



Full wwPDB EM Validation Report ⓘ

Nov 24, 2025 – 10:02 am GMT

PDB ID : 9T32 / pdb_00009t32
EMDB ID : EMD-55480
Title : The Cullin 2 RING VHL E3 ligase dimerised by the homoPROTAC CM11
Authors : Crowe, C.; Ciulli, A.
Deposited on : 2025-10-24
Resolution : 6.90 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.dev129
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

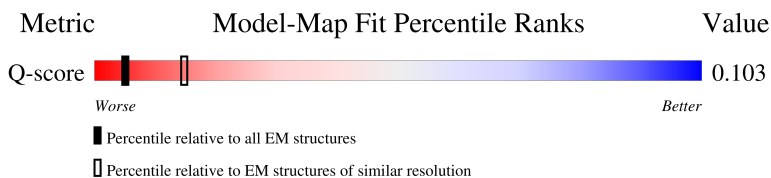
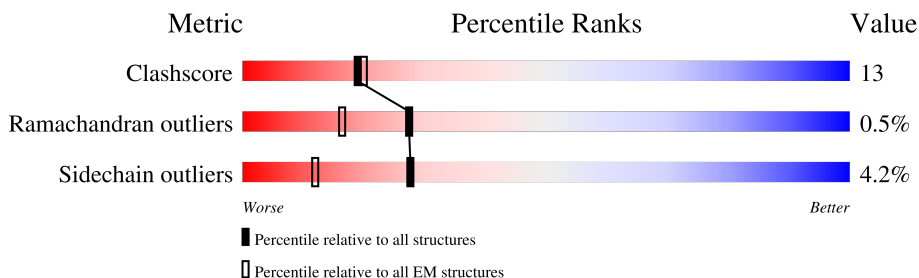
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.90 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.





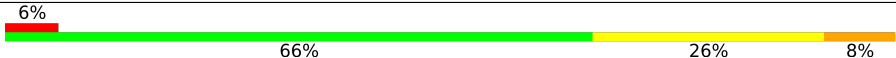
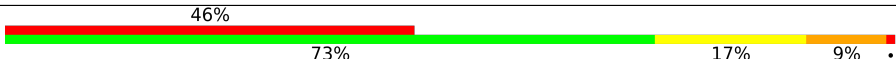
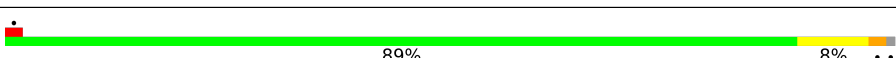
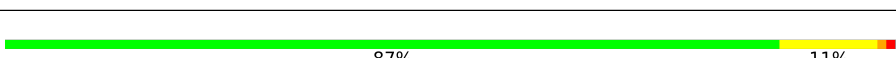
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	479 (6.40 - 7.40)

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	D	103	
1	F	103	
2	G	95	
2	J	95	

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Mol	Chain	Length	Quality of chain
3	E	655	
3	I	655	
4	R	89	
4	S	89	
5	C	141	
5	H	141	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 34854 atoms, of which 17356 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 Elongin-B.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	D	101	Total	C	H	N	O	S	0	0
			1585	504	794	134	150	3		
1	F	101	Total	C	H	N	O	S	0	0
			1585	504	794	134	150	3		

- Molecule 2 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	G	83	Total	C	H	N	O	S	0	0
			1322	428	660	106	123	5		
2	J	83	Total	C	H	N	O	S	0	0
			1322	428	660	106	123	5		

- Molecule 3 is a protein called Cullin-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	655	Total	C	H	N	O	S	0	0
			10708	3422	5337	901	1008	40		
3	I	655	Total	C	H	N	O	S	0	0
			10708	3422	5337	901	1008	40		

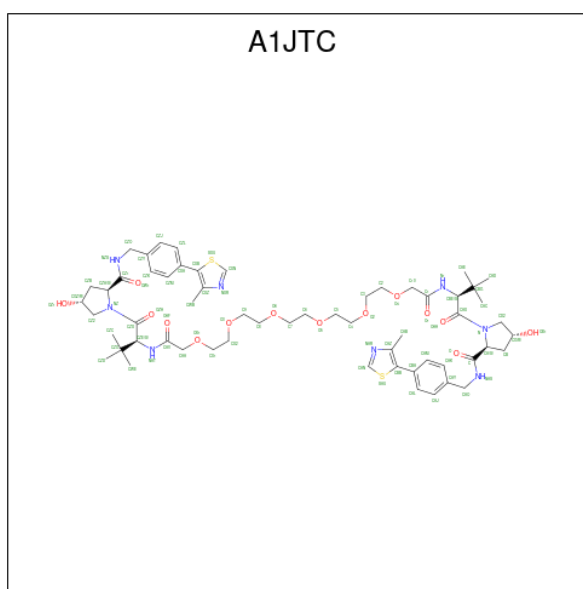
- Molecule 4 is a protein called E3 ubiquitin-protein ligase RBX1, N-terminally processed.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	R	89	Total	C	H	N	O	S	0	0
			1431	466	694	135	127	9		
4	S	89	Total	C	H	N	O	S	0	0
			1431	466	694	135	127	9		

- Molecule 5 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	H	140	Total	C	H	N	O	S	0	0
			2299	731	1152	209	206	1		
5	C	140	Total	C	H	N	O	S	0	0
			2299	731	1152	209	206	1		

- Molecule 6 is (2 {S},4 {R})-1-[(2 {S})-2-[2-[2-[2-[2-[2-[2-[(2 {S})-3,3-dimethyl-1-[(2 {S},4 {R})-2-[[4-(4-methyl-1,3-thiazol-5-yl)phenyl]methylcarbamoyl]-4-oxidanyl-pyrrolidin-1-yl]-1-oxidanylidene-butan-2-yl]amino]-2-oxidanylidene-ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethanoylamino]-3,3-dimethyl-butanoyl]- {N}-[[4-(4-methyl-1,3-thiazol-5-yl)phenyl]methyl]-4-oxidanyl-pyrrolidine-2-carboxamide (CCD ID: A1JTC) (formula: C₅₈H₈₂N₈O₁₄S₂) (labeled as "Ligand of Interest" by depositor).

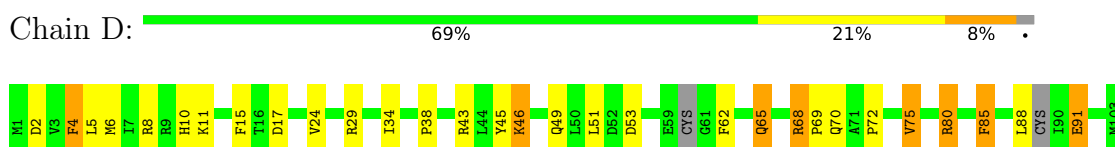


Mol	Chain	Residues	Atoms						AltConf
6	C	1	Total	C	H	N	O	S	0
			164	58	82	8	14	2	

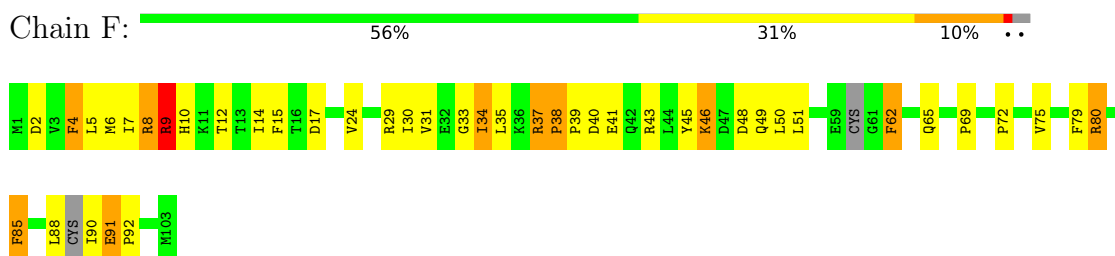
3 Residue-property plots [i](#)

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.

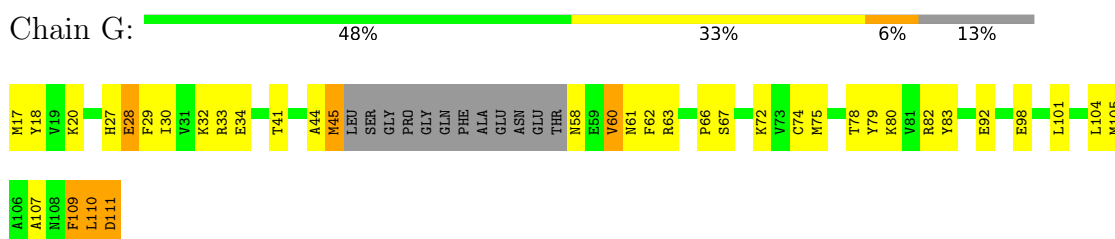
• Molecule 1: Elongin-B



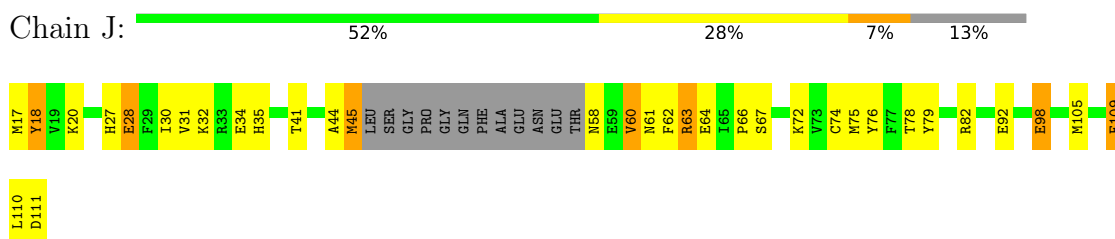
• Molecule 1: Elongin-B



• Molecule 2: Elongin-C

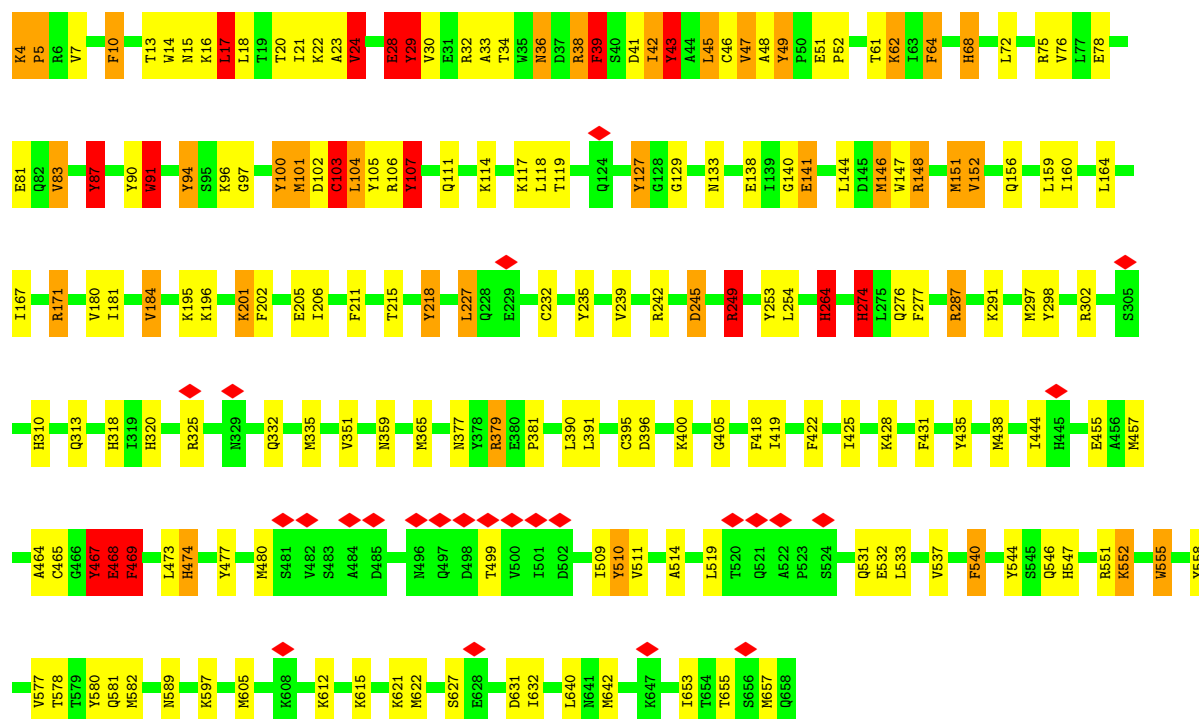


• Molecule 2: Elongin-C



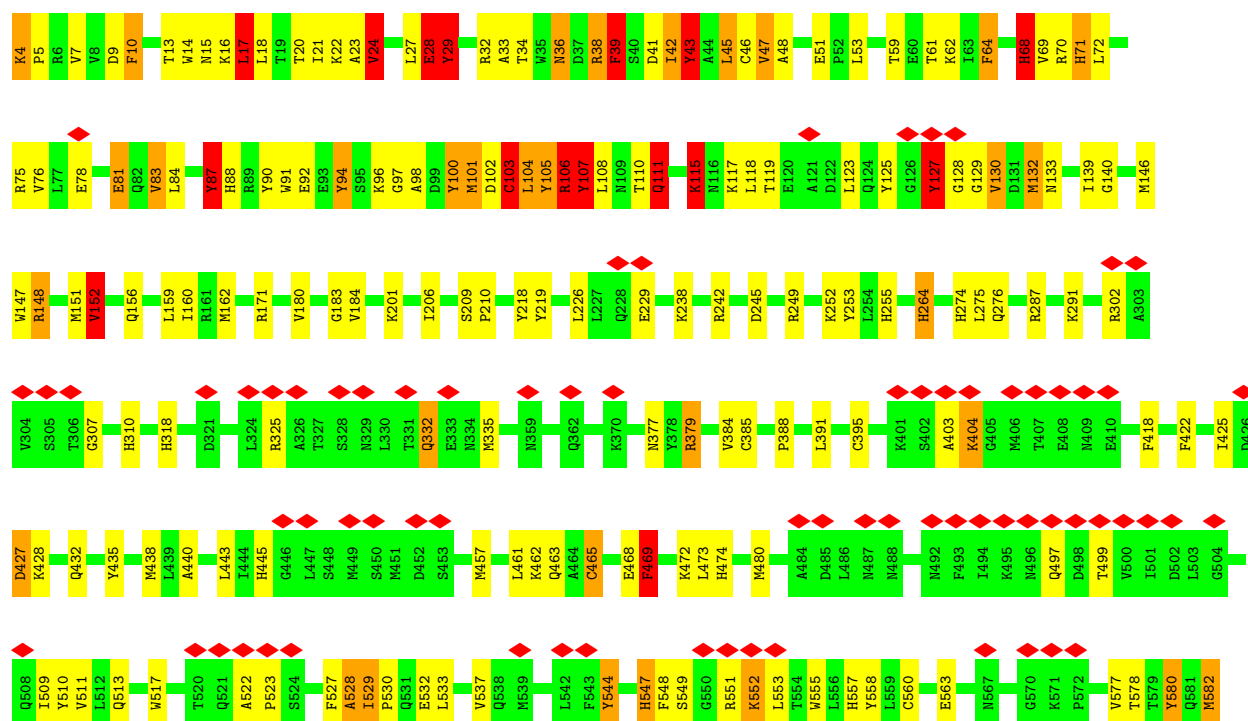
• Molecule 3: Cullin-2

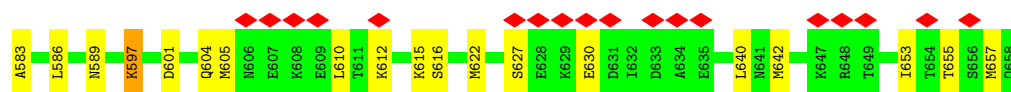
Chain E: 



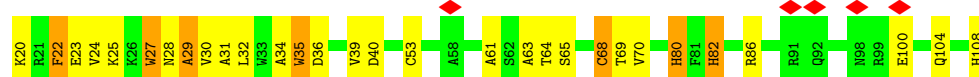
• Molecule 3: Cullin-2

Chain I: 





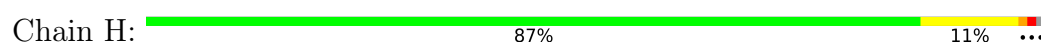
- Molecule 4: E3 ubiquitin-protein ligase RBX1, N-terminally processed



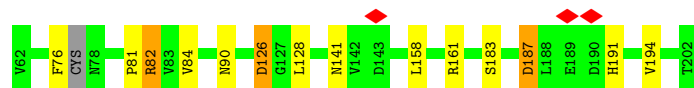
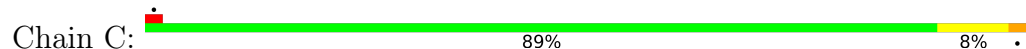
- Molecule 4: E3 ubiquitin-protein ligase RBX1, N-terminally processed



- Molecule 5: von Hippel-Lindau disease tumor suppressor



- Molecule 5: von Hippel-Lindau disease tumor suppressor



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68789	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	57	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.116	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0183	Depositor
Map size (Å)	444.0, 444.0, 444.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.74, 0.74, 0.74	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1JTC

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	D	0.97	0/805	1.75	17/1086 (1.6%)
1	F	0.96	0/805	1.82	18/1086 (1.7%)
2	G	0.96	0/676	1.74	11/914 (1.2%)
2	J	0.92	0/676	1.79	15/914 (1.6%)
3	E	0.83	0/5482	1.72	86/7390 (1.2%)
3	I	0.83	0/5482	1.73	98/7390 (1.3%)
4	R	0.94	0/759	1.83	15/1029 (1.5%)
4	S	0.93	0/759	1.92	17/1029 (1.7%)
5	C	0.96	0/1176	1.63	10/1604 (0.6%)
5	H	0.96	0/1176	1.62	12/1604 (0.7%)
All	All	0.88	0/17796	1.73	299/24046 (1.2%)

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
1	D	0	2
1	F	0	2
2	J	0	1
3	E	0	28
3	I	0	30
4	R	0	3
4	S	0	2
5	C	0	2
5	H	0	1
All	All	0	71

There are no bond length outliers.

All (299) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	32	LEU	N-CA-C	14.03	130.52	113.41
3	E	631	ASP	CA-C-N	11.64	136.81	120.98
3	E	631	ASP	C-N-CA	11.64	136.81	120.98
3	E	632	ILE	N-CA-C	11.09	123.17	109.30
3	E	104	LEU	N-CA-CB	-10.39	94.02	109.82
3	I	103	CYS	N-CA-C	-10.33	99.71	110.97
3	E	195	LYS	CA-C-N	10.28	134.06	120.28
3	E	195	LYS	C-N-CA	10.28	134.06	120.28
3	E	118	LEU	N-CA-C	-10.23	94.95	110.30
2	J	109	PHE	CA-CB-CG	10.21	124.01	113.80
4	R	32	LEU	N-CA-C	10.15	125.81	113.12
3	I	104	LEU	N-CA-CB	-10.11	94.45	109.82
1	D	85	PHE	CA-CB-CG	-10.10	103.70	113.80
2	J	35	HIS	CA-CB-CG	10.09	123.89	113.80
3	E	469	PHE	CA-CB-CG	-9.83	103.97	113.80
2	G	109	PHE	CA-CB-CG	9.71	123.50	113.80
4	R	65	SER	N-CA-C	9.41	122.40	111.11
3	I	133	ASN	CA-CB-CG	9.31	121.91	112.60
3	I	552	LYS	N-CA-C	9.23	123.15	109.59
5	C	187	ASP	CA-CB-CG	9.16	121.76	112.60
3	E	291	LYS	CB-CG-CD	8.99	131.97	111.30
3	I	291	LYS	CB-CG-CD	8.96	131.91	111.30
1	F	4	PHE	CA-CB-CG	-8.73	105.07	113.80
1	D	4	PHE	CA-CB-CG	-8.68	105.12	113.80
3	I	528	ALA	N-CA-C	-8.59	94.58	108.41
3	I	115	LYS	CB-CA-C	8.45	124.25	110.90
1	D	46	LYS	CA-CB-CG	-8.34	97.41	114.10
3	I	469	PHE	CA-CB-CG	-8.33	105.47	113.80
4	S	33	TRP	N-CA-C	8.30	121.13	108.52
3	E	468	GLU	CB-CA-C	-8.23	97.64	110.81
1	F	91	GLU	N-CA-C	-8.22	97.42	109.50
3	E	117	LYS	N-CA-C	-8.16	97.60	109.59
4	S	25	LYS	CB-CG-CD	8.04	129.79	111.30
3	E	39	PHE	CA-CB-CG	-8.00	105.80	113.80
3	I	549	SER	N-CA-C	7.91	118.69	108.24
4	R	82	HIS	CB-CG-CD2	-7.91	120.91	131.20
3	E	133	ASN	CA-CB-CG	7.91	120.51	112.60
3	E	264	HIS	CB-CG-CD2	-7.88	120.95	131.20
1	D	91	GLU	N-CA-C	-7.86	99.74	109.65
3	E	287	ARG	NE-CZ-NH2	7.74	126.16	119.20
5	C	82	ARG	NE-CZ-NH2	7.71	126.14	119.20
3	E	318	HIS	CB-CG-CD2	-7.52	121.43	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	547	HIS	N-CA-C	7.47	122.52	113.41
3	I	115	LYS	N-CA-C	-7.38	103.17	111.14
1	D	46	LYS	N-CA-C	-7.36	95.62	108.20
3	E	249	ARG	NE-CZ-NH2	7.29	125.76	119.20
3	I	252	LYS	CA-CB-CG	7.28	128.65	114.10
3	I	229	GLU	CA-CB-CG	7.25	128.61	114.10
3	E	196	LYS	N-CA-CB	-7.21	99.53	110.12
3	E	16	LYS	CG-CD-CE	7.20	127.86	111.30
3	I	28	GLU	N-CA-C	-7.19	103.38	111.07
3	I	377	ASN	CA-CB-CG	-7.17	105.43	112.60
3	E	15	ASN	CA-CB-CG	-7.14	105.46	112.60
3	I	589	ASN	OD1-CG-ND2	-7.08	115.52	122.60
1	F	46	LYS	N-CA-C	-7.07	96.12	108.20
3	I	16	LYS	CG-CD-CE	7.06	127.54	111.30
4	R	80	HIS	CB-CG-CD2	-7.02	122.08	131.20
3	E	377	ASN	CB-CA-C	7.01	123.13	110.72
3	I	39	PHE	CA-CB-CG	-6.99	106.81	113.80
3	I	201	LYS	CG-CD-CE	-6.97	95.26	111.30
2	J	61	ASN	CA-CB-CG	-6.94	105.66	112.60
3	I	379	ARG	NE-CZ-NH2	6.91	125.42	119.20
2	G	63	ARG	CA-C-N	6.89	132.99	122.37
2	G	63	ARG	C-N-CA	6.89	132.99	122.37
3	I	551	ARG	CA-C-N	6.88	131.15	121.24
3	I	551	ARG	C-N-CA	6.88	131.15	121.24
3	I	17	LEU	CA-C-N	6.88	129.83	120.54
3	I	17	LEU	C-N-CA	6.88	129.83	120.54
1	F	46	LYS	CA-CB-CG	-6.86	100.39	114.10
3	E	201	LYS	CG-CD-CE	-6.84	95.57	111.30
4	S	100	GLU	CB-CA-C	6.83	120.82	109.89
3	E	41	ASP	CA-CB-CG	6.79	119.39	112.60
3	I	101	MET	N-CA-C	-6.79	103.81	111.07
1	D	38	PRO	N-CA-CB	6.79	106.75	103.22
5	H	179	ASP	CA-CB-CG	6.78	119.38	112.60
1	D	80	ARG	NE-CZ-NH2	6.77	125.29	119.20
3	I	128	GLY	N-CA-C	6.77	120.39	110.38
1	F	34	ILE	CA-CB-CG2	6.76	122.00	110.50
1	F	80	ARG	NE-CZ-NH2	6.73	125.26	119.20
3	I	229	GLU	CB-CA-C	-6.68	96.24	109.67
5	C	90	ASN	CA-CB-CG	6.65	119.25	112.60
3	I	103	CYS	O-C-N	-6.63	115.13	122.03
3	I	15	ASN	CA-CB-CG	-6.60	106.00	112.60
3	I	529	ILE	N-CA-CB	-6.59	102.85	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	182	ARG	N-CA-C	6.59	119.30	111.33
3	I	117	LYS	N-CA-C	6.53	119.07	108.63
3	I	96	LYS	N-CA-C	-6.52	104.17	111.28
4	R	25	LYS	CB-CG-CD	6.52	126.29	111.30
3	I	47	VAL	CB-CA-C	6.50	121.95	111.29
3	E	17	LEU	CA-C-N	6.46	129.25	120.54
3	E	17	LEU	C-N-CA	6.46	129.25	120.54
3	I	529	ILE	CB-CA-C	6.45	118.09	110.68
4	S	65	SER	N-CA-C	6.43	117.98	110.97
3	E	597	LYS	CB-CG-CD	6.43	126.08	111.30
1	F	34	ILE	N-CA-CB	-6.42	100.63	111.23
1	D	46	LYS	N-CA-CB	6.42	120.97	110.37
3	I	597	LYS	CB-CG-CD	6.41	126.05	111.30
3	I	53	LEU	CA-C-N	6.40	128.13	120.14
3	I	53	LEU	C-N-CA	6.40	128.13	120.14
3	I	438	MET	CA-C-N	6.39	128.84	120.28
3	I	438	MET	C-N-CA	6.39	128.84	120.28
5	C	161	ARG	NE-CZ-NH2	6.37	124.93	119.20
3	I	68	HIS	CB-CG-CD2	-6.37	122.92	131.20
3	I	41	ASP	CA-CB-CG	6.34	118.94	112.60
1	D	65	GLN	CB-CA-C	6.30	120.62	110.09
3	I	45	LEU	N-CA-C	6.30	119.44	111.69
3	E	405	GLY	N-CA-C	-6.28	107.01	114.48
1	F	29	ARG	NE-CZ-NH2	6.26	124.83	119.20
3	E	597	LYS	CA-CB-CG	-6.25	101.60	114.10
3	I	53	LEU	N-CA-C	-6.24	105.94	112.93
2	G	61	ASN	CA-CB-CG	-6.21	106.39	112.60
3	I	253	TYR	N-CA-C	6.20	121.51	113.88
3	I	615	LYS	CA-CB-CG	-6.19	101.71	114.10
3	E	28	GLU	N-CA-C	-6.17	104.47	111.07
2	J	63	ARG	NE-CZ-NH2	6.17	124.75	119.20
3	E	103	CYS	O-C-N	-6.15	114.41	122.59
3	E	47	VAL	CB-CA-C	6.14	121.35	111.29
3	E	514	ALA	N-CA-C	6.13	119.60	111.75
2	J	45	MET	CG-SD-CE	6.13	114.39	100.90
3	E	101	MET	N-CA-C	-6.11	104.53	111.07
3	I	242	ARG	NE-CZ-NH2	6.08	124.67	119.20
2	J	63	ARG	CA-C-N	6.05	132.04	122.60
2	J	63	ARG	C-N-CA	6.05	132.04	122.60
3	E	245	ASP	CA-CB-CG	6.04	118.64	112.60
3	I	274	HIS	CB-CG-CD2	-6.03	123.36	131.20
5	H	143	ASP	CA-CB-CG	6.01	118.61	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	126	ASP	CA-CB-CG	6.00	118.60	112.60
3	I	332	GLN	N-CA-C	5.99	119.42	111.75
3	E	274	HIS	CB-CG-CD2	-5.99	123.42	131.20
3	E	302	ARG	CB-CG-CD	-5.99	97.53	111.30
3	E	264	HIS	CA-CB-CG	-5.96	107.84	113.80
3	E	377	ASN	CA-C-N	5.94	129.14	120.71
3	E	377	ASN	C-N-CA	5.94	129.14	120.71
1	D	38	PRO	CA-C-N	5.93	126.08	119.32
1	D	38	PRO	C-N-CA	5.93	126.08	119.32
2	G	45	MET	CG-SD-CE	5.91	113.91	100.90
3	E	359	ASN	OD1-CG-ND2	-5.91	116.69	122.60
3	I	547	HIS	N-CA-C	5.91	120.76	113.50
3	E	23	ALA	CA-C-N	5.89	132.58	121.97
3	E	23	ALA	C-N-CA	5.89	132.58	121.97
4	S	33	TRP	CA-CB-CG	5.88	124.77	113.60
1	D	10	HIS	CA-CB-CG	-5.85	107.95	113.80
3	E	103	CYS	N-CA-C	-5.83	98.38	110.80
3	E	467	TYR	CA-C-N	5.83	128.41	120.54
3	E	467	TYR	C-N-CA	5.83	128.41	120.54
3	E	615	LYS	CA-CB-CG	-5.82	102.45	114.10
5	H	186	GLU	CB-CG-CD	5.80	122.46	112.60
3	E	156	GLN	OE1-CD-NE2	-5.80	116.80	122.60
3	E	632	ILE	N-CA-CB	-5.79	103.19	110.31
3	I	111	GLN	OE1-CD-NE2	-5.79	116.81	122.60
2	G	58	ASN	CA-CB-CG	5.78	118.38	112.60
3	E	438	MET	CA-C-N	5.78	128.03	120.28
3	E	438	MET	C-N-CA	5.78	128.03	120.28
3	I	132	MET	CA-C-N	5.78	131.14	122.47
3	I	132	MET	C-N-CA	5.78	131.14	122.47
3	I	597	LYS	CA-CB-CG	-5.77	102.56	114.10
3	I	445	HIS	CB-CG-CD2	-5.76	123.71	131.20
3	I	549	SER	N-CA-CB	-5.76	101.99	110.97
1	F	65	GLN	CB-CA-C	5.75	119.69	110.09
3	E	274	HIS	CA-CB-CG	-5.74	108.06	113.80
4	R	70	VAL	N-CA-C	5.74	116.47	109.30
3	I	71	HIS	CB-CG-CD2	-5.74	123.74	131.20
3	E	184	VAL	CB-CA-C	-5.73	104.63	111.97
1	F	85	PHE	CA-CB-CG	-5.73	108.07	113.80
3	E	36	ASN	CA-CB-CG	5.71	118.31	112.60
4	R	100	GLU	CB-CA-C	5.69	119.38	109.65
5	H	76	PHE	CA-CB-CG	5.68	119.48	113.80
3	E	96	LYS	N-CA-C	-5.68	105.09	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	276	GLN	OE1-CD-NE2	-5.68	116.92	122.60
3	E	242	ARG	NE-CZ-NH1	-5.67	115.83	121.50
3	E	291	LYS	CA-CB-CG	-5.64	102.81	114.10
1	D	53	ASP	N-CA-C	5.64	118.16	111.33
5	C	76	PHE	CA-CB-CG	5.64	119.44	113.80
3	I	23	ALA	CA-C-N	5.61	132.07	121.97
3	I	23	ALA	C-N-CA	5.61	132.07	121.97
3	I	553	LEU	N-CA-C	-5.60	102.99	110.55
3	I	630	GLU	N-CA-CB	5.57	119.64	110.39
2	J	109	PHE	CA-C-N	5.57	130.10	120.58
2	J	109	PHE	C-N-CA	5.57	130.10	120.58
1	D	10	HIS	CB-CA-C	5.56	121.48	110.42
3	E	68	HIS	CB-CG-CD2	-5.56	123.97	131.20
4	S	105	LYS	CA-CB-CG	5.56	125.21	114.10
3	E	313	GLN	OE1-CD-NE2	-5.55	117.05	122.60
3	E	547	HIS	CB-CG-CD2	-5.55	123.99	131.20
4	R	64	THR	N-CA-C	5.54	119.21	112.23
2	J	60	VAL	N-CA-C	5.52	116.83	109.37
3	E	141	GLU	CA-C-N	5.51	127.60	120.44
3	E	141	GLU	C-N-CA	5.51	127.60	120.44
1	F	38	PRO	CA-C-N	5.50	125.59	119.32
1	F	38	PRO	C-N-CA	5.50	125.59	119.32
4	R	23	GLU	CA-C-N	5.49	127.93	120.63
4	R	23	GLU	C-N-CA	5.49	127.93	120.63
3	I	509	ILE	N-CA-C	5.49	116.95	108.44
3	E	171	ARG	NE-CZ-NH2	5.48	124.13	119.20
3	I	472	LYS	CB-CG-CD	5.47	123.88	111.30
4	S	78	ALA	N-CA-C	5.46	117.48	109.24
5	C	141	ASN	CA-CB-CG	5.45	118.05	112.60
2	J	105	MET	N-CA-C	-5.44	105.04	110.97
3	E	546	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	F	37	ARG	NE-CZ-NH2	5.42	124.08	119.20
3	I	152	VAL	CA-CB-CG2	5.42	119.62	110.40
3	I	597	LYS	CG-CD-CE	-5.42	98.84	111.30
4	S	45	CYS	CA-C-N	5.41	130.63	122.68
4	S	45	CYS	C-N-CA	5.41	130.63	122.68
4	S	108	HIS	CB-CG-CD2	-5.41	124.17	131.20
5	H	191	HIS	CA-C-N	5.39	126.58	119.84
5	H	191	HIS	C-N-CA	5.39	126.58	119.84
2	G	111	ASP	CA-CB-CG	-5.37	107.23	112.60
3	E	552	LYS	N-CA-C	5.37	122.23	110.80
3	E	468	GLU	CA-C-N	5.37	127.47	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	468	GLU	C-N-CA	5.37	127.47	120.28
3	E	291	LYS	CG-CD-CE	-5.35	99.00	111.30
3	I	529	ILE	CA-C-N	5.34	125.34	119.89
3	I	529	ILE	C-N-CA	5.34	125.34	119.89
3	E	45	LEU	N-CA-C	5.34	118.25	111.69
4	S	62	SER	CA-C-N	5.33	127.42	120.28
4	S	62	SER	C-N-CA	5.33	127.42	120.28
1	D	88	LEU	N-CA-C	5.33	117.17	110.24
3	I	461	LEU	CA-C-N	5.33	127.85	120.29
3	I	461	LEU	C-N-CA	5.33	127.85	120.29
2	J	110	LEU	N-CA-CB	-5.32	102.28	110.20
3	I	427	ASP	CA-CB-CG	5.31	117.91	112.60
3	I	522	ALA	CA-C-N	5.31	126.76	120.23
3	I	522	ALA	C-N-CA	5.31	126.76	120.23
3	I	463	GLN	OE1-CD-NE2	-5.30	117.30	122.60
2	G	60	VAL	N-CA-C	5.30	116.53	109.37
3	I	582	MET	N-CA-C	-5.29	105.40	111.07
3	I	156	GLN	OE1-CD-NE2	-5.29	117.31	122.60
3	I	612	LYS	CB-CG-CD	-5.29	99.14	111.30
3	E	531	GLN	OE1-CD-NE2	-5.28	117.33	122.60
3	I	9	ASP	CA-CB-CG	-5.27	107.33	112.60
3	E	227	LEU	CB-CA-C	-5.27	101.89	110.85
3	E	91	TRP	N-CA-C	-5.27	104.96	111.33
3	I	276	GLN	OE1-CD-NE2	-5.24	117.36	122.60
3	I	245	ASP	CA-CB-CG	5.23	117.83	112.60
4	R	39	VAL	N-CA-C	5.23	118.45	111.44
2	G	63	ARG	NE-CZ-NH2	5.23	123.91	119.20
3	E	195	LYS	CA-C-O	5.23	126.51	120.60
3	E	615	LYS	CB-CG-CD	5.22	123.31	111.30
2	J	61	ASN	OD1-CG-ND2	-5.20	117.40	122.60
3	I	68	HIS	CA-CB-CG	5.20	119.00	113.80
1	F	8	ARG	NE-CZ-NH2	5.20	123.88	119.20
4	R	40	ASP	N-CA-C	5.19	116.68	109.31
3	I	462	LYS	CB-CG-CD	-5.18	99.38	111.30
4	R	104	GLN	OE1-CD-NE2	-5.18	117.42	122.60
3	E	621	LYS	CA-CB-CG	-5.17	103.75	114.10
1	F	10	HIS	CA-CB-CG	-5.17	108.62	113.80
3	I	310	HIS	CB-CG-CD2	-5.17	124.47	131.20
3	I	513	GLN	OE1-CD-NE2	-5.17	117.43	122.60
3	E	540	PHE	CA-CB-CG	-5.16	108.64	113.80
3	I	497	GLN	OE1-CD-NE2	-5.15	117.45	122.60
3	I	465	CYS	CA-CB-SG	-5.14	102.57	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	46	ARG	N-CA-C	5.14	118.34	111.24
3	E	320	HIS	CB-CG-CD2	-5.14	124.52	131.20
3	E	379	ARG	CB-CG-CD	-5.14	99.48	111.30
3	I	318	HIS	CB-CG-CD2	-5.14	124.52	131.20
3	I	171	ARG	NE-CZ-NH2	5.13	123.82	119.20
2	J	58	ASN	OD1-CG-ND2	-5.13	117.47	122.60
3	I	255	HIS	CB-CG-CD2	-5.12	124.54	131.20
3	I	432	GLN	OE1-CD-NE2	-5.12	117.47	122.60
3	E	597	LYS	CG-CD-CE	-5.12	99.54	111.30
3	I	252	LYS	CB-CA-C	-5.11	102.16	110.85
1	D	29	ARG	NE-CZ-NH2	5.11	123.80	119.20
3	E	551	ARG	CB-CA-C	5.11	117.52	110.16
3	I	264	HIS	CB-CG-CD2	-5.11	124.56	131.20
2	J	58	ASN	CA-CB-CG	5.10	117.70	112.60
2	G	29	PHE	CA-CB-CG	-5.09	108.71	113.80
2	G	33	ARG	NE-CZ-NH2	5.09	123.78	119.20
3	I	106	ARG	NE-CZ-NH2	5.09	123.78	119.20
4	R	32	LEU	CA-C-O	-5.09	113.63	119.78
3	I	36	ASN	CA-CB-CG	5.08	117.68	112.60
3	I	100	TYR	CA-C-N	5.08	127.04	120.44
3	I	100	TYR	C-N-CA	5.08	127.04	120.44
3	I	287	ARG	NE-CZ-NH2	5.07	123.77	119.20
5	C	194	VAL	CA-C-N	5.07	127.08	120.28
5	C	194	VAL	C-N-CA	5.07	127.08	120.28
3	E	310	HIS	CB-CG-CD2	-5.07	124.61	131.20
3	I	70	ARG	NE-CZ-NH2	5.06	123.76	119.20
3	I	249	ARG	CD-NE-CZ	5.06	131.48	124.40
3	E	36	ASN	CA-C-N	5.06	128.47	120.89
3	E	36	ASN	C-N-CA	5.06	128.47	120.89
4	R	27	TRP	CB-CG-CD2	5.05	133.87	126.80
5	H	200	ARG	NE-CZ-NH2	5.05	123.75	119.20
4	S	32	LEU	CA-C-O	-5.04	113.71	119.41
4	S	22	PHE	N-CA-C	-5.03	100.08	110.80
1	F	33	GLY	CA-C-N	5.03	131.03	121.97
1	F	33	GLY	C-N-CA	5.03	131.03	121.97
3	I	249	ARG	NE-CZ-NH2	5.03	123.72	119.20
3	E	612	LYS	CB-CG-CD	-5.02	99.75	111.30
5	H	171	LYS	CA-C-N	5.02	126.11	119.84
5	H	171	LYS	C-N-CA	5.02	126.11	119.84
3	I	291	LYS	CA-CB-CG	-5.02	104.07	114.10
1	F	9	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	D	75	VAL	N-CA-C	-5.01	99.95	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	170	VAL	N-CA-C	5.01	115.50	108.89
3	E	474	HIS	CB-CG-CD2	-5.01	124.69	131.20
4	S	72	TRP	CA-CB-CG	5.01	123.11	113.60
5	H	107	ARG	NE-CZ-NH2	5.00	123.70	119.20
5	C	191	HIS	ND1-CE1-NE2	5.00	113.40	108.40

There are no chirality outliers.

All (71) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	C	187	ASP	Sidechain
5	C	82	ARG	Sidechain
1	D	68	ARG	Sidechain
1	D	8	ARG	Sidechain
3	E	100	TYR	Sidechain
3	E	103	CYS	Mainchain
3	E	105	TYR	Sidechain
3	E	107	TYR	Sidechain
3	E	127	TYR	Sidechain
3	E	148	ARG	Sidechain
3	E	218	TYR	Sidechain
3	E	249	ARG	Sidechain
3	E	264	HIS	Sidechain
3	E	274	HIS	Sidechain
3	E	287	ARG	Sidechain
3	E	29	TYR	Sidechain
3	E	298	TYR	Sidechain
3	E	32	ARG	Sidechain
3	E	325	ARG	Sidechain
3	E	379	ARG	Sidechain
3	E	38	ARG	Sidechain
3	E	43	TYR	Sidechain
3	E	467	TYR	Sidechain
3	E	469	PHE	Sidechain
3	E	474	HIS	Sidechain
3	E	49	TYR	Sidechain
3	E	510	TYR	Sidechain
3	E	558	TYR	Sidechain
3	E	64	PHE	Sidechain
3	E	87	TYR	Sidechain
3	E	90	TYR	Sidechain
3	E	94	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	F	62	PHE	Sidechain
1	F	9	ARG	Sidechain
5	H	182	ARG	Sidechain
3	I	100	TYR	Sidechain
3	I	103	CYS	Mainchain
3	I	105	TYR	Sidechain
3	I	107	TYR	Sidechain
3	I	115	LYS	Mainchain
3	I	125	TYR	Sidechain
3	I	127	TYR	Sidechain
3	I	148	ARG	Sidechain
3	I	218	TYR	Sidechain
3	I	219	TYR	Sidechain
3	I	264	HIS	Sidechain
3	I	29	TYR	Sidechain
3	I	302	ARG	Sidechain
3	I	32	ARG	Sidechain
3	I	325	ARG	Sidechain
3	I	379	ARG	Sidechain
3	I	38	ARG	Sidechain
3	I	43	TYR	Sidechain
3	I	469	PHE	Sidechain
3	I	474	HIS	Sidechain
3	I	510	TYR	Sidechain
3	I	544	TYR	Sidechain
3	I	558	TYR	Sidechain
3	I	580	TYR	Sidechain
3	I	64	PHE	Sidechain
3	I	68	HIS	Sidechain
3	I	87	TYR	Sidechain
3	I	90	TYR	Sidechain
3	I	92	GLU	Sidechain
3	I	94	TYR	Sidechain
2	J	18	TYR	Sidechain
4	R	61	ALA	Mainchain
4	R	82	HIS	Sidechain
4	R	86	ARG	Sidechain
4	S	22	PHE	Mainchain
4	S	91	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	D	791	794	791	37	0
1	F	791	794	791	57	0
2	G	662	660	656	56	0
2	J	662	660	656	57	0
3	E	5371	5337	5335	149	0
3	I	5371	5337	5335	151	0
4	R	737	694	692	13	0
4	S	737	694	692	22	0
5	C	1147	1152	1148	6	0
5	H	1147	1152	1148	12	0
6	C	82	82	0	0	0
All	All	17498	17356	17244	438	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 13.

All (438) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:44:ALA:HB2	3:E:106:ARG:HB3	1.37	1.07
2:J:44:ALA:HB2	3:I:106:ARG:HB3	1.35	1.06
1:D:62:PHE:CZ	1:D:75:VAL:HG22	2.11	0.86
3:I:395:CYS:SG	3:I:457:MET:HE2	2.20	0.81
1:F:15:PHE:HB2	2:J:31:VAL:HG12	1.62	0.81
1:F:62:PHE:CZ	1:F:75:VAL:HG22	2.16	0.80
2:G:44:ALA:HA	3:E:103:CYS:C	2.08	0.79
3:E:395:CYS:SG	3:E:457:MET:HE2	2.22	0.79
3:E:227:LEU:HD22	3:E:277:PHE:CD1	2.18	0.78
2:J:44:ALA:HA	3:I:103:CYS:C	2.11	0.76
3:I:418:PHE:CE1	3:I:457:MET:HE1	2.20	0.76
3:E:7:VAL:HA	3:E:48:ALA:HB1	1.70	0.74
2:J:41:THR:O	2:J:44:ALA:HB3	1.87	0.73
1:F:34:ILE:HD11	2:J:18:TYR:CE2	2.23	0.73
3:E:418:PHE:CD1	3:E:457:MET:HE1	2.23	0.72
3:I:428:LYS:HE2	3:I:465:CYS:SG	2.30	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:41:THR:O	2:G:44:ALA:HB3	1.88	0.72
3:I:418:PHE:CD1	3:I:457:MET:HE1	2.25	0.71
2:G:104:LEU:HA	5:H:162:CYS:SG	2.30	0.71
3:I:7:VAL:HA	3:I:48:ALA:HB1	1.73	0.70
3:E:24:VAL:HG22	3:E:97:GLY:HA2	1.73	0.70
2:G:44:ALA:HB2	3:E:106:ARG:CB	2.20	0.69
2:G:98:GLU:H	2:G:98:GLU:CD	2.00	0.69
2:J:44:ALA:HB2	3:I:106:ARG:CB	2.20	0.69
2:G:92:GLU:HB2	5:H:81:PRO:HG3	1.74	0.68
3:I:180:VAL:O	3:I:184:VAL:HG23	1.94	0.68
3:E:468:GLU:HG3	3:E:469:PHE:H	1.58	0.68
1:F:34:ILE:HG23	2:J:30:ILE:HG21	1.74	0.68
3:I:578:THR:HG21	3:I:657:MET:HB2	1.76	0.67
3:E:391:LEU:HD13	3:E:425:ILE:HD11	1.76	0.67
3:I:24:VAL:HG22	3:I:97:GLY:HA2	1.77	0.67
3:E:622:MET:SD	3:E:653:ILE:HD11	2.35	0.66
3:E:17:LEU:HD11	3:E:104:LEU:HD21	1.78	0.65
3:E:22:LYS:HE3	3:E:64:PHE:CD1	2.32	0.65
3:I:22:LYS:HE3	3:I:64:PHE:CD1	2.32	0.64
1:F:4:PHE:CD1	2:J:78:THR:CG2	2.81	0.64
3:I:148:ARG:HA	3:I:152:VAL:HG23	1.80	0.64
3:I:17:LEU:HD11	3:I:104:LEU:HD21	1.79	0.63
2:G:104:LEU:HB2	5:H:162:CYS:HB3	1.81	0.63
2:G:109:PHE:CD1	3:E:47:VAL:HG13	2.34	0.63
1:D:34:ILE:CG2	2:G:30:ILE:HG21	2.29	0.62
3:E:537:VAL:HG13	4:R:31:ALA:CB	2.29	0.62
1:D:34:ILE:HD11	2:G:18:TYR:CZ	2.33	0.62
3:E:180:VAL:O	3:E:184:VAL:HG23	2.00	0.62
3:E:45:LEU:HD23	3:E:46:CYS:HA	1.82	0.62
3:E:418:PHE:CE1	3:E:457:MET:HE1	2.35	0.62
1:F:35:LEU:HD13	1:F:79:PHE:CZ	2.36	0.61
2:G:44:ALA:HB1	3:E:104:LEU:O	2.01	0.61
1:F:4:PHE:CD1	2:J:78:THR:HG22	2.36	0.61
1:F:69:PRO:CB	2:J:79:TYR:HA	2.30	0.61
1:F:34:ILE:HD11	2:J:18:TYR:CD2	2.35	0.61
3:I:391:LEU:HD13	3:I:425:ILE:HD11	1.81	0.61
1:F:12:THR:HG21	1:F:35:LEU:HD11	1.82	0.60
3:E:10:PHE:HA	3:E:45:LEU:CD1	2.31	0.60
3:E:52:PRO:HD3	5:H:181:VAL:CG1	2.31	0.60
1:F:6:MET:HG2	1:F:15:PHE:CE1	2.35	0.60
2:J:44:ALA:HB1	3:I:104:LEU:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:87:TYR:CD1	3:E:87:TYR:C	2.80	0.60
2:J:17:MET:HE3	2:J:18:TYR:H	1.67	0.60
2:J:98:GLU:H	2:J:98:GLU:CD	2.10	0.59
3:I:605:MET:HE2	3:I:610:LEU:HA	1.83	0.59
1:F:14:ILE:HG21	1:F:34:ILE:HD13	1.84	0.59
3:I:10:PHE:HA	3:I:45:LEU:CD1	2.33	0.59
2:J:44:ALA:HA	3:I:103:CYS:O	2.01	0.59
3:E:14:TRP:CH2	3:E:61:THR:HA	2.39	0.58
3:I:468:GLU:HA	4:S:63:ALA:HB2	1.85	0.58
3:I:20:THR:HB	3:I:29:TYR:CE1	2.39	0.58
1:D:4:PHE:CD1	2:G:78:THR:HG22	2.38	0.58
3:E:52:PRO:HD3	5:H:181:VAL:HG12	1.85	0.58
1:F:34:ILE:CG1	2:J:18:TYR:CG	2.87	0.57
3:E:580:TYR:CD2	3:E:657:MET:HE3	2.39	0.57
3:I:45:LEU:HD23	3:I:46:CYS:HA	1.86	0.57
3:I:428:LYS:HB3	3:I:469:PHE:CD1	2.38	0.57
2:J:45:MET:HG2	3:I:39:PHE:CD2	2.40	0.57
3:I:622:MET:SD	3:I:653:ILE:HD11	2.44	0.57
3:E:444:ILE:HD11	3:E:519:LEU:HD11	1.87	0.56
3:I:428:LYS:HE2	3:I:465:CYS:HG	1.69	0.56
3:I:532:GLU:HG3	4:S:24:VAL:HG22	1.87	0.56
3:I:87:TYR:CD1	3:I:159:LEU:HD21	2.41	0.56
2:G:44:ALA:CA	3:E:103:CYS:C	2.78	0.56
3:I:10:PHE:CZ	3:I:14:TRP:CD1	2.94	0.56
1:F:15:PHE:CG	2:J:74:CYS:HB3	2.40	0.56
3:I:22:LYS:HE3	3:I:64:PHE:CE1	2.41	0.56
3:E:422:PHE:CE2	3:E:465:CYS:SG	2.98	0.55
3:E:227:LEU:HD23	3:E:235:TYR:CE1	2.42	0.55
2:G:44:ALA:HA	3:E:103:CYS:O	2.05	0.55
1:D:69:PRO:CB	2:G:79:TYR:HA	2.37	0.55
3:E:29:TYR:HA	3:E:33:ALA:HB3	1.89	0.55
1:F:69:PRO:HB3	2:J:79:TYR:HA	1.89	0.55
3:I:537:VAL:HG13	4:S:31:ALA:HB1	1.89	0.55
1:D:62:PHE:CE1	1:D:75:VAL:HG22	2.42	0.55
3:I:532:GLU:CG	4:S:24:VAL:HG22	2.37	0.54
3:I:555:TRP:CD2	3:I:557:HIS:CD2	2.95	0.54
1:F:69:PRO:HG3	2:J:82:ARG:HG2	1.89	0.54
2:G:107:ALA:CB	5:H:158:LEU:HG	2.37	0.54
3:I:332:GLN:HA	3:I:335:MET:HG2	1.88	0.54
3:E:13:THR:HG23	3:E:42:ILE:HA	1.90	0.54
3:I:118:LEU:H	3:I:130:VAL:HG11	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:13:THR:HG23	3:I:42:ILE:HA	1.89	0.54
1:D:34:ILE:HG12	2:G:18:TYR:CD1	2.43	0.54
1:F:4:PHE:CZ	2:J:82:ARG:HB2	2.43	0.54
3:E:20:THR:HB	3:E:29:TYR:CE1	2.42	0.53
3:E:580:TYR:CD2	3:E:605:MET:HE3	2.42	0.53
4:R:68:CYS:SG	4:R:80:HIS:HB3	2.48	0.53
2:J:18:TYR:CE2	2:J:32:LYS:HG3	2.43	0.53
3:I:45:LEU:HD23	3:I:45:LEU:C	2.33	0.53
3:I:640:LEU:CD2	4:S:22:PHE:CD2	2.91	0.53
1:F:7:ILE:HB	1:F:14:ILE:HB	1.91	0.53
3:I:97:GLY:C	3:I:101:MET:HE3	2.34	0.53
1:D:69:PRO:HG2	2:G:83:TYR:CE2	2.43	0.53
3:E:578:THR:HG21	3:E:655:THR:OG1	2.09	0.53
3:I:468:GLU:CA	4:S:63:ALA:HB2	2.39	0.53
1:F:14:ILE:CG2	1:F:34:ILE:HD13	2.38	0.53
1:F:69:PRO:HB2	2:J:79:TYR:HA	1.90	0.53
3:I:523:PRO:HB3	3:I:555:TRP:CE3	2.44	0.53
2:G:107:ALA:HB2	5:H:158:LEU:HG	1.90	0.53
2:J:44:ALA:CA	3:I:103:CYS:O	2.57	0.53
3:I:537:VAL:HG13	4:S:31:ALA:CB	2.38	0.53
2:J:44:ALA:CA	3:I:103:CYS:C	2.82	0.52
2:G:45:MET:HG2	3:E:39:PHE:CD2	2.43	0.52
3:E:227:LEU:HD21	3:E:274:HIS:HB3	1.92	0.52
1:F:35:LEU:HG	2:J:30:ILE:HD13	1.91	0.52
3:I:147:TRP:CE2	3:I:151:MET:HG3	2.45	0.52
3:E:232:CYS:SG	3:E:297:MET:HE1	2.49	0.52
3:E:480:MET:HA	3:E:480:MET:HE2	1.91	0.52
3:E:511:VAL:HG11	3:E:544:TYR:CZ	2.45	0.52
3:I:87:TYR:CD1	3:I:87:TYR:C	2.87	0.52
3:E:114:LYS:HE3	3:E:138:GLU:HG3	1.92	0.52
1:D:69:PRO:HB2	2:G:79:TYR:HA	1.91	0.52
3:E:10:PHE:CZ	3:E:14:TRP:CD1	2.98	0.52
1:D:4:PHE:CE2	1:D:69:PRO:HG3	2.45	0.51
3:E:48:ALA:HB3	3:E:51:GLU:O	2.11	0.51
2:J:109:PHE:CD1	3:I:47:VAL:HG13	2.45	0.51
3:E:45:LEU:HD23	3:E:45:LEU:C	2.35	0.51
3:E:435:TYR:CD2	3:E:473:LEU:HD13	2.46	0.51
1:F:2:ASP:HB2	1:F:4:PHE:CZ	2.46	0.51
2:J:72:LYS:HE2	2:J:75:MET:SD	2.50	0.51
3:E:13:THR:HG21	3:E:45:LEU:HD13	1.92	0.51
1:F:4:PHE:CD1	1:F:17:ASP:HB3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:580:TYR:CD2	3:I:605:MET:HE3	2.46	0.51
1:D:4:PHE:CE1	1:D:17:ASP:HB3	2.45	0.51
3:E:468:GLU:HG2	4:R:63:ALA:HA	1.92	0.51
1:D:4:PHE:CD1	2:G:78:THR:CG2	2.94	0.51
1:F:14:ILE:CD1	1:F:31:VAL:HG22	2.41	0.51
1:F:14:ILE:HD12	1:F:31:VAL:HG22	1.94	0.50
3:I:34:THR:HA	3:I:38:ARG:HB3	1.94	0.50
3:I:468:GLU:N	4:S:63:ALA:HB2	2.26	0.50
3:E:148:ARG:HA	3:E:152:VAL:HG23	1.93	0.50
3:E:38:ARG:HA	3:E:38:ARG:NH2	2.26	0.50
3:I:527:PHE:CZ	3:I:530:PRO:HD3	2.47	0.50
3:E:418:PHE:CD1	3:E:418:PHE:C	2.90	0.50
3:E:4:LYS:HE2	3:E:49:TYR:CE2	2.46	0.50
3:E:227:LEU:HD11	3:E:274:HIS:HB3	1.94	0.50
1:F:34:ILE:HG23	2:J:30:ILE:CG2	2.40	0.50
2:J:92:GLU:HB2	5:C:81:PRO:HG3	1.93	0.50
1:D:70:GLN:HB3	2:G:79:TYR:CD1	2.47	0.50
3:E:76:VAL:CG1	3:E:83:VAL:HA	2.42	0.50
3:E:97:GLY:C	3:E:101:MET:HE3	2.36	0.50
3:E:21:ILE:CG2	3:E:101:MET:HE2	2.41	0.50
3:E:46:CYS:HB2	3:E:107:TYR:CE1	2.47	0.50
2:G:44:ALA:CA	3:E:103:CYS:O	2.60	0.49
2:G:109:PHE:CE1	3:E:47:VAL:HG13	2.47	0.49
1:F:72:PRO:CD	2:J:75:MET:HG2	2.42	0.49
3:I:21:ILE:CG2	3:I:101:MET:HE2	2.41	0.49
1:D:5:LEU:HB3	1:D:75:VAL:HG23	1.95	0.49
3:E:351:VAL:HG22	3:E:365:MET:HE1	1.95	0.49
3:E:537:VAL:HG22	4:R:31:ALA:HB2	1.95	0.49
1:F:34:ILE:HG12	2:J:18:TYR:CG	2.48	0.49
3:I:115:LYS:C	5:C:183:SER:CB	2.85	0.49
3:I:640:LEU:HD23	4:S:22:PHE:CE2	2.48	0.49
3:I:29:TYR:HA	3:I:33:ALA:HB3	1.94	0.49
3:I:160:ILE:HD11	3:I:206:ILE:HG23	1.95	0.49
3:I:544:TYR:CE1	3:I:548:PHE:CD1	3.01	0.49
3:I:537:VAL:HG22	4:S:31:ALA:CB	2.43	0.49
3:E:211:PHE:CE2	3:E:254:LEU:HD11	2.47	0.49
1:D:4:PHE:CD1	1:D:17:ASP:HB3	2.48	0.49
1:D:80:ARG:HD3	1:D:85:PHE:CE1	2.48	0.49
3:E:29:TYR:CD1	3:E:29:TYR:C	2.90	0.48
1:D:45:TYR:HA	1:D:49:GLN:O	2.14	0.48
2:G:111:ASP:CB	3:E:111:GLN:HE22	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:76:VAL:CG1	3:I:83:VAL:HA	2.42	0.48
3:I:555:TRP:CZ3	3:I:557:HIS:HB2	2.49	0.48
3:E:147:TRP:CZ2	3:E:151:MET:SD	3.07	0.48
1:F:24:VAL:HG21	1:F:51:LEU:HB3	1.95	0.48
1:D:4:PHE:N	1:D:4:PHE:CD2	2.81	0.48
2:G:17:MET:HE3	2:G:18:TYR:H	1.78	0.48
2:G:44:ALA:HB1	3:E:103:CYS:O	2.14	0.48
3:E:91:TRP:HA	3:E:147:TRP:CE2	2.49	0.48
3:I:422:PHE:CD1	3:I:425:ILE:HD12	2.49	0.48
3:I:14:TRP:CH2	3:I:61:THR:HA	2.49	0.48
3:E:227:LEU:HD23	3:E:235:TYR:CD1	2.49	0.48
2:J:76:TYR:CG	5:C:158:LEU:HD13	2.49	0.48
1:F:4:PHE:HB3	2:J:78:THR:HG21	1.95	0.48
3:I:10:PHE:CD1	3:I:10:PHE:C	2.92	0.48
3:E:245:ASP:HB3	3:E:249:ARG:HH12	1.78	0.47
1:F:45:TYR:HA	1:F:49:GLN:O	2.13	0.47
2:G:44:ALA:CB	3:E:103:CYS:O	2.62	0.47
3:E:10:PHE:C	3:E:10:PHE:CD1	2.92	0.47
1:F:2:ASP:CB	1:F:4:PHE:CZ	2.98	0.47
1:D:34:ILE:HG23	2:G:30:ILE:HG21	1.95	0.47
2:G:32:LYS:HB3	2:G:34:GLU:CD	2.39	0.47
2:G:111:ASP:HB2	3:E:111:GLN:HE22	1.80	0.47
3:E:13:THR:HG23	3:E:42:ILE:CG1	2.44	0.47
1:F:37:ARG:HH21	1:F:41:GLU:CD	2.22	0.47
1:F:45:TYR:CG	1:F:88:LEU:HD22	2.49	0.47
3:I:17:LEU:HD21	3:I:104:LEU:HD21	1.95	0.47
3:I:84:LEU:O	3:I:184:VAL:HG22	2.14	0.47
1:D:46:LYS:HA	1:D:62:PHE:CZ	2.50	0.47
3:E:22:LYS:HE3	3:E:64:PHE:CE1	2.50	0.47
3:I:38:ARG:HA	3:I:38:ARG:NH2	2.29	0.47
3:I:435:TYR:CD2	3:I:473:LEU:HD13	2.50	0.47
1:F:14:ILE:HD13	1:F:34:ILE:HG21	1.97	0.47
1:F:15:PHE:CG	2:J:74:CYS:CB	2.98	0.47
1:F:46:LYS:HB2	1:F:51:LEU:HD21	1.97	0.46
2:J:44:ALA:HB1	3:I:103:CYS:O	2.15	0.46
4:S:72:TRP:CE3	4:S:105:LYS:HE3	2.50	0.46
4:S:72:TRP:CG	4:S:78:ALA:HB2	2.51	0.46
2:J:44:ALA:CB	3:I:103:CYS:O	2.63	0.46
3:I:102:ASP:CG	3:I:140:GLY:H	2.24	0.46
5:C:84:VAL:HG22	5:C:128:LEU:HD13	1.98	0.46
3:E:469:PHE:C	3:E:469:PHE:CD2	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:45:TYR:CD2	1:F:88:LEU:HD22	2.50	0.46
2:J:62:PHE:HA	3:I:43:TYR:CZ	2.51	0.46
1:D:11:LYS:HE2	2:G:27:HIS:CG	2.51	0.46
3:E:91:TRP:CZ3	3:E:144:LEU:HD22	2.50	0.46
3:E:171:ARG:HB3	3:E:218:TYR:CE2	2.50	0.46
3:I:115:LYS:O	5:C:183:SER:HB3	2.15	0.46
3:I:64:PHE:CE1	3:I:68:HIS:HB2	2.51	0.46
3:E:87:TYR:CD1	3:E:159:LEU:HD21	2.51	0.46
2:J:20:LYS:CE	2:J:30:ILE:HD11	2.45	0.46
3:I:529:ILE:HG22	3:I:533:LEU:HB2	1.98	0.46
3:I:616:SER:HB2	3:I:655:THR:CG2	2.46	0.46
3:E:160:ILE:HD11	3:E:206:ILE:HG23	1.98	0.46
3:I:530:PRO:HG3	3:I:583:ALA:CB	2.46	0.46
1:D:34:ILE:HG12	2:G:18:TYR:CG	2.51	0.46
1:F:8:ARG:HH22	1:F:92:PRO:HA	1.81	0.46
3:I:529:ILE:HG21	3:I:537:VAL:HG21	1.96	0.46
3:I:13:THR:HG21	3:I:45:LEU:HD13	1.98	0.45
3:I:46:CYS:SG	3:I:108:LEU:HD13	2.56	0.45
3:E:17:LEU:HD21	3:E:104:LEU:HD21	1.98	0.45
4:R:35:TRP:CD1	4:R:35:TRP:C	2.93	0.45
1:F:12:THR:CG2	1:F:35:LEU:HD11	2.46	0.45
1:F:30:ILE:HG23	2:J:18:TYR:CZ	2.51	0.45
2:J:109:PHE:CE1	3:I:47:VAL:HG13	2.52	0.45
2:G:104:LEU:CB	5:H:162:CYS:HB3	2.46	0.45
3:I:72:LEU:HD23	3:I:75:ARG:CZ	2.46	0.45
3:E:34:THR:HA	3:E:38:ARG:HB3	1.97	0.45
3:E:332:GLN:HA	3:E:335:MET:HG2	1.99	0.45
3:E:581:GLN:NE2	3:E:655:THR:HG23	2.31	0.45
1:F:6:MET:HG2	1:F:15:PHE:CZ	2.51	0.45
2:J:17:MET:C	2:J:18:TYR:CD1	2.95	0.45
3:E:39:PHE:CE1	3:E:104:LEU:O	2.69	0.45
3:E:52:PRO:CD	5:H:181:VAL:HG12	2.45	0.45
1:F:80:ARG:HB2	1:F:85:PHE:CE1	2.52	0.45
4:R:53:CYS:HB3	4:R:80:HIS:CB	2.47	0.45
3:I:115:LYS:O	5:C:183:SER:CB	2.65	0.45
3:I:418:PHE:CE1	3:I:457:MET:CE	2.97	0.45
3:I:537:VAL:HG22	4:S:31:ALA:HB3	1.97	0.45
1:D:2:ASP:HB3	1:D:4:PHE:CZ	2.52	0.45
3:I:46:CYS:HB2	3:I:107:TYR:CE1	2.52	0.45
1:F:48:ASP:OD1	1:F:90:ILE:HD12	2.17	0.45
3:I:42:ILE:CD1	3:I:46:CYS:SG	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:440:ALA:HA	3:I:517:TRP:CZ3	2.52	0.45
3:I:560:CYS:SG	4:S:30:VAL:HB	2.57	0.45
1:F:46:LYS:HA	1:F:62:PHE:CZ	2.52	0.45
2:J:111:ASP:CB	3:I:111:GLN:HE22	2.30	0.45
3:I:18:LEU:HD11	3:I:22:LYS:HE3	1.99	0.45
3:I:88:HIS:CE1	3:I:183:GLY:HA3	2.51	0.45
1:D:34:ILE:HD11	2:G:18:TYR:CE2	2.52	0.44
3:E:21:ILE:O	3:E:21:ILE:HG22	2.17	0.44
3:I:13:THR:HG23	3:I:42:ILE:CG1	2.47	0.44
3:I:577:VAL:HG12	3:I:653:ILE:HD12	1.98	0.44
3:E:18:LEU:HD11	3:E:22:LYS:HE3	1.99	0.44
3:E:87:TYR:CE2	3:E:152:VAL:HG22	2.52	0.44
3:E:94:TYR:CD1	3:E:147:TRP:CE3	3.05	0.44
3:I:582:MET:HG2	3:I:586:LEU:HD11	2.00	0.44
2:J:32:LYS:HB3	2:J:34:GLU:CD	2.43	0.44
2:J:111:ASP:CG	3:I:110:THR:HG21	2.43	0.44
3:I:29:TYR:CD1	3:I:29:TYR:C	2.94	0.44
3:I:107:TYR:CD1	3:I:107:TYR:C	2.96	0.44
1:D:24:VAL:HG21	1:D:51:LEU:HB3	1.99	0.44
3:I:28:GLU:CD	3:I:28:GLU:C	2.85	0.44
3:I:443:LEU:HD22	3:I:480:MET:HG3	2.00	0.44
3:E:235:TYR:CE2	3:E:239:VAL:HG21	2.52	0.44
2:J:20:LYS:HD3	2:J:28:GLU:HB3	1.99	0.44
2:J:27:HIS:HB2	2:J:67:SER:HB3	2.00	0.44
3:I:39:PHE:CE1	3:I:104:LEU:O	2.70	0.44
3:E:577:VAL:HG12	3:E:653:ILE:HD12	1.98	0.44
1:F:4:PHE:CE1	1:F:17:ASP:HB3	2.52	0.44
3:E:533:LEU:HD13	4:R:29:ALA:CB	2.47	0.44
3:E:642:MET:SD	4:R:20:LYS:HE3	2.58	0.44
1:F:43:ARG:HD3	1:F:50:LEU:HD13	1.99	0.44
3:I:102:ASP:HB3	3:I:106:ARG:HH12	1.82	0.44
1:F:4:PHE:CE2	1:F:69:PRO:HG3	2.53	0.43
3:E:45:LEU:HD23	3:E:46:CYS:CA	2.46	0.43
3:E:264:HIS:CD2	3:E:264:HIS:C	2.96	0.43
3:I:580:TYR:O	3:I:583:ALA:HB3	2.18	0.43
3:E:17:LEU:HD11	3:E:104:LEU:CD2	2.47	0.43
3:E:455:GLU:HB2	3:E:477:TYR:CZ	2.54	0.43
3:I:21:ILE:O	3:I:21:ILE:HG22	2.18	0.43
3:I:59:THR:OG1	3:I:132:MET:HE3	2.18	0.43
3:E:148:ARG:HD2	3:E:202:PHE:CD2	2.53	0.43
3:E:167:ILE:HG12	3:E:253:TYR:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:563:GLU:O	4:S:27:TRP:CE3	2.71	0.43
3:I:642:MET:SD	4:S:20:LYS:HE3	2.58	0.43
3:E:419:ILE:HG23	3:E:464:ALA:HB2	2.00	0.43
3:I:13:THR:HG23	3:I:42:ILE:CB	2.49	0.43
3:I:147:TRP:CZ2	3:I:151:MET:HG3	2.54	0.43
3:E:46:CYS:CB	3:E:107:TYR:CE1	3.02	0.43
3:E:396:ASP:OD1	3:E:400:LYS:HE3	2.19	0.43
3:E:509:ILE:HG21	3:E:540:PHE:CE1	2.54	0.43
4:R:69:THR:HG21	4:R:108:HIS:CG	2.53	0.43
2:J:60:VAL:HA	3:I:36:ASN:HA	2.00	0.43
3:I:123:LEU:HD11	3:I:130:VAL:CG2	2.49	0.43
1:D:43:ARG:HG3	1:D:85:PHE:CE1	2.53	0.43
3:I:24:VAL:CG2	3:I:97:GLY:HA2	2.46	0.43
3:I:418:PHE:CD1	3:I:418:PHE:C	2.96	0.43
2:G:72:LYS:HE2	2:G:75:MET:SD	2.58	0.43
2:G:80:LYS:HE3	5:H:155:VAL:CG1	2.49	0.43
3:E:428:LYS:CE	3:E:465:CYS:SG	3.07	0.43
3:E:467:TYR:CD2	3:E:467:TYR:C	2.96	0.43
1:F:48:ASP:HA	1:F:88:LEU:HD21	2.01	0.43
3:E:146:MET:HE2	3:E:146:MET:HA	2.01	0.42
1:F:34:ILE:HG23	2:J:30:ILE:CB	2.49	0.42
1:F:34:ILE:HG13	2:J:18:TYR:CG	2.53	0.42
3:I:39:PHE:CZ	3:I:42:ILE:HD13	2.54	0.42
3:I:528:ALA:HB2	3:I:604:GLN:CG	2.49	0.42
3:I:544:TYR:CZ	3:I:548:PHE:CB	3.02	0.42
4:S:79:PHE:CZ	4:S:95:PRO:HD2	2.53	0.42
1:D:6:MET:SD	1:D:15:PHE:CZ	3.12	0.42
1:D:72:PRO:CD	2:G:75:MET:HG2	2.49	0.42
3:E:5:PRO:O	3:E:49:TYR:CD2	2.72	0.42
3:E:21:ILE:C	3:E:24:VAL:HB	2.43	0.42
2:J:45:MET:HG2	3:I:39:PHE:CG	2.54	0.42
3:I:555:TRP:CE2	3:I:557:HIS:HD2	2.37	0.42
2:G:20:LYS:HD3	2:G:28:GLU:HB3	2.00	0.42
3:E:68:HIS:O	3:E:72:LEU:HD12	2.19	0.42
3:E:335:MET:CB	3:E:390:LEU:HD22	2.49	0.42
3:I:586:LEU:HD21	4:S:27:TRP:NE1	2.34	0.42
3:E:51:GLU:CD	3:E:52:PRO:HD2	2.44	0.42
3:E:138:GLU:HB2	3:E:141:GLU:HG3	1.99	0.42
3:E:164:LEU:CD2	3:E:211:PHE:HA	2.50	0.42
3:E:227:LEU:HD22	3:E:277:PHE:CG	2.54	0.42
3:E:431:PHE:CD1	3:E:431:PHE:C	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:66:PRO:HD3	3:I:4:LYS:HA	2.01	0.42
2:G:60:VAL:HA	3:E:36:ASN:HA	2.02	0.42
3:E:511:VAL:HG11	3:E:544:TYR:CE2	2.54	0.42
3:I:71:HIS:CD2	3:I:75:ARG:HH21	2.38	0.42
3:I:511:VAL:HG11	3:I:544:TYR:OH	2.19	0.42
3:I:586:LEU:HD21	4:S:27:TRP:CE2	2.54	0.42
3:I:597:LYS:HE2	3:I:601:ASP:OD2	2.19	0.42
3:E:38:ARG:HA	3:E:38:ARG:HH21	1.84	0.42
1:D:4:PHE:CD2	1:D:69:PRO:HD3	2.55	0.42
1:D:69:PRO:HB3	2:G:79:TYR:HA	2.00	0.42
2:G:66:PRO:HD3	3:E:4:LYS:HA	2.01	0.42
1:F:38:PRO:HA	1:F:39:PRO:HD3	1.93	0.42
1:F:40:ASP:C	1:F:80:ARG:HH11	2.28	0.42
3:I:21:ILE:HG23	3:I:101:MET:CG	2.50	0.42
3:I:127:TYR:CD1	3:I:127:TYR:N	2.87	0.42
3:E:422:PHE:CD1	3:E:425:ILE:HD12	2.54	0.42
3:I:17:LEU:HD22	3:I:17:LEU:HA	1.89	0.42
3:I:557:HIS:CE1	4:S:31:ALA:HB2	2.55	0.42
4:S:24:VAL:HA	4:S:27:TRP:CZ2	2.55	0.42
1:D:4:PHE:HD1	2:G:78:THR:CG2	2.31	0.42
2:G:27:HIS:HB2	2:G:67:SER:HB3	2.02	0.42
3:E:533:LEU:HD11	3:E:582:MET:SD	2.59	0.42
1:F:5:LEU:HB3	1:F:75:VAL:HG23	2.00	0.42
1:F:34:ILE:HG23	2:J:30:ILE:HD13	2.02	0.42
3:E:555:TRP:CD1	3:E:555:TRP:H	2.37	0.42
3:I:69:VAL:CG2	3:I:94:TYR:CE2	3.03	0.42
2:G:101:LEU:O	2:G:105:MET:HG3	2.20	0.41
3:E:100:TYR:N	3:E:100:TYR:CD1	2.84	0.41
3:E:102:ASP:HB3	3:E:106:ARG:HH12	1.85	0.41
3:E:181:ILE:HG21	3:E:253:TYR:CD1	2.54	0.41
3:E:201:LYS:HE2	3:E:205:GLU:OE1	2.19	0.41
3:E:532:GLU:HG2	4:R:24:VAL:HG22	2.02	0.41
3:I:39:PHE:CE1	3:I:42:ILE:HG23	2.55	0.41
3:I:385:CYS:SG	3:I:388:PRO:HD2	2.60	0.41
3:E:102:ASP:CG	3:E:140:GLY:H	2.27	0.41
3:E:171:ARG:HA	3:E:249:ARG:CZ	2.50	0.41
3:E:640:LEU:CD2	4:R:22:PHE:CE2	3.04	0.41
2:G:45:MET:HG2	3:E:39:PHE:CG	2.55	0.41
3:E:24:VAL:CG2	3:E:97:GLY:HA2	2.47	0.41
2:J:45:MET:SD	2:J:60:VAL:HG11	2.60	0.41
3:I:29:TYR:O	3:I:34:THR:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:81:GLU:HA	3:I:162:MET:SD	2.60	0.41
3:I:103:CYS:O	3:I:104:LEU:C	2.63	0.41
1:D:15:PHE:CZ	2:G:74:CYS:HB2	2.55	0.41
2:G:18:TYR:CE2	2:G:32:LYS:HG3	2.55	0.41
3:E:29:TYR:O	3:E:34:THR:N	2.54	0.41
3:I:404:LYS:HE3	3:I:404:LYS:HA	2.02	0.41
1:D:2:ASP:CB	1:D:4:PHE:CZ	3.04	0.41
1:D:72:PRO:HD2	2:G:75:MET:SD	2.61	0.41
1:F:6:MET:SD	1:F:15:PHE:CZ	3.14	0.41
3:I:27:LEU:O	3:I:27:LEU:HG	2.21	0.41
3:I:45:LEU:HD23	3:I:46:CYS:N	2.36	0.41
3:I:98:ALA:N	3:I:101:MET:HE3	2.36	0.41
3:E:332:GLN:HE21	3:E:381:PRO:HD2	1.84	0.41
3:E:589:ASN:HA	4:R:22:PHE:CD1	2.56	0.41
3:I:107:TYR:CD1	3:I:111:GLN:HG2	2.56	0.41
2:G:110:LEU:C	2:G:110:LEU:HD23	2.46	0.41
3:E:72:LEU:HD23	3:E:75:ARG:CZ	2.50	0.41
3:I:105:TYR:CD2	3:I:139:ILE:HG13	2.55	0.41
3:I:547:HIS:O	3:I:548:PHE:CD1	2.73	0.41
3:E:201:LYS:CE	3:E:205:GLU:CD	2.94	0.41
2:J:63:ARG:H	2:J:63:ARG:HD2	1.86	0.41
3:I:209:SER:HB3	3:I:210:PRO:HD3	2.02	0.41
3:I:555:TRP:HE3	3:I:557:HIS:H	1.67	0.41
1:D:11:LYS:HE3	2:G:27:HIS:CE1	2.56	0.41
1:D:65:GLN:O	1:D:68:ARG:HD3	2.21	0.41
3:E:114:LYS:HE3	3:E:138:GLU:CG	2.51	0.41
3:E:428:LYS:HB3	3:E:469:PHE:CD1	2.56	0.41
1:F:62:PHE:CE1	1:F:75:VAL:HG22	2.55	0.41
3:I:20:THR:CG2	3:I:29:TYR:CD1	3.04	0.41
3:I:87:TYR:CD1	3:I:159:LEU:CD2	3.04	0.41
3:I:226:LEU:HD22	3:I:238:LYS:HD3	2.02	0.41
3:I:640:LEU:HD12	3:I:640:LEU:HA	1.93	0.41
5:H:171:LYS:HE2	5:H:173:GLU:OE2	2.20	0.41
2:G:62:PHE:HA	3:E:43:TYR:CZ	2.56	0.41
3:I:48:ALA:HB3	3:I:51:GLU:O	2.20	0.41
3:E:39:PHE:CE1	3:E:42:ILE:CG2	3.04	0.40
3:E:103:CYS:O	3:E:104:LEU:C	2.63	0.40
3:E:396:ASP:CG	3:E:400:LYS:HE3	2.47	0.40
3:I:418:PHE:CE1	3:I:422:PHE:HB2	2.56	0.40
4:S:56:CYS:HB3	4:S:65:SER:HA	2.04	0.40
2:G:104:LEU:HD12	5:H:162:CYS:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:28:GLU:CD	3:E:28:GLU:C	2.89	0.40
3:I:275:LEU:HD11	3:I:307:GLY:HA2	2.02	0.40
3:E:171:ARG:CZ	3:E:215:THR:HG23	2.51	0.40
3:E:537:VAL:HG13	4:R:31:ALA:HB1	2.03	0.40
3:E:13:THR:HG23	3:E:42:ILE:CB	2.52	0.40
3:E:13:THR:HG23	3:E:42:ILE:HG12	2.03	0.40
3:E:62:LYS:C	3:E:62:LYS:HE3	2.47	0.40
2:J:64:GLU:N	2:J:64:GLU:CD	2.79	0.40
3:I:106:ARG:HA	3:I:106:ARG:NE	2.36	0.40
1:D:4:PHE:CZ	2:G:82:ARG:HG2	2.56	0.40
3:E:418:PHE:CE1	3:E:457:MET:CE	3.04	0.40
2:J:45:MET:CE	3:I:39:PHE:HB3	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	D	95/103 (92%)	91 (96%)	4 (4%)	0	100	100
1	F	95/103 (92%)	90 (95%)	5 (5%)	0	100	100
2	G	79/95 (83%)	75 (95%)	4 (5%)	0	100	100
2	J	79/95 (83%)	75 (95%)	4 (5%)	0	100	100
3	E	653/655 (100%)	622 (95%)	29 (4%)	2 (0%)	37	73
3	I	653/655 (100%)	621 (95%)	28 (4%)	4 (1%)	22	60
4	R	87/89 (98%)	69 (79%)	15 (17%)	3 (3%)	3	21
4	S	87/89 (98%)	70 (80%)	17 (20%)	0	100	100
5	C	136/141 (96%)	126 (93%)	10 (7%)	0	100	100
5	H	136/141 (96%)	125 (92%)	10 (7%)	1 (1%)	19	57
All	All	2100/2166 (97%)	1964 (94%)	126 (6%)	10 (0%)	27	64

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	R	36	ASP
5	H	192	PRO
3	E	129	GLY
3	I	403	ALA
3	E	24	VAL
3	I	24	VAL
4	R	29	ALA
4	R	34	ALA
3	I	129	GLY
3	I	130	VAL

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	D	86/91 (94%)	85 (99%)	1 (1%)	67	79
1	F	86/91 (94%)	84 (98%)	2 (2%)	45	64
2	G	74/84 (88%)	72 (97%)	2 (3%)	40	58
2	J	74/84 (88%)	72 (97%)	2 (3%)	40	58
3	E	600/600 (100%)	571 (95%)	29 (5%)	21	43
3	I	600/600 (100%)	571 (95%)	29 (5%)	21	43
4	R	78/78 (100%)	72 (92%)	6 (8%)	10	30
4	S	78/78 (100%)	72 (92%)	6 (8%)	10	30
5	C	131/132 (99%)	130 (99%)	1 (1%)	79	85
5	H	131/132 (99%)	128 (98%)	3 (2%)	45	64
All	All	1938/1970 (98%)	1857 (96%)	81 (4%)	27	46

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	91	GLU
2	G	28	GLU

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Mol	Chain	Res	Type
2	G	110	LEU
3	E	4	LYS
3	E	5	PRO
3	E	10	PHE
3	E	17	LEU
3	E	24	VAL
3	E	28	GLU
3	E	29	TYR
3	E	30	VAL
3	E	39	PHE
3	E	42	ILE
3	E	43	TYR
3	E	62	LYS
3	E	78	GLU
3	E	81	GLU
3	E	83	VAL
3	E	87	TYR
3	E	91	TRP
3	E	107	TYR
3	E	119	THR
3	E	127	TYR
3	E	146	MET
3	E	151	MET
3	E	152	VAL
3	E	468	GLU
3	E	499	THR
3	E	510	TYR
3	E	552	LYS
3	E	555	TRP
3	E	627	SER
4	R	22	PHE
4	R	27	TRP
4	R	28	ASN
4	R	30	VAL
4	R	35	TRP
4	R	68	CYS
1	F	9	ARG
1	F	91	GLU
2	J	28	GLU
2	J	98	GLU
3	I	4	LYS
3	I	5	PRO

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Mol	Chain	Res	Type
3	I	10	PHE
3	I	17	LEU
3	I	24	VAL
3	I	28	GLU
3	I	29	TYR
3	I	39	PHE
3	I	42	ILE
3	I	43	TYR
3	I	62	LYS
3	I	78	GLU
3	I	81	GLU
3	I	83	VAL
3	I	87	TYR
3	I	91	TRP
3	I	106	ARG
3	I	107	TYR
3	I	111	GLN
3	I	119	THR
3	I	127	TYR
3	I	146	MET
3	I	152	VAL
3	I	384	VAL
3	I	404	LYS
3	I	427	ASP
3	I	499	THR
3	I	552	LYS
3	I	627	SER
4	S	22	PHE
4	S	27	TRP
4	S	28	ASN
4	S	30	VAL
4	S	32	LEU
4	S	33	TRP
5	H	133	THR
5	H	173	GLU
5	H	182	ARG
5	C	126	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	35	HIS

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Mol	Chain	Res	Type
3	E	88	HIS
3	E	133	ASN
3	E	156	GLN
3	E	178	GLN
3	E	264	HIS
3	E	313	GLN
3	E	317	ASN
3	E	332	GLN
3	E	347	HIS
3	E	567	ASN
3	E	589	ASN
4	R	41	ASN
4	R	48	HIS
2	J	85	ASN
3	I	68	HIS
3	I	82	GLN
3	I	88	HIS
3	I	264	HIS
3	I	313	GLN
3	I	347	HIS
3	I	513	GLN
3	I	557	HIS
3	I	624	ASN
5	H	132	GLN
5	H	145	GLN
5	C	110	HIS
5	C	132	GLN
5	C	174	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	A1JTC	C	301	-	77,87,87	1.00	5 (6%)	98,120,120	1.11	7 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	A1JTC	C	301	-	-	9/83/107/107	0/6/6/6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	301	A1JTC	CXA-CXB	2.84	1.51	1.48
6	C	301	A1JTC	CZ2-CGZ	2.44	1.56	1.52
6	C	301	A1JTC	CBE-CAX	2.37	1.57	1.53
6	C	301	A1JTC	CBG-CBE	2.20	1.59	1.56
6	C	301	A1JTC	CZE-CZX	2.18	1.56	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	301	A1JTC	CZO-NZS-CZ1	2.86	126.46	122.34
6	C	301	A1JTC	CZG-CZE-NAT	-2.72	108.43	111.84
6	C	301	A1JTC	CWE-CZG-CZE	2.69	115.15	109.70
6	C	301	A1JTC	CGZ-CZ2-NZ	2.41	105.64	103.08
6	C	301	A1JTC	CZE-NAT-CAV	2.16	126.38	122.03
6	C	301	A1JTC	CZ1-CZA-NZ	2.10	118.33	112.56
6	C	301	A1JTC	CZX-CZE-NAT	2.01	109.53	107.34

There are no chirality outliers.

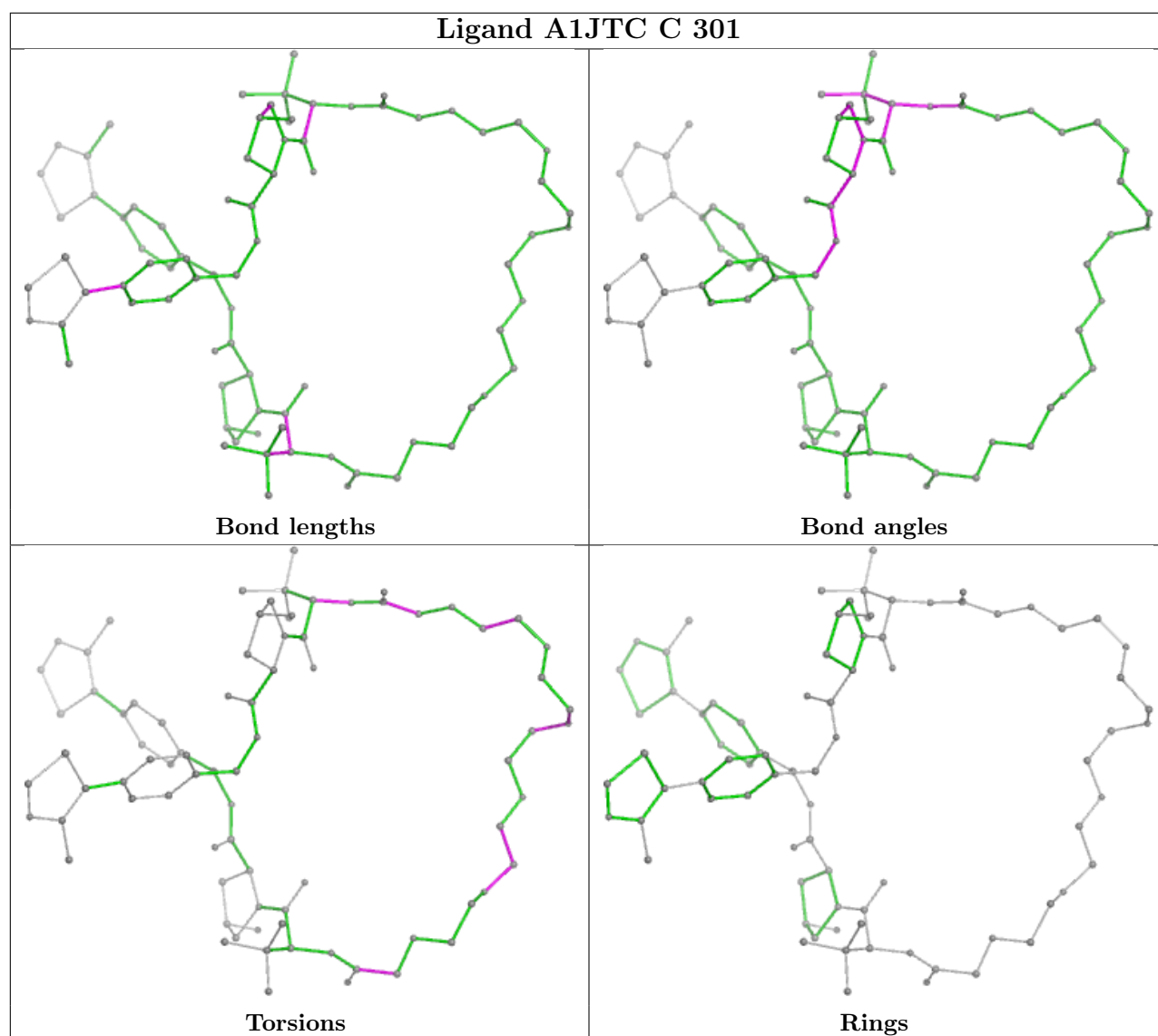
All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	301	A1JTC	C9-C8-O6-C7
6	C	301	A1JTC	O2-C4-C5-O5
6	C	301	A1JTC	N1-C1-C10-O4
6	C	301	A1JTC	O1-C1-C10-O4
6	C	301	A1JTC	OX1-CX1-CX2-O3
6	C	301	A1JTC	C6-C7-O6-C8
6	C	301	A1JTC	CZG-CZE-NAT-CAV
6	C	301	A1JTC	C5-C4-O2-C3
6	C	301	A1JTC	OX1-CAA-CAV-NAT

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

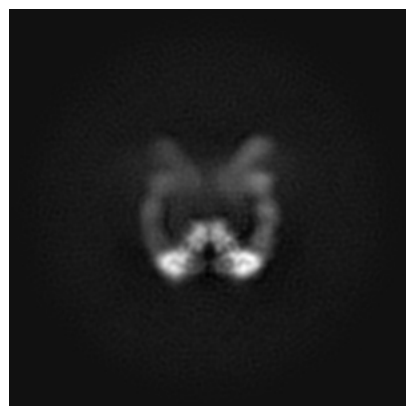
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55480. These allow visual inspection of the internal detail of the map and identification of artifacts.

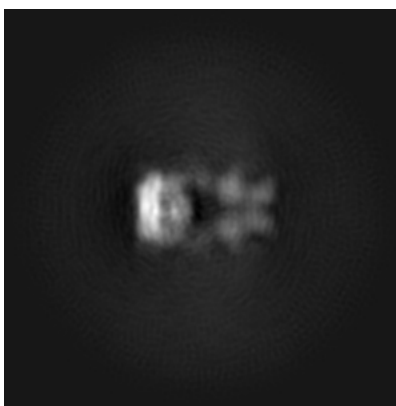
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

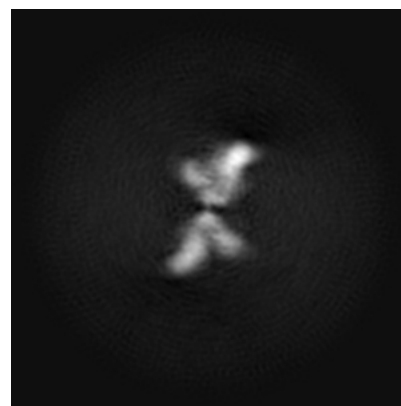
6.1.1 Primary map



X

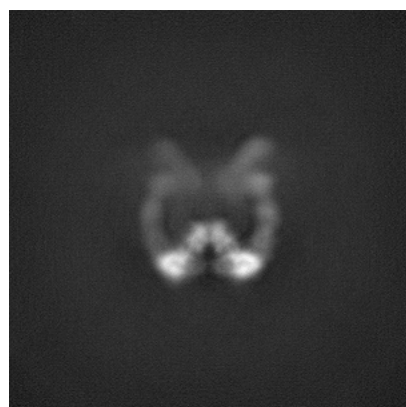


Y

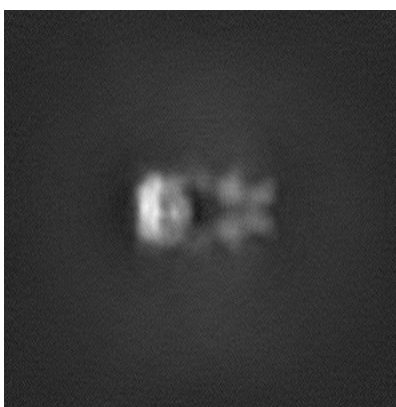


Z

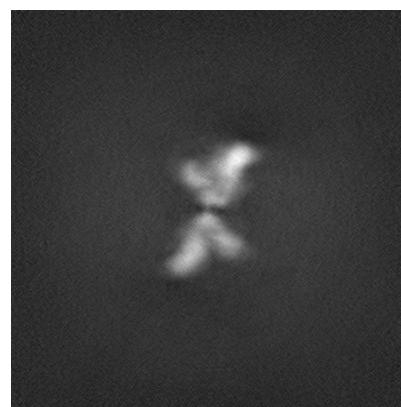
6.1.2 Raw map



X



Y

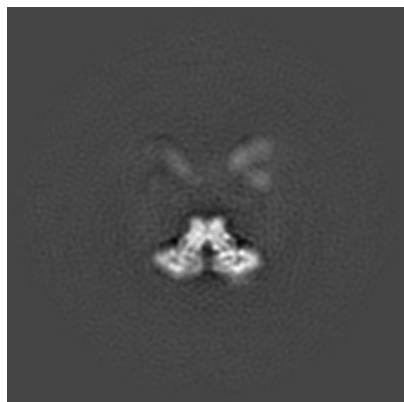


Z

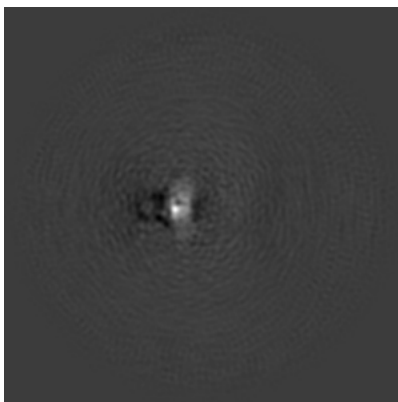
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

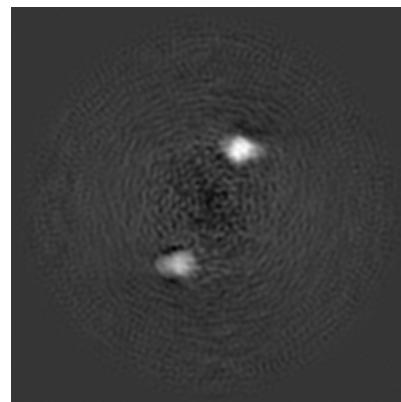
6.2.1 Primary map



X Index: 300

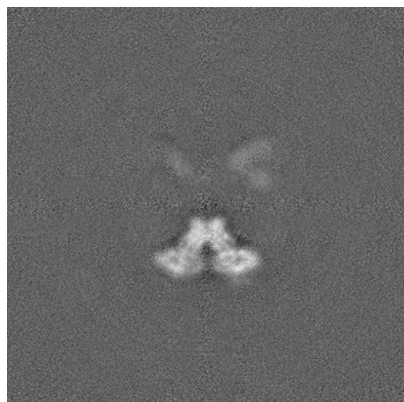


Y Index: 300

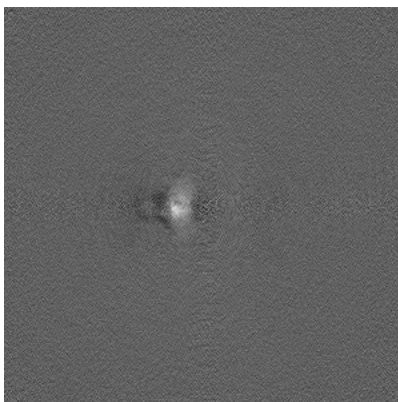


Z Index: 300

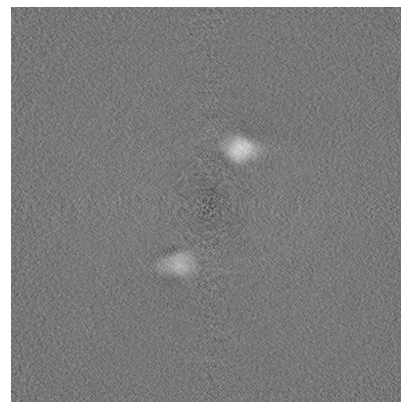
6.2.2 Raw map



X Index: 300



Y Index: 300

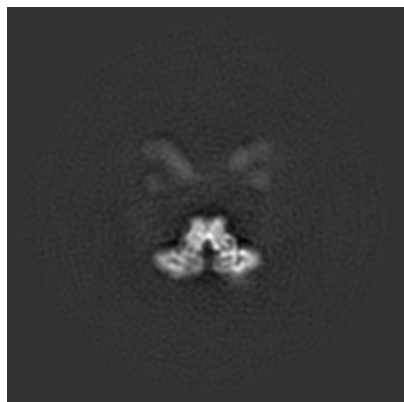


Z Index: 300

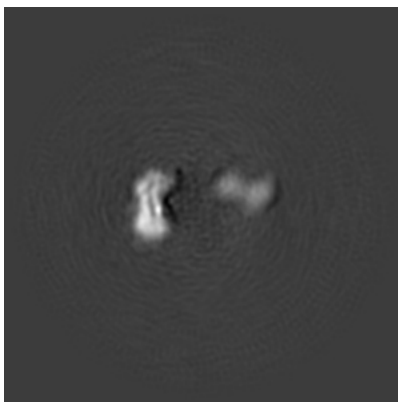
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

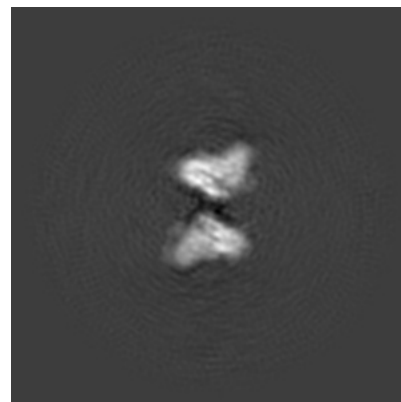
6.3.1 Primary map



X Index: 296

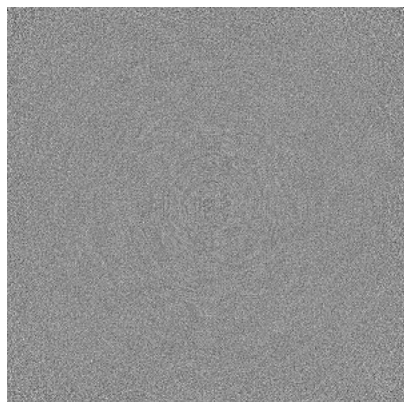


Y Index: 353

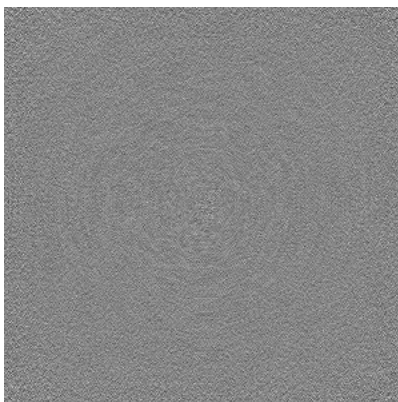


Z Index: 227

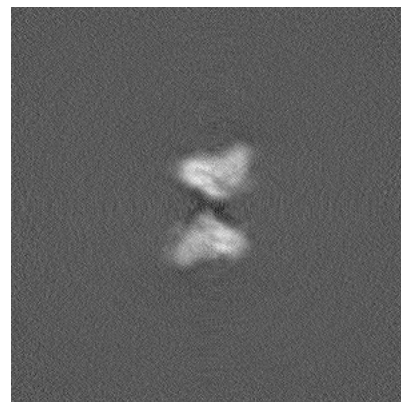
6.3.2 Raw map



X Index: 0



Y Index: 0

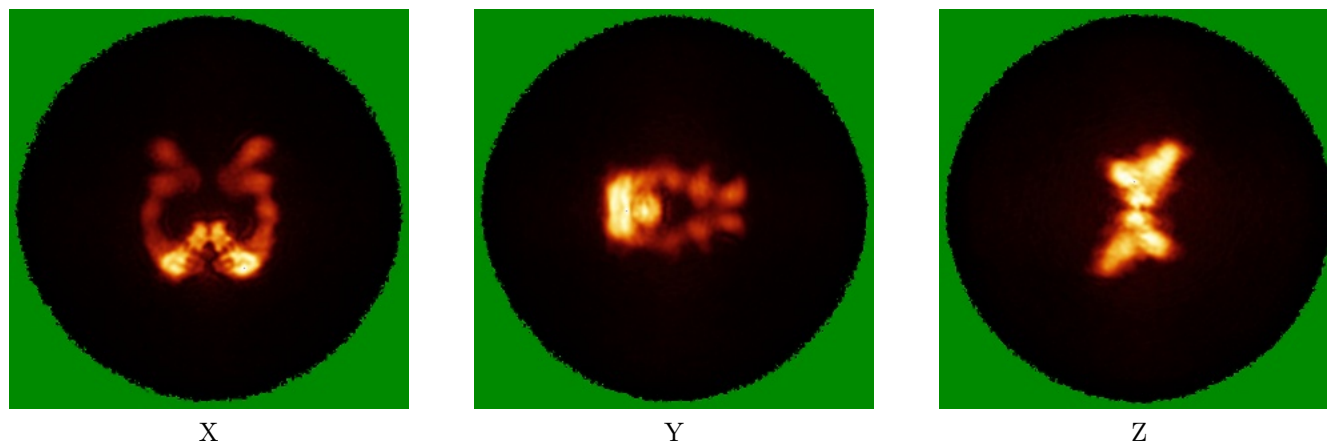


Z Index: 227

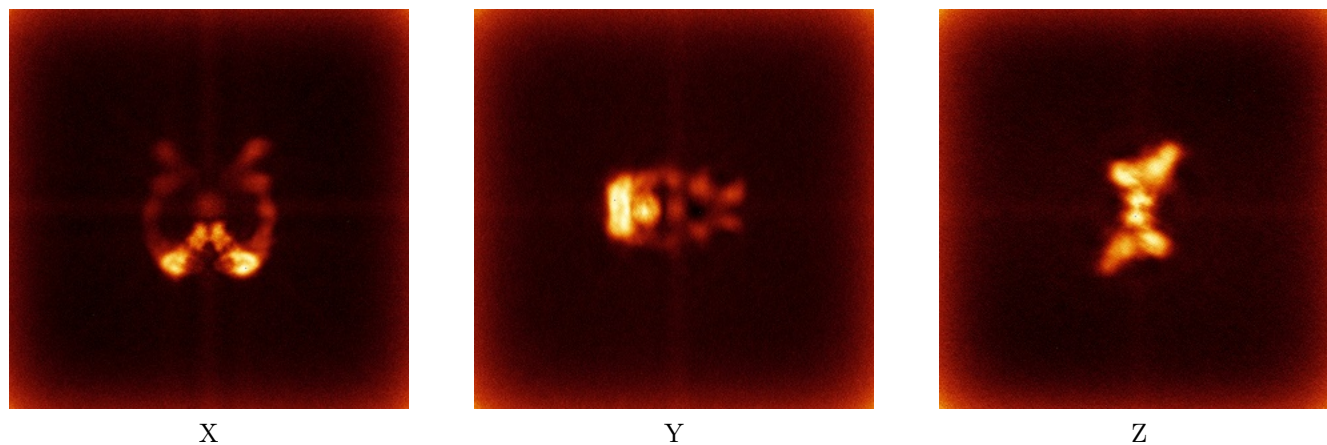
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



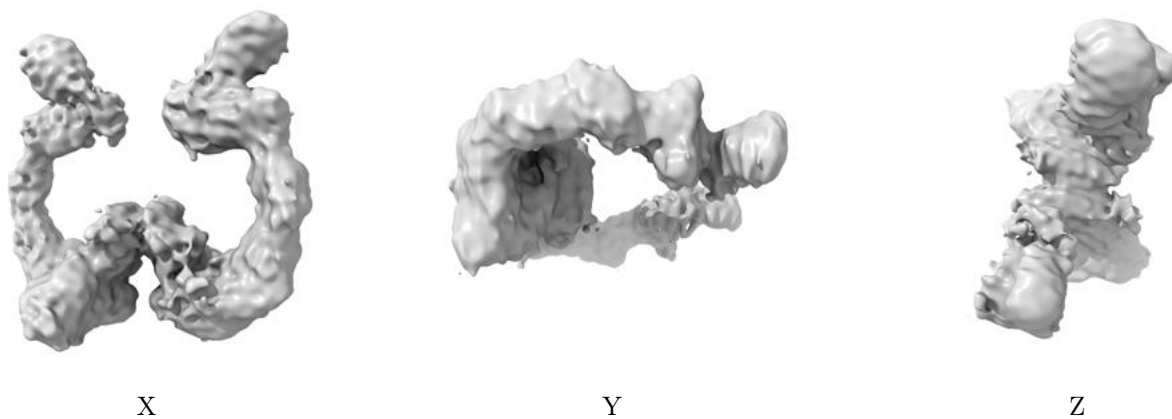
6.4.2 Raw map



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.

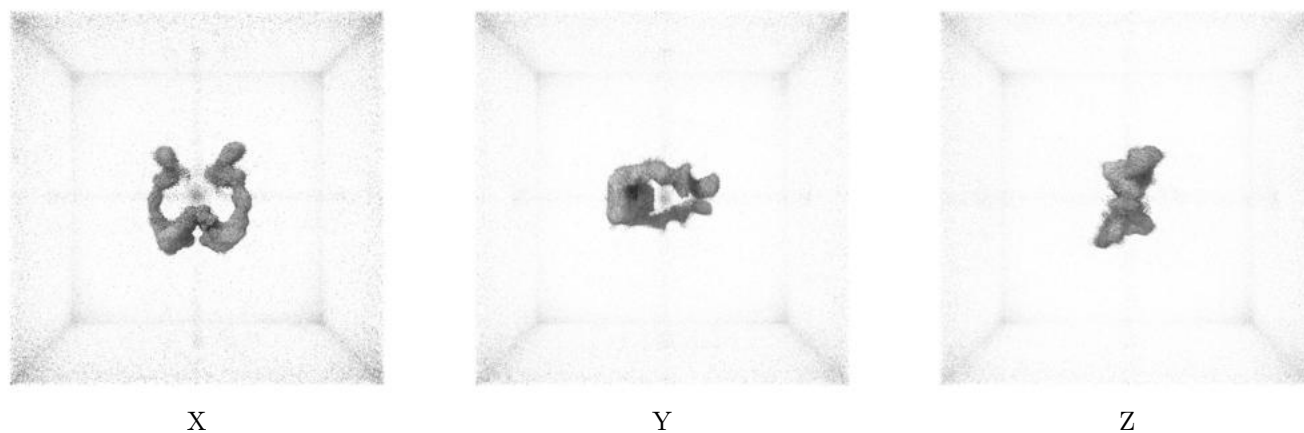
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0183. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

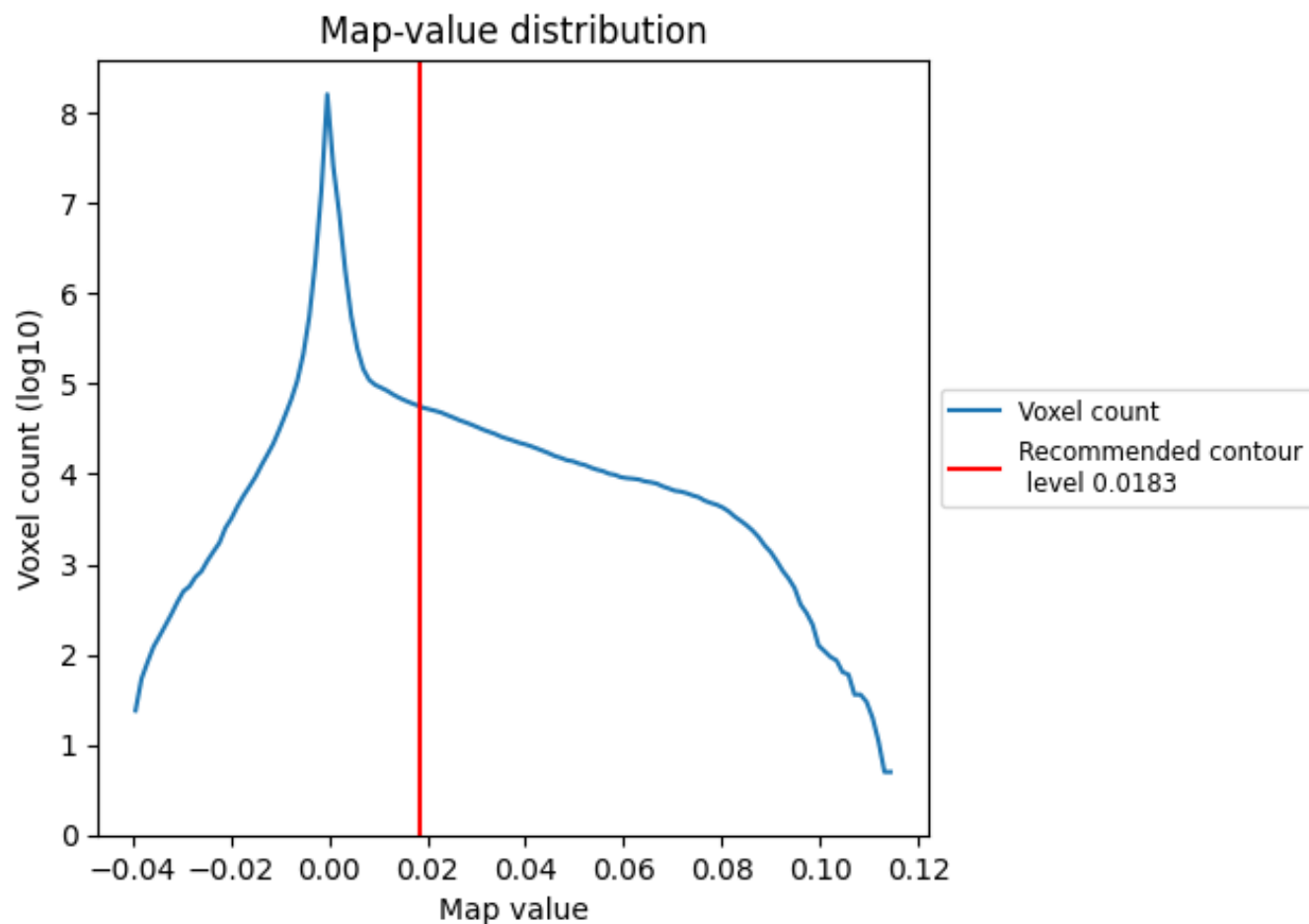
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

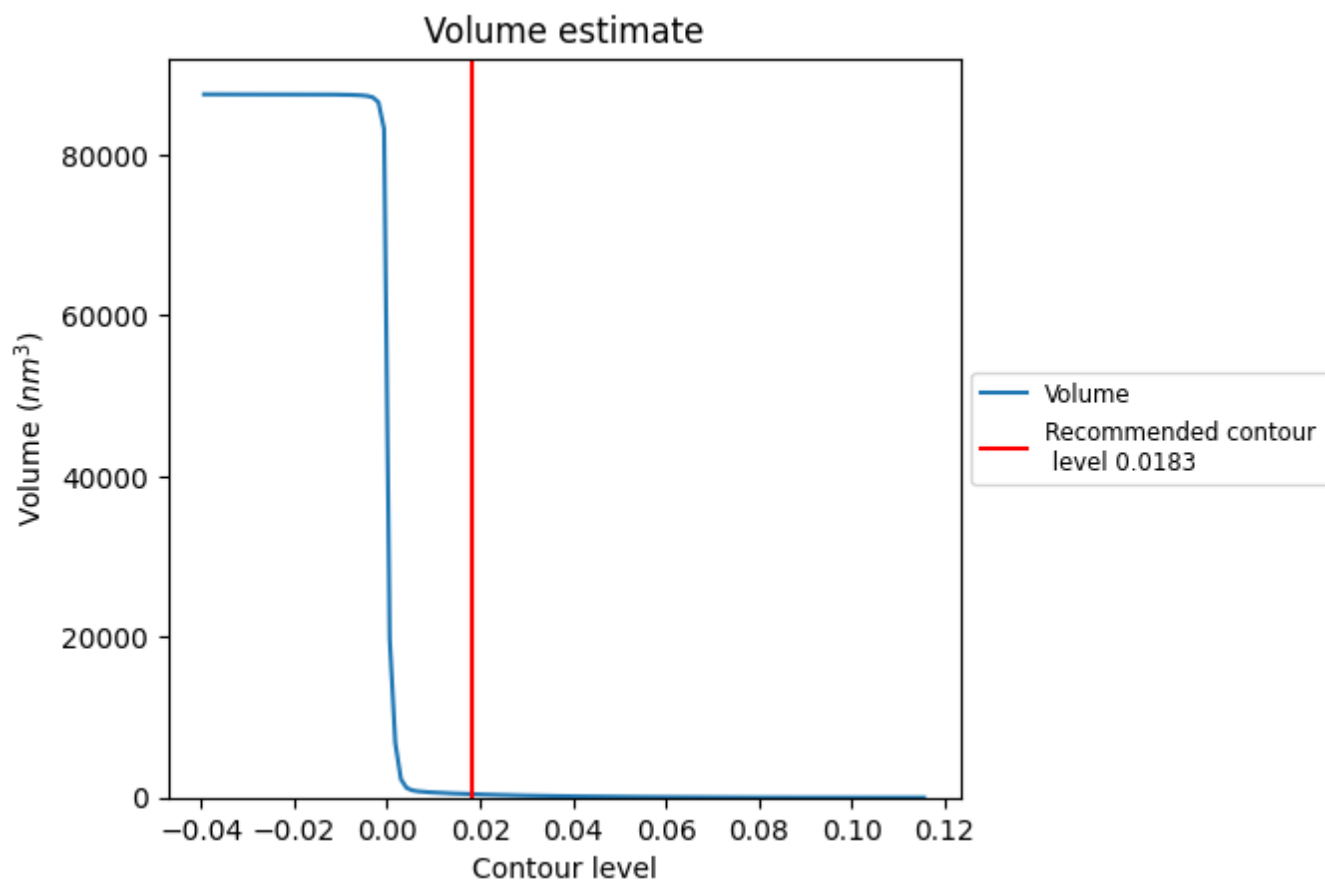
This section contains the results of statistical analysis of the map.

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.

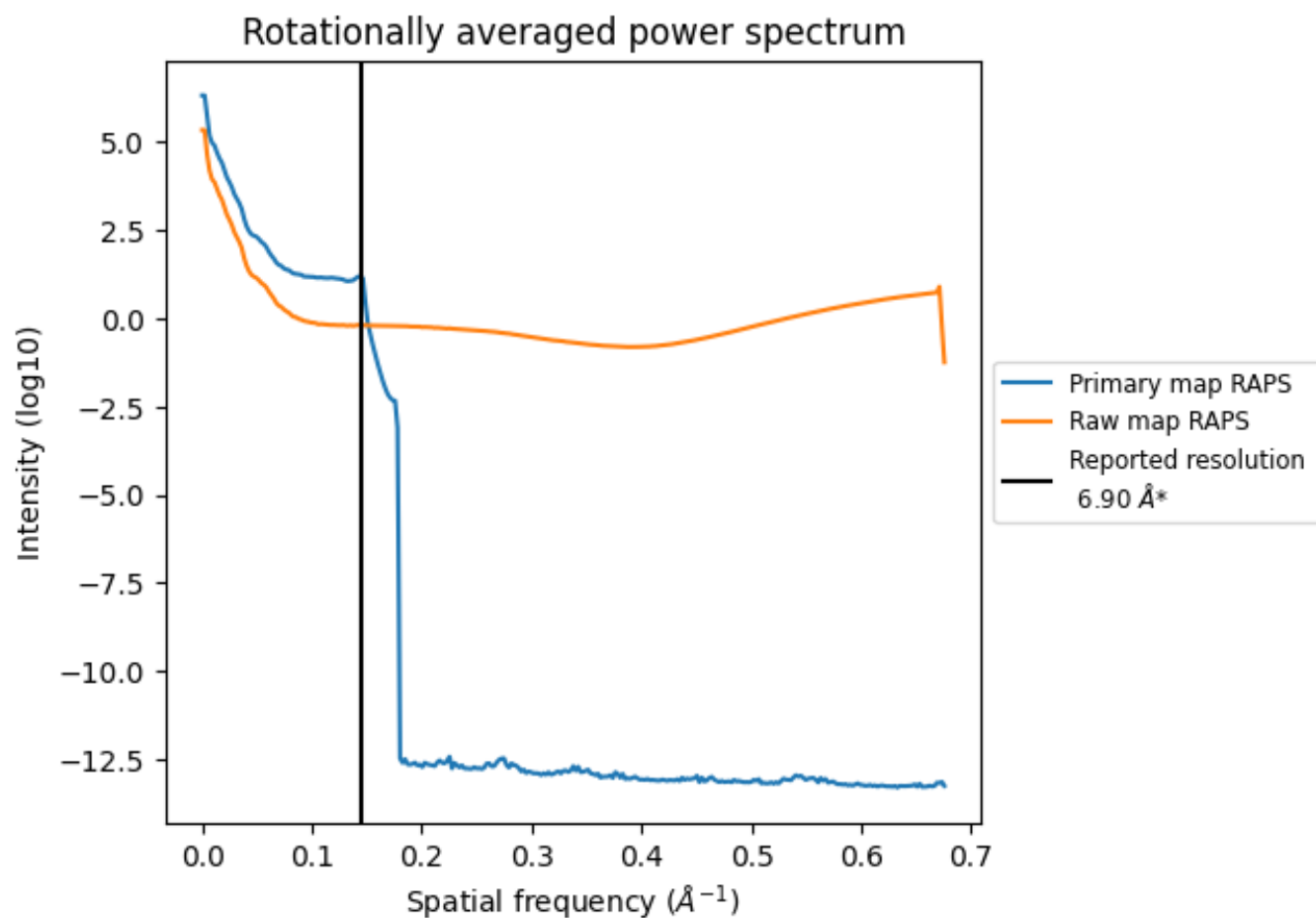
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 424 nm^3 ; this corresponds to an approximate mass of 383 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 ⓘ

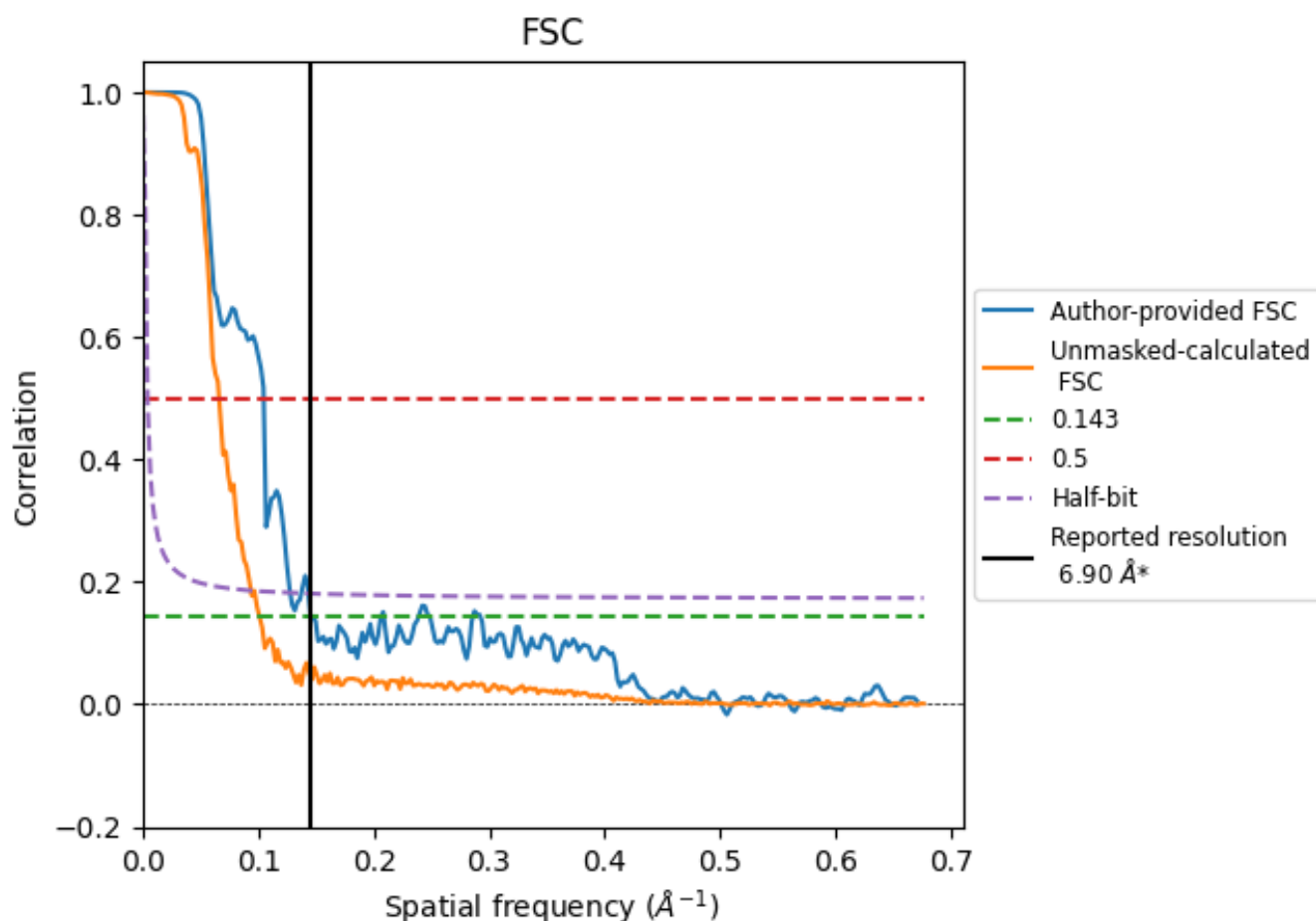


*Reported resolution corresponds to spatial frequency of 0.145 Å⁻¹

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 0.145 \AA^{-1}

8.2 Resolution estimates [i](#)

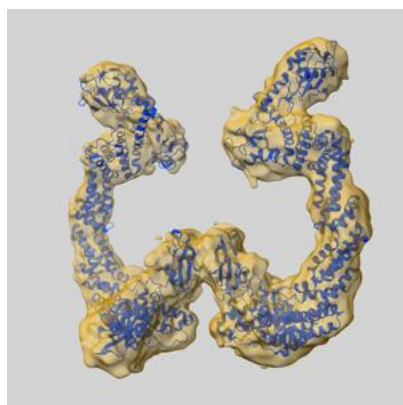
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.90	-	-
Author-provided FSC curve	6.82	9.53	7.82
Unmasked-calculated*	9.88	15.08	10.65

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.88 differs from the reported value 6.9 by more than 10 %

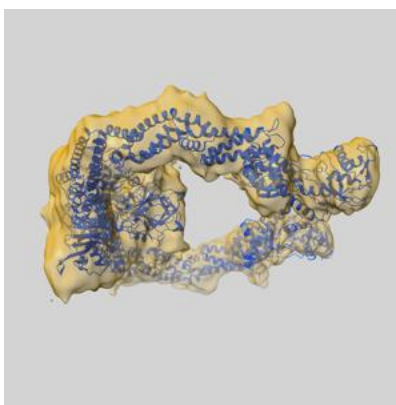
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55480 and PDB model 9T32. Per-residue inclusion information can be found in section [3](#) on page [6](#).

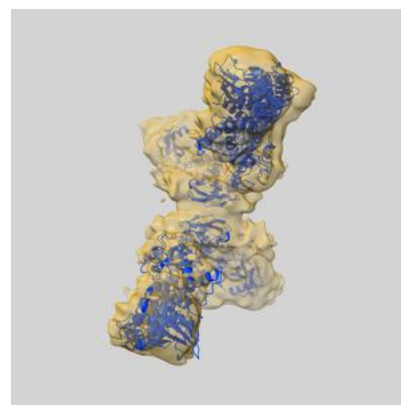
9.1 Map-model overlay [i](#)



X



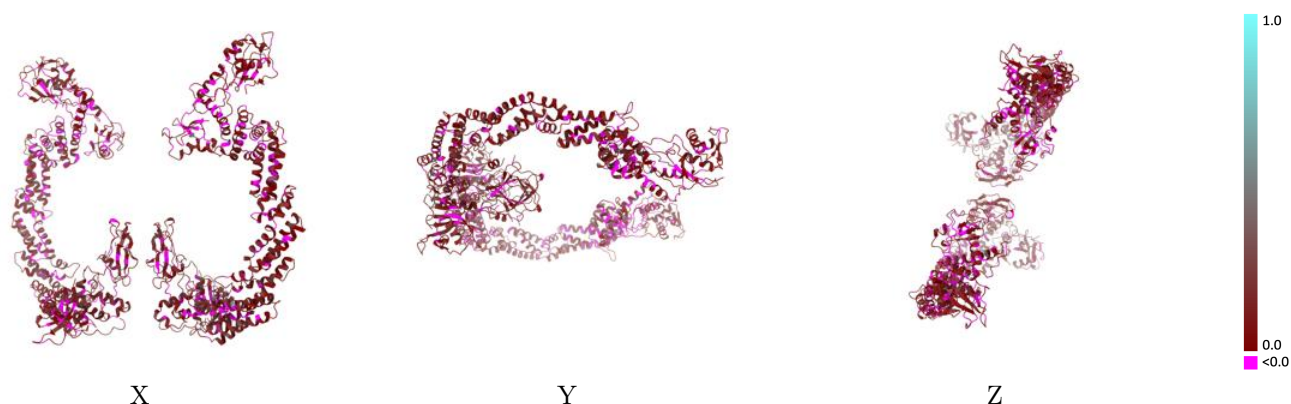
Y



Z

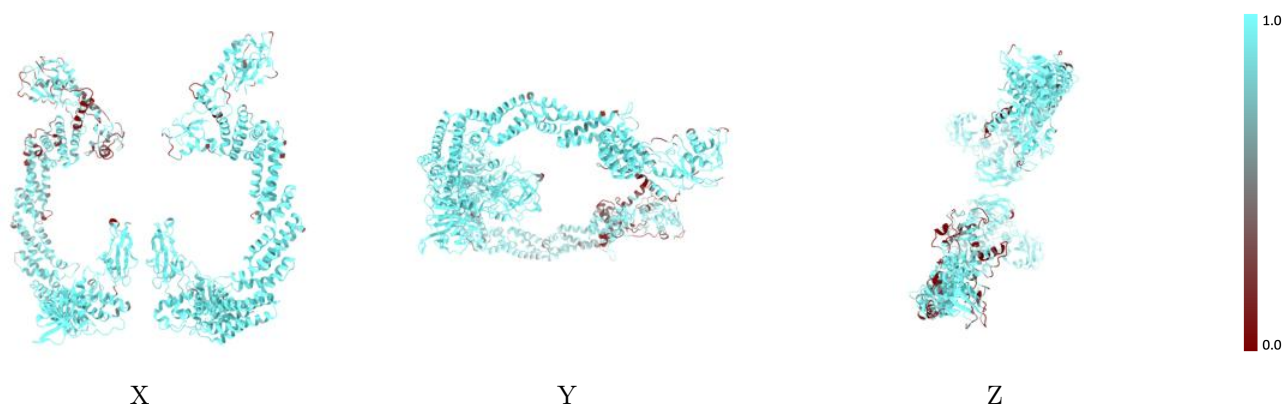
The images above show the 3D surface view of the map at the recommended contour level 0.0183 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



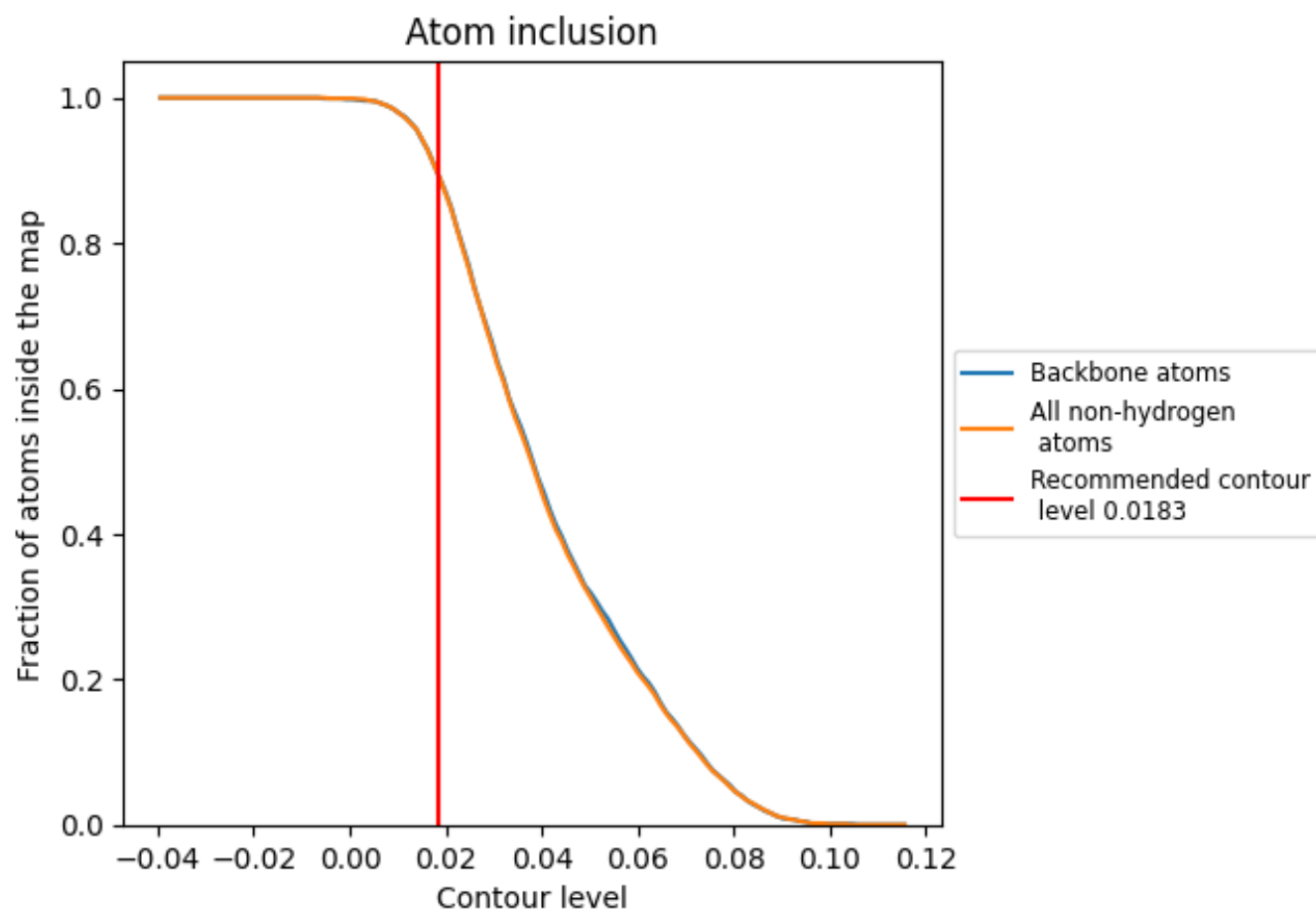
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0183).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 90% 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 (0.0183) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8970	<div></div> 0.1030
C	<div></div> 0.9470	<div></div> 0.1090
D	<div></div> 1.0000	<div></div> 0.1390
E	<div></div> 0.9500	<div></div> 0.0990
F	<div></div> 0.9990	<div></div> 0.1380
G	<div></div> 1.0000	<div></div> 0.1660
H	<div></div> 0.9850	<div></div> 0.1190
I	<div></div> 0.8250	<div></div> 0.0870
J	<div></div> 1.0000	<div></div> 0.1480
R	<div></div> 0.8870	<div></div> 0.0870
S	<div></div> 0.4860	<div></div> 0.0690

1.0

0.0

<0.0