Full wwPDB EM Validation Report ⓘ

Mar 12, 2024 – 02:52 PM JST

PDB ID	:	8JHZ
EMDB ID	:	EMD-36301
Title	:	Cryo-EM structure of the TcsH-TMPRSS2 complex
Authors	:	Zhou, R.; Liang, T.; Zhan, X.
Deposited on	:	2023-05-25
Resolution	:	3.20 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:

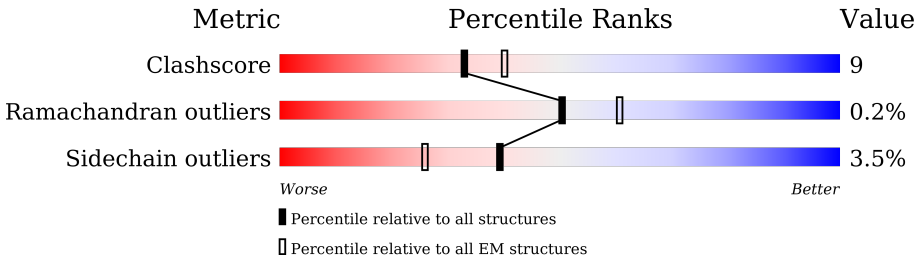
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

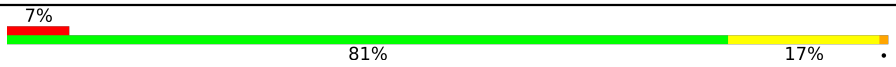
The reported resolution of this entry is 3.20 Å.

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	A	2626	
2	B	424	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 23814 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 Hemorrhagic toxin.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
1	A	2615	21144	13557	3425	4120	1	41	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1833	SER	LEU	conflict	UNP M9ZTT7
A	2619	HIS	-	expression tag	UNP M9ZTT7
A	2620	HIS	-	expression tag	UNP M9ZTT7
A	2621	HIS	-	expression tag	UNP M9ZTT7
A	2622	HIS	-	expression tag	UNP M9ZTT7
A	2623	HIS	-	expression tag	UNP M9ZTT7
A	2624	HIS	-	expression tag	UNP M9ZTT7
A	2625	HIS	-	expression tag	UNP M9ZTT7
A	2626	HIS	-	expression tag	UNP M9ZTT7

- Molecule 2 is a protein called Transmembrane protease serine 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	341	2669	1688	462	496	23	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	69	MET	-	initiating methionine	UNP O15393
B	70	GLY	-	expression tag	UNP O15393
B	71	ILE	-	expression tag	UNP O15393
B	72	LEU	-	expression tag	UNP O15393
B	73	PRO	-	expression tag	UNP O15393
B	74	SER	-	expression tag	UNP O15393
B	75	PRO	-	expression tag	UNP O15393
B	76	GLY	-	expression tag	UNP O15393

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Chain	Residue	Modelled	Actual	Comment	Reference
B	77	MET	-	expression tag	UNP O15393
B	78	PRO	-	expression tag	UNP O15393
B	79	ALA	-	expression tag	UNP O15393
B	80	LEU	-	expression tag	UNP O15393
B	81	LEU	-	expression tag	UNP O15393
B	82	SER	-	expression tag	UNP O15393
B	83	LEU	-	expression tag	UNP O15393
B	84	VAL	-	expression tag	UNP O15393
B	85	SER	-	expression tag	UNP O15393
B	86	LEU	-	expression tag	UNP O15393
B	87	LEU	-	expression tag	UNP O15393
B	88	SER	-	expression tag	UNP O15393
B	89	VAL	-	expression tag	UNP O15393
B	90	LEU	-	expression tag	UNP O15393
B	91	LEU	-	expression tag	UNP O15393
B	92	MET	-	expression tag	UNP O15393
B	93	GLY	-	expression tag	UNP O15393
B	94	CYS	-	expression tag	UNP O15393
B	95	VAL	-	expression tag	UNP O15393
B	96	ALA	-	expression tag	UNP O15393
B	97	GLU	-	expression tag	UNP O15393
B	98	THR	-	expression tag	UNP O15393
B	99	GLY	-	expression tag	UNP O15393
B	100	HIS	-	expression tag	UNP O15393
B	101	HIS	-	expression tag	UNP O15393
B	102	HIS	-	expression tag	UNP O15393
B	103	HIS	-	expression tag	UNP O15393
B	104	HIS	-	expression tag	UNP O15393
B	105	HIS	-	expression tag	UNP O15393
B	255	GLN	ARG	conflict	UNP O15393

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

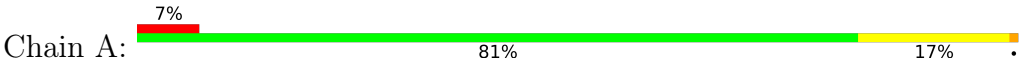
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
3	A	1	1	1	0

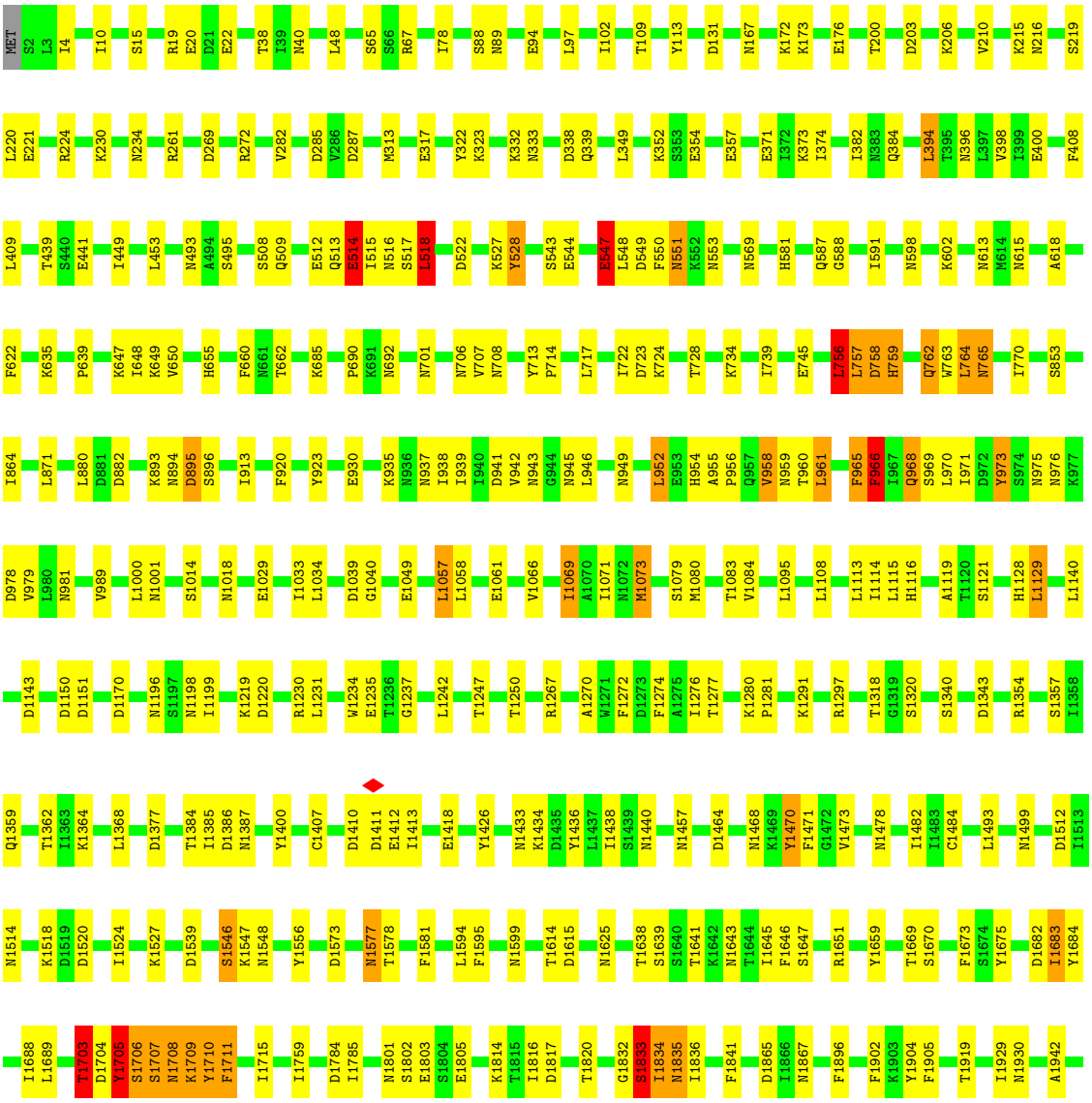
3 Residue-property plots (i)

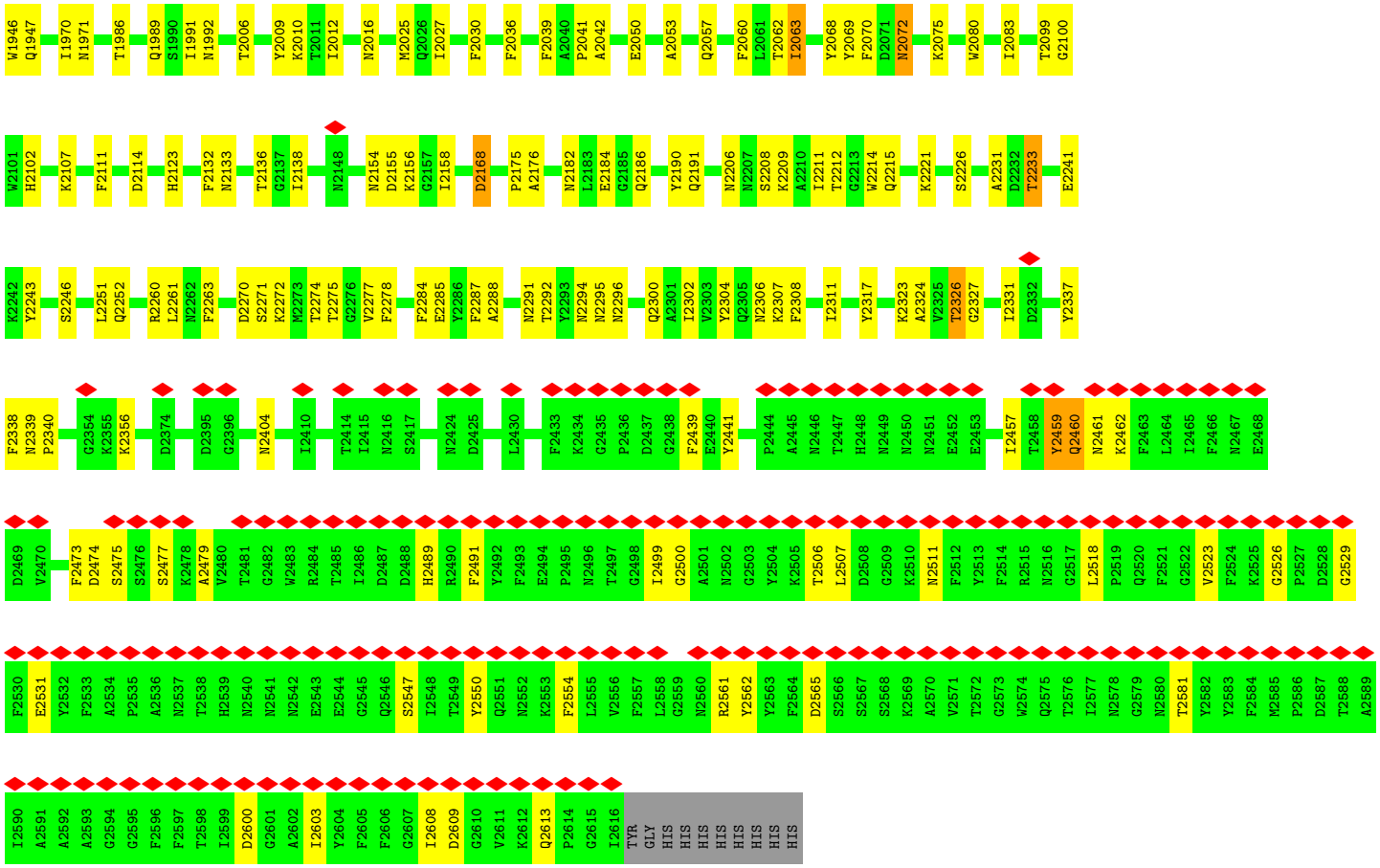
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Hemorrhagic toxin

Chain A:

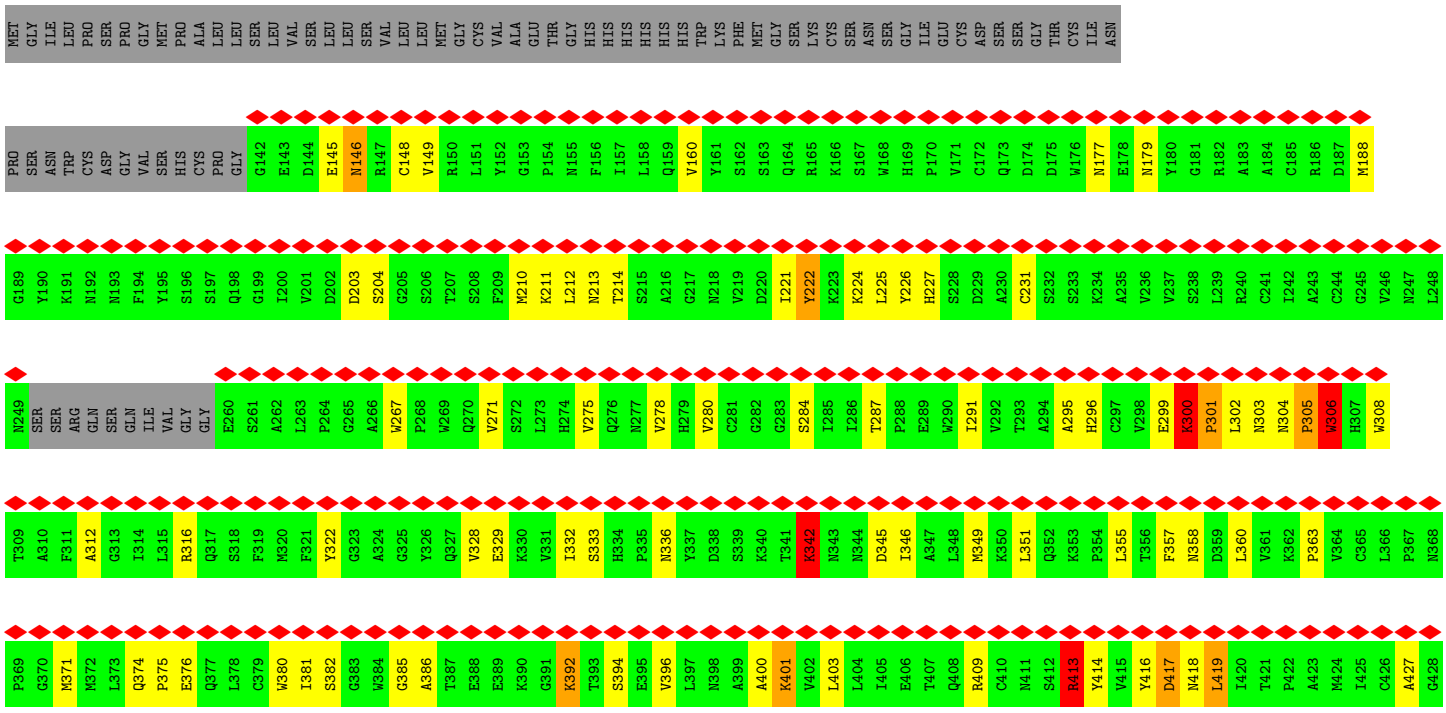


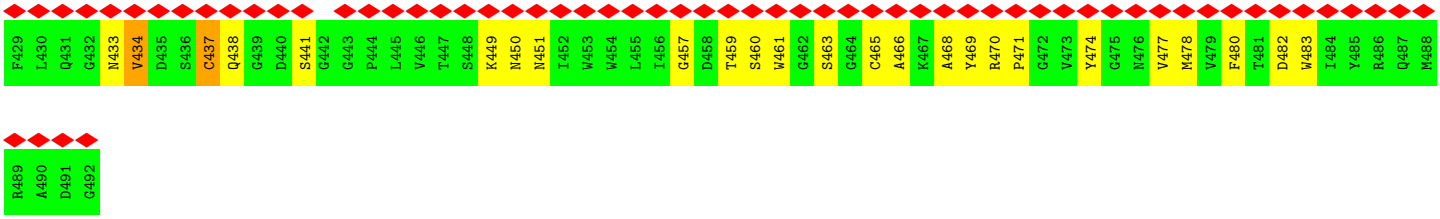




• Molecule 2: Transmembrane protease serine 2

Chain B:




F429 L430 Q431 G432 N433 V434 D435 S436 C437 Q438 G439 D440 S441 G442 G443 P444 L445 V446 T447 S448 K449 N450 N451 I452 W453 W454 L455 I456 G457 D458 T459 S460 W461 G462 S463 G464 C465 A466 K467 A468 Y469 R470 P471 G472 V473 Y474 G475 N476 V477 M478 V479 F480 T481 D482 W483 I484 Y485 R486 Q487 M488
R489 A490 D491 G492

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87378	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.00	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.558	Depositor
Minimum map value	-2.531	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	652.2, 652.2, 652.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

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

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	A	0.50	22/21600 (0.1%)	0.57	22/29255 (0.1%)
2	B	0.55	8/2740 (0.3%)	0.74	13/3724 (0.3%)
All	All	0.51	30/24340 (0.1%)	0.59	35/32979 (0.1%)

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	A	0	3
2	B	0	2
All	All	0	5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	304	ASN	C-O	-9.72	1.04	1.23
1	A	1833	SER	C-O	-9.71	1.04	1.23
1	A	1832	GLY	C-O	-9.40	1.08	1.23
1	A	1471	PHE	C-O	-9.06	1.06	1.23
1	A	1710	TYR	C-O	-8.11	1.07	1.23
1	A	1834	ILE	C-O	-7.89	1.08	1.23
1	A	1833	SER	CA-CB	-7.89	1.41	1.52
1	A	408	PHE	C-O	-7.72	1.08	1.23
1	A	1711	PHE	C-N	7.13	1.47	1.34
1	A	1709	LYS	C-O	-7.08	1.09	1.23
1	A	1707	SER	CA-CB	-6.91	1.42	1.52
1	A	514	GLU	C-O	-6.77	1.10	1.23
1	A	1711	PHE	C-O	-5.96	1.12	1.23
1	A	1833	SER	CB-OG	-5.92	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	513	GLN	C-O	-5.91	1.12	1.23
2	B	306	TRP	C-O	-5.91	1.12	1.23
2	B	413	ARG	C-O	-5.85	1.12	1.23
2	B	305	PRO	C-O	-5.80	1.11	1.23
1	A	287	ASP	CG-OD2	-5.78	1.12	1.25
1	A	516	ASN	C-O	-5.64	1.12	1.23
2	B	303	ASN	C-O	-5.64	1.12	1.23
2	B	301	PRO	C-O	-5.63	1.11	1.23
2	B	302	LEU	C-O	-5.52	1.12	1.23
1	A	1706	SER	CA-CB	-5.39	1.44	1.52
1	A	969	SER	CA-CB	-5.34	1.45	1.52
1	A	758	ASP	C-O	-5.19	1.13	1.23
1	A	543	SER	CA-CB	-5.19	1.45	1.52
1	A	547	GLU	CD-OE1	-5.16	1.20	1.25
2	B	342	LYS	CG-CD	-5.09	1.35	1.52
1	A	1704	ASP	C-O	-5.00	1.13	1.23

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	408	PHE	CB-CA-C	-14.12	82.17	110.40
1	A	959	ASN	CB-CA-C	-10.30	89.80	110.40
1	A	1471	PHE	CB-CA-C	-9.20	92.01	110.40
1	A	960	THR	CA-CB-OG1	-8.96	90.19	109.00
1	A	1835	ASN	CB-CA-C	-8.86	92.69	110.40
1	A	966	PHE	CB-CA-C	-7.81	94.78	110.40
2	B	342	LYS	CB-CG-CD	-7.66	91.69	111.60
2	B	305	PRO	N-CD-CG	-7.52	91.92	103.20
2	B	306	TRP	N-CA-CB	-7.41	97.26	110.60
2	B	300	LYS	CB-CA-C	-6.99	96.41	110.40
1	A	1704	ASP	CB-CA-C	-6.95	96.50	110.40
1	A	965	PHE	CB-CA-C	-6.74	96.92	110.40
2	B	305	PRO	CB-CA-C	-6.74	95.15	112.00
1	A	1703	THR	CA-CB-OG1	-6.70	94.94	109.00
1	A	2608	ILE	CB-CA-C	6.70	124.99	111.60
2	B	306	TRP	CB-CA-C	6.55	123.50	110.40
2	B	414	TYR	N-CA-C	-6.50	93.44	111.00
1	A	1708	ASN	CB-CA-C	-6.26	97.88	110.40
1	A	528	TYR	CB-CA-C	-6.26	97.88	110.40
2	B	342	LYS	CB-CA-C	6.21	122.81	110.40
2	B	299	GLU	C-N-CA	6.13	137.03	121.70
1	A	758	ASP	CB-CA-C	-6.05	98.29	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	414	TYR	C-N-CA	-5.94	106.84	121.70
1	A	518	LEU	CB-CG-CD2	-5.90	100.97	111.00
1	A	1705	TYR	CB-CA-C	-5.74	98.93	110.40
1	A	968	GLN	CB-CA-C	-5.66	99.08	110.40
1	A	1710	TYR	CB-CA-C	-5.53	99.34	110.40
1	A	758	ASP	N-CA-CB	-5.37	100.94	110.60
2	B	305	PRO	N-CA-CB	-5.22	96.85	102.60
1	A	762	GLN	CB-CA-C	-5.21	99.97	110.40
1	A	512	GLU	CB-CA-C	-5.19	100.03	110.40
1	A	960	THR	CB-CA-C	-5.13	97.75	111.60
2	B	299	GLU	O-C-N	5.06	130.79	122.70
1	A	1833	SER	CA-C-O	-5.03	109.53	120.10
2	B	413	ARG	CB-CA-C	5.03	120.46	110.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1703	THR	Mainchain
1	A	1833	SER	Mainchain
1	A	756	LEU	Mainchain
2	B	300	LYS	Mainchain
2	B	306	TRP	Mainchain

5.2 Too-close contacts (i)

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	A	21144	0	20628	374	0
2	B	2669	0	2561	58	0
3	A	1	0	0	0	0
All	All	23814	0	23189	431	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 9.

All (431) 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:A:2308:PHE:CZ	1:A:2331:ILE:HD13	1.37	1.56
1:A:2326:THR:CB	1:A:2340:PRO:HA	1.49	1.42
1:A:2308:PHE:HZ	1:A:2331:ILE:CD1	1.32	1.39
1:A:2326:THR:OG1	1:A:2340:PRO:CA	1.75	1.33
1:A:655:HIS:HE1	1:A:759:HIS:CE1	1.51	1.28
1:A:2460:GLN:HB2	1:A:2474:ASP:O	1.12	1.26
1:A:655:HIS:CE1	1:A:759:HIS:CE1	2.18	1.19
1:A:2326:THR:OG1	1:A:2340:PRO:HA	1.37	1.14
1:A:2308:PHE:CE2	1:A:2331:ILE:HD13	1.84	1.11
1:A:2099:THR:O	1:A:2102:HIS:NE2	1.82	1.11
1:A:2070:PHE:CD1	1:A:2075:LYS:O	2.03	1.11
1:A:2460:GLN:CB	1:A:2474:ASP:O	1.99	1.11
1:A:2308:PHE:CZ	1:A:2331:ILE:CD1	2.17	1.10
1:A:2070:PHE:CE1	1:A:2075:LYS:O	2.08	1.06
1:A:2326:THR:CG2	1:A:2340:PRO:HA	1.87	1.03
1:A:2060:PHE:CZ	1:A:2083:ILE:HD13	1.94	1.02
1:A:2060:PHE:HZ	1:A:2083:ILE:HD13	1.23	1.00
1:A:1836:ILE:HD12	1:A:1841:PHE:CD2	1.97	1.00
1:A:1073:MET:CE	1:A:1484:CYS:SG	2.52	0.98
1:A:1705:TYR:CD2	1:A:1759:ILE:HD13	1.99	0.97
1:A:2326:THR:OG1	1:A:2340:PRO:N	1.95	0.97
2:B:300:LYS:HB3	2:B:301:PRO:CD	1.94	0.94
1:A:2460:GLN:HG2	1:A:2477:SER:N	1.82	0.94
1:A:2326:THR:CB	1:A:2340:PRO:CA	2.39	0.91
1:A:1675:TYR:O	1:A:1708:ASN:OD1	1.90	0.90
2:B:300:LYS:HB3	2:B:301:PRO:HD3	1.54	0.90
2:B:300:LYS:O	2:B:300:LYS:NZ	2.03	0.90
1:A:2460:GLN:HB3	1:A:2477:SER:HA	1.53	0.90
2:B:419:LEU:HD23	2:B:461:TRP:CH2	2.06	0.90
1:A:655:HIS:CE1	1:A:759:HIS:HE1	1.87	0.88
1:A:765:ASN:O	1:A:765:ASN:ND2	2.07	0.88
1:A:547:GLU:OE1	1:A:547:GLU:N	2.06	0.88
1:A:2308:PHE:HE2	1:A:2331:ILE:HG21	1.40	0.87
2:B:371:MET:O	2:B:449:LYS:NZ	2.07	0.86
2:B:416:TYR:OH	2:B:471:PRO:O	1.91	0.86
1:A:1073:MET:HE3	1:A:1484:CYS:SG	2.16	0.86
1:A:1073:MET:HE1	1:A:1484:CYS:SG	2.16	0.85
1:A:1836:ILE:HD12	1:A:1841:PHE:HD2	1.40	0.84
1:A:2460:GLN:HG2	1:A:2477:SER:H	1.40	0.83
1:A:2506:THR:OG1	1:A:2511:ASN:OD1	1.96	0.83
1:A:2063:ILE:CG2	1:A:2068:TYR:HE2	1.92	0.82
1:A:2327:GLY:O	1:A:2337:TYR:CD1	2.33	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2460:GLN:HA	1:A:2473:PHE:HB2	1.60	0.82
1:A:1682:ASP:OD1	1:A:1708:ASN:ND2	2.14	0.81
1:A:2326:THR:HG21	1:A:2340:PRO:HA	1.61	0.81
1:A:528:TYR:CE2	1:A:660:PHE:HA	2.15	0.80
1:A:2603:ILE:HD12	1:A:2603:ILE:O	1.81	0.80
2:B:419:LEU:HD23	2:B:461:TRP:CZ2	2.17	0.80
2:B:328:VAL:HG21	2:B:349:MET:HE3	1.64	0.80
1:A:2550:TYR:OH	1:A:2554:PHE:O	2.00	0.79
2:B:419:LEU:CD2	2:B:461:TRP:CH2	2.66	0.78
1:A:2099:THR:O	1:A:2102:HIS:CD2	2.38	0.77
1:A:930:GLU:HG3	1:A:966:PHE:HD1	1.50	0.77
1:A:591:ILE:HD13	1:A:759:HIS:HA	1.67	0.77
1:A:2006:THR:HG21	1:A:2010:LYS:HD2	1.67	0.77
1:A:764:LEU:HD23	1:A:764:LEU:N	2.00	0.76
1:A:1436:TYR:O	1:A:1440:ASN:ND2	2.19	0.76
1:A:961:LEU:O	1:A:961:LEU:HD22	1.86	0.75
1:A:930:GLU:HG3	1:A:966:PHE:CD1	2.21	0.74
1:A:2326:THR:OG1	1:A:2340:PRO:CB	2.36	0.73
1:A:2291:ASN:H	1:A:2296:ASN:HA	1.54	0.73
1:A:2326:THR:HB	1:A:2340:PRO:HA	1.61	0.72
1:A:1705:TYR:CD2	1:A:1759:ILE:CD1	2.73	0.72
1:A:4:ILE:HD13	1:A:976:ASN:HD21	1.54	0.72
1:A:2295:ASN:HB2	1:A:2302:ILE:HD13	1.72	0.72
2:B:291:ILE:HD12	2:B:351:LEU:HD21	1.71	0.71
2:B:437:CYS:SG	2:B:438:GLN:N	2.63	0.71
1:A:1108:LEU:HD12	1:A:1113:LEU:HB3	1.71	0.71
1:A:2326:THR:OG1	1:A:2340:PRO:CG	2.39	0.71
1:A:2060:PHE:HZ	1:A:2083:ILE:CD1	2.03	0.71
1:A:2461:ASN:ND2	1:A:2475:SER:HA	2.06	0.71
1:A:2308:PHE:CE2	1:A:2331:ILE:HG21	2.26	0.70
1:A:528:TYR:HE2	1:A:660:PHE:HA	1.57	0.70
1:A:2288:ALA:HB1	1:A:2292:THR:HG21	1.75	0.69
1:A:2295:ASN:HD21	1:A:2300:GLN:HB3	1.57	0.69
1:A:756:LEU:HD12	1:A:756:LEU:O	1.93	0.69
1:A:2460:GLN:CB	1:A:2477:SER:HA	2.22	0.68
1:A:38:THR:HG22	1:A:40:ASN:H	1.57	0.68
1:A:2176:ALA:HB2	1:A:2184:GLU:HG3	1.75	0.68
1:A:2057:GLN:NE2	1:A:2072:ASN:O	2.27	0.67
1:A:2233:THR:O	1:A:2233:THR:OG1	2.11	0.67
1:A:527:LYS:NZ	1:A:701:ASN:OD1	2.27	0.66
2:B:457:GLY:HA2	2:B:477:VAL:HG23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLU:OE2	1:A:224:ARG:NH2	2.29	0.66
1:A:384:GLN:OE1	1:A:509:GLN:NE2	2.28	0.66
1:A:2327:GLY:O	1:A:2337:TYR:HA	1.96	0.65
1:A:354:GLU:HB2	1:A:357:GLU:HG3	1.78	0.65
1:A:2243:TYR:OH	1:A:2272:LYS:NZ	2.24	0.65
1:A:2308:PHE:HZ	1:A:2331:ILE:HD11	1.51	0.65
1:A:591:ILE:CD1	1:A:759:HIS:HA	2.27	0.64
1:A:1548:ASN:ND2	1:A:1599:ASN:O	2.30	0.64
1:A:1478:ASN:ND2	1:A:1520:ASP:OD2	2.30	0.64
1:A:15:SER:HB3	1:A:67:ARG:HH21	1.63	0.64
1:A:509:GLN:O	1:A:514:GLU:HG2	1.98	0.64
1:A:2460:GLN:HA	1:A:2473:PHE:CB	2.29	0.63
1:A:551:ASN:O	1:A:553:ASN:ND2	2.31	0.63
2:B:385:GLY:O	2:B:394:SER:N	2.31	0.63
1:A:971:ILE:O	1:A:971:ILE:HG22	1.99	0.62
2:B:291:ILE:CD1	2:B:351:LEU:HD21	2.28	0.62
1:A:2489:HIS:ND1	2:B:322:TYR:OH	2.33	0.62
1:A:942:VAL:HG23	1:A:943:ASN:H	1.63	0.62
1:A:2356:LYS:NZ	1:A:2404:ASN:O	2.32	0.62
1:A:2561:ARG:NE	1:A:2609:ASP:O	2.32	0.62
1:A:647:LYS:HG3	1:A:692:ASN:HB2	1.81	0.61
1:A:2060:PHE:CE2	1:A:2083:ILE:HG21	2.34	0.61
1:A:1069:ILE:HD12	1:A:1457:ASN:HB2	1.80	0.61
1:A:2439:PHE:HB2	1:A:2479:ALA:HB3	1.82	0.61
2:B:295:ALA:N	2:B:345:ASP:OD1	2.33	0.61
1:A:20:GLU:OE2	1:A:67:ARG:NH1	2.33	0.61
1:A:518:LEU:HD23	1:A:518:LEU:O	2.01	0.61
1:A:757:LEU:HG	1:A:757:LEU:O	2.00	0.61
1:A:1638:THR:HG22	1:A:1639:SER:H	1.64	0.61
1:A:2154:ASN:OD1	1:A:2158:ILE:N	2.34	0.61
1:A:2460:GLN:HG2	1:A:2477:SER:CA	2.30	0.61
1:A:762:GLN:O	1:A:762:GLN:HG3	2.00	0.60
1:A:1340:SER:N	1:A:1343:ASP:OD1	2.27	0.60
1:A:2460:GLN:CG	1:A:2477:SER:HA	2.32	0.60
1:A:2326:THR:HG21	1:A:2340:PRO:CA	2.30	0.60
1:A:1546:SER:OG	1:A:1547:LYS:N	2.35	0.60
1:A:2063:ILE:O	1:A:2063:ILE:HG13	2.01	0.60
1:A:2294:ASN:HB3	1:A:2302:ILE:HD11	1.83	0.60
1:A:1071:ILE:HG12	1:A:1473:VAL:HG23	1.83	0.59
1:A:94:GLU:OE2	1:A:94:GLU:N	2.34	0.59
1:A:2278:PHE:HB2	1:A:2287:PHE:HE2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:ASN:ND2	1:A:745:GLU:OE1	2.35	0.59
1:A:1946:TRP:O	1:A:1947:GLN:NE2	2.36	0.59
2:B:203:ASP:OD1	2:B:203:ASP:N	2.33	0.59
1:A:1386:ASP:N	1:A:1386:ASP:OD2	2.34	0.59
1:A:551:ASN:H	1:A:551:ASN:ND2	2.00	0.58
2:B:463:SER:O	2:B:463:SER:OG	2.15	0.58
1:A:1247:THR:O	1:A:1250:THR:OG1	2.16	0.58
1:A:2063:ILE:CG2	1:A:2068:TYR:CE2	2.82	0.58
1:A:439:THR:HG23	1:A:441:GLU:H	1.69	0.58
1:A:763:TRP:N	1:A:763:TRP:CD1	2.72	0.57
2:B:482:ASP:OD1	2:B:483:TRP:N	2.37	0.57
1:A:2009:TYR:HE2	1:A:2016:ASN:HB3	1.69	0.57
1:A:722:ILE:HD11	1:A:734:LYS:HD3	1.87	0.57
1:A:2060:PHE:HE2	1:A:2083:ILE:HG21	1.70	0.57
1:A:2072:ASN:OD1	1:A:2072:ASN:N	2.36	0.56
1:A:1578:THR:HG22	1:A:1835:ASN:ND2	2.20	0.56
1:A:1493:LEU:HD21	1:A:1524:ILE:HD13	1.86	0.56
1:A:1706:SER:O	1:A:1706:SER:OG	2.21	0.56
1:A:1970:ILE:HG22	1:A:1971:ASN:ND2	2.20	0.56
1:A:2460:GLN:CG	1:A:2477:SER:CA	2.84	0.56
1:A:1242:LEU:O	1:A:1267:ARG:NH1	2.39	0.56
1:A:48:LEU:HD22	1:A:78:ILE:HG23	1.88	0.56
1:A:2326:THR:OG1	1:A:2340:PRO:CD	2.54	0.56
2:B:465:CYS:O	2:B:466:ALA:HB3	2.05	0.56
1:A:1836:ILE:CD1	1:A:1841:PHE:CD2	2.82	0.56
1:A:354:GLU:N	1:A:357:GLU:OE2	2.27	0.56
1:A:1196:ASN:OD1	1:A:1198:ASN:ND2	2.40	0.56
1:A:1235:GLU:OE1	1:A:1280:LYS:NZ	2.31	0.55
1:A:528:TYR:CD2	1:A:660:PHE:HA	2.41	0.55
1:A:2063:ILE:HG21	1:A:2068:TYR:HE2	1.71	0.55
2:B:358:ASN:OD1	2:B:360:LEU:N	2.36	0.55
2:B:211:LYS:N	2:B:226:TYR:O	2.38	0.55
1:A:2063:ILE:HG23	1:A:2068:TYR:HE2	1.72	0.55
2:B:177:ASN:OD1	2:B:179:ASN:N	2.35	0.55
1:A:2461:ASN:N	1:A:2473:PHE:O	2.29	0.54
1:A:1539:ASP:HB2	1:A:1556:TYR:HB3	1.89	0.54
1:A:515:ILE:HG23	1:A:708:ASN:HD21	1.72	0.54
2:B:346:ILE:HG21	2:B:480:PHE:CD2	2.42	0.54
1:A:1865:ASP:OD1	1:A:1867:ASN:ND2	2.40	0.54
1:A:1986:THR:O	1:A:1989:GLN:NE2	2.41	0.54
1:A:2327:GLY:N	1:A:2338:PHE:O	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:342:LYS:O	2:B:345:ASP:HB2	2.08	0.54
1:A:2457:ILE:HD11	1:A:2459:TYR:HD2	1.73	0.53
1:A:167:ASN:OD1	1:A:167:ASN:N	2.41	0.53
1:A:2062:THR:O	1:A:2062:THR:HG23	2.08	0.53
1:A:613:ASN:OD1	1:A:613:ASN:N	2.39	0.53
1:A:65:SER:OG	1:A:67:ARG:HG2	2.09	0.53
1:A:2211:ILE:HD12	1:A:2215:GLN:HG3	1.91	0.53
1:A:2613:GLN:OE1	1:A:2613:GLN:HA	2.08	0.53
1:A:1196:ASN:HD22	1:A:1199:ILE:HG13	1.74	0.53
1:A:2036:PHE:O	1:A:2075:LYS:HA	2.09	0.53
1:A:2326:THR:HG1	1:A:2340:PRO:N	2.02	0.53
2:B:413:ARG:HB3	2:B:417:ASP:HB2	1.91	0.52
1:A:313:MET:O	1:A:317:GLU:HG3	2.09	0.52
1:A:1079:SER:O	1:A:1083:THR:HG23	2.09	0.52
1:A:2461:ASN:HD21	1:A:2475:SER:CA	2.23	0.52
2:B:336:ASN:OD1	2:B:336:ASN:O	2.27	0.52
1:A:618:ALA:HB3	1:A:635:LYS:HD3	1.90	0.52
1:A:2460:GLN:HB3	1:A:2473:PHE:HB3	1.92	0.52
1:A:2168:ASP:OD1	1:A:2209:LYS:NZ	2.35	0.52
1:A:882:ASP:OD1	1:A:882:ASP:N	2.39	0.52
1:A:893:LYS:HD3	1:A:895:ASP:H	1.76	0.51
1:A:2308:PHE:CZ	1:A:2331:ILE:HD11	2.34	0.51
1:A:2042:ALA:HB2	1:A:2050:GLU:HB2	1.92	0.51
1:A:2231:ALA:O	1:A:2233:THR:HG22	2.10	0.51
2:B:271:VAL:HG12	2:B:312:ALA:HB2	1.93	0.51
1:A:396:ASN:O	1:A:400:GLU:HG2	2.11	0.51
1:A:880:LEU:HD11	1:A:913:ILE:HG13	1.92	0.51
1:A:2308:PHE:CE1	1:A:2317:TYR:HB2	2.46	0.51
1:A:713:TYR:HB3	1:A:714:PRO:HD3	1.93	0.51
1:A:1578:THR:O	1:A:1581:PHE:HB3	2.11	0.51
1:A:2461:ASN:HD21	1:A:2475:SER:HA	1.76	0.51
2:B:328:VAL:HG21	2:B:349:MET:CE	2.38	0.51
1:A:1673:PHE:CZ	1:A:1688:ILE:HD13	2.46	0.50
1:A:2246:SER:HB3	1:A:2252:GLN:HG3	1.94	0.50
1:A:1359:GLN:O	1:A:1362:THR:OG1	2.28	0.50
1:A:1196:ASN:ND2	1:A:1199:ILE:HG13	2.27	0.50
1:A:216:ASN:OD1	1:A:219:SER:N	2.40	0.50
1:A:1651:ARG:HD3	1:A:1684:TYR:O	2.11	0.50
1:A:374:ILE:HG12	1:A:382:ILE:O	2.11	0.50
1:A:508:SER:O	1:A:508:SER:OG	2.30	0.49
1:A:1387:ASN:N	1:A:1387:ASN:OD1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1548:ASN:HD21	1:A:1599:ASN:HD22	1.60	0.49
2:B:146:ASN:N	2:B:146:ASN:OD1	2.44	0.49
2:B:278:VAL:O	2:B:280:VAL:HG23	2.12	0.49
1:A:1833:SER:O	1:A:1833:SER:OG	2.27	0.49
1:A:2274:THR:HG22	1:A:2275:THR:H	1.77	0.49
1:A:2459:TYR:CE1	1:A:2462:LYS:HE3	2.47	0.49
1:A:966:PHE:CD2	1:A:966:PHE:C	2.84	0.49
1:A:989:VAL:HG12	1:A:1000:LEU:HD11	1.94	0.49
1:A:2284:PHE:HB2	1:A:2324:ALA:HB3	1.94	0.49
1:A:2175:PRO:O	1:A:2182:ASN:ND2	2.41	0.49
1:A:1115:LEU:HB2	1:A:1281:PRO:HD3	1.95	0.49
1:A:1128:HIS:NE2	1:A:1150:ASP:O	2.39	0.49
1:A:973:TYR:O	1:A:973:TYR:CD1	2.65	0.49
1:A:1709:LYS:O	1:A:1709:LYS:HG2	2.12	0.49
1:A:2523:VAL:HG21	1:A:2562:TYR:CD2	2.48	0.49
1:A:2461:ASN:HD21	1:A:2475:SER:CB	2.25	0.49
2:B:468:ALA:O	2:B:469:TYR:HB2	2.13	0.49
1:A:1039:ASP:N	1:A:1039:ASP:OD1	2.45	0.48
1:A:1573:ASP:OD2	1:A:1573:ASP:N	2.31	0.48
2:B:275:VAL:HB	2:B:280:VAL:HG21	1.94	0.48
1:A:1340:SER:OG	1:A:1343:ASP:OD2	2.29	0.48
1:A:322:TYR:HD2	1:A:349:LEU:HD12	1.78	0.48
1:A:954:HIS:O	1:A:958:VAL:HG22	2.13	0.48
1:A:2460:GLN:CG	1:A:2477:SER:H	2.18	0.48
1:A:550:PHE:HD1	1:A:587:GLN:NE2	2.11	0.48
1:A:2461:ASN:ND2	1:A:2475:SER:CA	2.76	0.48
1:A:871:LEU:HB3	1:A:981:ASN:HD22	1.79	0.48
1:A:1377:ASP:HB3	1:A:1384:THR:HB	1.95	0.48
1:A:588:GLY:HA2	1:A:613:ASN:HD22	1.79	0.47
1:A:756:LEU:HD23	1:A:770:ILE:HG13	1.96	0.47
1:A:871:LEU:HD13	1:A:920:PHE:HE1	1.79	0.47
1:A:2107:LYS:HD3	1:A:2138:ILE:HD13	1.95	0.47
1:A:88:SER:OG	1:A:89:ASN:OD1	2.32	0.47
1:A:206:LYS:HG3	1:A:220:LEU:HD12	1.96	0.47
1:A:323:LYS:NZ	1:A:352:LYS:O	2.29	0.47
1:A:549:ASP:HB3	1:A:551:ASN:HD21	1.80	0.47
1:A:973:TYR:HE1	1:A:978:ASP:OD2	1.97	0.47
1:A:1410:ASP:OD2	1:A:1412:GLU:HG2	2.14	0.47
2:B:380:TRP:CZ2	2:B:401:LYS:HD2	2.49	0.47
1:A:22:GLU:OE2	1:A:22:GLU:N	2.47	0.47
1:A:550:PHE:CD1	1:A:587:GLN:NE2	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2461:ASN:HD21	1:A:2475:SER:HB3	1.79	0.47
1:A:515:ILE:HG23	1:A:708:ASN:ND2	2.29	0.47
1:A:968:GLN:O	1:A:968:GLN:HG3	2.13	0.47
1:A:685:LYS:HD3	1:A:728:THR:HG23	1.96	0.47
1:A:717:LEU:HD23	1:A:739:ILE:HD13	1.97	0.47
1:A:935:LYS:O	1:A:935:LYS:HG2	2.14	0.47
1:A:648:ILE:HG13	1:A:690:PRO:HG3	1.97	0.47
1:A:200:THR:OG1	1:A:203:ASP:OD1	2.20	0.47
1:A:2261:LEU:HB2	1:A:2263:PHE:HE2	1.79	0.47
1:A:409:LEU:HD13	1:A:449:ILE:HD12	1.98	0.46
1:A:1577:ASN:OD1	1:A:1577:ASN:N	2.48	0.46
1:A:551:ASN:ND2	1:A:551:ASN:N	2.60	0.46
1:A:591:ILE:HD11	1:A:759:HIS:O	2.15	0.46
1:A:1115:LEU:HD13	1:A:1281:PRO:HG3	1.98	0.46
1:A:2326:THR:OG1	1:A:2340:PRO:HG3	2.13	0.46
1:A:394:LEU:O	1:A:398:VAL:HG23	2.16	0.46
1:A:2100:GLY:O	1:A:2102:HIS:HD2	1.98	0.46
1:A:2460:GLN:CG	1:A:2477:SER:N	2.69	0.46
2:B:213:ASN:O	2:B:224:LYS:NZ	2.39	0.46
1:A:109:THR:O	1:A:113:TYR:HD2	1.99	0.46
1:A:941:ASP:HB3	1:A:946:LEU:HD13	1.97	0.46
1:A:1272:PHE:HB2	1:A:1274:PHE:CE2	2.51	0.46
1:A:1711:PHE:N	1:A:1711:PHE:CD2	2.84	0.46
1:A:1904:TYR:O	1:A:1919:THR:HA	2.16	0.46
1:A:2284:PHE:O	1:A:2323:LYS:HA	2.15	0.46
1:A:2080:TRP:CH2	1:A:2111:PHE:HZ	2.34	0.46
2:B:149:VAL:HG12	2:B:160:VAL:HG22	1.98	0.46
2:B:400:ALA:HB1	2:B:434:VAL:HG13	1.97	0.46
1:A:493:ASN:OD1	1:A:495:SER:OG	2.30	0.45
1:A:518:LEU:HD22	1:A:707:VAL:CG2	2.47	0.45
1:A:1645:ILE:HD11	1:A:1651:ARG:HB3	1.97	0.45
1:A:2441:TYR:HD2	1:A:2459:TYR:CD2	2.35	0.45
1:A:317:GLU:OE1	1:A:333:ASN:HB2	2.16	0.45
1:A:894:ASN:O	1:A:896:SER:N	2.38	0.45
1:A:1433:ASN:HB3	1:A:1436:TYR:HB3	1.97	0.45
1:A:2460:GLN:CG	1:A:2474:ASP:O	2.64	0.45
1:A:210:VAL:HG23	1:A:215:LYS:O	2.17	0.45
2:B:450:ASN:OD1	2:B:450:ASN:O	2.33	0.45
1:A:230:LYS:O	1:A:234:ASN:ND2	2.50	0.45
1:A:549:ASP:OD1	1:A:549:ASP:N	2.48	0.45
1:A:1033:ILE:HG13	1:A:1034:LEU:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1594:LEU:HD23	1:A:1595:PHE:CE2	2.52	0.45
1:A:1896:PHE:HB2	1:A:1905:PHE:CE2	2.52	0.45
1:A:1802:SER:O	1:A:1802:SER:OG	2.27	0.45
1:A:2326:THR:HB	1:A:2339:ASN:O	2.17	0.45
2:B:357:PHE:CZ	2:B:363:PRO:HG3	2.52	0.45
1:A:2271:SER:O	1:A:2271:SER:OG	2.35	0.45
1:A:2291:ASN:N	1:A:2296:ASN:HA	2.28	0.45
1:A:1669:THR:O	1:A:1669:THR:OG1	2.35	0.44
1:A:1902:PHE:HB2	1:A:1942:ALA:HB3	1.99	0.44
1:A:549:ASP:HB3	1:A:551:ASN:ND2	2.33	0.44
1:A:871:LEU:HD13	1:A:920:PHE:CE1	2.52	0.44
1:A:2025:MET:HE3	1:A:2050:GLU:HG3	1.99	0.44
1:A:2221:LYS:HD3	1:A:2251:LEU:HD23	1.99	0.44
1:A:10:ILE:HD13	1:A:19:ARG:HH22	1.83	0.44
1:A:173:LYS:HD2	1:A:173:LYS:HA	1.82	0.44
1:A:1129:LEU:HA	1:A:1129:LEU:HD23	1.64	0.44
1:A:2326:THR:CG2	1:A:2340:PRO:CA	2.77	0.44
2:B:386:ALA:HB2	2:B:392:LYS:O	2.17	0.44
1:A:1066:VAL:O	1:A:1518:LYS:NZ	2.38	0.44
1:A:706:ASN:OD1	1:A:706:ASN:N	2.51	0.44
1:A:2190:TYR:O	1:A:2208:SER:HA	2.17	0.44
1:A:1220:ASP:OD2	1:A:1220:ASP:N	2.41	0.44
1:A:1669:THR:O	1:A:1670:SER:OG	2.34	0.44
1:A:2016:ASN:HB2	1:A:2053:ALA:HB3	1.99	0.44
2:B:392:LYS:N	2:B:392:LYS:HD2	2.33	0.44
1:A:15:SER:HB3	1:A:67:ARG:NH2	2.29	0.44
1:A:622:PHE:CE1	1:A:639:PRO:HD3	2.53	0.44
1:A:1140:LEU:HD11	1:A:1219:LYS:HE3	1.99	0.44
1:A:1411:ASP:N	1:A:1411:ASP:OD2	2.40	0.44
1:A:2459:TYR:CD1	1:A:2462:LYS:HE3	2.53	0.44
2:B:222:TYR:HA	2:B:225:LEU:CD2	2.48	0.44
1:A:723:ASP:OD2	1:A:724:LYS:N	2.51	0.43
1:A:1014:SER:O	1:A:1018:ASN:ND2	2.50	0.43
1:A:1049:GLU:OE2	1:A:1058:LEU:HD11	2.17	0.43
2:B:465:CYS:O	2:B:466:ALA:CB	2.66	0.43
1:A:102:ILE:HG23	1:A:131:ASP:HB2	2.00	0.43
1:A:338:ASP:OD2	1:A:339:GLN:N	2.49	0.43
1:A:518:LEU:HD22	1:A:707:VAL:HG21	1.99	0.43
1:A:2191:GLN:HB3	1:A:2206:ASN:HA	2.00	0.43
1:A:2277:VAL:HA	1:A:2285:GLU:O	2.18	0.43
1:A:1991:ILE:HG22	1:A:1992:ASN:ND2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:923:TYR:OH	1:A:970:LEU:HD11	2.18	0.43
1:A:1614:THR:OG1	1:A:1615:ASP:N	2.52	0.43
1:A:2080:TRP:CH2	1:A:2111:PHE:CZ	3.06	0.43
1:A:1270:ALA:C	1:A:1272:PHE:H	2.21	0.43
1:A:2156:LYS:HE3	1:A:2156:LYS:HB3	1.77	0.43
1:A:2212:THR:OG1	1:A:2226:SER:HA	2.18	0.43
1:A:2241:GLU:OE1	1:A:2272:LYS:HE3	2.19	0.43
1:A:2295:ASN:HD21	1:A:2300:GLN:CB	2.29	0.43
1:A:1029:GLU:H	1:A:1029:GLU:CD	2.22	0.43
1:A:1237:GLY:N	1:A:1277:THR:OG1	2.51	0.43
1:A:765:ASN:ND2	1:A:765:ASN:C	2.71	0.43
1:A:941:ASP:HB2	1:A:945:ASN:O	2.18	0.43
1:A:942:VAL:HG23	1:A:943:ASN:N	2.32	0.43
1:A:949:ASN:ND2	1:A:1040:GLY:O	2.52	0.43
1:A:1119:ALA:HB1	1:A:1242:LEU:HD11	2.00	0.43
1:A:2123:HIS:HB2	1:A:2132:PHE:HE2	1.83	0.43
1:A:2457:ILE:CD1	1:A:2459:TYR:HD2	2.32	0.43
2:B:433:ASN:O	2:B:434:VAL:HG23	2.19	0.43
1:A:2311:ILE:O	1:A:2311:ILE:HG13	2.19	0.43
1:A:975:ASN:ND2	1:A:976:ASN:O	2.52	0.43
1:A:2499:ILE:HG22	1:A:2500:GLY:N	2.34	0.43
2:B:376:GLU:OE1	2:B:403:LEU:HD23	2.19	0.42
1:A:1114:ILE:HD13	1:A:2260:ARG:HH22	1.84	0.42
1:A:2609:ASP:OD1	1:A:2609:ASP:N	2.48	0.42
1:A:1095:LEU:H	1:A:1095:LEU:HD23	1.84	0.42
1:A:1385:ILE:HG22	1:A:1386:ASP:H	1.83	0.42
1:A:1464:ASP:OD2	1:A:1468:ASN:HB2	2.19	0.42
2:B:221:ILE:O	2:B:225:LEU:HD22	2.19	0.42
1:A:1080:MET:O	1:A:1084:VAL:HG23	2.19	0.42
1:A:1219:LYS:O	1:A:1297:ARG:NH1	2.53	0.42
1:A:1834:ILE:HD13	1:A:1834:ILE:HG21	1.70	0.42
1:A:756:LEU:H	1:A:756:LEU:HG	1.77	0.42
1:A:1242:LEU:HD23	1:A:1242:LEU:HA	1.72	0.42
1:A:1929:ILE:HG22	1:A:1930:ASN:OD1	2.20	0.42
1:A:2027:ILE:HD11	1:A:2041:PRO:HG3	2.00	0.42
1:A:2531:GLU:OE2	1:A:2547:SER:OG	2.26	0.42
2:B:221:ILE:HG23	2:B:222:TYR:CE1	2.54	0.42
2:B:409:ARG:HA	2:B:409:ARG:NE	2.34	0.42
1:A:261:ARG:NH2	1:A:453:LEU:O	2.53	0.42
1:A:2526:GLY:N	1:A:2529:GLY:O	2.46	0.42
2:B:316:ARG:NE	2:B:396:VAL:HG12	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2133:ASN:HB3	1:A:2136:THR:HG22	2.02	0.42
1:A:2523:VAL:HB	1:A:2562:TYR:CE2	2.55	0.42
2:B:267:TRP:CZ2	2:B:380:TRP:CE3	3.07	0.42
1:A:97:LEU:HD12	1:A:282:VAL:HB	2.02	0.42
1:A:1234:TRP:CZ3	1:A:1276:ILE:HG12	2.55	0.42
1:A:1683:ILE:HG23	1:A:1710:TYR:CE1	2.55	0.42
1:A:1470:TYR:N	1:A:1470:TYR:CD2	2.88	0.42
1:A:2010:LYS:HD3	1:A:2012:ILE:HD11	2.02	0.42
2:B:213:ASN:OD1	2:B:214:THR:N	2.53	0.42
2:B:222:TYR:HA	2:B:225:LEU:HD23	2.02	0.42
1:A:269:ASP:O	1:A:272:ARG:HG2	2.19	0.41
1:A:971:ILE:O	1:A:971:ILE:CG2	2.66	0.41
1:A:1170:ASP:O	1:A:1231:LEU:HD12	2.20	0.41
1:A:955:ALA:HB3	1:A:956:PRO:HD3	2.02	0.41
1:A:518:LEU:CD2	1:A:707:VAL:HG21	2.50	0.41
1:A:581:HIS:HA	1:A:649:LYS:O	2.20	0.41
1:A:961:LEU:HD22	1:A:961:LEU:C	2.33	0.41
1:A:1357:SER:OG	1:A:1364:LYS:HD2	2.20	0.41
1:A:882:ASP:HB3	1:A:979:VAL:O	2.20	0.41
1:A:1001:ASN:OD1	1:A:1001:ASN:N	2.53	0.41
1:A:1151:ASP:OD2	1:A:1230:ARG:NH2	2.53	0.41
1:A:1434:LYS:O	1:A:1438:ILE:HG12	2.21	0.41
1:A:1140:LEU:HG	1:A:1143:ASP:HA	2.01	0.41
1:A:1354:ARG:HG2	1:A:1368:LEU:HD23	2.02	0.41
1:A:1410:ASP:OD1	1:A:1413:ILE:HB	2.20	0.41
1:A:1512:ASP:O	1:A:1514:ASN:ND2	2.54	0.41
1:A:1527:LYS:HE3	1:A:1527:LYS:HB2	1.67	0.41
1:A:2030:PHE:HB2	1:A:2039:PHE:HE2	1.84	0.41
2:B:296:HIS:ND1	2:B:342:LYS:HE2	2.36	0.41
2:B:374:GLN:HB2	2:B:375:PRO:HD2	2.01	0.41
1:A:1418:GLU:O	1:A:1426:TYR:HA	2.21	0.41
2:B:210:MET:HB3	2:B:225:LEU:HB3	2.03	0.41
2:B:427:ALA:HB3	2:B:474:TYR:CE1	2.56	0.41
1:A:1320:SER:O	1:A:1320:SER:OG	2.39	0.41
1:A:952:LEU:HD13	1:A:1625:ASN:OD1	2.20	0.41
1:A:1805:GLU:HB2	1:A:1816:ILE:HD13	2.02	0.41
1:A:2060:PHE:CE1	1:A:2069:TYR:HB2	2.56	0.41
1:A:2214:TRP:CE3	1:A:2221:LYS:HE2	2.56	0.41
1:A:2306:ASN:O	1:A:2307:LYS:HD3	2.21	0.41
1:A:2491:PHE:CE2	1:A:2518:LEU:HD13	2.55	0.41
1:A:172:LYS:O	1:A:176:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:864:ILE:HG22	1:A:973:TYR:CE2	2.56	0.41
1:A:1057:LEU:O	1:A:1061:GLU:HG3	2.21	0.41
1:A:2182:ASN:HB2	1:A:2186:GLN:HB3	2.03	0.41
1:A:569:ASN:ND2	1:A:602:LYS:HA	2.35	0.40
1:A:1029:GLU:OE1	1:A:1029:GLU:N	2.40	0.40
1:A:1801:ASN:OD1	1:A:1803:GLU:HG2	2.21	0.40
1:A:2260:ARG:HD2	1:A:2260:ARG:N	2.37	0.40
1:A:332:LYS:HE2	1:A:332:LYS:HB2	1.90	0.40
1:A:758:ASP:OD2	1:A:759:HIS:N	2.54	0.40
1:A:1689:LEU:HD12	1:A:1715:ILE:HB	2.03	0.40
2:B:212:LEU:HG	2:B:213:ASN:N	2.36	0.40
2:B:275:VAL:HG23	2:B:308:TRP:CE3	2.56	0.40
1:A:4:ILE:HD13	1:A:976:ASN:ND2	2.30	0.40
1:A:1291:LYS:HA	1:A:1318:THR:OG1	2.22	0.40
1:A:371:GLU:OE2	1:A:373:LYS:HE3	2.21	0.40
1:A:544:GLU:H	1:A:544:GLU:HG2	1.42	0.40
1:A:2292:THR:N	1:A:2295:ASN:O	2.54	0.40
1:A:2491:PHE:CZ	1:A:2518:LEU:HD13	2.56	0.40
1:A:1116:HIS:HB3	1:A:1121:SER:HB3	2.04	0.40
1:A:1814:LYS:O	1:A:1820:THR:HA	2.22	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	A	2612/2626 (100%)	2499 (96%)	109 (4%)	4 (0%)	47 79
2	B	337/424 (80%)	300 (89%)	34 (10%)	3 (1%)	17 56
All	All	2949/3050 (97%)	2799 (95%)	143 (5%)	7 (0%)	50 79

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1707	SER
2	B	300	LYS
1	A	1703	THR
2	B	145	GLU
1	A	1705	TYR
2	B	305	PRO
1	A	895	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2352/2362 (100%)	2290 (97%)	62 (3%)	46 76
2	B	290/360 (81%)	259 (89%)	31 (11%)	6 27
All	All	2642/2722 (97%)	2549 (96%)	93 (4%)	39 69

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	285	ASP
1	A	394	LEU
1	A	514	GLU
1	A	518	LEU
1	A	522	ASP
1	A	547	GLU
1	A	548	LEU
1	A	551	ASN
1	A	615	ASN
1	A	650	VAL
1	A	662	THR
1	A	756	LEU
1	A	757	LEU
1	A	759	HIS
1	A	764	LEU
1	A	765	ASN
1	A	853	SER

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Mol	Chain	Res	Type
1	A	937	ASN
1	A	938	ILE
1	A	939	ILE
1	A	952	LEU
1	A	958	VAL
1	A	961	LEU
1	A	965	PHE
1	A	966	PHE
1	A	973	TYR
1	A	1057	LEU
1	A	1069	ILE
1	A	1073	MET
1	A	1129	LEU
1	A	1400	TYR
1	A	1407	CYS
1	A	1470	TYR
1	A	1482	ILE
1	A	1499	ASN
1	A	1546	SER
1	A	1577	ASN
1	A	1641	THR
1	A	1643	ASN
1	A	1646	PHE
1	A	1647	SER
1	A	1659	TYR
1	A	1683	ILE
1	A	1705	TYR
1	A	1784	ASP
1	A	1785	ILE
1	A	1817	ASP
1	A	2063	ILE
1	A	2072	ASN
1	A	2114	ASP
1	A	2155	ASP
1	A	2168	ASP
1	A	2233	THR
1	A	2270	ASP
1	A	2304	TYR
1	A	2326	THR
1	A	2459	TYR
1	A	2460	GLN
1	A	2507	LEU

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Mol	Chain	Res	Type
1	A	2565	ASP
1	A	2581	THR
1	A	2600	ASP
2	B	146	ASN
2	B	148	CYS
2	B	188	MET
2	B	204	SER
2	B	222	TYR
2	B	227	HIS
2	B	231	CYS
2	B	284	SER
2	B	287	THR
2	B	306	TRP
2	B	329	GLU
2	B	332	ILE
2	B	333	SER
2	B	342	LYS
2	B	355	LEU
2	B	381	ILE
2	B	382	SER
2	B	392	LYS
2	B	401	LYS
2	B	413	ARG
2	B	417	ASP
2	B	418	ASN
2	B	419	LEU
2	B	434	VAL
2	B	437	CYS
2	B	441	SER
2	B	451	ASN
2	B	459	THR
2	B	460	SER
2	B	470	ARG
2	B	478	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	404	ASN
1	A	529	GLN
1	A	551	ASN
1	A	553	ASN

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Mol	Chain	Res	Type
1	A	585	GLN
1	A	603	ASN
1	A	606	ASN
1	A	611	GLN
1	A	692	ASN
1	A	814	ASN
1	A	852	ASN
1	A	859	ASN
1	A	879	ASN
1	A	937	ASN
1	A	949	ASN
1	A	976	ASN
1	A	1188	HIS
1	A	1196	ASN
1	A	1198	ASN
1	A	1214	ASN
1	A	1446	ASN
1	A	1457	ASN
1	A	1514	ASN
1	A	1548	ASN
1	A	1576	HIS
1	A	1792	HIS
1	A	1867	ASN
1	A	1868	ASN
1	A	1909	ASN
1	A	1959	ASN
1	A	1971	ASN
1	A	1992	ASN
1	A	1993	ASN
1	A	2022	ASN
1	A	2026	GLN
1	A	2047	ASN
1	A	2057	GLN
1	A	2058	ASN
1	A	2160	GLN
1	A	2294	ASN
1	A	2461	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	$\#\|Z\| > 2$
1	SEP	A	517	1	8,9,10	1.54	2 (25%)	8,12,14	2.01	2 (25%)

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
1	SEP	A	517	1	-	4/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	517	SEP	P-OG	2.40	1.67	1.60
1	A	517	SEP	P-O3P	-2.22	1.46	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	517	SEP	OG-P-O1P	3.87	117.34	106.47
1	A	517	SEP	OG-CB-CA	2.95	111.02	108.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	517	SEP	N-CA-CB-OG
1	A	517	SEP	CB-OG-P-O2P
1	A	517	SEP	CB-OG-P-O3P
1	A	517	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

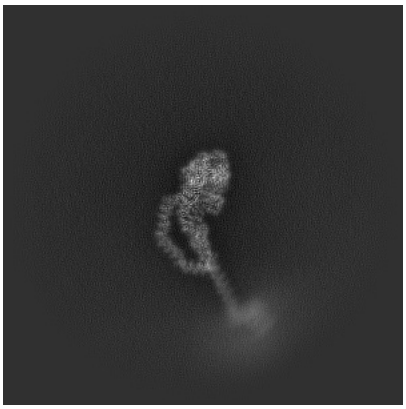
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36301. These allow visual inspection of the internal detail of the map and identification of artifacts.

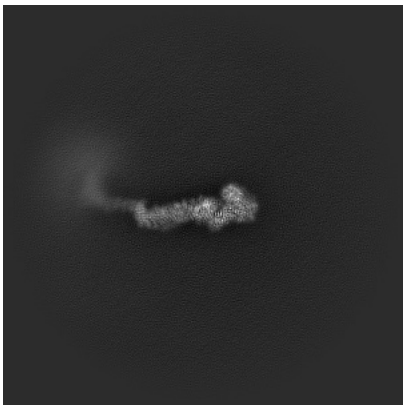
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

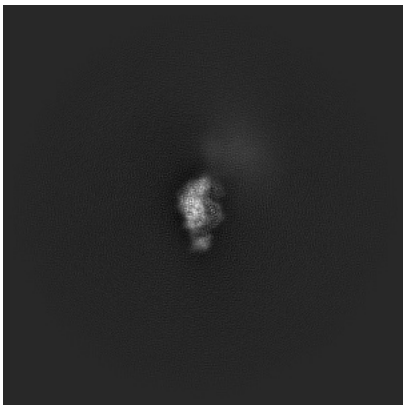
6.1.1 Primary map



X

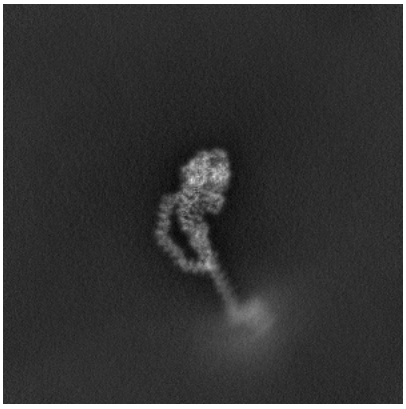


Y

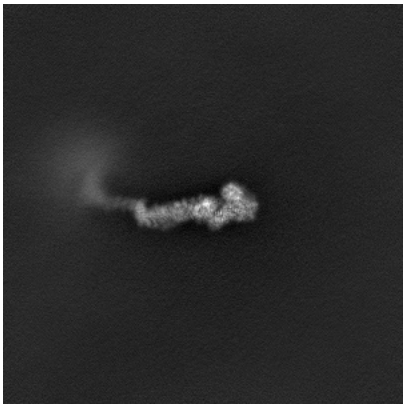


Z

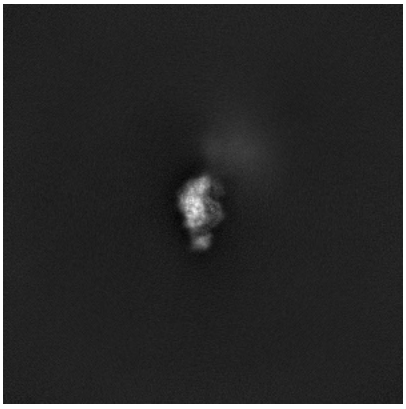
6.1.2 Raw map



X



Y



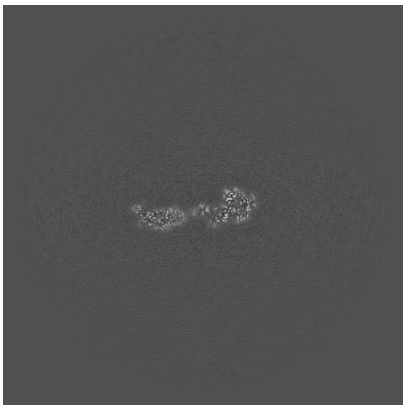
Z

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

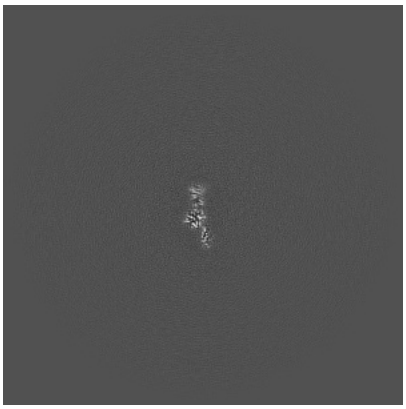
6.2 Central slices (i)

6.2.1 Primary map

X Index: 300

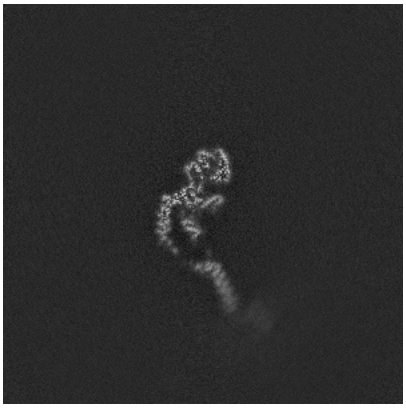


Y Index: 300

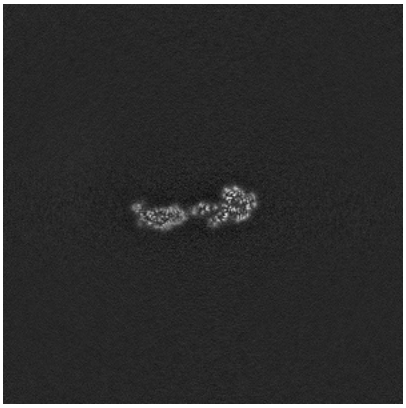


Z Index: 300

6.2.2 Raw map



X Index: 300



Y Index: 300

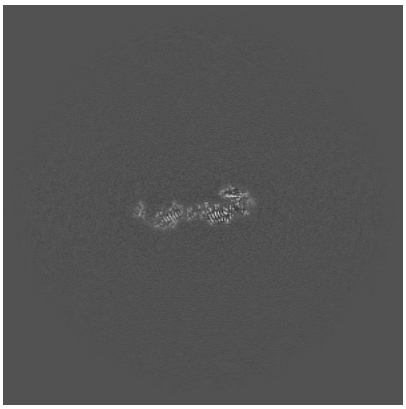
Z Index: 300

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

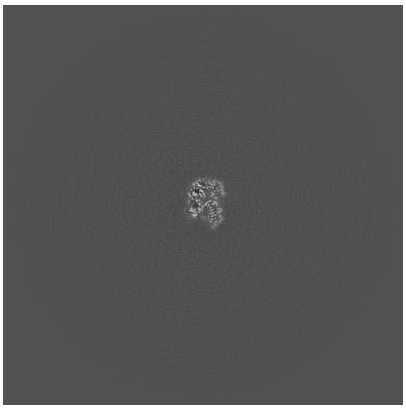
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 286



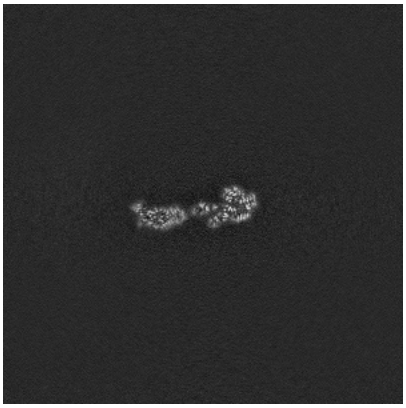
Y Index: 292



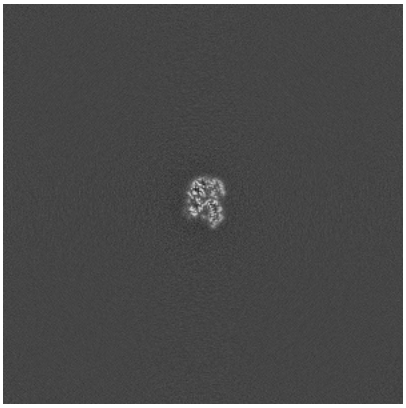
Z Index: 340

6.3.2 Raw map

X Index: 285



Y Index: 301

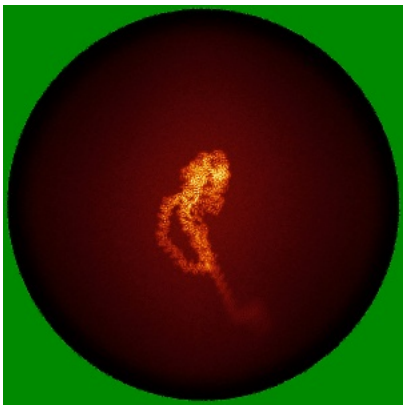


Z Index: 340

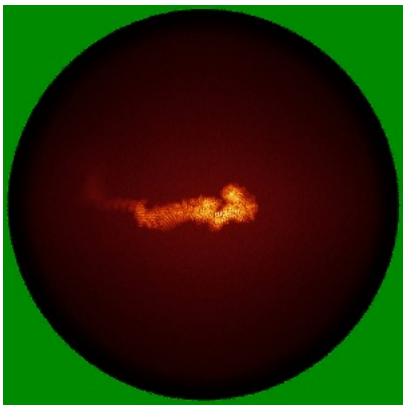
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

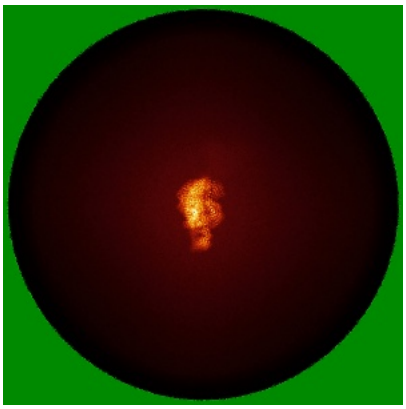
6.4.1 Primary map



X



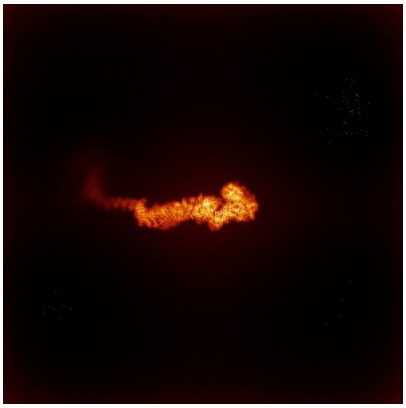
Y



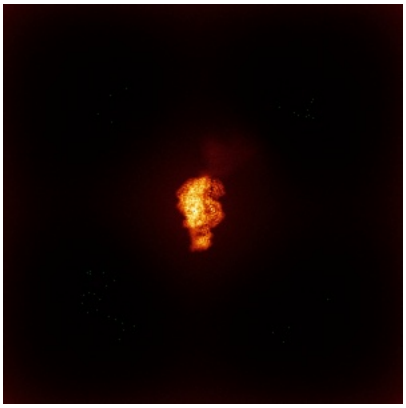
Z

6.4.2 Raw map

X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. 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

X Y Z

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.

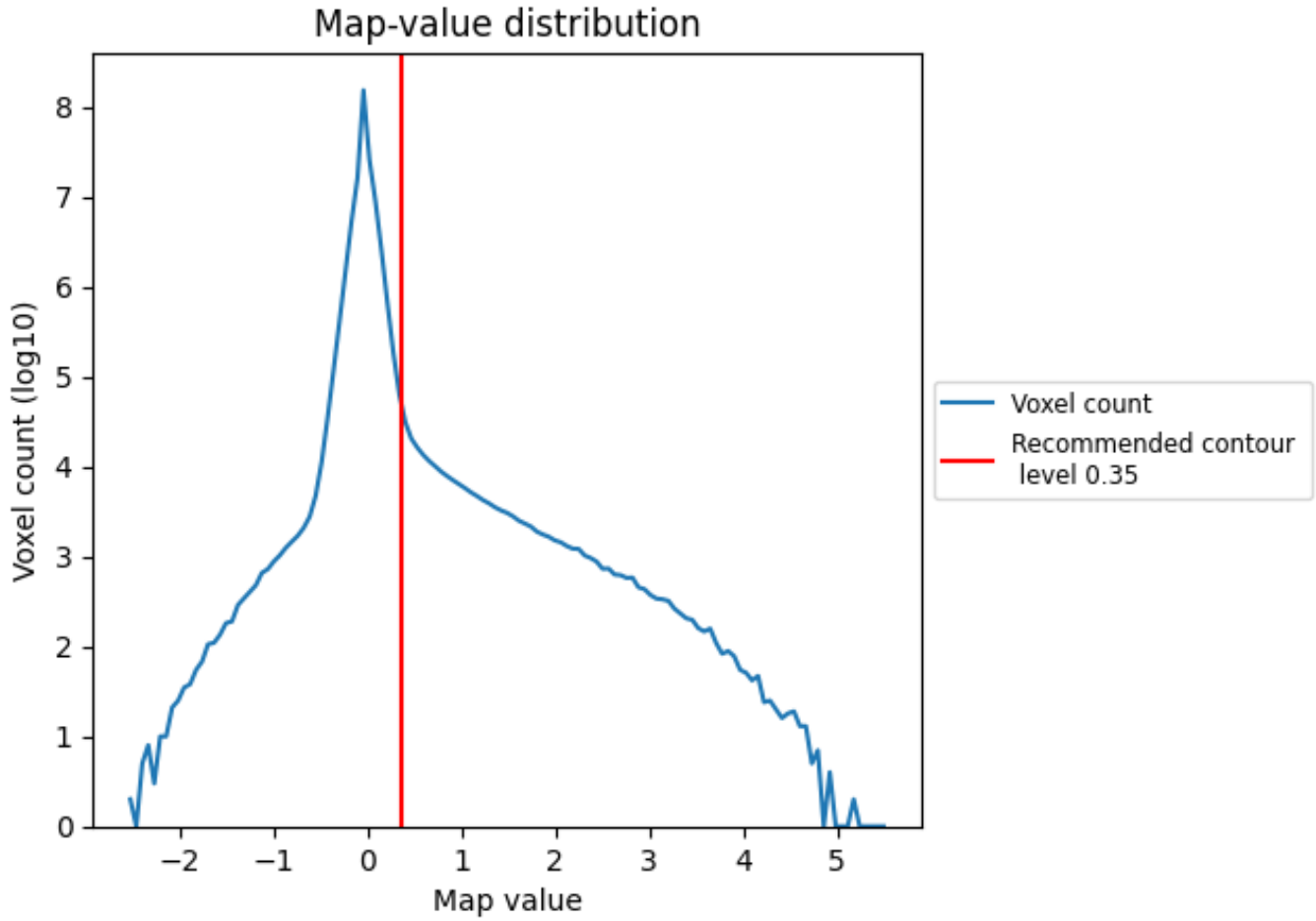
6.6 Mask visualisation (i)

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

7 Map analysis

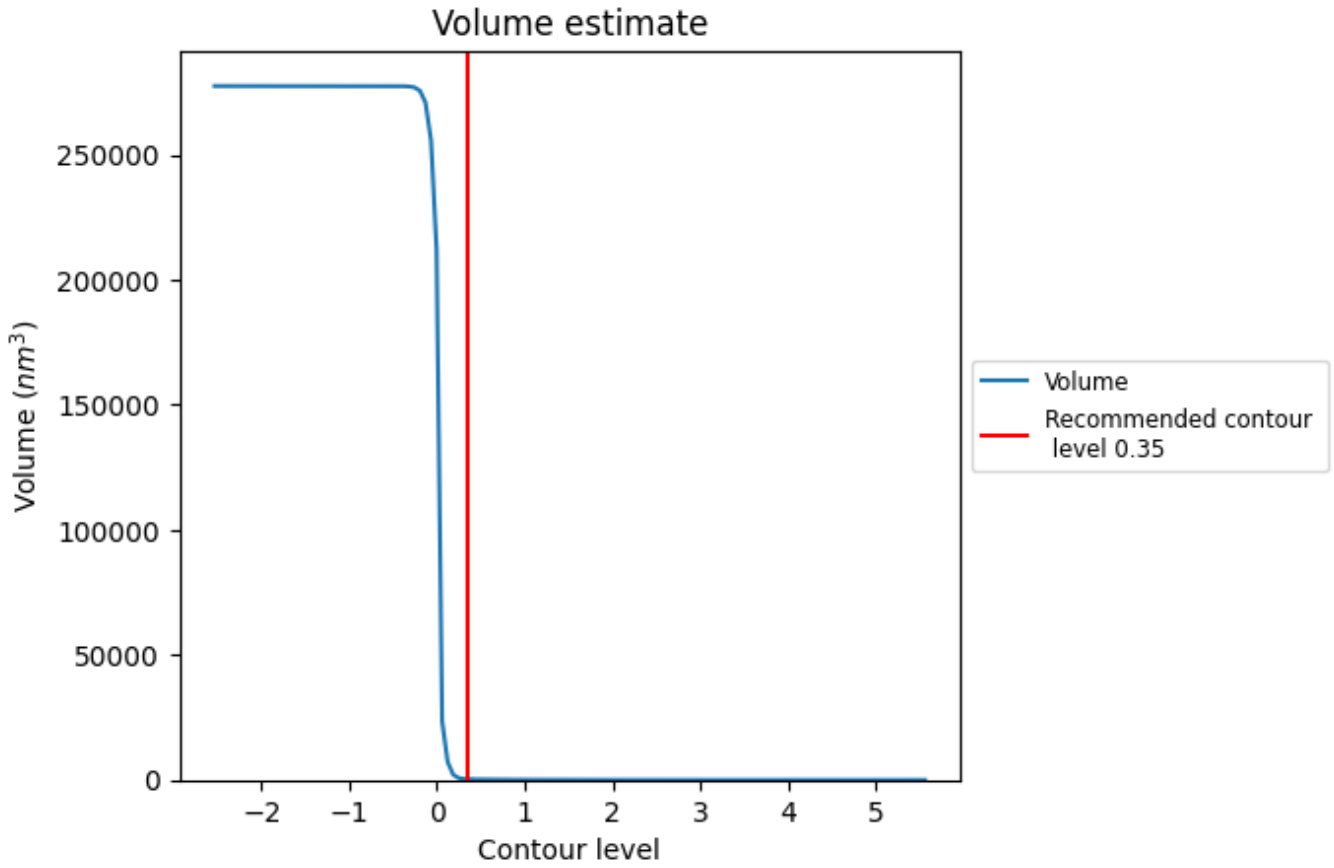
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

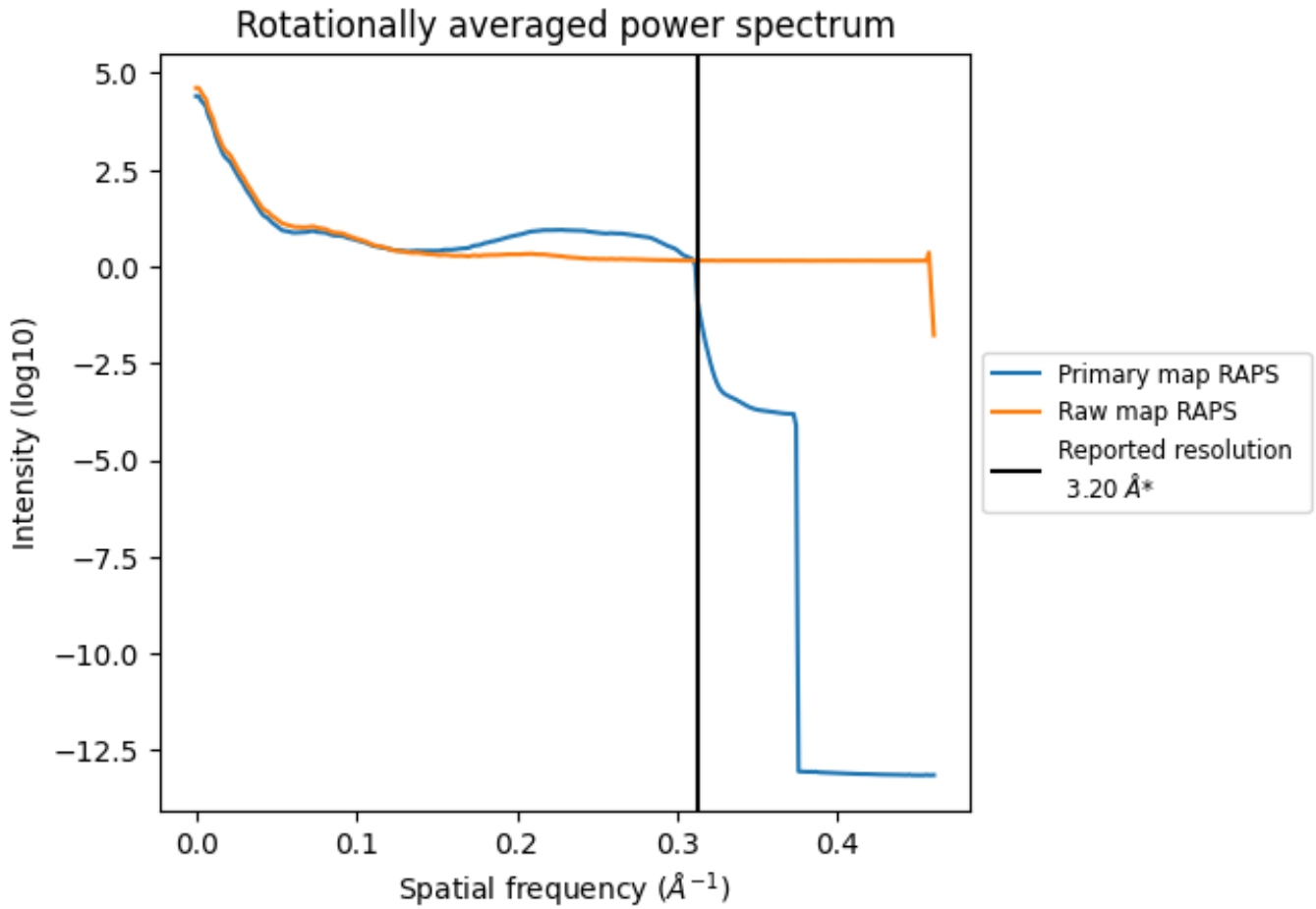
7.2 Volume estimate



The volume at the recommended contour level is 325 nm^3; this corresponds to an approximate mass of 293 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 (i)

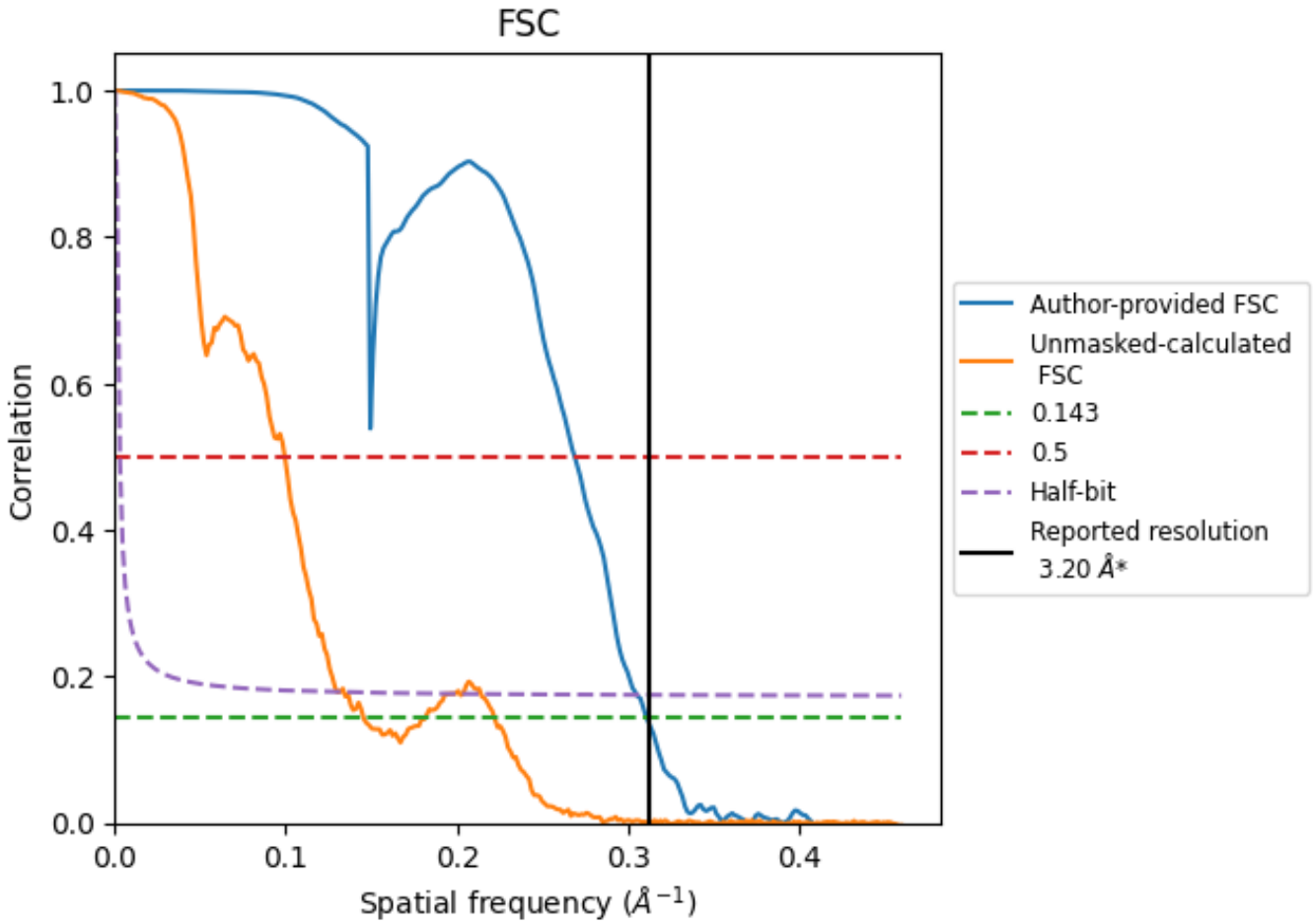


*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

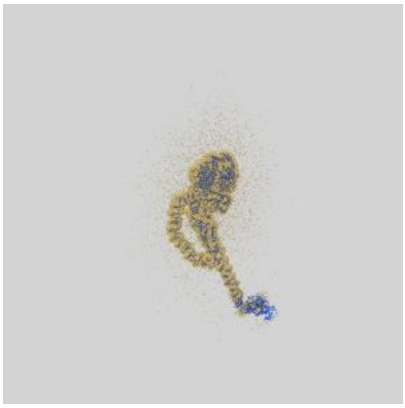
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.21	3.72	3.28
Unmasked-calculated*	6.87	10.06	7.67

*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 6.87 differs from the reported value 3.2 by more than 10 %

9 Map-model fit

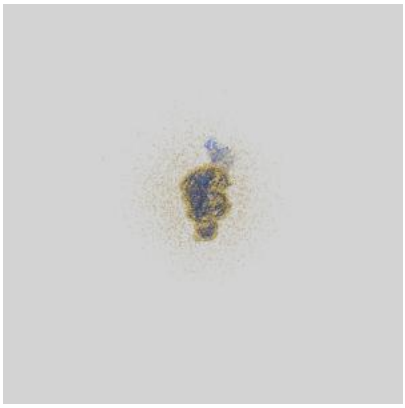
This section contains information regarding the fit between EMDB map EMD-36301 and PDB model 8JHZ. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay



X

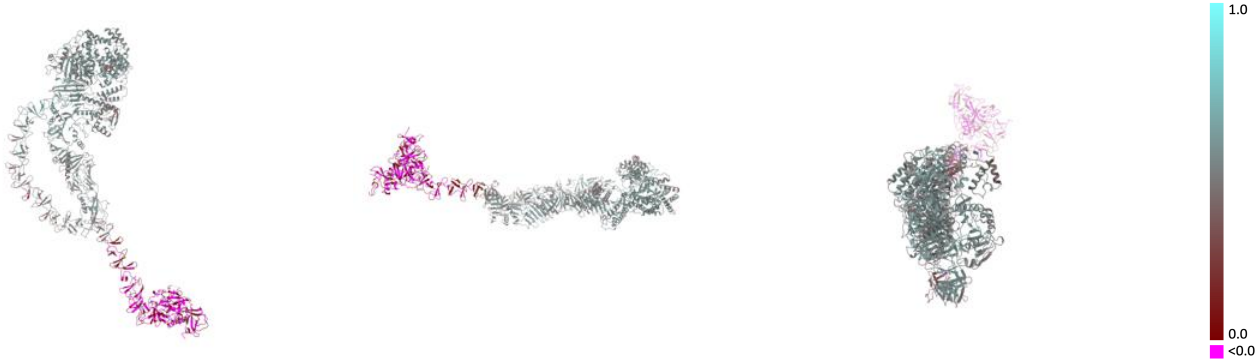
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 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.

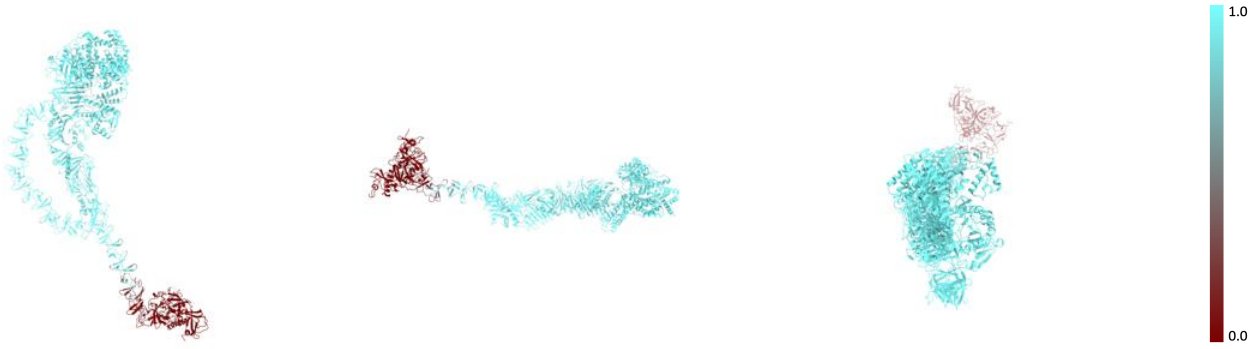
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

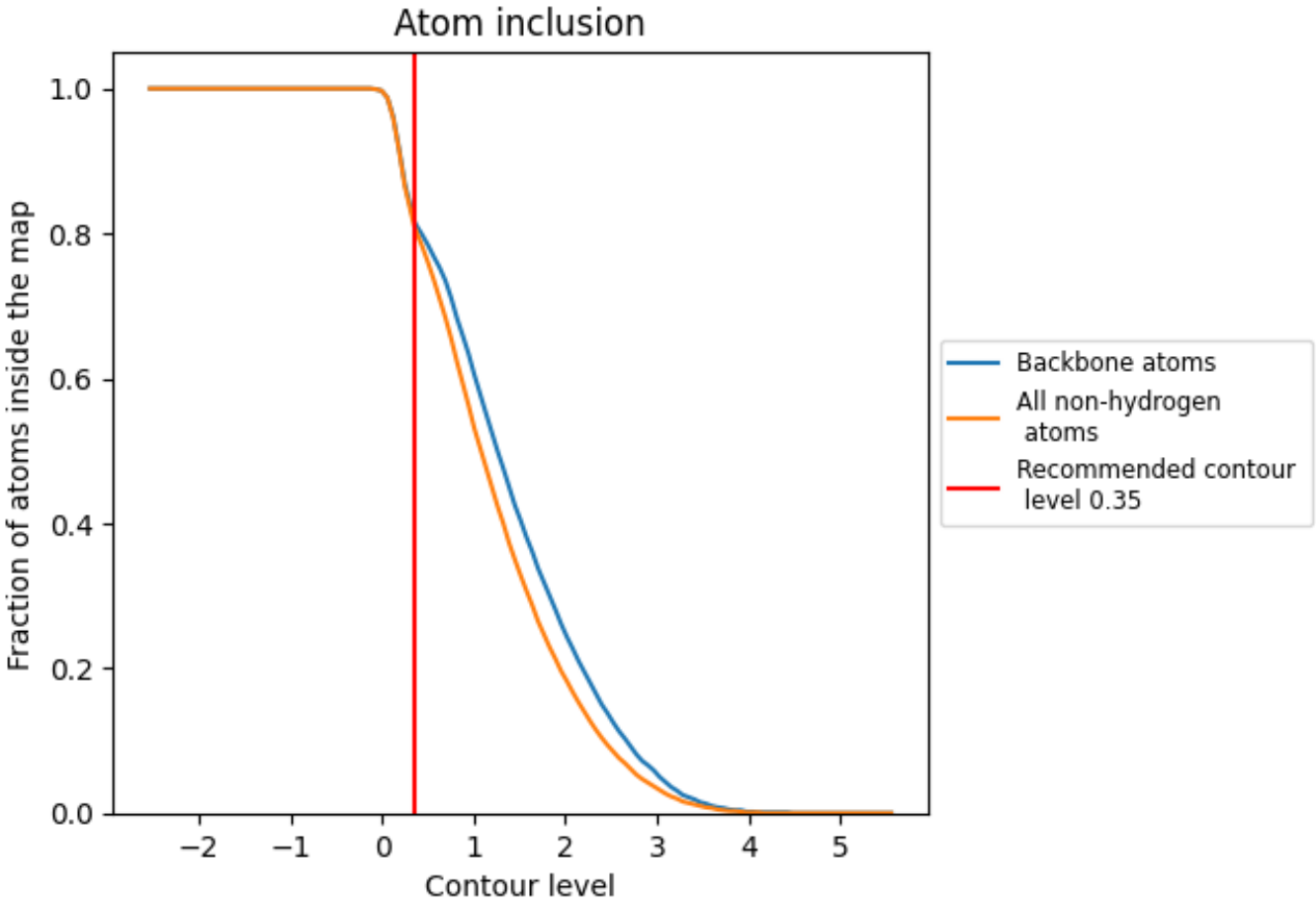
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 81% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8110	0.4040
A	0.9100	0.4560
B	0.0210	-0.0020