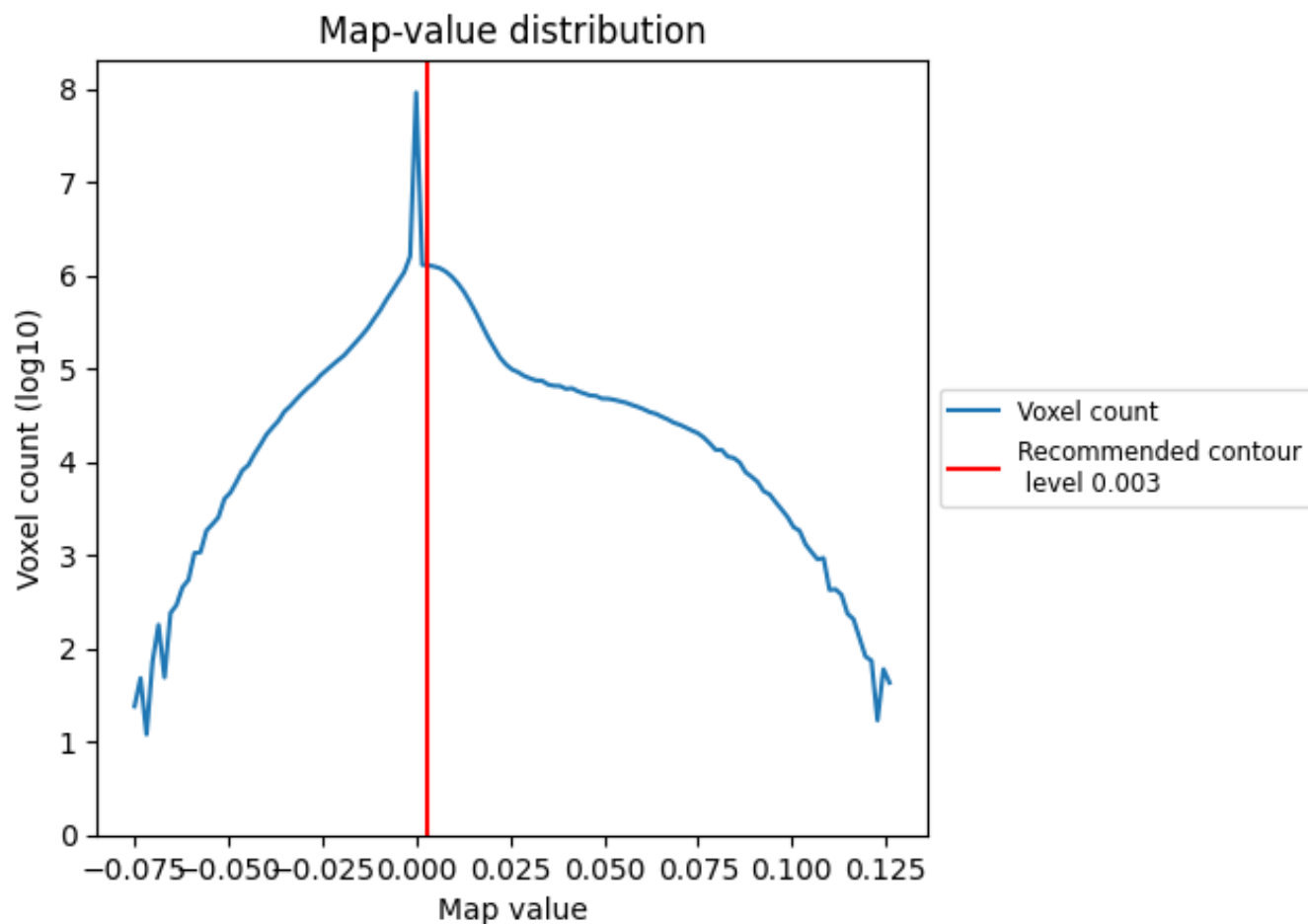
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

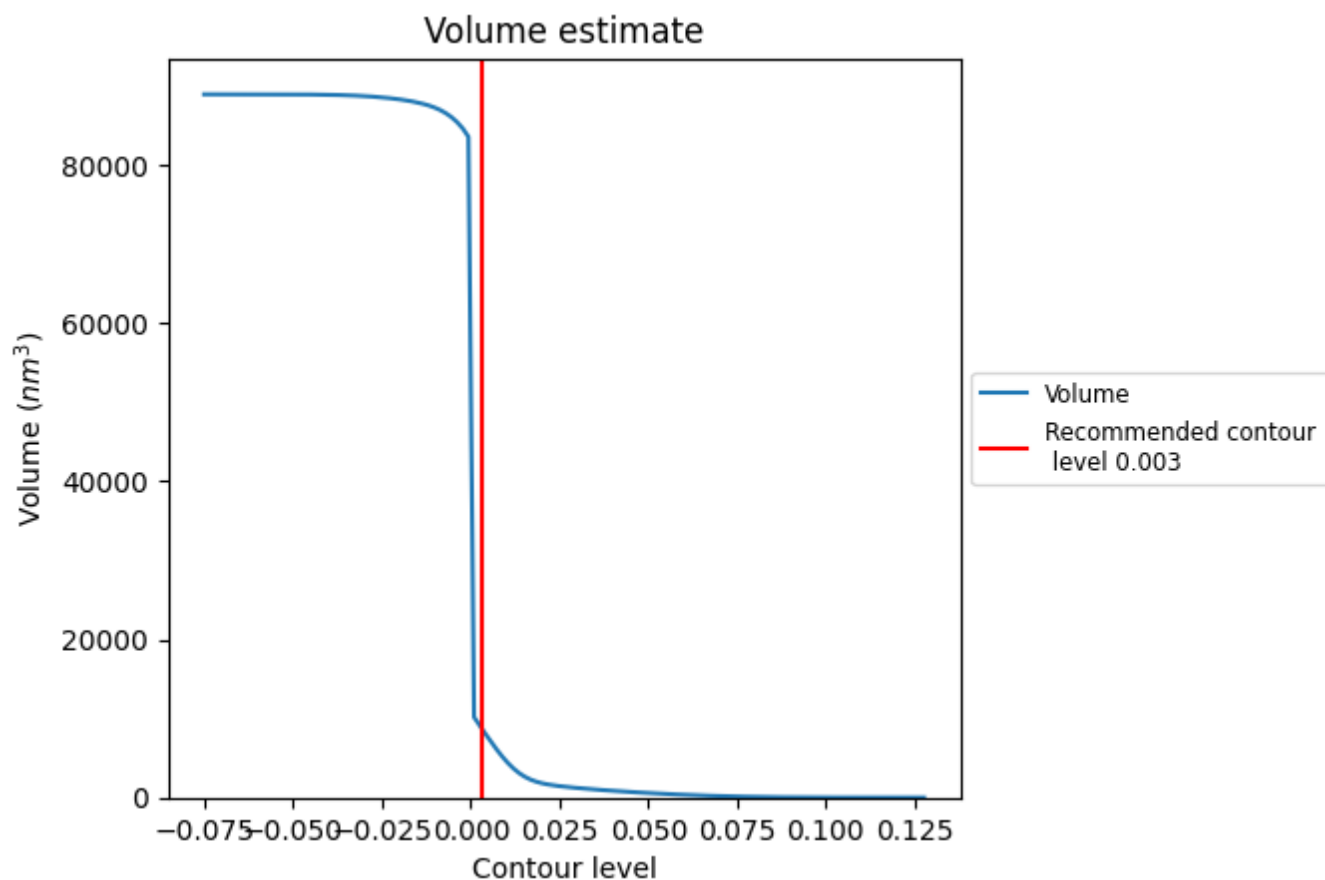
This section contains the results of statistical analysis of the map.

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.

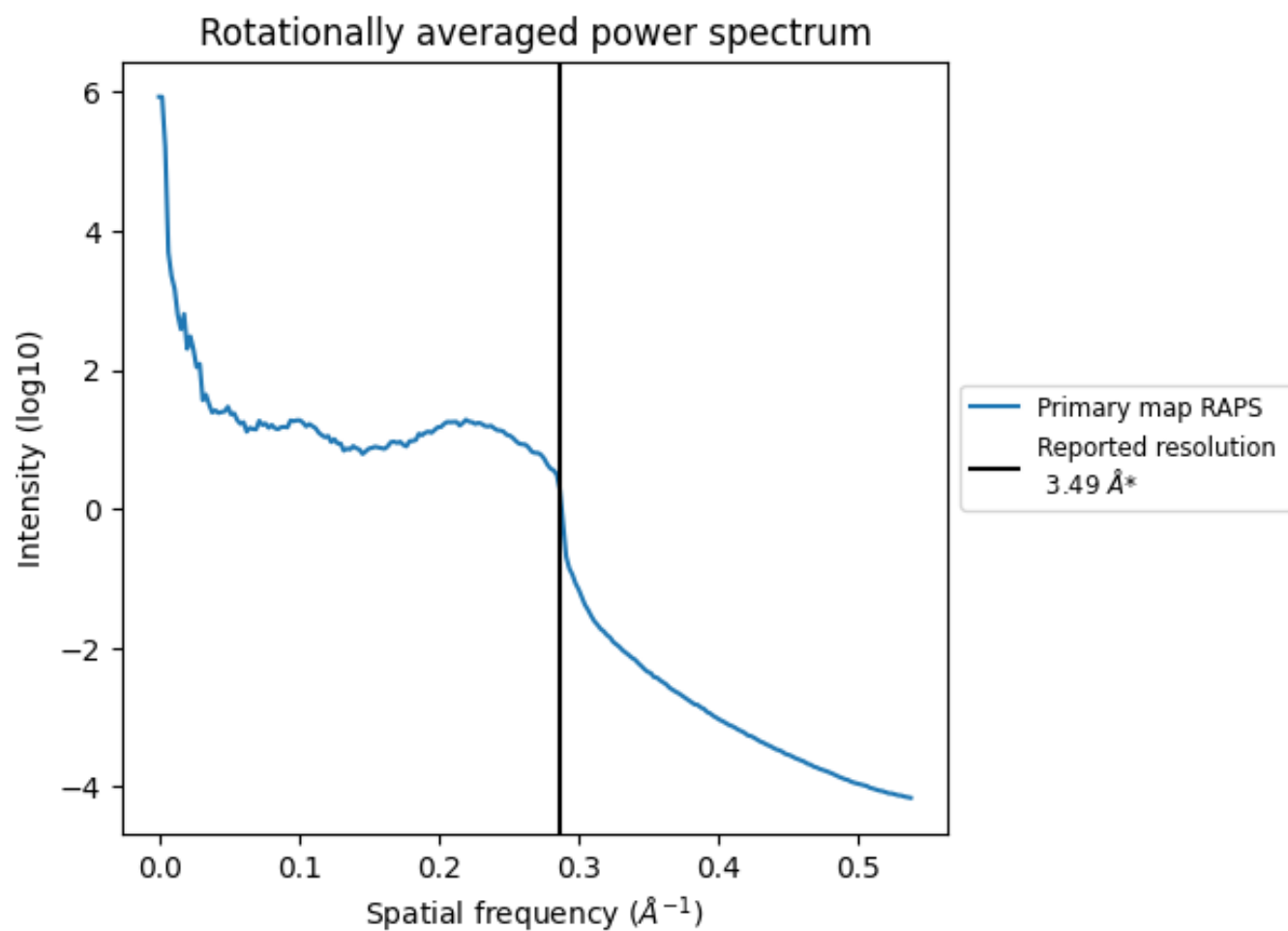
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 8826 nm³; this corresponds to an approximate mass of 7973 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 0.287 Å⁻¹

8 Fourier-Shell correlation ⓘ

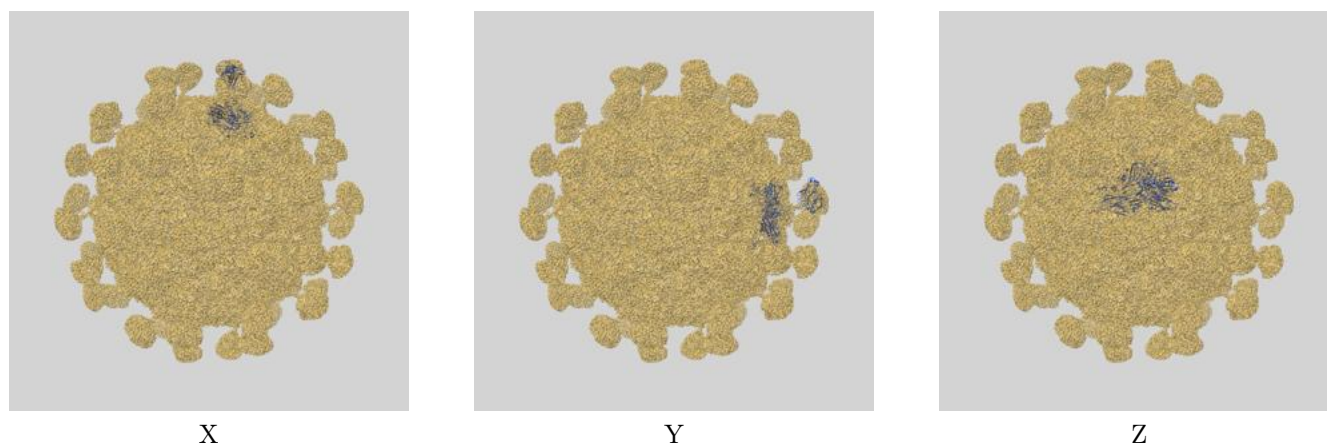
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

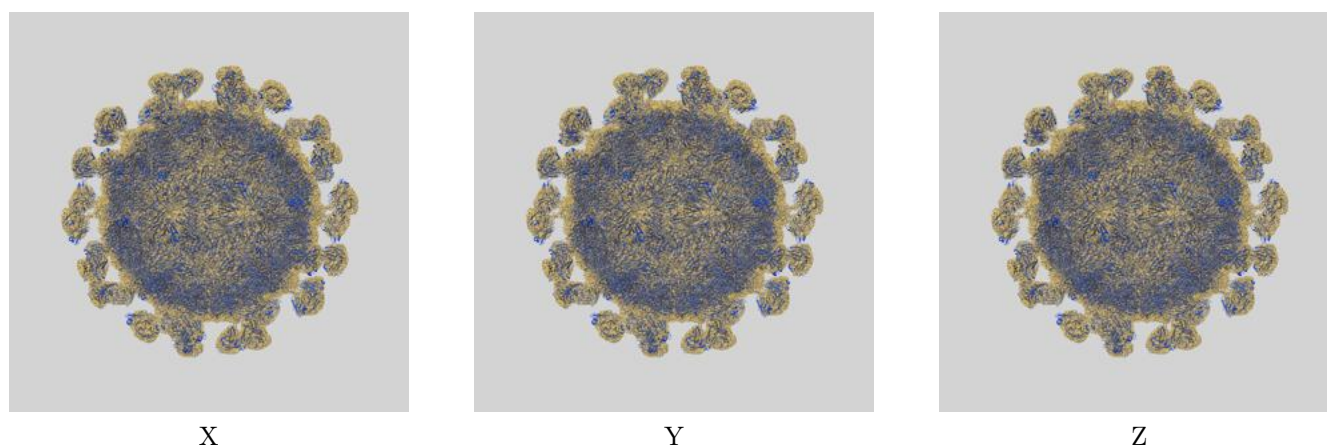
This section contains information regarding the fit between EMDB map EMD-30565 and PDB model 7D3R. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

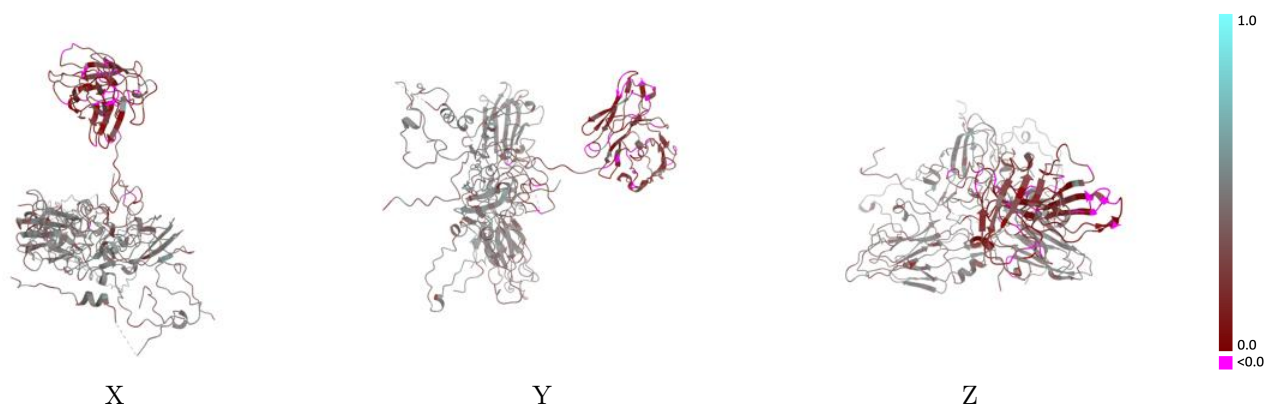


9.1.2 Map-model assembly overlay [i](#)



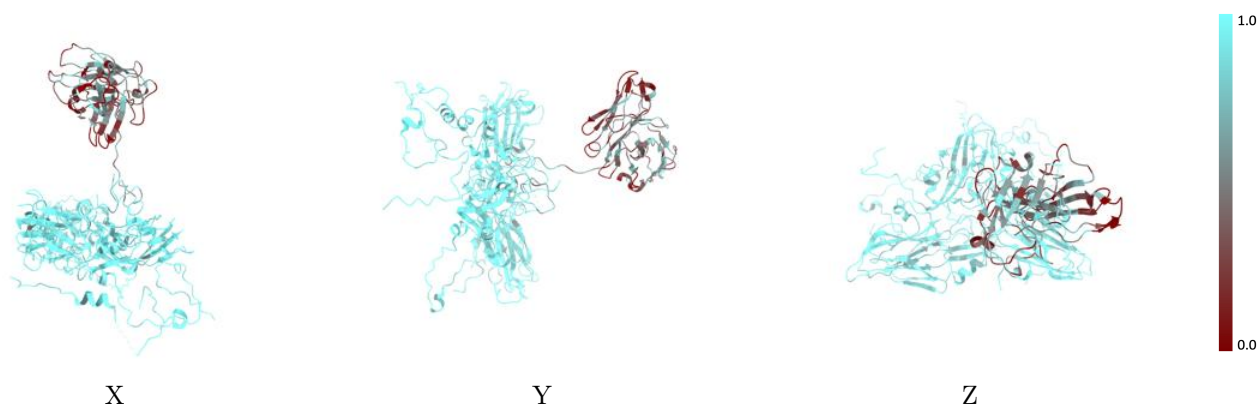
The images above show the 3D surface view of the map at the recommended contour level 0.003 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



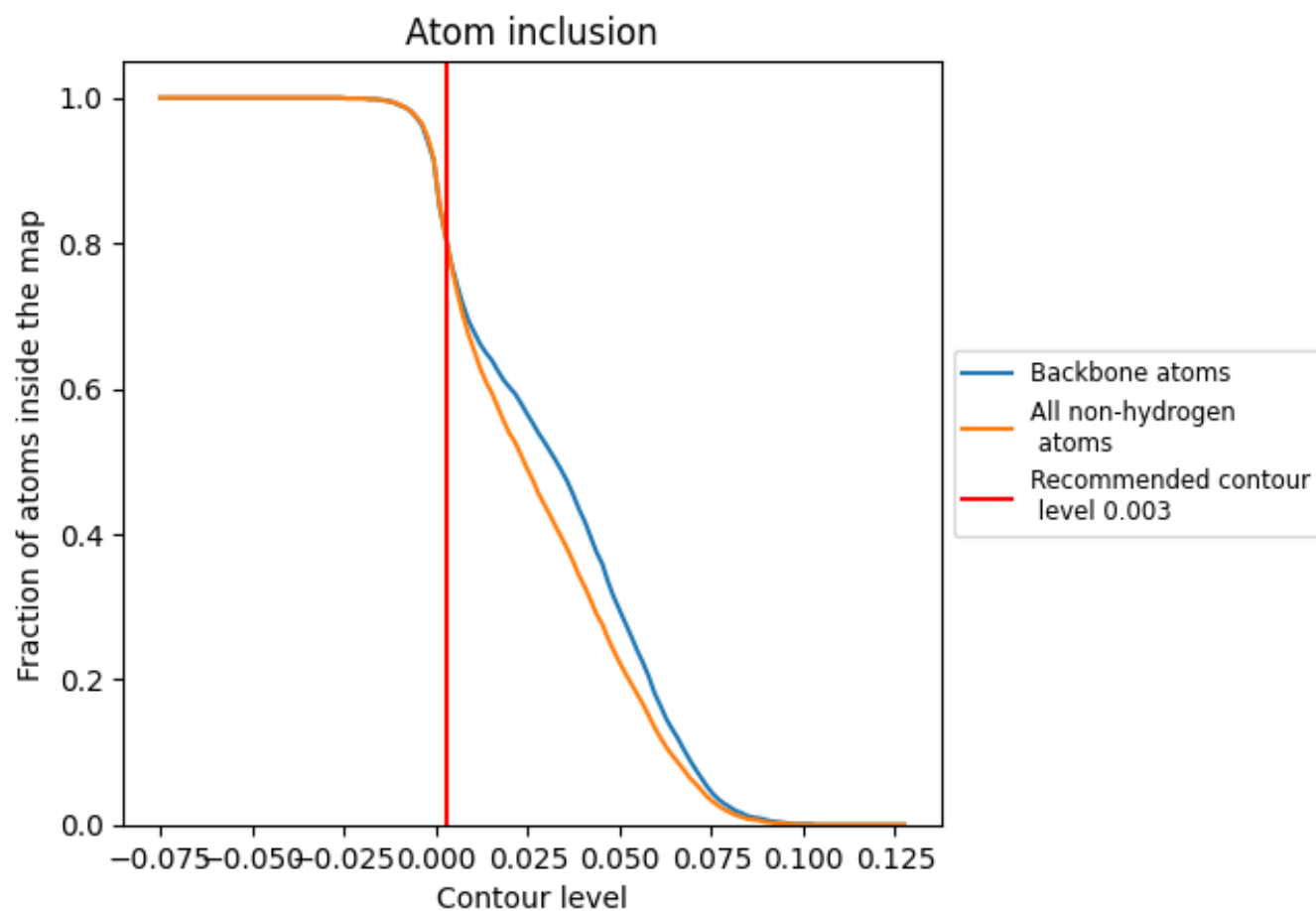
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.003).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 80% 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 (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8000	0.3630
1	0.9230	0.4310
2	0.9140	0.4230
3	0.9250	0.4290
4	0.8950	0.4130
H	0.5470	0.2160
L	0.3630	0.1410

1.0

0.0

<0.0