



Full wwPDB EM Validation Report ⓘ

Mar 15, 2026 – 06:36 AM UTC

PDB ID : 7JTI / pdb_00007jti
EMDB ID : EMD-22474
Title : Interphotoreceptor retinoid-binding protein (IRBP) in complex with a monoclonal antibody (F3F5 mAb5)
Authors : Sears, A.E.; Albiez, S.; Gulati, S.; Wang, B.; Kiser, P.; Kovacik, L.; Engel, A.; Stahlberg, H.; Palczewski, K.
Deposited on : 2020-08-17
Resolution : 7.40 Å (reported)
Based on initial model : 1J7X

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

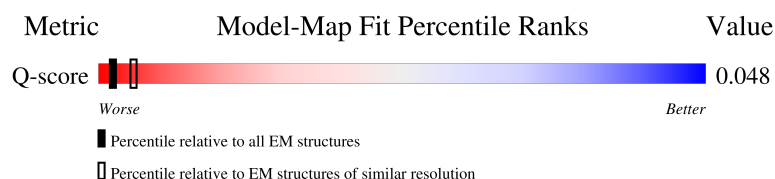
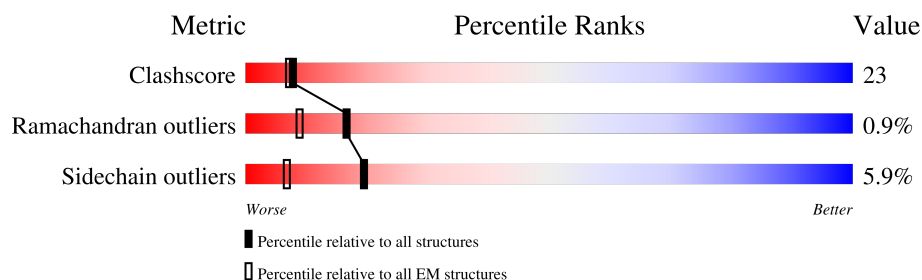
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.40 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	412 (6.90 - 7.90)

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	L	210	28% 58% 30% 11% .
2	H	221	23% 50% 40% 9% .
3	A	303	35% 73% 24% ..
4	B	309	77% 82% 16% .

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Mol	Chain	Length	Quality of chain
5	C	300	33% 87% 11%
6	D	296	64% 82% 14%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12432 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 mAb5 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	210	Total	C	N	O	S	0	0
			1589	994	266	323	6		

- Molecule 2 is a protein called mAb5 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	221	Total	C	N	O	S	0	0
			1672	1065	270	328	9		

- Molecule 3 is a protein called Retinol-binding protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	303	Total	C	N	O	S	0	0
			2346	1485	396	461	4		

- Molecule 4 is a protein called Retinol-binding protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	309	Total	C	N	O	S	0	0
			2285	1465	367	447	6		

- Molecule 5 is a protein called Retinol-binding protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	300	Total	C	N	O	S	0	0
			2278	1446	383	439	10		

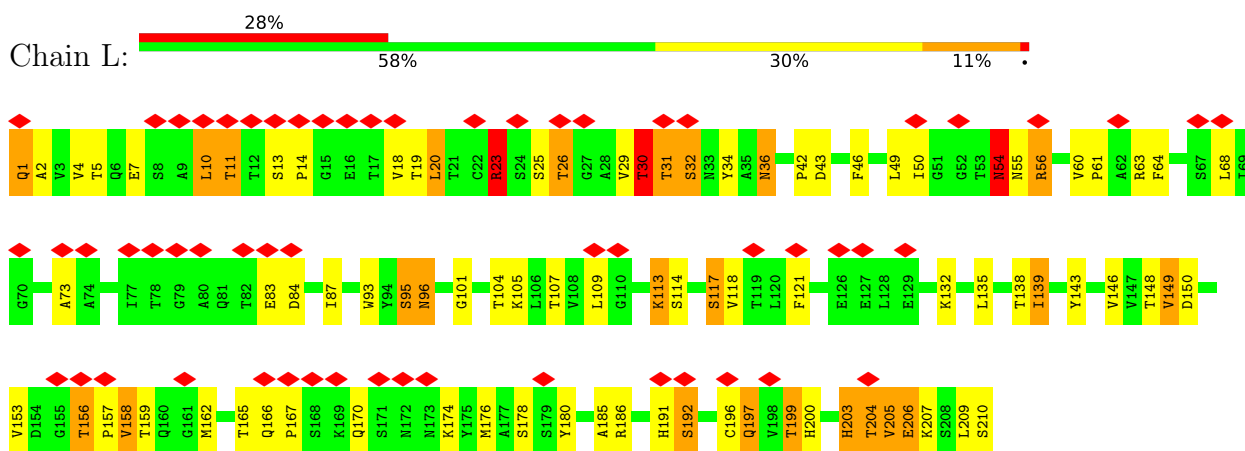
- Molecule 6 is a protein called Retinol-binding protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	296	Total	C	N	O	S	0	0
			2262	1435	375	442	10		

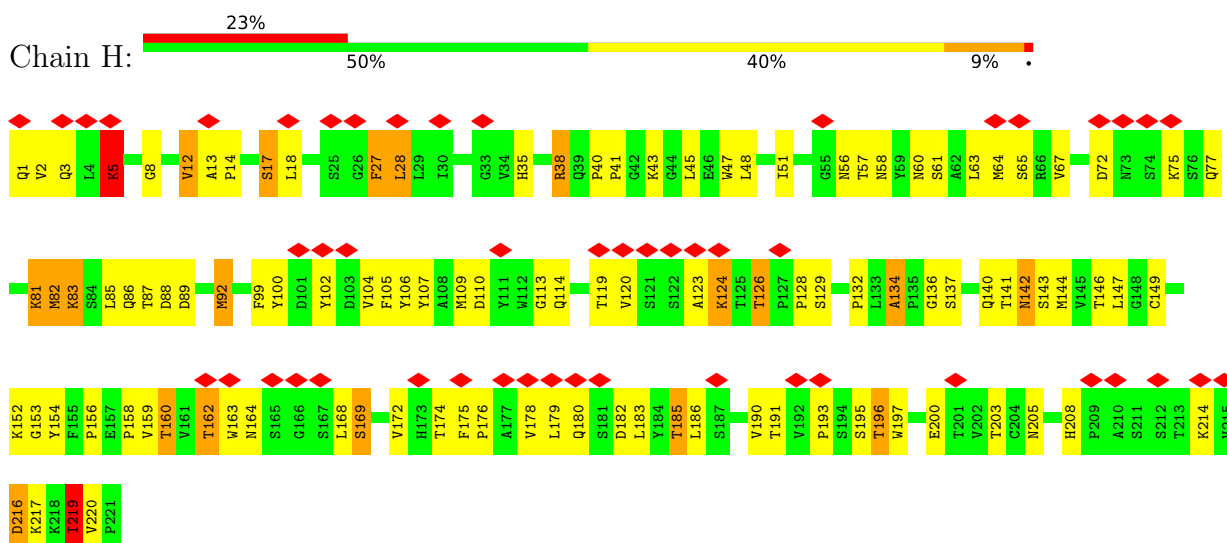
3 Residue-property plots

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: mAb5 Fab light chain

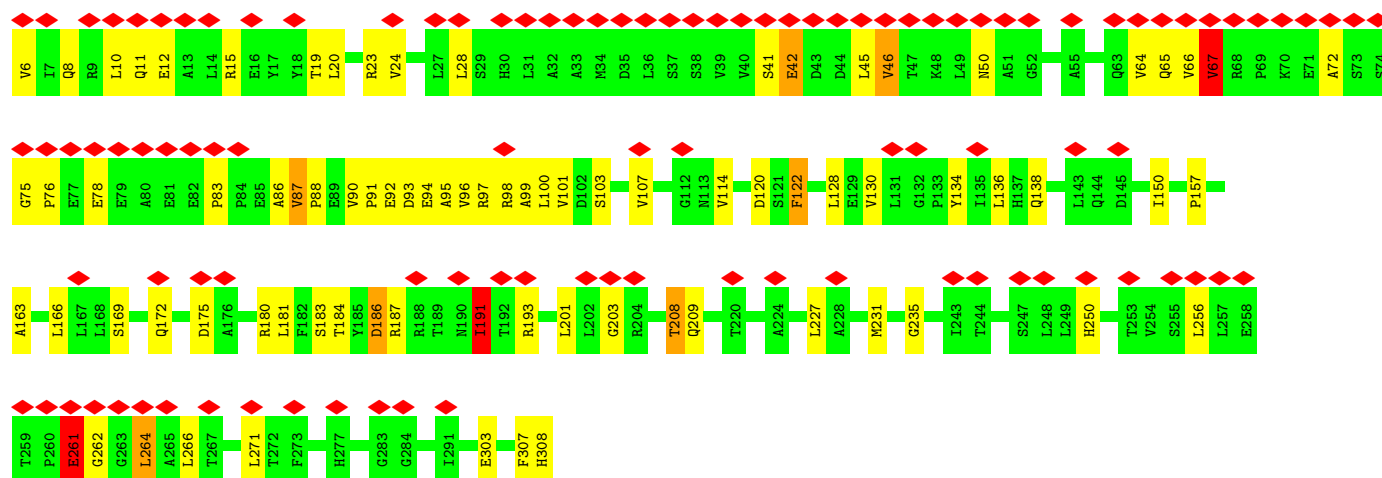


- Molecule 2: mAb5 Fab heavy chain

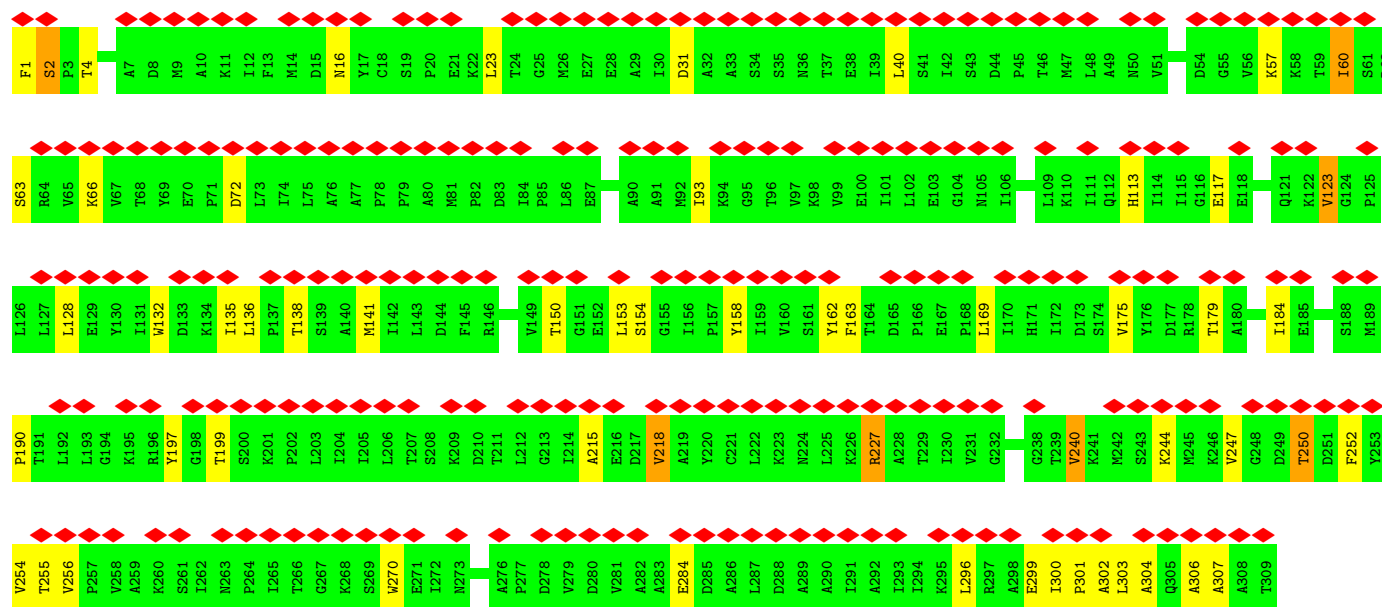
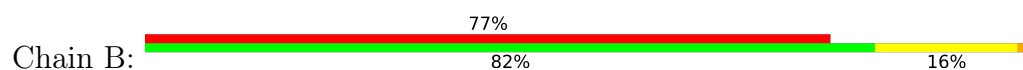


- Molecule 3: Retinol-binding protein 3

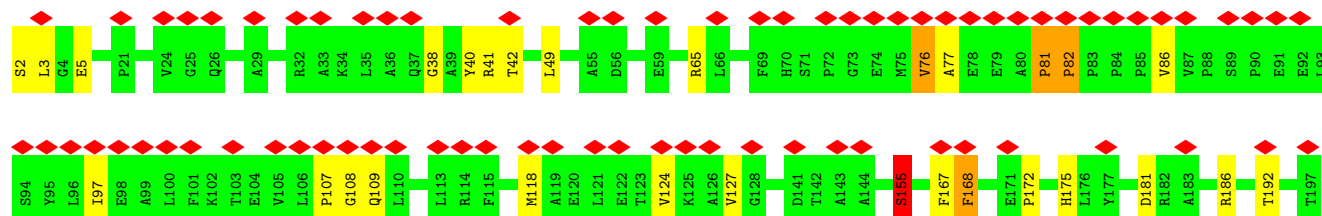
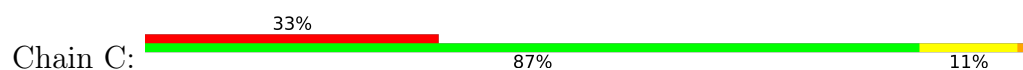


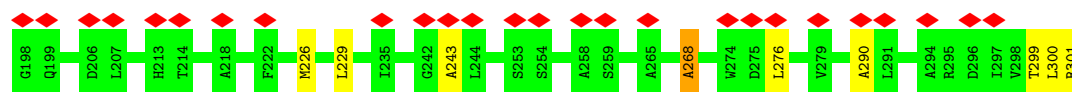


• Molecule 4: Retinol-binding protein 3

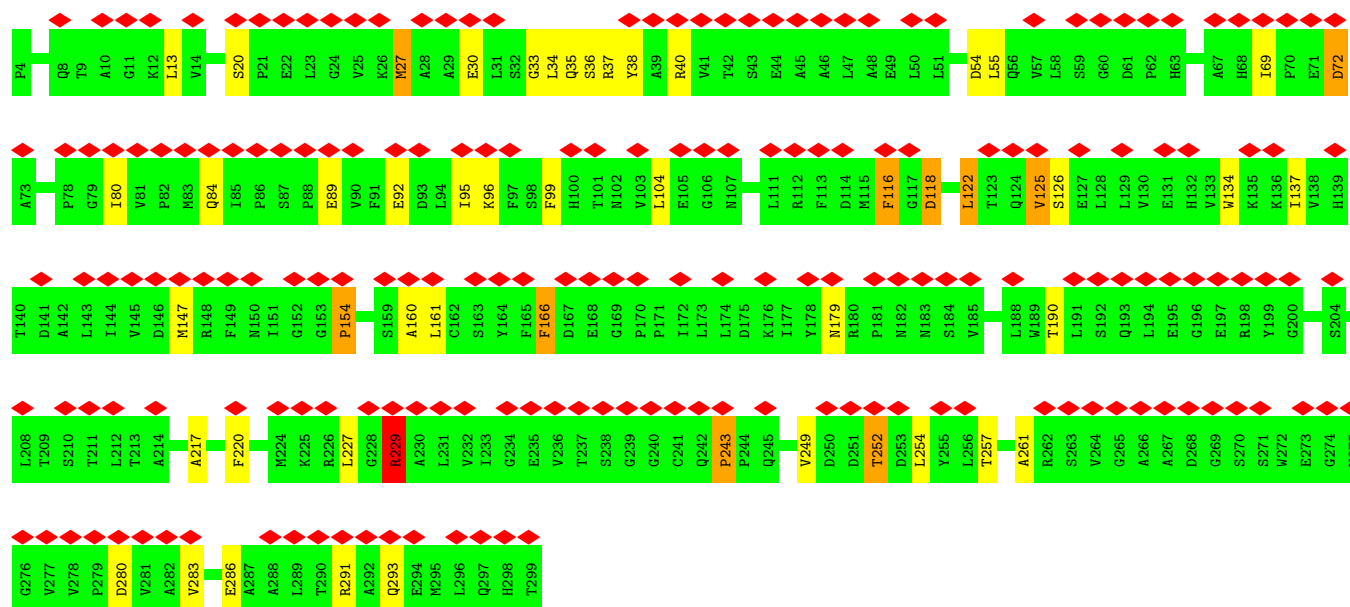
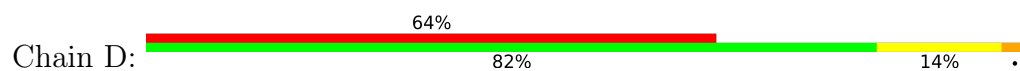


• Molecule 5: Retinol-binding protein 3





• Molecule 6: Retinol-binding protein 3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17900	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	60000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	4.328	Depositor
Minimum map value	-1.114	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.73	Depositor
Map size (Å)	398.87997, 398.87997, 398.87997	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.662, 1.662, 1.662	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	L	1.00	0/1627	2.09	58/2224 (2.6%)
2	H	1.02	0/1718	2.11	64/2351 (2.7%)
3	A	1.01	1/2397 (0.0%)	1.51	15/3277 (0.5%)
4	B	0.73	1/2326 (0.0%)	0.89	1/3175 (0.0%)
5	C	0.84	0/2329	1.44	8/3178 (0.3%)
6	D	0.96	2/2309 (0.1%)	1.51	15/3143 (0.5%)
All	All	0.93	4/12706 (0.0%)	1.59	161/17348 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	1
5	C	0	2
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	116	PHE	C-O	-8.32	1.14	1.23
4	B	240	VAL	CA-CB	5.53	1.61	1.54
3	A	261	GLU	CA-C	5.17	1.60	1.52
6	D	229	ARG	CD-NE	5.00	1.53	1.46

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	42	GLU	CB-CG-CD	-11.81	92.53	112.60
3	A	186	ASP	CA-CB-CG	11.68	124.28	112.60
2	H	58	ASN	CA-CB-CG	9.76	122.36	112.60
1	L	2	ALA	N-CA-C	-8.94	91.76	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	36	ASN	OD1-CG-ND2	8.87	131.47	122.60
5	C	155	SER	CA-C-N	8.77	133.27	120.90
5	C	155	SER	C-N-CA	8.77	133.27	120.90
2	H	88	ASP	CA-CB-CG	8.52	121.12	112.60
3	A	261	GLU	CA-C-O	8.37	134.38	120.65
1	L	83	GLU	CB-CG-CD	8.25	126.62	112.60
2	H	195	SER	CA-C-N	8.12	131.49	120.44
2	H	195	SER	C-N-CA	8.12	131.49	120.44
2	H	110	ASP	N-CA-C	8.06	123.46	112.90
1	L	30	THR	CA-C-N	8.04	131.06	120.28
1	L	30	THR	C-N-CA	8.04	131.06	120.28
2	H	196	THR	N-CA-C	7.87	119.64	111.14
1	L	42	PRO	CA-C-N	7.67	136.20	121.54
1	L	42	PRO	C-N-CA	7.67	136.20	121.54
3	A	42	GLU	CB-CA-C	-7.43	99.21	110.88
3	A	264	LEU	N-CA-C	7.43	120.98	110.50
2	H	5	LYS	CB-CA-C	-7.39	98.32	110.14
2	H	197	TRP	CB-CA-C	7.31	118.84	108.68
1	L	23	ARG	CD-NE-CZ	7.26	134.57	124.40
2	H	60	ASN	N-CA-C	-7.22	99.13	109.96
6	D	154	PRO	CA-C-N	7.08	130.07	120.38
6	D	154	PRO	C-N-CA	7.08	130.07	120.38
2	H	38	ARG	CB-CG-CD	7.06	127.55	111.30
6	D	27	MET	CG-SD-CE	-7.06	85.37	100.90
1	L	30	THR	N-CA-CB	-7.02	100.52	111.05
2	H	57	THR	CA-CB-OG1	-6.93	99.20	109.60
1	L	166	GLN	N-CA-C	-6.93	101.06	109.72
2	H	169	SER	CA-C-O	6.87	126.46	118.90
2	H	110	ASP	CA-CB-CG	6.86	119.46	112.60
2	H	160	THR	CA-CB-OG1	-6.85	99.33	109.60
1	L	30	THR	CA-CB-CG2	6.80	122.06	110.50
2	H	8	GLY	O-C-N	6.80	128.57	121.77
2	H	220	VAL	O-C-N	6.76	127.01	121.40
2	H	219	ILE	CB-CA-C	6.75	120.23	110.98
3	A	87	VAL	N-CA-CB	6.69	114.72	110.50
2	H	86	GLN	N-CA-C	-6.67	99.18	109.52
1	L	43	ASP	CB-CA-C	6.66	123.67	110.42
2	H	129	SER	CA-C-O	-6.53	113.27	120.38
3	A	191	ILE	CA-CB-CG2	6.51	121.57	110.50
1	L	7	GLU	CA-C-O	-6.51	114.65	121.55
1	L	26	THR	N-CA-CB	-6.34	99.86	110.39
2	H	174	THR	CB-CA-C	6.33	120.92	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	2	ALA	CA-C-O	6.30	129.52	120.51
3	A	262	GLY	N-CA-C	6.24	127.97	113.18
1	L	26	THR	N-CA-C	6.23	120.14	112.54
1	L	150	ASP	CA-CB-CG	6.22	118.82	112.60
2	H	87	THR	CA-CB-OG1	-6.17	100.34	109.60
2	H	152	LYS	N-CA-C	6.17	119.76	109.95
2	H	89	ASP	N-CA-C	-6.17	105.40	113.17
2	H	182	ASP	CA-CB-CG	-6.16	106.44	112.60
2	H	196	THR	CA-CB-OG1	-6.14	100.39	109.60
2	H	113	GLY	N-CA-C	-6.09	102.79	112.66
1	L	101	GLY	N-CA-C	-6.07	103.31	112.60
1	L	7	GLU	CB-CG-CD	6.07	122.92	112.60
2	H	109	MET	N-CA-C	-6.05	96.50	107.75
1	L	29	VAL	N-CA-C	-6.04	100.99	109.21
2	H	5	LYS	N-CA-CB	6.01	120.20	110.77
6	D	80	ILE	CA-C-N	5.99	126.18	120.43
6	D	80	ILE	C-N-CA	5.99	126.18	120.43
1	L	32	SER	O-C-N	5.98	130.38	122.43
2	H	176	PRO	CA-C-N	5.96	130.91	122.09
2	H	176	PRO	C-N-CA	5.96	130.91	122.09
1	L	31	THR	CB-CA-C	5.94	120.65	110.79
2	H	56	ASN	OD1-CG-ND2	-5.92	116.68	122.60
2	H	92	MET	N-CA-C	-5.92	99.64	109.46
1	L	84	ASP	CA-CB-CG	-5.91	106.69	112.60
1	L	54	ASN	N-CA-C	5.87	121.41	112.54
1	L	191	HIS	CA-CB-CG	-5.86	107.94	113.80
2	H	136	GLY	N-CA-C	-5.84	99.34	113.18
2	H	203	THR	O-C-N	5.84	130.39	123.27
4	B	240	VAL	N-CA-CB	5.84	118.48	110.54
1	L	148	THR	CA-CB-OG1	-5.83	100.86	109.60
2	H	110	ASP	CA-C-N	5.82	131.71	122.74
2	H	110	ASP	C-N-CA	5.82	131.71	122.74
1	L	121	PHE	CA-CB-CG	5.78	119.58	113.80
1	L	4	VAL	CA-C-O	-5.78	114.39	120.57
1	L	19	THR	CA-C-O	-5.75	114.15	120.36
6	D	27	MET	N-CA-C	5.75	117.54	111.28
2	H	5	LYS	CA-CB-CG	5.73	125.57	114.10
6	D	20	SER	CA-C-N	5.71	125.56	119.28
6	D	20	SER	C-N-CA	5.71	125.56	119.28
2	H	159	VAL	N-CA-CB	5.70	122.48	111.93
6	D	118	ASP	CA-CB-CG	5.69	118.29	112.60
2	H	216	ASP	CA-C-O	-5.69	114.00	120.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	134	ALA	CB-CA-C	5.68	117.42	108.84
1	L	26	THR	CA-CB-OG1	-5.68	101.08	109.60
2	H	28	LEU	CA-C-O	-5.67	114.51	120.80
1	L	31	THR	CA-CB-CG2	5.67	120.13	110.50
2	H	123	ALA	CA-C-N	5.67	129.52	121.42
2	H	123	ALA	C-N-CA	5.67	129.52	121.42
2	H	119	THR	CA-C-O	-5.66	114.09	120.32
3	A	46	VAL	CB-CA-C	-5.63	104.77	111.97
6	D	118	ASP	N-CA-C	5.62	117.59	110.33
6	D	72	ASP	CA-CB-CG	5.62	118.22	112.60
1	L	54	ASN	CB-CG-ND2	5.59	124.78	116.40
2	H	126	THR	O-C-N	5.59	127.74	121.32
2	H	77	GLN	CA-C-O	5.57	127.06	120.66
2	H	152	LYS	N-CA-CB	-5.56	101.95	110.85
1	L	170	GLN	N-CA-C	-5.55	102.25	110.46
1	L	87	ILE	CA-C-O	-5.51	114.64	120.48
1	L	205	VAL	N-CA-CB	5.50	119.14	112.10
5	C	82	PRO	N-CA-C	5.49	117.40	110.70
2	H	65	SER	N-CA-C	5.48	117.34	111.36
1	L	26	THR	OG1-CB-CG2	5.46	120.23	109.30
5	C	167	PHE	CA-CB-CG	-5.45	108.35	113.80
1	L	178	SER	N-CA-CB	-5.45	101.38	111.13
5	C	290	ALA	N-CA-C	5.43	117.20	111.28
1	L	56	ARG	NE-CZ-NH1	5.42	126.92	121.50
1	L	13	SER	CB-CA-C	5.41	118.56	109.32
1	L	30	THR	CA-CB-OG1	-5.38	101.52	109.60
1	L	31	THR	N-CA-CB	-5.38	102.20	110.12
3	A	303	GLU	CB-CA-C	-5.38	102.44	110.88
2	H	185	THR	CA-CB-CG2	5.36	119.61	110.50
1	L	23	ARG	N-CA-CB	-5.34	101.54	110.83
1	L	104	THR	N-CA-CB	5.33	119.64	110.68
1	L	143	TYR	CA-CB-CG	-5.32	104.32	113.90
2	H	149	CYS	O-C-N	5.31	129.84	123.36
1	L	32	SER	CA-C-O	-5.31	112.41	119.10
2	H	126	THR	CA-C-N	5.31	123.53	119.66
2	H	126	THR	C-N-CA	5.31	123.53	119.66
2	H	185	THR	N-CA-CB	5.31	120.63	111.13
1	L	185	ALA	CA-C-N	5.30	127.33	120.44
1	L	185	ALA	C-N-CA	5.30	127.33	120.44
5	C	118	MET	O-C-N	-5.29	116.47	123.13
2	H	176	PRO	CB-CA-C	5.28	117.99	111.23
1	L	186	ARG	CD-NE-CZ	5.27	131.78	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	192	SER	N-CA-C	5.26	119.45	112.72
2	H	149	CYS	CA-C-O	-5.25	113.83	120.28
5	C	168	PHE	CA-CB-CG	-5.23	108.57	113.80
6	D	122	LEU	O-C-N	-5.21	116.59	122.12
2	H	169	SER	N-CA-C	-5.20	106.90	114.12
1	L	174	LYS	N-CA-C	-5.19	103.06	110.59
2	H	109	MET	CA-C-O	-5.18	115.25	120.84
1	L	205	VAL	CA-C-O	-5.16	115.26	120.31
2	H	124	LYS	CA-C-O	-5.15	115.18	121.05
2	H	174	THR	CA-CB-OG1	-5.15	101.87	109.60
1	L	55	ASN	CA-CB-CG	5.14	117.74	112.60
1	L	117	SER	N-CA-C	-5.14	100.80	109.07
3	A	175	ASP	N-CA-C	5.12	116.54	110.19
1	L	73	ALA	N-CA-C	-5.12	102.17	110.32
2	H	182	ASP	CA-C-O	-5.12	114.23	120.12
2	H	163	TRP	CA-C-O	5.12	125.78	120.30
1	L	158	VAL	O-C-N	5.11	128.76	122.83
6	D	166	PHE	CA-CB-CG	-5.11	108.69	113.80
1	L	25	SER	CA-C-O	5.09	125.82	119.97
6	D	190	THR	N-CA-CB	5.08	117.52	110.26
1	L	43	ASP	O-C-N	5.06	129.32	122.59
3	A	122	PHE	CA-CB-CG	-5.06	108.74	113.80
5	C	268	ALA	N-CA-C	5.06	116.79	111.28
3	A	86	ALA	CA-C-N	5.06	123.42	120.24
3	A	86	ALA	C-N-CA	5.06	123.42	120.24
3	A	208	THR	CB-CA-C	-5.03	101.69	110.09
2	H	179	LEU	CA-C-O	-5.02	115.13	120.40
1	L	63	ARG	CD-NE-CZ	5.01	131.41	124.40
2	H	27	PHE	CA-C-O	-5.01	115.87	121.23
2	H	51	ILE	N-CA-CB	5.01	118.63	111.82
6	D	280	ASP	CA-CB-CG	-5.01	107.59	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	261	GLU	Peptide
5	C	40	TYR	Sidechain
5	C	65	ARG	Sidechain

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	L	1589	0	1530	84	0
2	H	1672	0	1633	88	0
3	A	2346	0	2301	330	0
4	B	2285	0	2320	164	0
5	C	2278	0	2256	156	0
6	D	2262	0	2243	98	0
All	All	12432	0	12283	559	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 23.

All (559) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:96:ASN:HA	3:A:103:SER:CB	1.29	1.60
3:A:308:HIS:CE1	5:C:3:LEU:HD13	1.30	1.58
3:A:15:ARG:CZ	4:B:306:ALA:HB3	1.23	1.57
3:A:235:GLY:CA	5:C:42:THR:HG23	1.33	1.54
5:C:301:ARG:CG	6:D:33:GLY:CA	1.79	1.52
5:C:301:ARG:CG	6:D:33:GLY:HA2	1.30	1.51
3:A:209:GLN:HA	5:C:41:ARG:CD	1.36	1.51
2:H:106:TYR:CD1	3:A:93:ASP:OD2	1.67	1.47
1:L:96:ASN:CA	3:A:103:SER:HB3	1.42	1.46
3:A:8:GLN:CB	4:B:296:LEU:HD23	1.46	1.43
3:A:8:GLN:HB2	4:B:296:LEU:CD2	1.47	1.41
3:A:12:GLU:N	4:B:303:LEU:HD21	1.28	1.40
3:A:15:ARG:HD2	4:B:307:ALA:N	1.07	1.39
3:A:235:GLY:HA3	5:C:42:THR:CG2	1.49	1.39
3:A:308:HIS:CE1	5:C:3:LEU:CD1	2.07	1.38
3:A:15:ARG:CZ	4:B:306:ALA:CB	2.01	1.37
3:A:308:HIS:HE1	5:C:3:LEU:CD1	1.36	1.36
5:C:301:ARG:HG2	6:D:33:GLY:CA	0.91	1.36
3:A:15:ARG:NH2	4:B:306:ALA:HB3	1.35	1.35
3:A:24:VAL:CG1	4:B:307:ALA:HB1	1.55	1.35
3:A:12:GLU:CA	4:B:303:LEU:HD11	1.58	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:8:GLN:N	4:B:296:LEU:HD21	1.41	1.30
3:A:12:GLU:HA	4:B:303:LEU:CD1	1.59	1.30
3:A:8:GLN:CB	4:B:296:LEU:CD2	2.04	1.29
5:C:301:ARG:OXT	6:D:33:GLY:CA	1.81	1.28
3:A:15:ARG:CD	4:B:307:ALA:N	1.97	1.28
1:L:96:ASN:CA	3:A:103:SER:CB	2.03	1.27
1:L:95:SER:O	3:A:103:SER:N	1.61	1.27
5:C:299:THR:O	6:D:38:TYR:CE2	1.86	1.26
1:L:95:SER:C	3:A:103:SER:N	1.89	1.25
5:C:107:PRO:CB	6:D:40:ARG:NH2	1.90	1.24
3:A:209:GLN:NE2	5:C:41:ARG:CZ	2.01	1.23
5:C:108:GLY:O	6:D:36:SER:HB2	1.04	1.22
5:C:299:THR:CG2	6:D:37:ARG:HE	1.45	1.22
5:C:301:ARG:C	6:D:33:GLY:C	2.08	1.20
5:C:108:GLY:O	6:D:36:SER:CB	1.88	1.20
5:C:301:ARG:HB3	6:D:33:GLY:O	1.39	1.19
3:A:15:ARG:HD2	4:B:306:ALA:C	1.68	1.18
5:C:300:LEU:HD23	6:D:38:TYR:OH	1.39	1.18
5:C:301:ARG:C	6:D:33:GLY:O	1.86	1.18
4:B:141:MET:HG2	4:B:197:TYR:CZ	1.80	1.17
3:A:235:GLY:O	5:C:42:THR:HA	1.45	1.17
2:H:106:TYR:HD1	3:A:93:ASP:OD2	0.84	1.16
5:C:301:ARG:C	6:D:33:GLY:CA	2.18	1.16
3:A:12:GLU:CG	4:B:303:LEU:HD13	1.75	1.14
3:A:15:ARG:HG3	4:B:307:ALA:CA	1.76	1.14
3:A:24:VAL:HG11	4:B:307:ALA:HB1	1.20	1.14
2:H:106:TYR:HB3	3:A:95:ALA:HB3	1.30	1.14
3:A:209:GLN:CA	5:C:41:ARG:HD3	1.78	1.14
2:H:106:TYR:CB	3:A:95:ALA:HB3	1.78	1.13
5:C:299:THR:CG2	6:D:37:ARG:NE	2.00	1.13
2:H:106:TYR:HA	3:A:96:VAL:N	1.63	1.13
3:A:12:GLU:HG3	4:B:303:LEU:HD22	1.22	1.13
3:A:8:GLN:H	4:B:296:LEU:CD2	1.59	1.13
5:C:301:ARG:CB	6:D:33:GLY:O	1.97	1.12
1:L:95:SER:O	3:A:103:SER:CB	1.98	1.12
5:C:301:ARG:C	6:D:33:GLY:HA3	1.75	1.11
5:C:301:ARG:HG2	6:D:33:GLY:HA3	1.14	1.11
3:A:209:GLN:CA	5:C:41:ARG:CD	2.26	1.11
3:A:11:GLN:C	4:B:303:LEU:HD21	1.77	1.10
5:C:301:ARG:OXT	6:D:33:GLY:HA3	1.43	1.09
3:A:15:ARG:HG3	4:B:307:ALA:HA	1.27	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:107:TYR:CG	3:A:96:VAL:HG13	1.89	1.08
3:A:209:GLN:HE21	5:C:41:ARG:CZ	1.62	1.08
5:C:107:PRO:HB2	6:D:40:ARG:NH2	1.50	1.07
3:A:8:GLN:OE1	4:B:300:ILE:HG13	1.52	1.07
3:A:12:GLU:N	4:B:303:LEU:CD2	2.18	1.05
4:B:141:MET:HG2	4:B:197:TYR:OH	1.57	1.04
2:H:107:TYR:CD1	3:A:96:VAL:HG13	1.93	1.04
3:A:15:ARG:HD2	4:B:307:ALA:H	1.22	1.03
5:C:299:THR:OG1	6:D:37:ARG:NE	1.77	1.03
2:H:104:VAL:O	3:A:93:ASP:CB	2.04	1.02
5:C:301:ARG:CA	6:D:33:GLY:O	2.08	1.02
3:A:15:ARG:HG3	4:B:307:ALA:CB	1.89	1.02
1:L:96:ASN:HB3	3:A:103:SER:CA	1.89	1.02
5:C:301:ARG:CB	6:D:33:GLY:C	2.33	1.01
1:L:96:ASN:CB	3:A:103:SER:CB	2.37	1.01
3:A:308:HIS:NE2	5:C:3:LEU:HB2	1.76	1.01
5:C:301:ARG:OXT	6:D:33:GLY:N	1.92	1.01
2:H:106:TYR:HA	3:A:96:VAL:H	1.14	1.01
3:A:15:ARG:CG	4:B:307:ALA:HB2	1.90	1.00
5:C:301:ARG:CB	6:D:33:GLY:CA	2.39	1.00
3:A:15:ARG:NE	4:B:306:ALA:HB3	1.77	1.00
3:A:209:GLN:HA	5:C:41:ARG:HD2	1.43	1.00
1:L:96:ASN:HB3	3:A:103:SER:CB	1.91	0.99
2:H:104:VAL:O	3:A:93:ASP:HB2	1.58	0.99
3:A:208:THR:O	5:C:41:ARG:CD	2.11	0.99
3:A:8:GLN:CD	4:B:299:GLU:HB2	1.86	0.99
4:B:141:MET:CG	4:B:197:TYR:CZ	2.44	0.99
3:A:308:HIS:HE1	5:C:3:LEU:CG	1.74	0.99
3:A:308:HIS:ND1	5:C:3:LEU:HD13	1.78	0.99
3:A:308:HIS:CE1	5:C:3:LEU:HB2	1.98	0.98
5:C:299:THR:HG23	6:D:37:ARG:HE	1.23	0.98
2:H:106:TYR:CD1	3:A:93:ASP:CG	2.42	0.97
5:C:301:ARG:HB3	6:D:33:GLY:C	1.88	0.97
1:L:95:SER:O	3:A:103:SER:CA	2.11	0.97
3:A:15:ARG:NH2	4:B:306:ALA:CB	2.17	0.97
3:A:12:GLU:HG2	4:B:303:LEU:CD1	1.94	0.97
3:A:8:GLN:OE1	4:B:300:ILE:N	1.97	0.97
2:H:104:VAL:O	3:A:93:ASP:OD2	1.83	0.97
1:L:96:ASN:CB	3:A:103:SER:HA	1.96	0.96
3:A:12:GLU:HG2	4:B:303:LEU:HD13	1.00	0.96
3:A:308:HIS:CE1	5:C:3:LEU:CG	2.48	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:96:ASN:HB3	3:A:103:SER:HB2	1.47	0.96
3:A:11:GLN:HB2	4:B:303:LEU:HD23	1.45	0.96
3:A:208:THR:O	5:C:41:ARG:HD2	1.63	0.95
5:C:301:ARG:CD	6:D:33:GLY:HA2	1.96	0.95
2:H:162:THR:HG22	2:H:205:ASN:HB2	1.49	0.95
1:L:96:ASN:HA	3:A:103:SER:HB2	1.44	0.95
1:L:96:ASN:CB	3:A:103:SER:HB2	1.97	0.94
5:C:301:ARG:O	6:D:33:GLY:O	1.85	0.94
3:A:12:GLU:H	4:B:303:LEU:HD21	1.24	0.94
3:A:308:HIS:CE1	5:C:3:LEU:CB	2.49	0.94
5:C:300:LEU:HD23	6:D:38:TYR:HH	1.08	0.94
5:C:300:LEU:HD22	6:D:54:ASP:OD1	1.66	0.93
2:H:142:ASN:HD22	2:H:143:SER:H	1.13	0.93
4:B:250:THR:HG23	4:B:252:PHE:H	1.33	0.93
5:C:301:ARG:CG	6:D:33:GLY:HA3	1.68	0.93
3:A:308:HIS:CE1	5:C:3:LEU:H	1.86	0.92
5:C:107:PRO:HB2	6:D:40:ARG:HH22	1.17	0.92
5:C:300:LEU:CD2	6:D:54:ASP:OD1	2.17	0.92
3:A:209:GLN:HA	5:C:41:ARG:HD3	0.94	0.92
3:A:6:VAL:N	4:B:296:LEU:HD11	1.84	0.92
3:A:8:GLN:CG	4:B:299:GLU:HB2	2.01	0.91
3:A:15:ARG:CG	4:B:307:ALA:CA	2.47	0.91
4:B:113:HIS:HD2	4:B:150:THR:HG23	1.36	0.91
1:L:95:SER:C	3:A:103:SER:CA	2.44	0.91
3:A:12:GLU:HG3	4:B:303:LEU:CD2	2.00	0.91
5:C:301:ARG:CA	6:D:33:GLY:HA3	2.00	0.91
1:L:34:TYR:OH	3:A:98:ARG:N	2.03	0.91
5:C:301:ARG:OXT	6:D:30:GLU:O	1.88	0.90
3:A:8:GLN:HB3	4:B:296:LEU:HG	1.53	0.90
2:H:142:ASN:ND2	2:H:143:SER:H	1.70	0.90
1:L:96:ASN:CB	3:A:103:SER:CA	2.51	0.89
5:C:301:ARG:CZ	6:D:34:LEU:N	2.36	0.89
3:A:235:GLY:O	5:C:42:THR:CA	2.21	0.88
3:A:15:ARG:HD2	4:B:307:ALA:CA	2.03	0.88
2:H:40:PRO:HB2	2:H:43:LYS:HE2	1.56	0.87
3:A:8:GLN:NE2	4:B:299:GLU:C	2.31	0.87
3:A:8:GLN:N	4:B:296:LEU:CD2	2.27	0.87
3:A:15:ARG:CG	4:B:307:ALA:CB	2.51	0.87
1:L:95:SER:C	3:A:103:SER:HB3	2.01	0.86
3:A:15:ARG:CD	4:B:307:ALA:CA	2.53	0.86
3:A:8:GLN:HG2	4:B:299:GLU:HB2	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:15:ARG:CG	4:B:307:ALA:HA	2.04	0.85
4:B:247:VAL:O	4:B:250:THR:HG22	1.75	0.85
5:C:299:THR:HA	6:D:35:GLN:CB	1.89	0.85
1:L:34:TYR:OH	3:A:94:GLU:O	1.95	0.85
3:A:208:THR:CB	5:C:41:ARG:CZ	2.54	0.85
5:C:299:THR:HG21	6:D:37:ARG:NE	1.61	0.85
2:H:106:TYR:CA	3:A:96:VAL:H	1.90	0.85
3:A:8:GLN:CD	4:B:299:GLU:CB	2.49	0.84
5:C:300:LEU:CD2	6:D:38:TYR:OH	2.25	0.84
5:C:301:ARG:CB	6:D:33:GLY:HA3	2.05	0.84
3:A:209:GLN:NE2	5:C:41:ARG:NH1	2.24	0.84
1:L:95:SER:HA	3:A:99:ALA:O	1.78	0.84
3:A:8:GLN:HB3	4:B:296:LEU:CD2	2.04	0.83
3:A:208:THR:HB	5:C:41:ARG:CZ	2.08	0.83
2:H:104:VAL:O	3:A:93:ASP:CG	2.20	0.83
3:A:11:GLN:OE1	4:B:300:ILE:HG23	1.78	0.83
3:A:12:GLU:CG	4:B:303:LEU:CD1	2.52	0.83
3:A:209:GLN:CA	5:C:41:ARG:HD2	2.01	0.83
3:A:208:THR:OG1	5:C:41:ARG:NH1	2.11	0.82
1:L:96:ASN:N	3:A:103:SER:HB3	1.93	0.82
3:A:15:ARG:NH2	4:B:303:LEU:HA	1.95	0.82
3:A:208:THR:OG1	5:C:41:ARG:NH2	2.11	0.82
2:H:105:PHE:O	3:A:95:ALA:N	2.13	0.81
3:A:8:GLN:CA	4:B:296:LEU:HD21	2.10	0.81
2:H:105:PHE:HD2	3:A:91:PRO:C	1.87	0.81
3:A:24:VAL:HG12	4:B:307:ALA:HB1	1.59	0.81
5:C:301:ARG:HH12	6:D:34:LEU:HB3	1.44	0.81
3:A:208:THR:O	5:C:41:ARG:NE	1.94	0.81
3:A:209:GLN:HE21	5:C:41:ARG:NH1	1.77	0.81
5:C:301:ARG:CG	6:D:33:GLY:C	2.54	0.81
3:A:24:VAL:HG11	4:B:307:ALA:CB	2.07	0.81
3:A:8:GLN:OE1	4:B:296:LEU:O	1.97	0.81
3:A:8:GLN:HE22	4:B:299:GLU:C	1.88	0.80
4:B:93:ILE:HD12	4:B:123:VAL:HG21	1.64	0.80
1:L:96:ASN:HB3	3:A:103:SER:HA	1.56	0.80
3:A:8:GLN:HB3	4:B:296:LEU:CG	2.11	0.80
4:B:175:VAL:HG23	4:B:184:ILE:HB	1.64	0.80
3:A:11:GLN:HB2	4:B:303:LEU:CD2	2.12	0.80
5:C:301:ARG:NH1	6:D:34:LEU:HB3	1.97	0.80
4:B:16:ASN:OD1	4:B:179:THR:HG22	1.83	0.79
2:H:107:TYR:CD2	3:A:96:VAL:HG13	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:163:PHE:HB3	4:B:227:ARG:NH1	1.98	0.79
3:A:11:GLN:CB	4:B:303:LEU:HD23	2.11	0.79
5:C:301:ARG:NH1	6:D:34:LEU:O	2.14	0.79
3:A:235:GLY:CA	5:C:42:THR:CG2	2.29	0.79
4:B:153:LEU:HD21	4:B:175:VAL:HG21	1.64	0.79
1:L:165:THR:HG22	2:H:178:VAL:HG13	1.65	0.79
3:A:15:ARG:HD3	4:B:303:LEU:O	1.83	0.78
4:B:117:GLU:CG	4:B:158:TYR:HE1	1.96	0.78
4:B:117:GLU:HG2	4:B:158:TYR:HE1	1.48	0.78
3:A:12:GLU:CA	4:B:303:LEU:CD1	2.37	0.77
4:B:113:HIS:CD2	4:B:150:THR:HG23	2.19	0.77
2:H:105:PHE:CD2	3:A:91:PRO:C	2.62	0.77
3:A:8:GLN:CA	4:B:296:LEU:CD2	2.62	0.77
3:A:235:GLY:HA2	5:C:42:THR:HG23	1.62	0.77
2:H:105:PHE:CG	3:A:97:ARG:HG3	2.19	0.77
1:L:95:SER:C	3:A:103:SER:CB	2.56	0.77
1:L:34:TYR:CE2	3:A:99:ALA:HB2	2.20	0.77
1:L:34:TYR:CD2	3:A:99:ALA:HB2	2.19	0.76
1:L:34:TYR:HE2	3:A:99:ALA:H	1.32	0.76
3:A:15:ARG:CB	4:B:307:ALA:HB2	2.16	0.76
4:B:175:VAL:CG2	4:B:184:ILE:HB	2.15	0.76
4:B:141:MET:HG2	4:B:197:TYR:CE2	2.21	0.76
3:A:15:ARG:NH2	4:B:303:LEU:O	2.17	0.75
2:H:107:TYR:CD2	3:A:99:ALA:HB3	2.21	0.75
3:A:8:GLN:OE1	4:B:300:ILE:CG1	2.35	0.74
1:L:96:ASN:CA	3:A:103:SER:CA	2.66	0.74
3:A:15:ARG:NE	4:B:306:ALA:CB	2.43	0.74
3:A:208:THR:CB	5:C:41:ARG:NH1	2.51	0.74
2:H:105:PHE:O	3:A:94:GLU:N	2.09	0.74
3:A:307:PHE:O	5:C:2:SER:HB3	1.88	0.74
3:A:209:GLN:HE21	5:C:41:ARG:NH2	1.86	0.73
5:C:300:LEU:CD2	6:D:38:TYR:HH	1.95	0.73
5:C:299:THR:O	6:D:38:TYR:CD2	2.42	0.73
3:A:8:GLN:CB	4:B:296:LEU:CG	2.65	0.73
1:L:34:TYR:CE2	3:A:99:ALA:CB	2.72	0.72
3:A:11:GLN:CB	4:B:303:LEU:CD2	2.68	0.72
1:L:34:TYR:HE2	3:A:99:ALA:CB	2.02	0.72
1:L:95:SER:O	3:A:103:SER:HB3	1.73	0.72
3:A:208:THR:HB	5:C:41:ARG:NH1	2.04	0.72
6:D:252:THR:HG23	6:D:254:LEU:H	1.54	0.72
3:A:15:ARG:CD	4:B:307:ALA:HB2	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:235:GLY:C	5:C:42:THR:HG23	2.14	0.70
3:A:8:GLN:H	4:B:296:LEU:HD21	0.66	0.70
5:C:301:ARG:O	6:D:33:GLY:C	2.31	0.69
2:H:107:TYR:HD2	3:A:99:ALA:HB3	1.56	0.69
3:A:6:VAL:N	4:B:296:LEU:CD1	2.55	0.69
2:H:35:HIS:HD2	2:H:47:TRP:HE1	1.41	0.69
2:H:100:TYR:CB	3:A:96:VAL:HG11	2.22	0.69
2:H:193:PRO:O	2:H:196:THR:HB	1.93	0.69
4:B:141:MET:CG	4:B:197:TYR:CE2	2.76	0.69
2:H:106:TYR:HD1	3:A:93:ASP:CG	1.82	0.69
4:B:227:ARG:CG	4:B:227:ARG:HH11	2.05	0.68
3:A:24:VAL:CG1	4:B:307:ALA:CB	2.52	0.68
1:L:93:TRP:CZ2	3:A:99:ALA:O	2.34	0.68
3:A:11:GLN:C	4:B:303:LEU:CD2	2.63	0.68
2:H:106:TYR:HB2	3:A:95:ALA:HB3	1.73	0.68
3:A:15:ARG:HH21	4:B:303:LEU:C	2.02	0.68
3:A:15:ARG:HB2	4:B:307:ALA:HB2	1.74	0.68
3:A:28:LEU:CD1	4:B:304:ALA:HA	2.24	0.68
3:A:50:ASN:HD21	3:A:64:VAL:H	1.42	0.68
3:A:6:VAL:HG11	3:A:45:LEU:HD21	1.77	0.67
4:B:132:TRP:CE3	4:B:135:ILE:HD11	2.29	0.67
2:H:107:TYR:CD1	3:A:96:VAL:CG1	2.74	0.67
1:L:34:TYR:HH	3:A:98:ARG:H	1.41	0.67
2:H:107:TYR:CE1	3:A:96:VAL:HG13	2.29	0.67
4:B:93:ILE:CD1	4:B:123:VAL:HG21	2.24	0.67
3:A:6:VAL:HG13	3:A:256:LEU:HD13	1.77	0.66
3:A:308:HIS:CG	5:C:3:LEU:H	2.12	0.66
4:B:113:HIS:HD2	4:B:150:THR:CG2	2.07	0.66
1:L:96:ASN:CG	3:A:103:SER:HA	2.20	0.66
2:H:35:HIS:CD2	2:H:47:TRP:HE1	2.13	0.66
1:L:113:LYS:O	1:L:113:LYS:HE2	1.96	0.66
3:A:67:VAL:HA	3:A:76:PRO:HD3	1.75	0.66
5:C:3:LEU:HG	5:C:49:LEU:HD21	1.76	0.66
3:A:15:ARG:CD	4:B:307:ALA:CB	2.74	0.66
5:C:299:THR:HA	6:D:35:GLN:HB3	1.76	0.66
5:C:107:PRO:HB3	6:D:40:ARG:NH2	2.05	0.66
1:L:95:SER:O	3:A:99:ALA:O	2.14	0.65
3:A:208:THR:OG1	5:C:41:ARG:CZ	2.43	0.65
3:A:15:ARG:CZ	4:B:306:ALA:HB1	2.21	0.65
3:A:308:HIS:CE1	5:C:3:LEU:N	2.64	0.65
3:A:28:LEU:HD12	4:B:304:ALA:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:96:ASN:OD1	3:A:103:SER:HA	1.96	0.65
2:H:105:PHE:HD2	3:A:92:GLU:N	1.95	0.65
4:B:117:GLU:HG2	4:B:158:TYR:CE1	2.31	0.64
5:C:299:THR:O	6:D:38:TYR:CZ	2.46	0.64
3:A:8:GLN:CD	4:B:299:GLU:C	2.65	0.64
3:A:28:LEU:HD12	4:B:304:ALA:CB	2.27	0.64
5:C:97:ILE:HD11	5:C:127:VAL:HB	1.79	0.64
5:C:300:LEU:HD23	6:D:54:ASP:OD1	1.98	0.63
2:H:106:TYR:HB3	3:A:95:ALA:CB	2.18	0.63
3:A:180:ARG:HH11	3:A:183:SER:HB2	1.63	0.63
2:H:38:ARG:HG2	2:H:48:LEU:HD21	1.80	0.63
3:A:15:ARG:NH1	4:B:306:ALA:CB	2.60	0.63
1:L:199:THR:HG23	1:L:204:THR:OG1	1.99	0.63
2:H:83:LYS:HB2	2:H:83:LYS:NZ	2.14	0.62
3:A:28:LEU:HD12	4:B:304:ALA:HB2	1.80	0.62
3:A:235:GLY:HA3	5:C:42:THR:HG23	0.63	0.62
3:A:28:LEU:HD12	4:B:304:ALA:CA	2.30	0.62
3:A:172:GLN:HE22	3:A:181:LEU:HD21	1.64	0.62
6:D:27:MET:HE1	6:D:55:LEU:CD2	2.29	0.62
5:C:301:ARG:NH1	6:D:34:LEU:CA	2.63	0.62
3:A:15:ARG:NH2	4:B:303:LEU:CA	2.61	0.61
6:D:27:MET:HE1	6:D:55:LEU:HD22	1.82	0.61
3:A:8:GLN:NE2	4:B:299:GLU:HB3	2.15	0.61
3:A:6:VAL:CG2	3:A:261:GLU:HG3	2.31	0.61
2:H:107:TYR:CE1	3:A:96:VAL:CG1	2.84	0.61
1:L:34:TYR:CE2	3:A:96:VAL:CA	2.77	0.61
1:L:192:SER:O	1:L:210:SER:HA	2.01	0.61
5:C:109:GLN:N	6:D:40:ARG:HH11	1.98	0.60
3:A:307:PHE:C	5:C:2:SER:HB3	2.26	0.60
1:L:95:SER:CA	3:A:99:ALA:O	2.50	0.60
4:B:254:VAL:HG12	4:B:256:VAL:HG23	1.82	0.60
5:C:301:ARG:NH1	6:D:34:LEU:N	2.49	0.60
4:B:1:PHE:O	4:B:2:SER:CB	2.50	0.59
5:C:301:ARG:CA	6:D:33:GLY:CA	2.70	0.59
3:A:209:GLN:NE2	5:C:41:ARG:NH2	2.46	0.59
5:C:301:ARG:NH1	6:D:34:LEU:CB	2.66	0.59
3:A:8:GLN:CD	4:B:300:ILE:N	2.60	0.59
5:C:301:ARG:CZ	6:D:34:LEU:H	2.15	0.59
2:H:100:TYR:CD1	3:A:91:PRO:HB3	2.37	0.58
3:A:8:GLN:CG	4:B:299:GLU:CB	2.79	0.58
3:A:8:GLN:NE2	4:B:299:GLU:CB	2.65	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:34:TYR:CE2	3:A:96:VAL:HA	2.39	0.58
1:L:118:VAL:HG12	1:L:207:LYS:HG3	1.85	0.58
4:B:1:PHE:O	4:B:2:SER:HB2	2.04	0.58
4:B:117:GLU:CG	4:B:158:TYR:CE1	2.85	0.58
1:L:96:ASN:HA	3:A:103:SER:HB3	0.65	0.57
3:A:308:HIS:HE1	5:C:3:LEU:CD2	2.17	0.57
6:D:95:ILE:HD12	6:D:125:VAL:HG21	1.86	0.57
2:H:2:VAL:HG13	2:H:27:PHE:CD1	2.39	0.57
3:A:15:ARG:CD	4:B:307:ALA:H	1.90	0.57
4:B:141:MET:HG3	4:B:197:TYR:CZ	2.35	0.57
3:A:308:HIS:ND1	5:C:2:SER:OG	2.29	0.57
3:A:12:GLU:CB	4:B:303:LEU:CD1	2.83	0.57
1:L:96:ASN:N	3:A:103:SER:CA	2.68	0.56
2:H:18:LEU:O	2:H:81:LYS:HD2	2.05	0.56
3:A:15:ARG:NH2	4:B:303:LEU:C	2.63	0.56
3:A:191:ILE:HG22	3:A:193:ARG:H	1.70	0.56
3:A:307:PHE:O	5:C:2:SER:CB	2.52	0.56
3:A:12:GLU:H	4:B:303:LEU:CD2	2.04	0.56
4:B:117:GLU:HG3	4:B:158:TYR:HE1	1.69	0.56
1:L:149:VAL:HA	1:L:197:GLN:O	2.05	0.56
3:A:209:GLN:C	5:C:41:ARG:CD	2.78	0.56
2:H:67:VAL:HG12	2:H:82:MET:HG3	1.89	0.55
2:H:1:GLN:OE1	2:H:1:GLN:N	2.32	0.55
2:H:104:VAL:C	3:A:93:ASP:CG	2.68	0.55
3:A:307:PHE:O	5:C:5:GLU:OE1	2.25	0.55
4:B:23:LEU:HD22	4:B:60:ILE:HD11	1.89	0.55
4:B:227:ARG:HH11	4:B:227:ARG:HG3	1.71	0.55
3:A:184:THR:HB	3:A:271:LEU:HD11	1.89	0.55
3:A:208:THR:C	5:C:41:ARG:HD2	2.30	0.55
1:L:10:LEU:HD23	1:L:20:LEU:HD22	1.89	0.55
3:A:308:HIS:HE2	5:C:3:LEU:HB2	1.66	0.55
2:H:164:ASN:ND2	2:H:168:LEU:HD22	2.21	0.55
3:A:209:GLN:C	5:C:41:ARG:HD2	2.32	0.55
6:D:96:LYS:HA	6:D:99:PHE:CE2	2.42	0.54
3:A:10:LEU:HD13	3:A:266:LEU:HD22	1.90	0.54
3:A:114:VAL:CG1	3:A:150:ILE:HD13	2.38	0.54
3:A:209:GLN:NE2	5:C:41:ARG:NE	2.53	0.54
3:A:10:LEU:CD1	3:A:266:LEU:HD22	2.36	0.54
5:C:301:ARG:CZ	6:D:33:GLY:C	2.81	0.54
3:A:208:THR:HG1	5:C:41:ARG:HH12	1.52	0.54
1:L:96:ASN:N	3:A:103:SER:CB	2.63	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:169:LEU:CD2	4:B:190:PRO:HD3	2.38	0.54
5:C:301:ARG:HG2	6:D:33:GLY:HA2	0.54	0.54
1:L:32:SER:HB2	3:A:98:ARG:NH2	2.07	0.53
2:H:100:TYR:HB2	3:A:96:VAL:HG11	1.88	0.53
4:B:215:ALA:HA	4:B:218:VAL:HG12	1.89	0.53
5:C:301:ARG:NH2	6:D:33:GLY:HA2	2.22	0.53
4:B:141:MET:CG	4:B:197:TYR:OH	2.44	0.53
5:C:301:ARG:NH2	6:D:34:LEU:H	2.06	0.53
3:A:12:GLU:CG	4:B:303:LEU:HD22	2.15	0.53
1:L:95:SER:O	3:A:103:SER:OG	2.26	0.53
2:H:107:TYR:HD2	3:A:99:ALA:CB	2.21	0.53
5:C:181:ASP:H	5:C:186:ARG:HB3	1.73	0.53
5:C:76:VAL:HG13	5:C:77:ALA:H	1.73	0.53
5:C:301:ARG:C	6:D:30:GLU:O	2.51	0.53
1:L:1:GLN:HA	1:L:1:GLN:OE1	2.08	0.53
4:B:23:LEU:CD2	4:B:60:ILE:HD11	2.38	0.53
3:A:6:VAL:HG13	3:A:256:LEU:CD1	2.39	0.52
1:L:200:HIS:HB3	1:L:203:HIS:CE1	2.45	0.52
2:H:106:TYR:CG	3:A:93:ASP:CG	2.79	0.52
3:A:67:VAL:HG12	3:A:75:GLY:HA3	1.91	0.52
5:C:301:ARG:NH2	6:D:33:GLY:CA	2.72	0.52
2:H:107:TYR:CE2	3:A:96:VAL:O	2.62	0.52
5:C:301:ARG:NH1	6:D:34:LEU:C	2.67	0.52
5:C:107:PRO:CB	6:D:40:ARG:HH21	2.13	0.52
6:D:166:PHE:CZ	6:D:227:LEU:HD13	2.44	0.52
4:B:66:LYS:HB3	4:B:255:THR:OG1	2.10	0.52
4:B:141:MET:HG3	4:B:197:TYR:CE2	2.45	0.52
2:H:100:TYR:HB2	3:A:96:VAL:HG21	1.93	0.51
1:L:197:GLN:HG2	1:L:204:THR:HG23	1.92	0.51
3:A:8:GLN:HE22	4:B:300:ILE:HA	1.76	0.51
1:L:46:PHE:CE1	2:H:45:LEU:HD11	2.46	0.51
5:C:243:ALA:HB3	5:C:276:LEU:HD13	1.92	0.51
3:A:209:GLN:HA	5:C:41:ARG:NE	2.16	0.50
2:H:144:MET:HB3	2:H:191:THR:HG22	1.93	0.50
3:A:8:GLN:CB	4:B:296:LEU:HD21	2.09	0.50
1:L:113:LYS:HE2	1:L:113:LYS:C	2.36	0.50
1:L:167:PRO:HA	1:L:176:MET:O	2.10	0.50
2:H:107:TYR:OH	3:A:100:LEU:HB2	2.12	0.50
5:C:168:PHE:CZ	5:C:229:LEU:HD13	2.47	0.50
3:A:12:GLU:CG	4:B:303:LEU:CD2	2.80	0.50
1:L:34:TYR:HE2	3:A:99:ALA:N	2.06	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:56:ARG:HD3	1:L:64:PHE:O	2.11	0.50
2:H:132:PRO:HD3	2:H:217:LYS:HE2	1.93	0.50
3:A:15:ARG:HD3	4:B:307:ALA:HB2	1.93	0.50
2:H:205:ASN:HD22	2:H:216:ASP:CG	2.20	0.50
2:H:107:TYR:CZ	3:A:96:VAL:CG1	2.95	0.49
3:A:15:ARG:CD	4:B:306:ALA:C	2.60	0.49
1:L:95:SER:C	3:A:99:ALA:O	2.55	0.49
1:L:153:VAL:HG23	1:L:158:VAL:HG22	1.93	0.49
3:A:42:GLU:OE2	3:A:66:VAL:HG21	2.12	0.49
3:A:8:GLN:OE1	4:B:300:ILE:CA	2.60	0.49
3:A:15:ARG:CD	4:B:306:ALA:HB3	2.40	0.49
1:L:5:THR:OG1	1:L:23:ARG:NE	2.46	0.49
6:D:122:LEU:HD13	6:D:160:ALA:CB	2.42	0.49
3:A:12:GLU:CB	4:B:303:LEU:HD13	2.39	0.49
3:A:67:VAL:HG21	3:A:72:ALA:HA	1.95	0.49
3:A:8:GLN:NE2	4:B:299:GLU:O	2.39	0.49
3:A:20:LEU:HD13	3:A:23:ARG:CZ	2.42	0.49
1:L:30:THR:HG22	1:L:32:SER:HB2	1.96	0.48
2:H:100:TYR:CD1	3:A:91:PRO:CB	2.96	0.48
3:A:169:SER:HB2	3:A:201:LEU:HD11	1.94	0.48
1:L:34:TYR:HD2	3:A:99:ALA:HB2	1.75	0.48
3:A:11:GLN:CB	4:B:303:LEU:HD21	2.44	0.48
3:A:235:GLY:O	5:C:42:THR:CB	2.61	0.48
4:B:169:LEU:HD22	4:B:190:PRO:HD3	1.95	0.48
5:C:301:ARG:HH21	6:D:33:GLY:HA2	1.78	0.48
1:L:54:ASN:HD22	1:L:54:ASN:C	2.22	0.48
2:H:107:TYR:CE2	3:A:99:ALA:HB3	2.49	0.48
2:H:107:TYR:CE2	3:A:96:VAL:HG13	2.48	0.48
6:D:179:ASN:HA	6:D:261:ALA:HB2	1.95	0.48
3:A:66:VAL:HB	3:A:264:LEU:HD23	1.96	0.48
5:C:175:HIS:CD2	5:C:268:ALA:CB	2.96	0.48
6:D:229:ARG:HG3	6:D:229:ARG:HH11	1.79	0.48
3:A:11:GLN:CA	4:B:303:LEU:HD21	2.39	0.48
4:B:158:TYR:O	4:B:162:TYR:HD2	1.96	0.47
1:L:32:SER:CB	3:A:98:ARG:NH2	2.70	0.47
2:H:63:LEU:HD22	2:H:82:MET:HE2	1.96	0.47
1:L:117:SER:O	1:L:139:ILE:HA	2.14	0.47
2:H:107:TYR:CD2	3:A:99:ALA:CB	2.96	0.47
3:A:65:GLN:HB3	3:A:76:PRO:HG2	1.95	0.47
4:B:135:ILE:HD12	4:B:135:ILE:C	2.39	0.47
5:C:299:THR:HA	6:D:35:GLN:HB2	1.86	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:46:VAL:CG2	3:A:264:LEU:HD21	2.44	0.47
6:D:249:VAL:O	6:D:252:THR:HG22	2.15	0.47
1:L:153:VAL:HG23	1:L:158:VAL:CG2	2.45	0.47
3:A:15:ARG:CD	4:B:303:LEU:O	2.60	0.47
2:H:172:VAL:HG22	2:H:190:VAL:HG23	1.96	0.47
3:A:19:THR:HA	3:A:187:ARG:HB2	1.97	0.47
3:A:172:GLN:HA	3:A:208:THR:HG22	1.96	0.47
5:C:107:PRO:HB2	6:D:40:ARG:HH21	1.66	0.47
5:C:301:ARG:NH2	6:D:34:LEU:N	2.61	0.47
2:H:164:ASN:HD22	2:H:168:LEU:HD22	1.80	0.47
1:L:60:VAL:HA	1:L:61:PRO:HD3	1.83	0.46
2:H:100:TYR:CB	3:A:96:VAL:HG21	2.45	0.46
2:H:107:TYR:CZ	3:A:96:VAL:HG13	2.50	0.46
3:A:208:THR:C	5:C:41:ARG:CD	2.87	0.46
5:C:175:HIS:CD2	5:C:268:ALA:HB1	2.50	0.46
3:A:308:HIS:CE1	5:C:3:LEU:HD22	2.51	0.46
6:D:95:ILE:CD1	6:D:125:VAL:HG21	2.46	0.46
3:A:90:VAL:HG11	3:A:130:VAL:HG11	1.98	0.46
3:A:209:GLN:C	5:C:41:ARG:HD3	2.39	0.46
3:A:87:VAL:CG1	3:A:88:PRO:HD3	2.45	0.46
3:A:19:THR:HG23	3:A:20:LEU:HG	1.97	0.46
6:D:134:TRP:CE3	6:D:137:ILE:HD11	2.50	0.46
3:A:308:HIS:CE1	5:C:3:LEU:CD2	2.95	0.46
5:C:109:GLN:H	6:D:40:ARG:HH11	1.61	0.46
3:A:107:VAL:HG23	3:A:138:GLN:HE21	1.81	0.46
2:H:104:VAL:C	3:A:93:ASP:OD2	2.56	0.45
3:A:8:GLN:OE1	4:B:299:GLU:C	2.58	0.45
1:L:34:TYR:CE2	3:A:99:ALA:N	2.75	0.45
2:H:99:PHE:HD1	2:H:102:TYR:CZ	2.34	0.45
3:A:209:GLN:HE22	5:C:38:GLY:CA	2.29	0.45
3:A:87:VAL:HG12	3:A:88:PRO:HD3	1.99	0.45
3:A:308:HIS:CG	5:C:2:SER:HG	2.30	0.45
5:C:168:PHE:CD2	5:C:192:THR:HG21	2.51	0.45
2:H:128:PRO:HB3	2:H:154:TYR:HB3	1.98	0.45
2:H:41:PRO:O	2:H:43:LYS:HD3	2.17	0.45
3:A:66:VAL:HG22	3:A:67:VAL:N	2.32	0.45
6:D:89:GLU:HA	6:D:92:GLU:HG2	1.98	0.45
1:L:96:ASN:CA	3:A:103:SER:HB2	2.06	0.45
3:A:8:GLN:HB2	4:B:296:LEU:HD23	0.59	0.45
3:A:186:ASP:HB3	3:A:191:ILE:HG12	1.99	0.45
5:C:108:GLY:O	6:D:36:SER:OG	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:203:HIS:ND1	1:L:203:HIS:C	2.76	0.44
2:H:92:MET:HE3	2:H:92:MET:HB3	1.85	0.44
4:B:135:ILE:HD12	4:B:136:LEU:N	2.32	0.44
4:B:215:ALA:HA	4:B:218:VAL:CG1	2.47	0.44
5:C:124:VAL:HA	5:C:127:VAL:HG22	1.99	0.44
4:B:138:THR:OG1	4:B:141:MET:SD	2.76	0.44
4:B:244:LYS:HG3	4:B:255:THR:CG2	2.47	0.44
3:A:122:PHE:HZ	3:A:227:LEU:HD22	1.82	0.44
3:A:307:PHE:O	5:C:2:SER:CA	2.66	0.44
4:B:227:ARG:NH1	4:B:227:ARG:HG3	2.31	0.44
1:L:132:LYS:HA	1:L:132:LYS:HD2	1.77	0.44
2:H:40:PRO:HA	2:H:41:PRO:HD3	1.88	0.44
2:H:134:ALA:HB2	2:H:219:ILE:CD1	2.48	0.44
2:H:5:LYS:HB2	2:H:5:LYS:NZ	2.31	0.44
4:B:117:GLU:HG3	4:B:154:SER:O	2.17	0.44
2:H:100:TYR:HB3	3:A:96:VAL:HG11	1.96	0.44
3:A:12:GLU:HA	4:B:303:LEU:HD11	0.66	0.44
3:A:250:HIS:CD2	3:A:271:LEU:HD23	2.52	0.44
5:C:97:ILE:CD1	5:C:127:VAL:HB	2.47	0.44
1:L:5:THR:HG23	1:L:23:ARG:NH2	2.32	0.44
1:L:113:LYS:HG2	1:L:114:SER:N	2.33	0.44
2:H:107:TYR:CD2	3:A:96:VAL:HA	2.52	0.44
3:A:12:GLU:CA	4:B:303:LEU:CD2	2.95	0.44
2:H:18:LEU:HB2	2:H:85:LEU:HD11	2.00	0.43
3:A:209:GLN:HE22	5:C:38:GLY:HA3	1.83	0.43
1:L:138:THR:HB	2:H:175:PHE:CZ	2.53	0.43
4:B:132:TRP:CZ3	4:B:135:ILE:HD11	2.53	0.43
1:L:34:TYR:HE2	3:A:99:ALA:HB3	1.79	0.43
5:C:107:PRO:CB	6:D:40:ARG:HH22	1.78	0.43
2:H:12:VAL:HG23	2:H:120:VAL:HG22	2.01	0.43
3:A:308:HIS:CG	5:C:2:SER:N	2.49	0.43
6:D:283:VAL:HG11	6:D:291:ARG:HG3	2.01	0.43
1:L:34:TYR:OH	3:A:97:ARG:N	2.52	0.43
3:A:186:ASP:HB3	3:A:191:ILE:CG1	2.49	0.43
3:A:15:ARG:NH2	4:B:302:ALA:O	2.51	0.43
3:A:128:LEU:HD22	3:A:163:ALA:HB1	2.01	0.43
3:A:256:LEU:HD12	3:A:264:LEU:CB	2.48	0.43
6:D:118:ASP:HB3	6:D:154:PRO:HG2	2.00	0.43
6:D:243:PRO:CG	6:D:261:ALA:HB3	2.49	0.43
3:A:172:GLN:HA	3:A:208:THR:CG2	2.49	0.43
3:A:308:HIS:ND1	5:C:3:LEU:CD1	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:106:TYR:HA	3:A:95:ALA:HB3	2.00	0.42
2:H:156:PRO:O	2:H:208:HIS:HE1	2.01	0.42
3:A:8:GLN:CD	4:B:296:LEU:O	2.62	0.42
6:D:69:ILE:HG22	6:D:72:ASP:HB2	2.00	0.42
1:L:96:ASN:CA	3:A:103:SER:HA	2.40	0.42
1:L:162:MET:HA	1:L:180:TYR:O	2.19	0.42
3:A:46:VAL:CG2	3:A:264:LEU:CD2	2.97	0.42
6:D:243:PRO:CD	6:D:261:ALA:HB3	2.49	0.42
1:L:11:THR:HA	1:L:107:THR:O	2.20	0.42
4:B:163:PHE:HB3	4:B:227:ARG:HH11	1.81	0.42
5:C:301:ARG:CZ	6:D:33:GLY:HA2	2.49	0.42
1:L:14:PRO:HD3	1:L:109:LEU:O	2.19	0.42
1:L:196:CYS:O	1:L:206:GLU:HA	2.20	0.42
2:H:106:TYR:CA	3:A:95:ALA:HB3	2.43	0.42
4:B:117:GLU:HG3	4:B:158:TYR:CE1	2.51	0.42
4:B:300:ILE:N	4:B:301:PRO:HD2	2.34	0.42
2:H:153:GLY:HA2	2:H:183:LEU:HB3	2.02	0.42
3:A:166:LEU:HD12	3:A:201:LEU:CD1	2.50	0.42
6:D:104:LEU:HD13	6:D:293:GLN:HE21	1.84	0.42
6:D:229:ARG:HH11	6:D:229:ARG:CG	2.33	0.42
2:H:72:ASP:HB3	2:H:75:LYS:HB2	2.01	0.42
5:C:81:PRO:HG3	5:C:155:SER:OG	2.20	0.41
6:D:116:PHE:CE2	6:D:217:ALA:HA	2.54	0.41
3:A:307:PHE:O	5:C:2:SER:HA	2.20	0.41
1:L:203:HIS:CE1	1:L:205:VAL:HG23	2.55	0.41
2:H:13:ALA:HA	2:H:14:PRO:HD3	1.92	0.41
3:A:136:LEU:HD13	3:A:203:GLY:CA	2.49	0.41
6:D:122:LEU:O	6:D:126:SER:HB2	2.20	0.41
3:A:101:VAL:HG21	3:A:134:TYR:HB2	2.02	0.41
4:B:169:LEU:HD21	4:B:190:PRO:HD3	2.02	0.41
3:A:169:SER:HB3	3:A:201:LEU:HD21	2.03	0.41
3:A:308:HIS:OXT	5:C:3:LEU:N	2.30	0.41
3:A:186:ASP:H	3:A:191:ILE:HB	1.84	0.41
3:A:209:GLN:O	5:C:41:ARG:CD	2.69	0.41
5:C:97:ILE:HD11	5:C:127:VAL:CB	2.50	0.41
3:A:6:VAL:HG23	3:A:261:GLU:HG3	2.03	0.41
4:B:57:LYS:HE2	4:B:63:SER:CA	2.51	0.41
2:H:17:SER:OG	2:H:81:LYS:HE3	2.20	0.41
4:B:270:TRP:CD1	4:B:270:TRP:H	2.38	0.40
1:L:156:THR:HA	1:L:157:PRO:HD2	1.90	0.40
3:A:42:GLU:OE2	3:A:66:VAL:CG2	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:147:MET:HE1	6:D:220:PHE:HD2	1.85	0.40
6:D:161:LEU:HB3	6:D:220:PHE:CE1	2.56	0.40
3:A:10:LEU:CD1	3:A:266:LEU:CD2	2.99	0.40
2:H:104:VAL:HG23	3:A:93:ASP:OD2	2.21	0.40
3:A:120:ASP:O	3:A:157:PRO:HD2	2.21	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	L	208/210 (99%)	198 (95%)	9 (4%)	1 (0%)	24	63
2	H	219/221 (99%)	209 (95%)	7 (3%)	3 (1%)	9	40
3	A	301/303 (99%)	281 (93%)	16 (5%)	4 (1%)	9	42
4	B	307/309 (99%)	298 (97%)	8 (3%)	1 (0%)	36	72
5	C	298/300 (99%)	275 (92%)	19 (6%)	4 (1%)	9	42
6	D	294/296 (99%)	280 (95%)	12 (4%)	2 (1%)	18	56
All	All	1627/1639 (99%)	1541 (95%)	71 (4%)	15 (1%)	16	51

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	64	MET
5	C	155	SER
5	C	172	PRO
6	D	84	GLN
6	D	243	PRO
2	H	137	SER
3	A	83	PRO

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Mol	Chain	Res	Type
4	B	2	SER
3	A	67	VAL
5	C	81	PRO
1	L	95	SER
2	H	142	ASN
3	A	78	GLU
3	A	191	ILE
5	C	82	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	L	178/178 (100%)	149 (84%)	29 (16%)	2	10
2	H	192/192 (100%)	166 (86%)	26 (14%)	4	14
3	A	258/258 (100%)	255 (99%)	3 (1%)	63	75
4	B	245/259 (95%)	232 (95%)	13 (5%)	20	41
5	C	243/243 (100%)	240 (99%)	3 (1%)	63	75
6	D	248/248 (100%)	242 (98%)	6 (2%)	43	64
All	All	1364/1378 (99%)	1284 (94%)	80 (6%)	19	39

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	GLN
1	L	10	LEU
1	L	11	THR
1	L	18	VAL
1	L	20	LEU
1	L	23	ARG
1	L	26	THR
1	L	30	THR
1	L	31	THR
1	L	36	ASN

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Mol	Chain	Res	Type
1	L	49	LEU
1	L	50	ILE
1	L	54	ASN
1	L	68	LEU
1	L	96	ASN
1	L	105	LYS
1	L	113	LYS
1	L	135	LEU
1	L	139	ILE
1	L	146	VAL
1	L	149	VAL
1	L	156	THR
1	L	159	THR
1	L	197	GLN
1	L	199	THR
1	L	203	HIS
1	L	204	THR
1	L	206	GLU
1	L	209	LEU
2	H	3	GLN
2	H	5	LYS
2	H	12	VAL
2	H	17	SER
2	H	28	LEU
2	H	61	SER
2	H	81	LYS
2	H	82	MET
2	H	83	LYS
2	H	114	GLN
2	H	124	LYS
2	H	126	THR
2	H	140	GLN
2	H	141	THR
2	H	146	THR
2	H	147	LEU
2	H	158	PRO
2	H	160	THR
2	H	162	THR
2	H	169	SER
2	H	180	GLN
2	H	185	THR
2	H	186	LEU

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Mol	Chain	Res	Type
2	H	200	GLU
2	H	214	LYS
2	H	219	ILE
3	A	41	SER
3	A	67	VAL
3	A	231	MET
4	B	4	THR
4	B	31	ASP
4	B	40	LEU
4	B	60	ILE
4	B	72	ASP
4	B	123	VAL
4	B	128	LEU
4	B	199	THR
4	B	218	VAL
4	B	227	ARG
4	B	240	VAL
4	B	250	THR
4	B	284	GLU
5	C	76	VAL
5	C	86	VAL
5	C	226	MET
6	D	13	LEU
6	D	125	VAL
6	D	229	ARG
6	D	252	THR
6	D	257	THR
6	D	286	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	54	ASN
1	L	200	HIS
2	H	35	HIS
2	H	77	GLN
2	H	142	ASN
2	H	180	GLN
2	H	208	HIS
3	A	50	ASN
3	A	138	GLN
3	A	144	GLN

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Mol	Chain	Res	Type
3	A	190	ASN
3	A	209	GLN
3	A	218	HIS
3	A	250	HIS
3	A	252	HIS
4	B	113	HIS
5	C	17	HIS
5	C	133	GLN
5	C	137	GLN
5	C	175	HIS
6	D	102	ASN
6	D	293	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-22474. These allow visual inspection of the internal detail of the map and identification of artifacts.

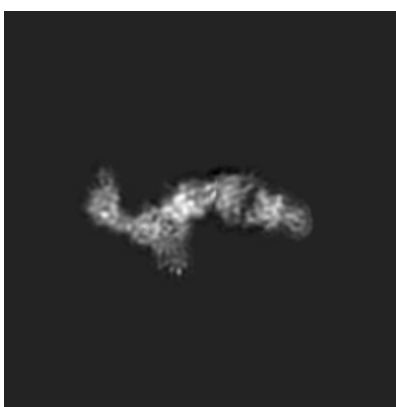
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

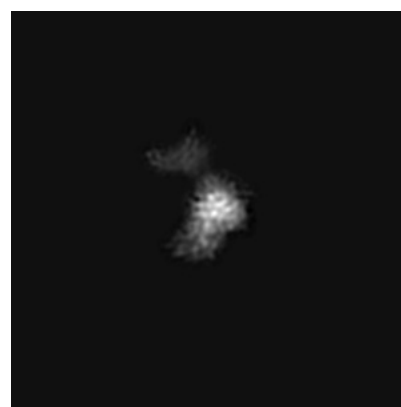
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

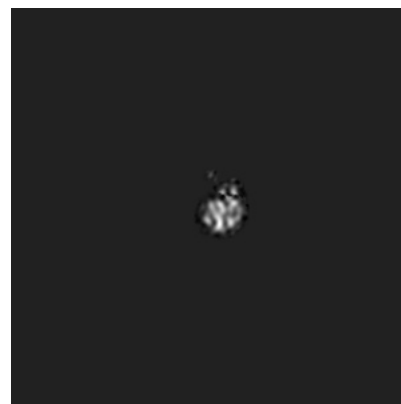
6.2.1 Primary map



X Index: 120



Y Index: 120



Z Index: 120

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

6.3 Largest variance slices [i](#)

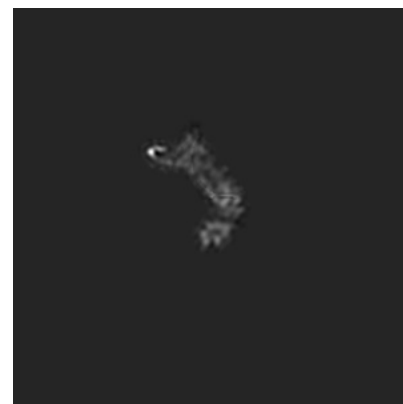
6.3.1 Primary map



X Index: 120



Y Index: 123

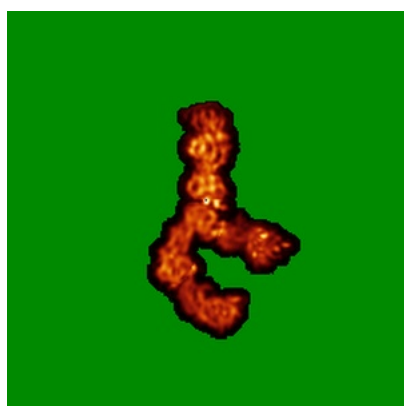


Z Index: 105

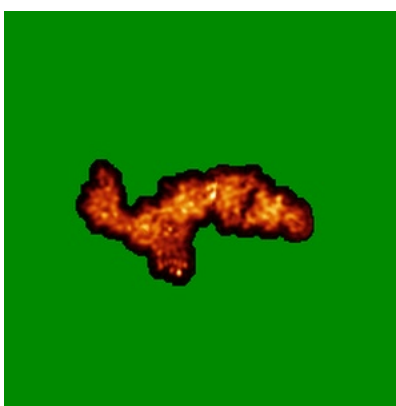
The images above show the largest variance slices of the map in three orthogonal directions.

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

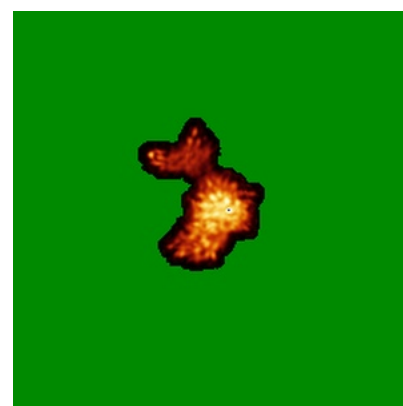
6.4.1 Primary map



X



Y

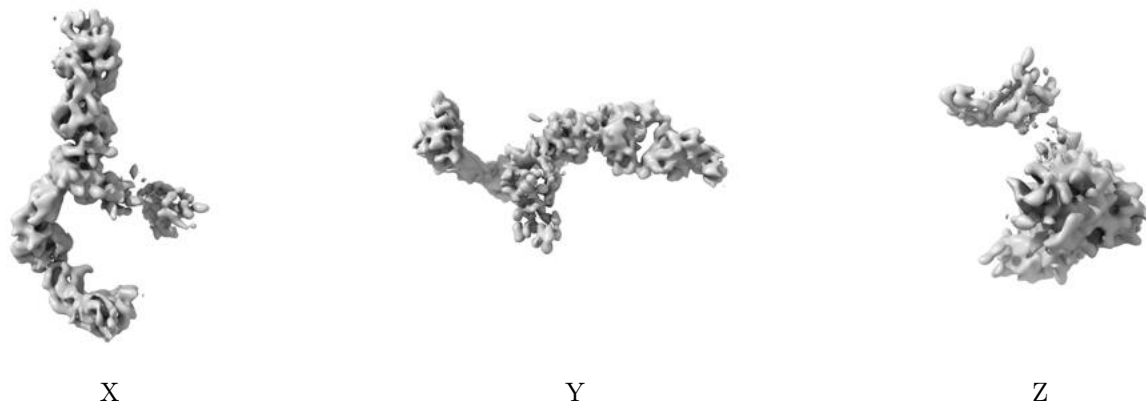


Z

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

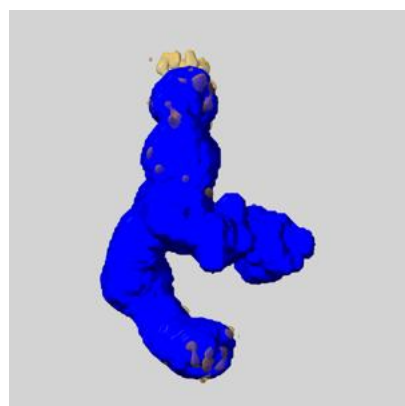
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

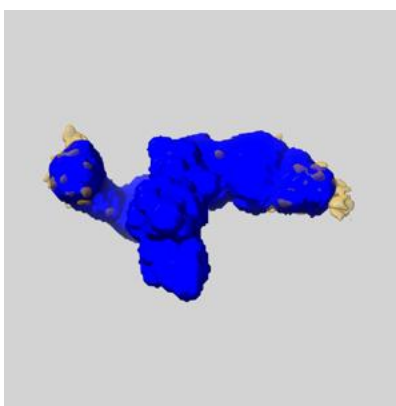
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

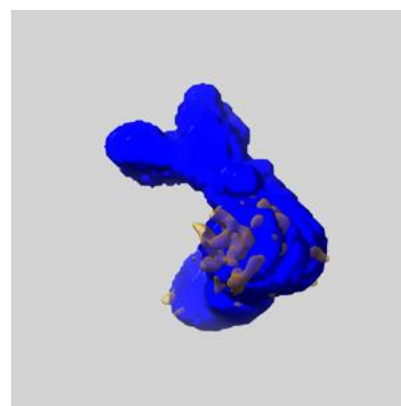
6.6.1 emd_22474_msk_1.map [i](#)



X



Y

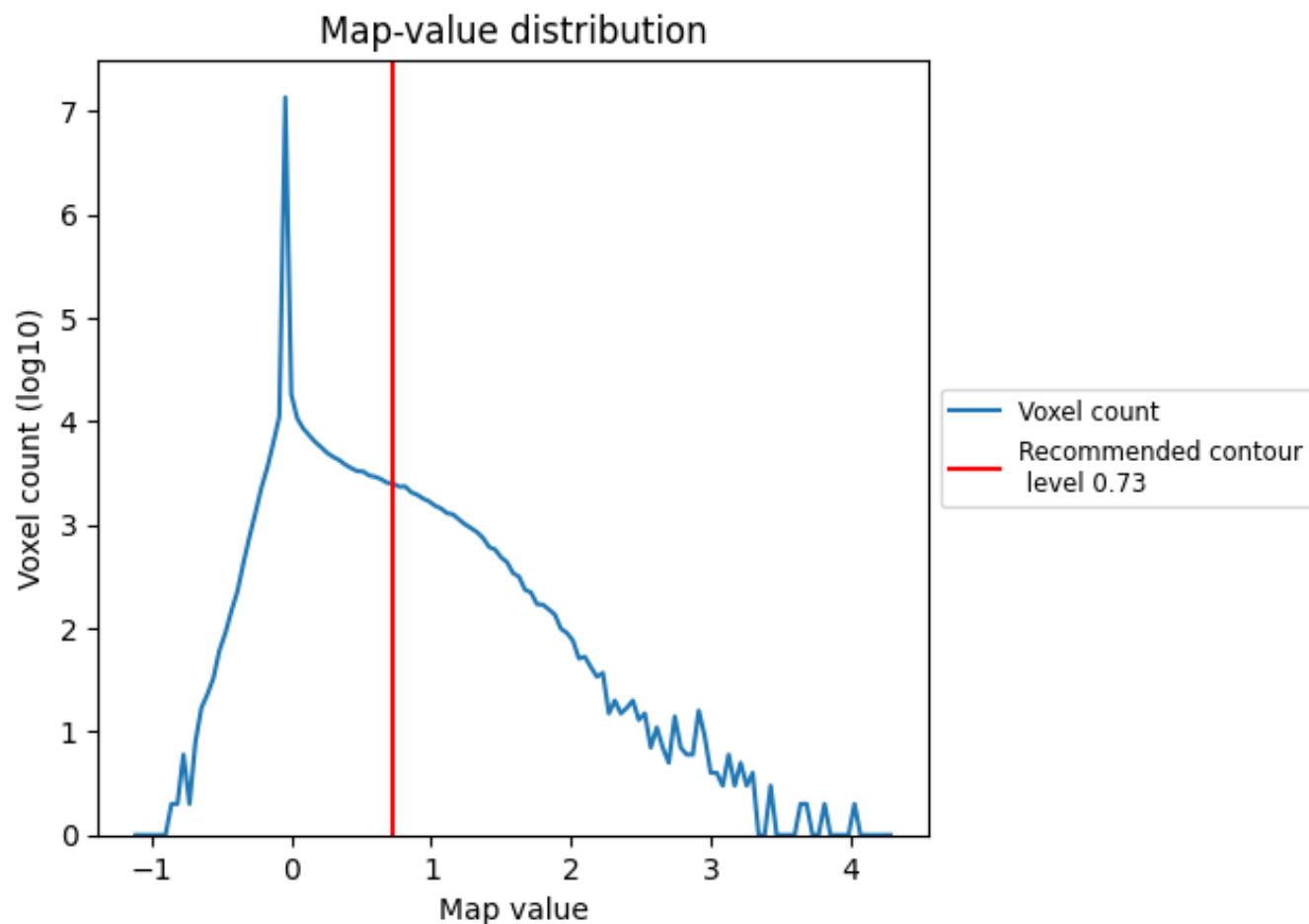


Z

7 Map analysis [i](#)

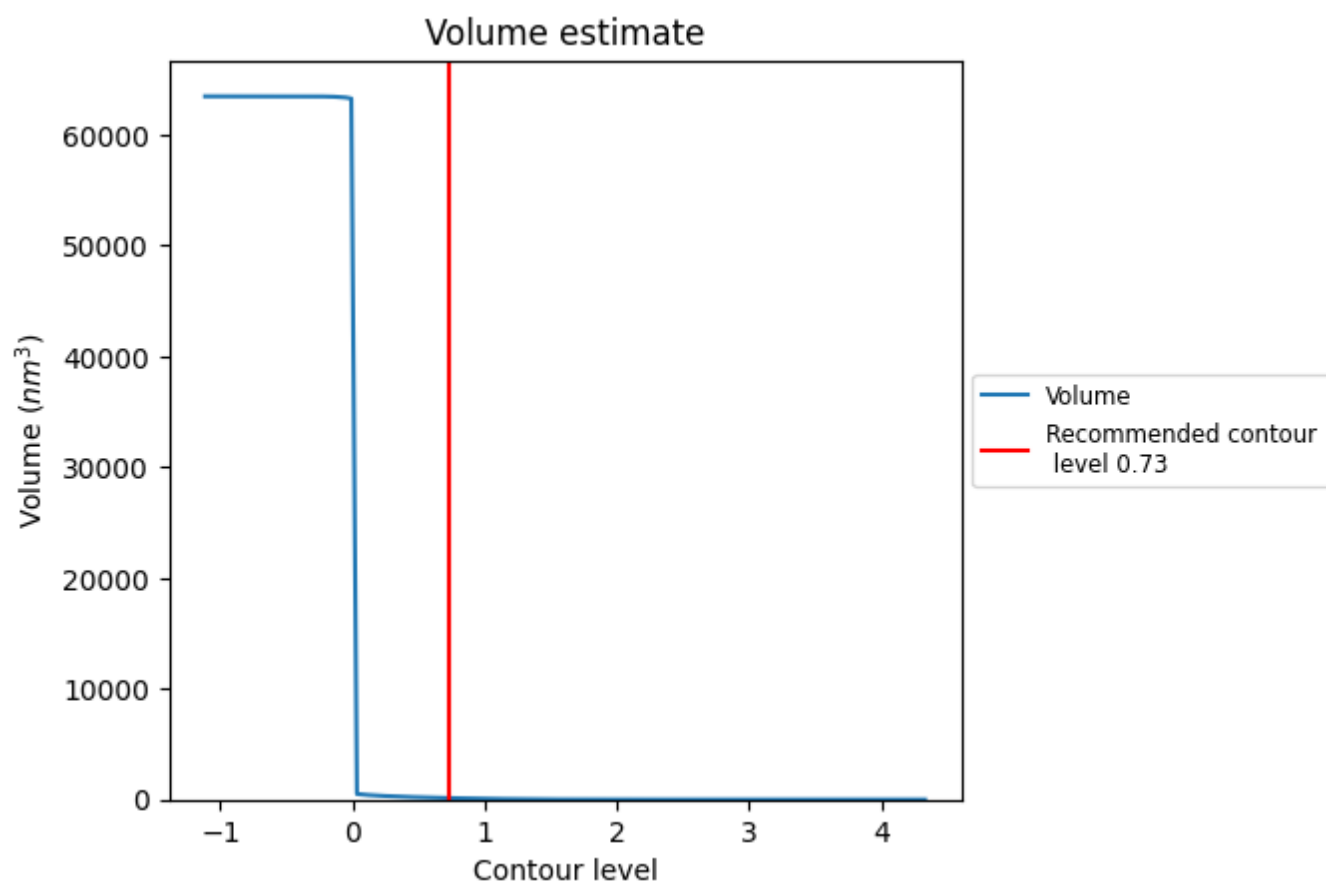
This section contains the results of statistical analysis of the map.

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.

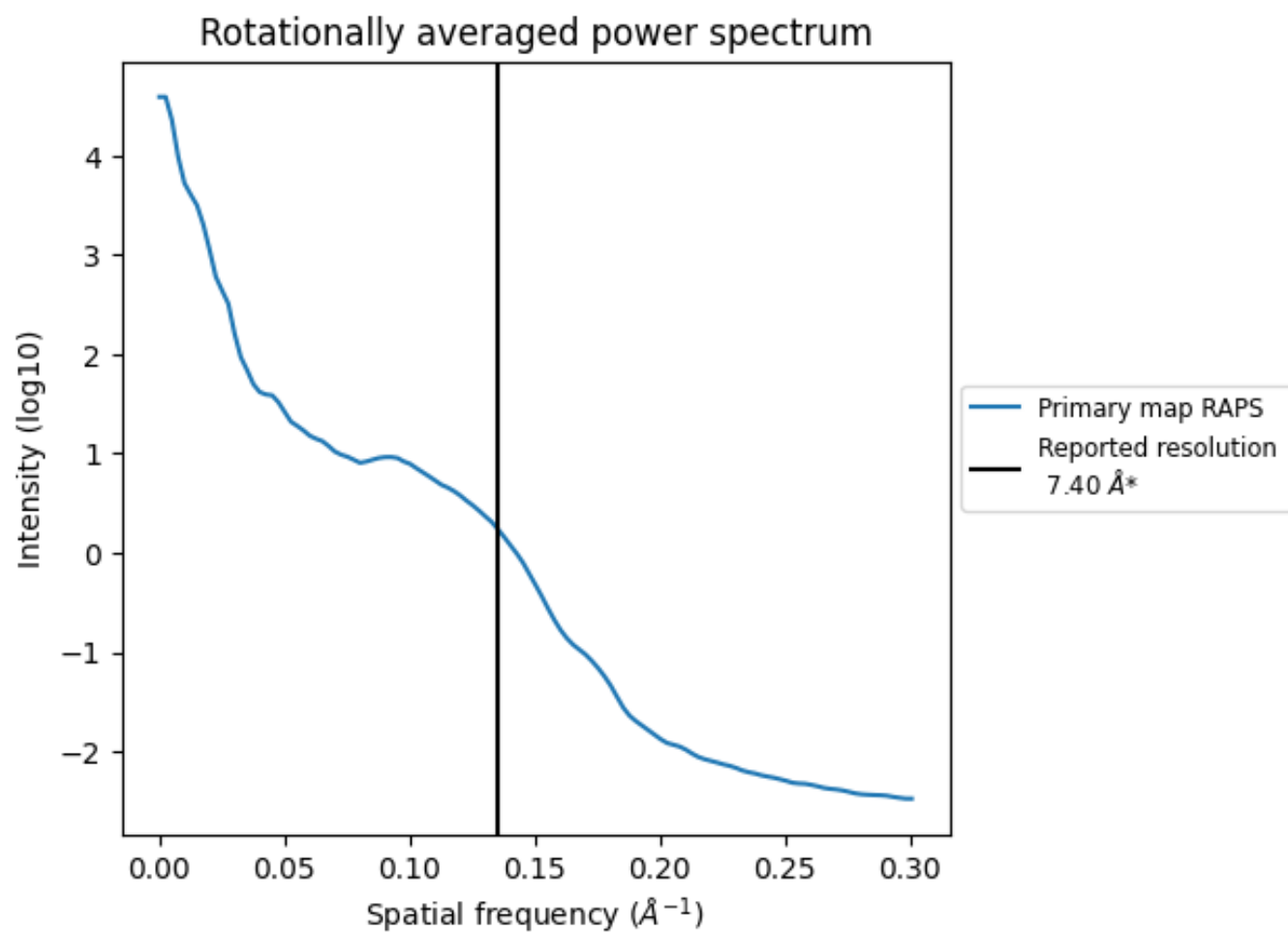
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 135 nm^3 ; this corresponds to an approximate mass of 122 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 ⓘ

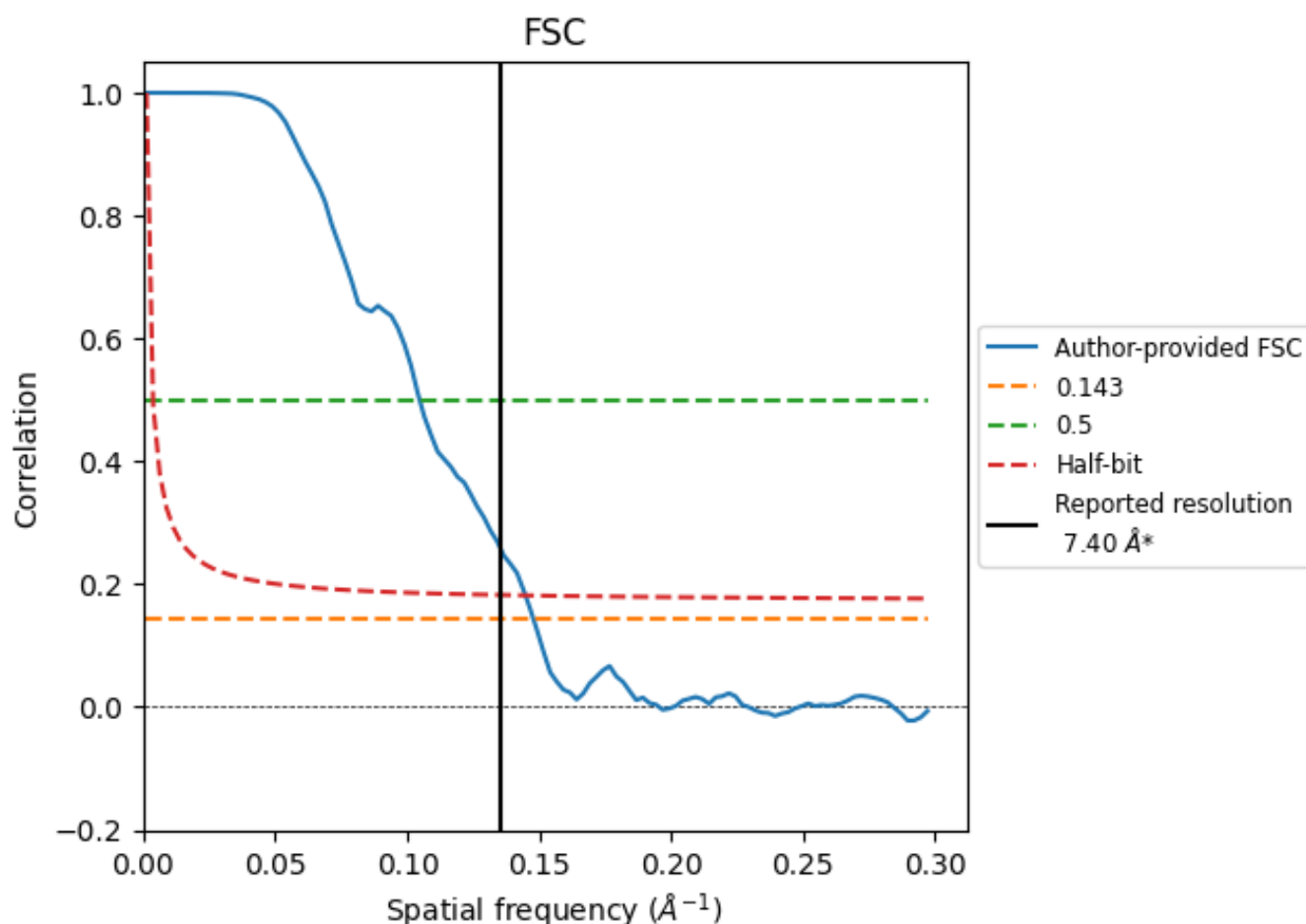


*Reported resolution corresponds to spatial frequency of 0.135 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.135 Å⁻¹

8.2 Resolution estimates [i](#)

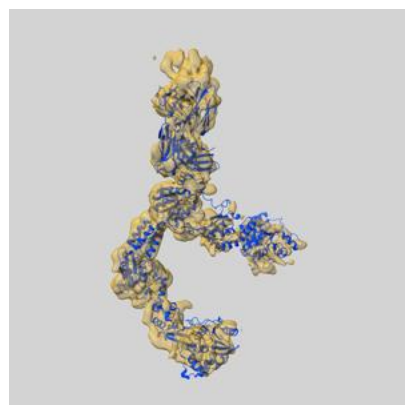
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	7.40	-
Author-provided FSC curve	6.77	9.54	6.91
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.5 CUT-OFF 9.54 differs from the reported value 7.4 by more than 10 %

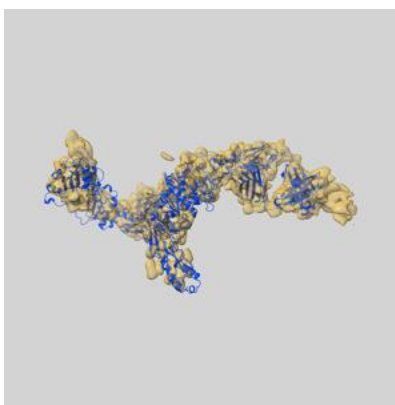
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22474 and PDB model 7JTI. Per-residue inclusion information can be found in section 3 on page 5.

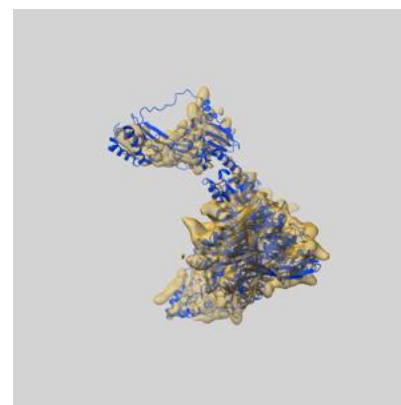
9.1 Map-model overlay [i](#)



X



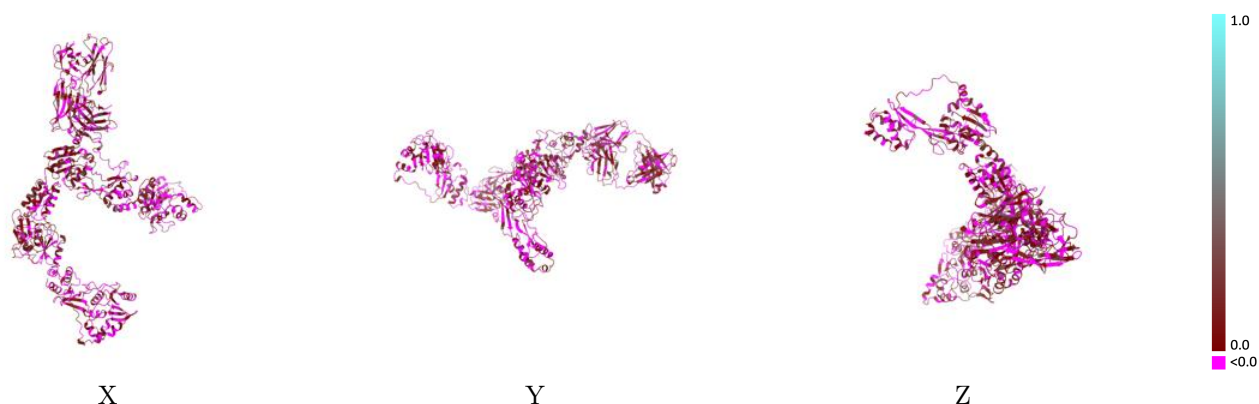
Y



Z

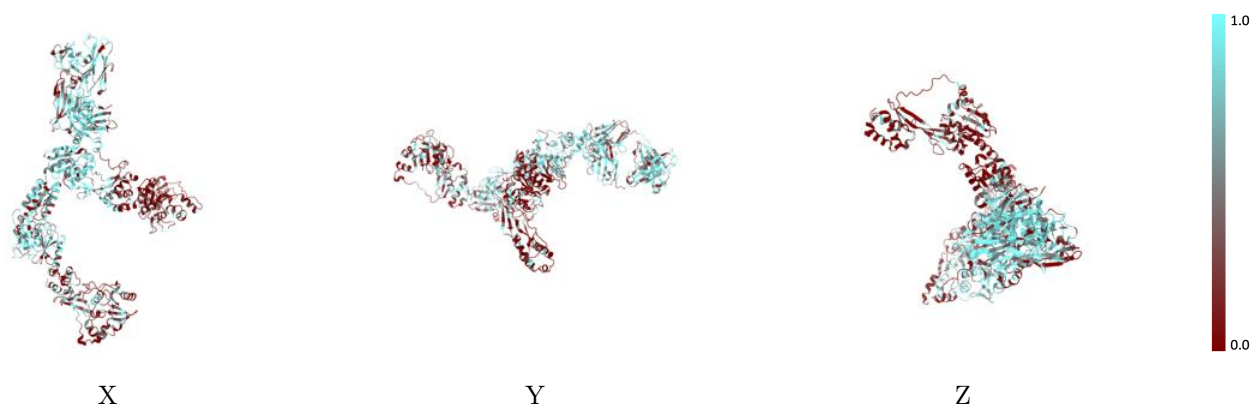
The images above show the 3D surface view of the map at the recommended contour level 0.73 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



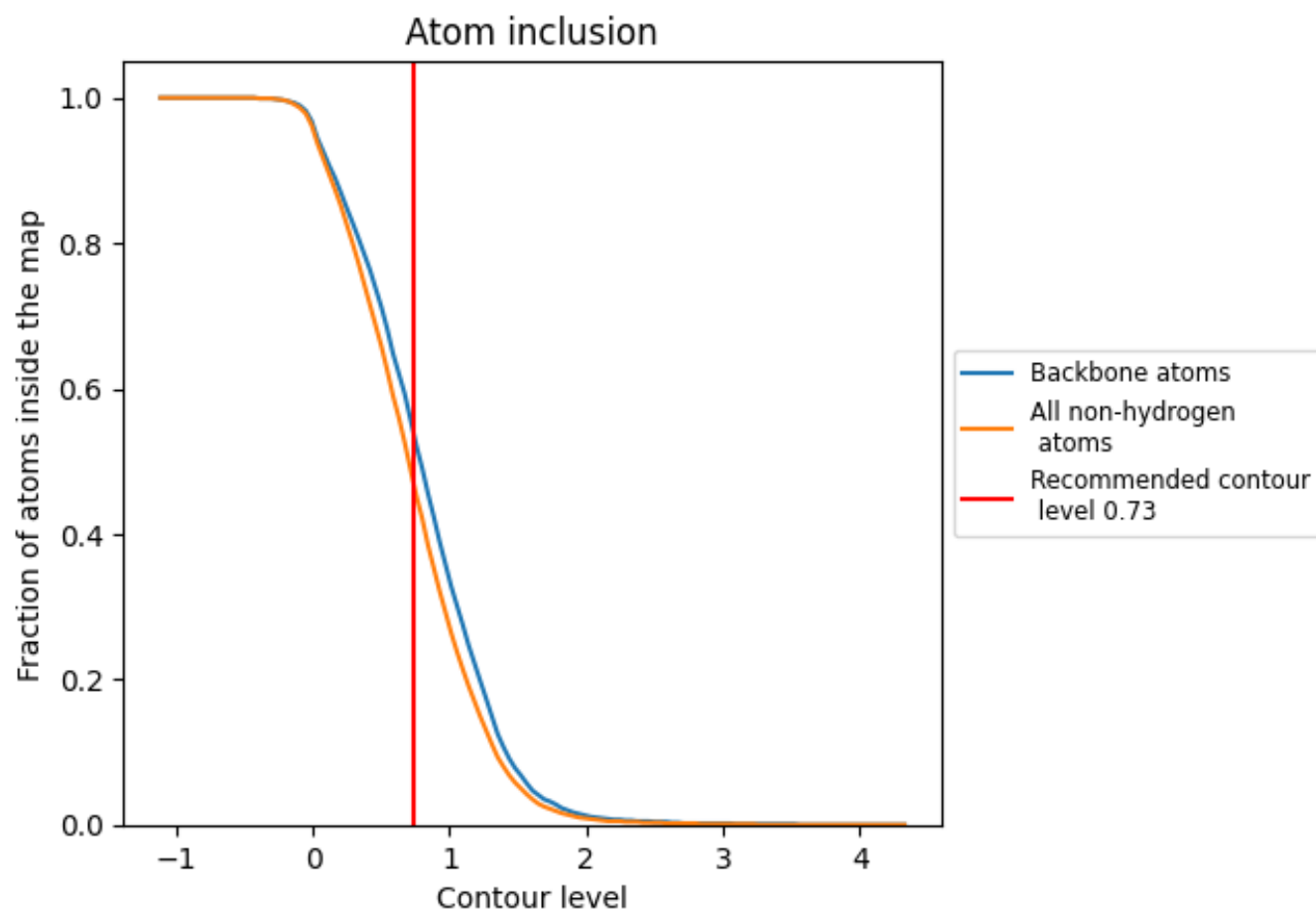
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.73).

9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 48% 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 (0.73) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4750	0.0480
A	0.5690	0.0740
B	0.2060	0.0240
C	0.5760	0.0620
D	0.3170	0.0150
H	0.6480	0.0750
L	0.6230	0.0460

1.0

0.0

<0.0