



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:19 PM UTC

PDB ID : 8YYV / pdb_00008yyv
EMDB ID : EMD-39680
Title : A dimeric STAT1-DNA complex
Authors : Sugiyama, A.; Minami, M.; Sugita, Y.; Ose, T.
Deposited on : 2024-04-04
Resolution : 3.07 Å(reported)
Based on initial model : 1BF5

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

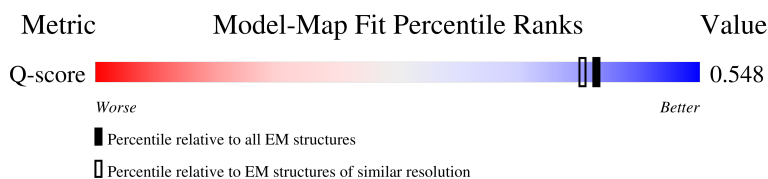
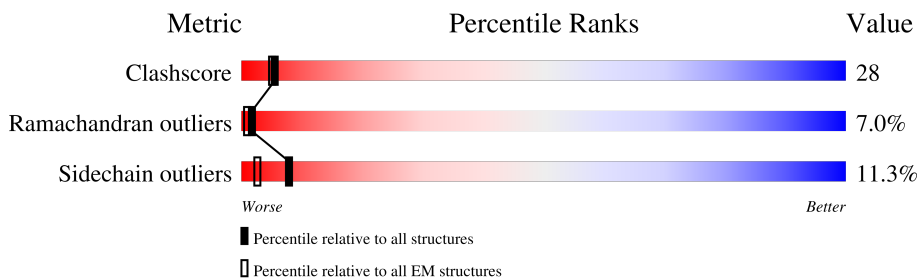
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.07 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13977 (2.57 - 3.57)

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	A	776	
2	C	18	
3	B	18	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5249 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 Signal transducer and activator of transcription 1-alpha/beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	553	Total	C	N	O	P	S	0	0
			4511	2880	774	836	1	20		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	initiating methionine	UNP P42224
A	-24	ASN	-	expression tag	UNP P42224
A	-23	HIS	-	expression tag	UNP P42224
A	-22	LYS	-	expression tag	UNP P42224
A	-21	HIS	-	expression tag	UNP P42224
A	-20	HIS	-	expression tag	UNP P42224
A	-19	HIS	-	expression tag	UNP P42224
A	-18	HIS	-	expression tag	UNP P42224
A	-17	HIS	-	expression tag	UNP P42224
A	-16	HIS	-	expression tag	UNP P42224
A	-15	HIS	-	expression tag	UNP P42224
A	-14	HIS	-	expression tag	UNP P42224
A	-13	HIS	-	expression tag	UNP P42224
A	-12	HIS	-	expression tag	UNP P42224
A	-11	SER	-	expression tag	UNP P42224
A	-10	SER	-	expression tag	UNP P42224
A	-9	GLY	-	expression tag	UNP P42224
A	-8	GLU	-	expression tag	UNP P42224
A	-7	ASN	-	expression tag	UNP P42224
A	-6	LEU	-	expression tag	UNP P42224
A	-5	TYR	-	expression tag	UNP P42224
A	-4	PHE	-	expression tag	UNP P42224
A	-3	GLN	-	expression tag	UNP P42224
A	-2	GLY	-	expression tag	UNP P42224
A	-1	HIS	-	expression tag	UNP P42224
A	0	MET	-	expression tag	UNP P42224

- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*CP*AP*GP*TP*TP*TP*CP*CP*CP

*GP*TP*AP*AP*AP*TP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	18	Total	C	N	O	P	0	0
			366	175	65	108	18		

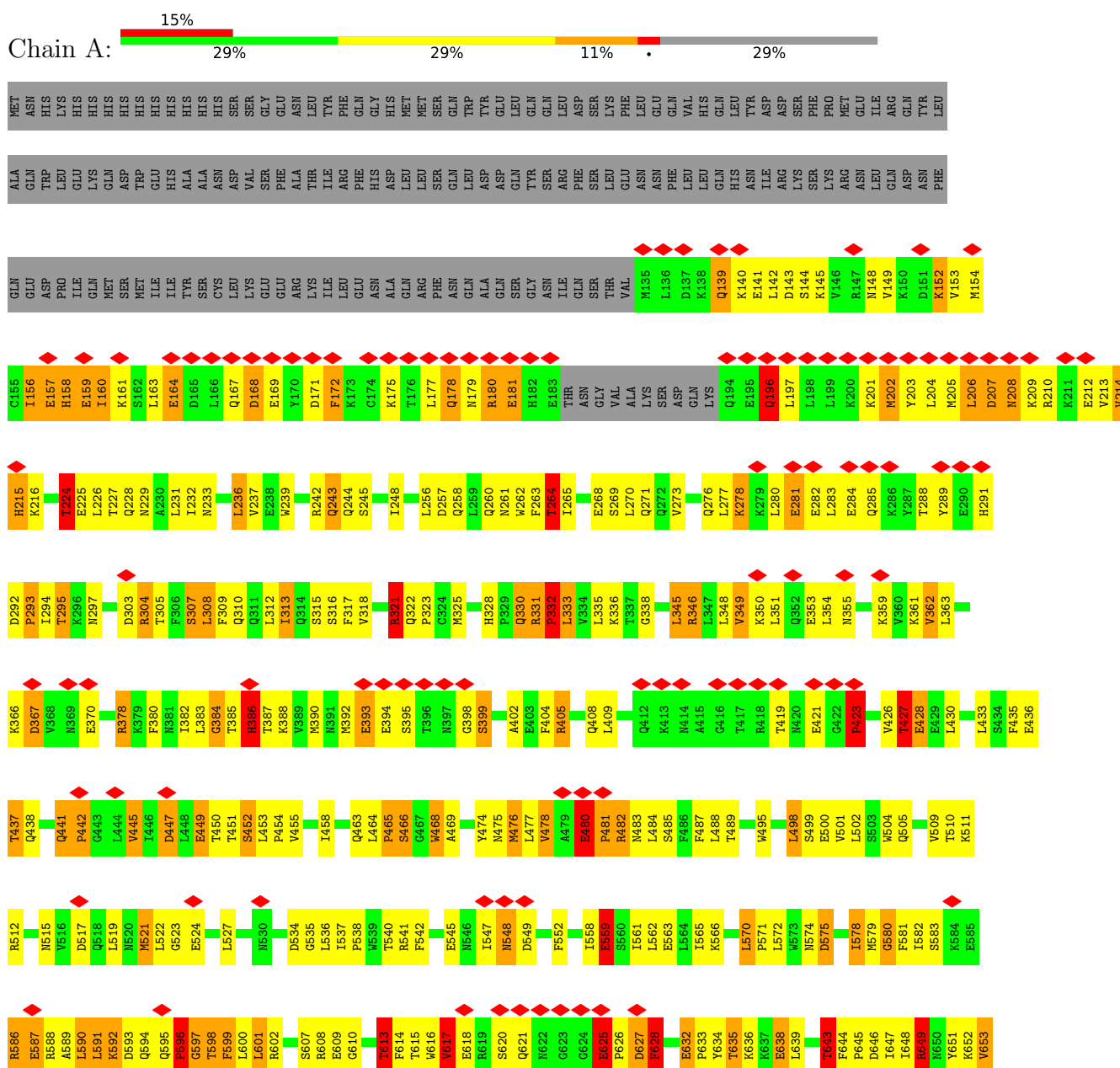
- Molecule 3 is a DNA chain called DNA (5'-D(P*TP*GP*CP*AP*TP*TP*TP*AP*CP*GP*GP*GP*AP*AP*AP*CP*TP*G)-3').

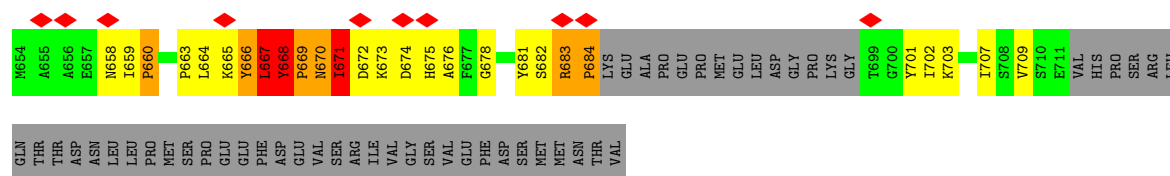
Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	18	Total	C	N	O	P	0	0
			372	177	69	108	18		

3 Residue-property plots

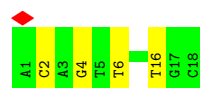
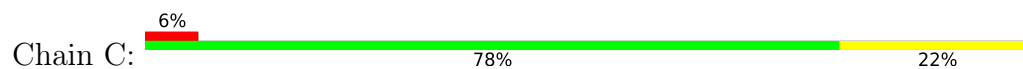
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Signal transducer and activator of transcription 1-alpha/beta

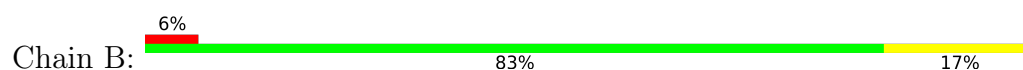




- Molecule 2: DNA (5'-D(P*AP*CP*AP*GP*TP*TP*TP*CP*CP*CP*GP*TP*AP*AP*AP*T P*GP*C)-3')



- Molecule 3: DNA (5'-D(P*TP*GP*CP*AP*TP*TP*TP*AP*CP*GP*GP*GP*AP*AP*AP*C P*TP*G)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	115824	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	18000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	7.667	Depositor
Minimum map value	-6.063	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.432	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	213.84001, 108.240005, 161.04001	wwPDB
Map dimensions	162, 82, 122	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.85	4/4589 (0.1%)	1.82	111/6206 (1.8%)
2	C	0.45	0/409	1.28	4/628 (0.6%)
3	B	0.43	0/417	1.25	3/642 (0.5%)
All	All	0.80	4/5415 (0.1%)	1.74	118/7476 (1.6%)

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	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	427	THR	C-O	5.61	1.31	1.24
1	A	466	SER	CA-CB	-5.44	1.44	1.53
1	A	427	THR	CA-C	5.29	1.59	1.52
1	A	315	SER	CA-CB	-5.17	1.45	1.53

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	427	THR	OG1-CB-CG2	-12.16	84.99	109.30
1	A	635	THR	CA-CB-OG1	-10.99	93.11	109.60
1	A	590	LEU	N-CA-CB	-9.98	95.18	111.06
1	A	599	PHE	N-CA-CB	-9.83	93.33	111.13
1	A	668	TYR	N-CA-CB	9.66	127.56	110.37
1	A	346	ARG	CB-CA-C	-9.50	94.42	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	ARG	CB-CA-C	-8.41	97.19	110.14
1	A	227	THR	CA-CB-OG1	-8.31	97.13	109.60
1	A	164	GLU	CB-CG-CD	8.26	126.64	112.60
1	A	335	LEU	N-CA-CB	-8.19	97.08	111.08
1	A	468	TRP	N-CA-C	-8.19	102.18	112.90
1	A	428	GLU	CB-CA-C	-8.16	92.81	111.83
1	A	271	GLN	N-CA-CB	8.16	122.30	110.06
1	A	304	ARG	CA-CB-CG	-7.95	98.20	114.10
1	A	214	VAL	N-CA-CB	7.92	119.82	110.55
1	A	264	THR	CA-CB-OG1	-7.80	97.90	109.60
1	A	427	THR	CA-C-N	7.76	134.05	122.87
1	A	427	THR	C-N-CA	7.76	134.05	122.87
1	A	244	GLN	CB-CA-C	-7.70	95.10	110.42
1	A	214	VAL	CB-CA-C	-7.66	102.17	111.97
1	A	643	THR	CA-CB-OG1	-7.64	98.14	109.60
1	A	427	THR	CA-CB-OG1	7.61	121.02	109.60
1	A	330	GLN	CA-C-N	-7.58	114.51	122.85
1	A	330	GLN	C-N-CA	-7.58	114.51	122.85
1	A	592	LYS	CB-CA-C	7.46	124.22	111.46
3	B	10	DG	C4'-C3'-O3'	-7.24	99.14	110.00
1	A	596	PRO	N-CA-CB	-7.21	95.68	103.25
1	A	563	GLU	N-CA-CB	7.20	120.81	110.16
1	A	617	VAL	CB-CA-C	-7.17	99.94	110.62
1	A	242	ARG	N-CA-CB	7.01	121.01	110.22
1	A	280	LEU	N-CA-CB	-7.01	99.42	110.28
1	A	310	GLN	CB-CA-C	6.83	121.60	110.88
1	A	307	SER	O-C-N	6.82	129.18	122.09
1	A	349	VAL	N-CA-CB	-6.59	105.69	112.28
1	A	540	THR	N-CA-C	-6.55	104.06	111.07
1	A	229	ASN	CA-CB-CG	-6.52	106.08	112.60
1	A	602	ARG	CA-CB-CG	-6.52	101.05	114.10
1	A	427	THR	CA-C-O	6.46	129.75	120.51
2	C	2	DC	O3'-P-O5'	-6.44	94.34	104.00
1	A	441	GLN	CB-CA-C	6.37	118.53	110.76
1	A	559	GLU	CB-CA-C	6.37	121.36	110.79
1	A	423	PRO	N-CA-CB	-6.33	96.60	103.25
1	A	651	TYR	CA-C-O	-6.31	114.87	121.55
1	A	671	ILE	CB-CA-C	6.28	118.67	110.12
1	A	613	THR	OG1-CB-CG2	-6.21	96.88	109.30
1	A	332	PRO	N-CA-CB	-6.14	96.80	103.25
1	A	304	ARG	N-CA-CB	6.14	118.87	109.91
1	A	521	MET	CG-SD-CE	-6.12	87.43	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	674	ASP	CB-CA-C	6.03	121.24	110.81
1	A	313	ILE	O-C-N	5.99	128.00	121.83
2	C	6	DT	O3'-P-O5'	5.98	112.97	104.00
1	A	602	ARG	CB-CA-C	-5.93	99.74	111.60
1	A	378	ARG	CA-CB-CG	-5.92	102.25	114.10
1	A	385	THR	CA-CB-OG1	-5.90	100.76	109.60
1	A	268	GLU	N-CA-CB	5.87	118.53	110.01
1	A	208	ASN	CA-CB-CG	-5.85	106.75	112.60
1	A	312	LEU	CB-CA-C	-5.85	101.46	110.81
1	A	586	ARG	N-CA-C	-5.85	105.91	113.16
3	B	2	DG	O3'-P-O5'	-5.84	95.24	104.00
1	A	209	LYS	N-CA-CB	5.84	118.70	110.12
1	A	449	GLU	CB-CG-CD	5.82	122.50	112.60
1	A	449	GLU	CB-CA-C	-5.80	98.88	110.42
1	A	158	HIS	CB-CA-C	5.79	121.95	110.42
1	A	487	PHE	CA-CB-CG	-5.79	108.01	113.80
1	A	304	ARG	CB-CA-C	-5.78	102.06	110.96
1	A	592	LYS	N-CA-CB	-5.78	102.88	111.43
1	A	244	GLN	N-CA-CB	5.78	120.25	110.49
1	A	345	LEU	CA-C-O	-5.72	114.90	121.82
1	A	570	LEU	O-C-N	5.70	125.55	120.48
1	A	587	GLU	N-CA-C	-5.69	106.01	113.12
1	A	668	TYR	CB-CA-C	-5.68	98.98	110.17
1	A	524	GLU	N-CA-C	-5.66	105.87	112.89
1	A	465	PRO	N-CD-CG	-5.66	94.72	103.20
3	B	4	DA	O3'-P-O5'	-5.64	95.54	104.00
1	A	243	GLN	N-CA-CB	5.62	118.46	110.13
1	A	563	GLU	CB-CG-CD	5.58	122.08	112.60
1	A	570	LEU	CA-C-N	5.56	124.75	118.97
1	A	570	LEU	C-N-CA	5.56	124.75	118.97
1	A	524	GLU	CB-CA-C	5.54	121.57	109.99
1	A	627	ASP	N-CA-C	-5.54	106.36	113.01
1	A	480	GLU	N-CA-CB	5.51	120.18	110.37
1	A	628	PHE	N-CA-CB	-5.49	101.21	110.49
1	A	625	GLU	CB-CG-CD	5.49	121.93	112.60
1	A	156	ILE	O-C-N	5.47	127.25	121.89
1	A	678	GLY	O-C-N	5.46	129.79	122.70
1	A	388	LYS	CB-CA-C	5.44	120.94	109.79
1	A	609	GLU	N-CA-C	-5.42	106.66	113.28
1	A	617	VAL	N-CA-C	5.42	116.28	108.48
1	A	362	VAL	CB-CA-C	-5.41	103.61	111.68
1	A	660	PRO	N-CA-CB	-5.39	97.00	102.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	638	GLU	CB-CG-CD	5.33	121.66	112.60
1	A	317	PHE	CB-CA-C	5.31	119.00	110.29
1	A	317	PHE	N-CA-CB	-5.29	101.25	109.87
1	A	308	LEU	N-CA-CB	5.27	117.65	110.01
2	C	4	DG	O3'-P-O5'	-5.25	96.12	104.00
1	A	566	LYS	N-CA-C	-5.24	105.64	111.36
1	A	666	TYR	N-CA-CB	-5.23	101.76	110.80
2	C	16	DT	O3'-P-O5'	-5.20	96.20	104.00
1	A	178	GLN	N-CA-CB	5.17	117.51	110.01
1	A	433	LEU	N-CA-CB	5.17	117.61	110.17
1	A	601	LEU	N-CA-CB	-5.17	102.44	110.55
1	A	224	THR	O-C-N	5.15	128.02	122.15
1	A	592	LYS	N-CA-C	-5.15	103.94	111.30
1	A	207	ASP	CB-CA-C	5.14	120.65	110.42
1	A	152	LYS	CB-CA-C	5.14	119.42	110.68
1	A	643	THR	OG1-CB-CG2	5.12	119.55	109.30
1	A	281	GLU	N-CA-CB	5.12	117.64	110.12
1	A	278	LYS	N-CA-CB	-5.11	102.47	110.44
1	A	157	GLU	CB-CG-CD	5.11	121.28	112.60
1	A	563	GLU	CB-CA-C	-5.10	102.18	110.85
1	A	559	GLU	N-CA-C	-5.08	105.74	111.28
1	A	632	GLU	CB-CA-C	-5.04	100.23	110.17
1	A	312	LEU	N-CA-CB	5.04	117.45	109.94
1	A	331	ARG	CD-NE-CZ	-5.03	117.36	124.40
1	A	297	ASN	CB-CA-C	5.03	118.44	109.29
1	A	437	THR	CA-CB-OG1	-5.03	102.06	109.60
1	A	635	THR	OG1-CB-CG2	5.02	119.34	109.30
1	A	590	LEU	CB-CA-C	5.02	116.87	109.29

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	180	ARG	Sidechain
1	A	196	GLN	Peptide
1	A	321	ARG	Sidechain
1	A	404	PHE	Peptide
1	A	427	THR	Peptide
1	A	489	THR	Peptide
1	A	591	LEU	Peptide
1	A	593	ASP	Peptide
1	A	649	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	A	4511	0	4527	283	0
2	C	366	0	204	0	0
3	B	372	0	204	0	0
All	All	5249	0	4935	283	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 28.

All (283) 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:663:PRO:O	1:A:664:LEU:HD23	1.53	1.09
1:A:618:GLU:H	1:A:626:PRO:HG2	1.22	1.03
1:A:428:GLU:HG3	1:A:428:GLU:O	1.61	1.00
1:A:521:MET:CE	1:A:581:PHE:HB3	1.93	0.97
1:A:521:MET:HE3	1:A:581:PHE:HB3	1.47	0.97
1:A:618:GLU:H	1:A:626:PRO:CG	1.77	0.96
1:A:332:PRO:O	1:A:333:LEU:HG	1.65	0.96
1:A:649:ARG:HD3	1:A:681:TYR:CZ	2.01	0.95
1:A:668:TYR:HB3	1:A:669:PRO:HD3	1.49	0.93
1:A:664:LEU:O	1:A:673:LYS:NZ	2.04	0.90
1:A:599:PHE:HA	1:A:615:THR:O	1.72	0.88
1:A:164:GLU:O	1:A:168:ASP:OD1	1.91	0.87
1:A:428:GLU:O	1:A:428:GLU:CG	2.24	0.82
1:A:579:MET:HE1	1:A:590:LEU:HD21	1.62	0.81
1:A:362:VAL:O	1:A:363:LEU:HD23	1.82	0.79
1:A:594:GLN:HE21	1:A:595:GLN:HG2	1.47	0.78
1:A:594:GLN:NE2	1:A:595:GLN:CG	2.48	0.77
1:A:594:GLN:HE21	1:A:595:GLN:CG	1.99	0.76
1:A:292:ASP:O	1:A:294:ILE:N	2.20	0.76
1:A:598:THR:O	1:A:616:TRP:HA	1.87	0.74
1:A:683:ARG:HB3	1:A:684:PRO:HD3	1.68	0.74
1:A:649:ARG:HD3	1:A:681:TYR:CE1	2.23	0.73
1:A:370:GLU:OE2	1:A:485:SER:OG	2.06	0.73
1:A:405:ARG:HH11	1:A:405:ARG:HB2	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:GLN:NE2	1:A:595:GLN:HG2	2.05	0.71
1:A:178:GLN:NE2	1:A:179:ASN:OD1	2.21	0.71
1:A:627:ASP:O	1:A:628:PHE:HB2	1.91	0.71
1:A:618:GLU:N	1:A:626:PRO:CG	2.54	0.71
1:A:386:HIS:O	1:A:387:THR:C	2.33	0.70
1:A:618:GLU:N	1:A:626:PRO:HG2	2.01	0.70
1:A:594:GLN:NE2	1:A:595:GLN:HG3	2.07	0.70
1:A:598:THR:HA	1:A:666:TYR:O	1.92	0.69
1:A:214:VAL:HG13	1:A:215:HIS:N	2.08	0.69
1:A:214:VAL:CG1	1:A:215:HIS:N	2.55	0.69
1:A:309:PHE:CZ	1:A:313:ILE:HD11	2.28	0.69
1:A:643:THR:OG1	1:A:645:PRO:HD2	1.93	0.69
1:A:437:THR:OG1	1:A:438:GLN:N	2.25	0.69
1:A:600:LEU:C	1:A:601:LEU:HD23	2.18	0.68
1:A:207:ASP:O	1:A:208:ASN:C	2.37	0.68
1:A:594:GLN:CG	1:A:595:GLN:H	2.05	0.68
1:A:441:GLN:HG2	1:A:442:PRO:HD2	1.76	0.68
1:A:484:LEU:N	1:A:484:LEU:HD23	2.08	0.68
1:A:620:SER:O	1:A:621:GLN:HB3	1.92	0.68
1:A:158:HIS:O	1:A:160:ILE:N	2.27	0.68
1:A:172:PHE:O	1:A:175:LYS:HG2	1.94	0.68
1:A:309:PHE:CE2	1:A:313:ILE:CD1	2.76	0.68
1:A:598:THR:HG23	1:A:666:TYR:HB2	1.74	0.68
1:A:316:SER:OG	1:A:348:LEU:N	2.25	0.67
1:A:316:SER:O	1:A:318:VAL:HG13	1.94	0.67
1:A:168:ASP:O	1:A:171:ASP:N	2.28	0.67
1:A:332:PRO:HD2	1:A:468:TRP:CH2	2.30	0.66
1:A:158:HIS:O	1:A:159:GLU:C	2.37	0.66
1:A:163:LEU:HD22	1:A:213:VAL:HG21	1.76	0.66
1:A:350:LYS:HE2	1:A:398:GLY:HA3	1.77	0.65
1:A:594:GLN:HG2	1:A:595:GLN:N	2.11	0.65
1:A:626:PRO:HB2	1:A:628:PHE:H	1.60	0.65
1:A:591:LEU:O	1:A:628:PHE:HE1	1.80	0.64
1:A:390:MET:HG2	1:A:402:ALA:HB2	1.79	0.63
1:A:666:TYR:HA	1:A:671:ILE:O	1.98	0.63
1:A:670:ASN:O	1:A:670:ASN:ND2	2.32	0.63
1:A:203:TYR:O	1:A:204:LEU:C	2.42	0.63
1:A:464:LEU:C	1:A:464:LEU:HD23	2.24	0.62
1:A:270:LEU:O	1:A:273:VAL:N	2.33	0.62
1:A:239:TRP:CZ2	1:A:256:LEU:HD21	2.34	0.62
1:A:309:PHE:CE2	1:A:313:ILE:HD11	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:LEU:HD12	1:A:676:ALA:HB1	1.80	0.62
1:A:495:TRP:HB2	1:A:527:LEU:HD11	1.81	0.61
1:A:595:GLN:O	1:A:597:GLY:N	2.33	0.61
1:A:480:GLU:OE2	1:A:482:ARG:HG3	2.00	0.61
1:A:537:ILE:N	1:A:537:ILE:HD12	2.15	0.61
1:A:332:PRO:O	1:A:333:LEU:CG	2.46	0.60
1:A:378:ARG:HH11	1:A:380:PHE:HZ	1.49	0.60
1:A:421:GLU:C	1:A:423:PRO:HD3	2.27	0.60
1:A:292:ASP:HB3	1:A:295:THR:OG1	2.01	0.60
1:A:600:LEU:O	1:A:601:LEU:HD23	2.02	0.60
1:A:154:MET:O	1:A:157:GLU:N	2.33	0.59
1:A:325:MET:HE3	1:A:328:HIS:CD2	2.37	0.59
1:A:515:ASN:OD1	1:A:517:ASP:N	2.36	0.59
1:A:232:ILE:HG22	1:A:233:ASN:OD1	2.03	0.59
1:A:362:VAL:C	1:A:363:LEU:HD23	2.28	0.59
1:A:547:ILE:O	1:A:549:ASP:N	2.36	0.59
1:A:635:THR:OG1	1:A:636:LYS:N	2.34	0.59
1:A:649:ARG:HD3	1:A:681:TYR:CE2	2.37	0.59
1:A:547:ILE:O	1:A:548:ASN:C	2.46	0.58
1:A:309:PHE:CE2	1:A:313:ILE:HD12	2.37	0.58
1:A:353:GLU:OE1	1:A:353:GLU:N	2.36	0.58
1:A:167:GLN:OE1	1:A:283:LEU:HD13	2.04	0.58
1:A:332:PRO:HD2	1:A:468:TRP:HH2	1.67	0.58
1:A:512:ARG:NH1	1:A:574:ASN:O	2.36	0.58
1:A:634:TYR:HB3	1:A:639:LEU:CD1	2.33	0.58
1:A:570:LEU:N	1:A:571:PRO:CD	2.68	0.57
1:A:683:ARG:CB	1:A:684:PRO:HD3	2.35	0.57
1:A:597:GLY:O	1:A:666:TYR:N	2.34	0.57
1:A:180:ARG:O	1:A:181:GLU:HB2	2.04	0.57
1:A:239:TRP:CE2	1:A:256:LEU:HD21	2.40	0.57
1:A:613:THR:CG2	1:A:614:PHE:N	2.68	0.56
1:A:158:HIS:O	1:A:161:LYS:N	2.34	0.56
1:A:284:GLU:HB2	1:A:294:ILE:HD11	1.87	0.56
1:A:292:ASP:O	1:A:295:THR:N	2.38	0.56
1:A:664:LEU:HB2	1:A:673:LYS:NZ	2.20	0.56
1:A:201:LYS:O	1:A:202:MET:HB2	2.05	0.56
1:A:515:ASN:OD1	1:A:515:ASN:C	2.49	0.56
1:A:260:GLN:O	1:A:264:THR:HG22	2.06	0.56
1:A:668:TYR:HB3	1:A:669:PRO:CD	2.30	0.56
1:A:652:LYS:O	1:A:653:VAL:HB	2.06	0.56
1:A:591:LEU:O	1:A:628:PHE:CE1	2.59	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LYS:HA	1:A:281:GLU:HB2	1.88	0.55
1:A:599:PHE:CA	1:A:615:THR:O	2.51	0.55
1:A:316:SER:HG	1:A:348:LEU:H	1.54	0.55
1:A:451:THR:HG21	1:A:482:ARG:HD2	1.89	0.55
1:A:143:ASP:O	1:A:144:SER:C	2.50	0.54
1:A:139:GLN:O	1:A:143:ASP:HB2	2.07	0.54
1:A:203:TYR:O	1:A:206:LEU:N	2.41	0.54
1:A:480:GLU:N	1:A:481:PRO:HD2	2.22	0.54
1:A:239:TRP:CE2	1:A:256:LEU:CD2	2.91	0.54
1:A:152:LYS:O	1:A:156:ILE:HG12	2.07	0.54
1:A:582:ILE:HD11	1:A:586:ARG:HD3	1.90	0.54
1:A:649:ARG:CD	1:A:681:TYR:CE2	2.90	0.54
1:A:441:GLN:CG	1:A:442:PRO:HD2	2.38	0.54
1:A:480:GLU:CD	1:A:480:GLU:O	2.51	0.54
1:A:345:LEU:HD21	1:A:435:PHE:CG	2.42	0.54
1:A:350:LYS:O	1:A:350:LYS:HG2	2.08	0.54
1:A:393:GLU:N	1:A:393:GLU:OE2	2.39	0.54
1:A:668:TYR:CD1	1:A:668:TYR:C	2.82	0.54
1:A:505:GLN:OE1	1:A:505:GLN:HA	2.07	0.53
1:A:463:GLN:O	1:A:464:LEU:C	2.52	0.53
1:A:363:LEU:HD12	1:A:366:LYS:HD3	1.91	0.53
1:A:588:ARG:O	1:A:590:LEU:N	2.42	0.53
1:A:648:ILE:HG23	1:A:664:LEU:HD12	1.90	0.53
1:A:145:LYS:O	1:A:148:ASN:HB3	2.09	0.53
1:A:572:LEU:HD12	1:A:572:LEU:H	1.73	0.52
1:A:383:LEU:O	1:A:384:GLY:O	2.26	0.52
1:A:142:LEU:O	1:A:143:ASP:C	2.52	0.52
1:A:224:THR:HG22	1:A:308:LEU:HD13	1.92	0.52
1:A:236:LEU:O	1:A:237:VAL:C	2.52	0.51
1:A:596:PRO:HA	1:A:617:VAL:O	2.10	0.51
1:A:161:LYS:O	1:A:164:GLU:N	2.44	0.51
1:A:474:TYR:C	1:A:476:MET:H	2.18	0.51
1:A:542:PHE:O	1:A:542:PHE:CG	2.64	0.51
1:A:618:GLU:N	1:A:626:PRO:HG3	2.25	0.50
1:A:228:GLN:NE2	1:A:308:LEU:HD22	2.26	0.50
1:A:466:SER:O	1:A:469:ALA:HB3	2.12	0.50
1:A:228:GLN:HE22	1:A:308:LEU:HD22	1.77	0.50
1:A:141:GLU:O	1:A:142:LEU:C	2.55	0.49
1:A:359:LYS:CG	1:A:387:THR:HG23	2.42	0.49
1:A:626:PRO:C	1:A:628:PHE:H	2.18	0.49
1:A:359:LYS:HG3	1:A:387:THR:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:GLU:O	1:A:500:GLU:HG3	2.13	0.49
1:A:304:ARG:O	1:A:305:THR:C	2.54	0.49
1:A:649:ARG:CD	1:A:681:TYR:CZ	2.86	0.49
1:A:140:LYS:O	1:A:141:GLU:C	2.56	0.48
1:A:331:ARG:HG3	1:A:468:TRP:CE3	2.48	0.48
1:A:480:GLU:OE2	1:A:480:GLU:O	2.31	0.48
1:A:618:GLU:C	1:A:626:PRO:HG3	2.38	0.48
1:A:345:LEU:HD12	1:A:345:LEU:N	2.29	0.48
1:A:617:VAL:HG12	1:A:628:PHE:CD1	2.48	0.48
1:A:260:GLN:NE2	1:A:346:ARG:HH21	2.12	0.48
1:A:277:LEU:HD23	1:A:277:LEU:HA	1.62	0.48
1:A:594:GLN:HG2	1:A:595:GLN:HG2	1.96	0.48
1:A:168:ASP:O	1:A:171:ASP:HB3	2.14	0.48
1:A:393:GLU:O	1:A:395:SER:N	2.46	0.48
1:A:474:TYR:O	1:A:476:MET:N	2.47	0.48
1:A:419:THR:HG22	1:A:419:THR:O	2.13	0.48
1:A:586:ARG:O	1:A:586:ARG:HG2	2.13	0.48
1:A:480:GLU:O	1:A:482:ARG:N	2.46	0.47
1:A:552:PHE:CD1	1:A:608:ARG:HG2	2.49	0.47
1:A:668:TYR:CD1	1:A:668:TYR:O	2.67	0.47
1:A:627:ASP:O	1:A:628:PHE:CB	2.62	0.47
1:A:330:GLN:O	1:A:331:ARG:HD2	2.13	0.47
1:A:294:ILE:O	1:A:294:ILE:HG13	2.14	0.47
1:A:172:PHE:HA	1:A:175:LYS:HD3	1.96	0.47
1:A:501:VAL:O	1:A:504:TRP:N	2.48	0.47
1:A:536:LEU:O	1:A:538:PRO:HD3	2.15	0.47
1:A:316:SER:OG	1:A:348:LEU:HB2	2.15	0.47
1:A:485:SER:HB3	1:A:488:LEU:HD12	1.97	0.47
1:A:643:THR:HG1	1:A:645:PRO:HD2	1.80	0.47
1:A:582:ILE:HD11	1:A:586:ARG:HH11	1.80	0.47
1:A:598:THR:CG2	1:A:666:TYR:HB2	2.42	0.47
1:A:153:VAL:HG21	1:A:269:SER:HB3	1.97	0.46
1:A:596:PRO:HG3	1:A:618:GLU:O	2.14	0.46
1:A:578:ILE:HG22	1:A:580:GLY:N	2.31	0.46
1:A:668:TYR:CB	1:A:669:PRO:HD3	2.29	0.46
1:A:480:GLU:H	1:A:481:PRO:HD2	1.79	0.46
1:A:617:VAL:CG1	1:A:628:PHE:CD1	2.98	0.46
1:A:207:ASP:O	1:A:210:ARG:N	2.48	0.46
1:A:308:LEU:HD23	1:A:308:LEU:HA	1.54	0.46
1:A:351:LEU:HB2	1:A:354:LEU:HD22	1.98	0.46
1:A:257:ASP:O	1:A:258:GLN:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ASP:C	1:A:294:ILE:N	2.73	0.46
1:A:435:PHE:N	1:A:435:PHE:CD1	2.83	0.46
1:A:594:GLN:HG2	1:A:595:GLN:H	1.71	0.46
1:A:355:ASN:CG	1:A:392:MET:HG3	2.40	0.46
1:A:570:LEU:N	1:A:571:PRO:HD3	2.30	0.46
1:A:288:THR:HG22	1:A:289:TYR:H	1.79	0.46
1:A:362:VAL:HG12	1:A:363:LEU:N	2.31	0.46
1:A:292:ASP:O	1:A:293:PRO:C	2.59	0.46
1:A:231:LEU:O	1:A:231:LEU:HD12	2.15	0.45
1:A:366:LYS:O	1:A:367:ASP:HB2	2.16	0.45
1:A:168:ASP:O	1:A:169:GLU:C	2.59	0.45
1:A:703:LYS:H	1:A:703:LYS:HD2	1.80	0.45
1:A:322:GLN:HB3	1:A:323:PRO:CD	2.47	0.45
1:A:361:LYS:HG3	1:A:363:LEU:HD21	1.99	0.45
1:A:480:GLU:O	1:A:481:PRO:C	2.59	0.45
1:A:552:PHE:CZ	1:A:607:SER:O	2.70	0.45
1:A:156:ILE:CG2	1:A:276:GLN:NE2	2.79	0.45
1:A:331:ARG:HG2	1:A:464:LEU:HD21	1.99	0.45
1:A:626:PRO:C	1:A:628:PHE:N	2.75	0.45
1:A:673:LYS:C	1:A:675:HIS:H	2.25	0.45
1:A:303:ASP:O	1:A:307:SER:OG	2.32	0.45
1:A:578:ILE:HG22	1:A:580:GLY:H	1.81	0.45
1:A:588:ARG:C	1:A:590:LEU:H	2.25	0.45
1:A:474:TYR:C	1:A:476:MET:N	2.75	0.45
1:A:527:LEU:HA	1:A:527:LEU:HD23	1.68	0.45
1:A:338:GLY:O	1:A:408:GLN:NE2	2.50	0.44
1:A:668:TYR:CB	1:A:669:PRO:CD	2.92	0.44
1:A:261:ASN:O	1:A:262:TRP:C	2.58	0.44
1:A:308:LEU:O	1:A:309:PHE:C	2.58	0.44
1:A:349:VAL:HG12	1:A:349:VAL:O	2.17	0.44
1:A:139:GLN:OE1	1:A:139:GLN:N	2.48	0.44
1:A:292:ASP:C	1:A:294:ILE:H	2.25	0.44
1:A:510:THR:OG1	1:A:511:LYS:N	2.49	0.44
1:A:522:LEU:O	1:A:523:GLY:C	2.59	0.44
1:A:156:ILE:HG22	1:A:276:GLN:NE2	2.32	0.44
1:A:638:GLU:H	1:A:638:GLU:CD	2.23	0.44
1:A:644:PHE:N	1:A:645:PRO:CD	2.81	0.44
1:A:269:SER:O	1:A:273:VAL:HG23	2.17	0.44
1:A:452:SER:OG	1:A:453:LEU:O	2.36	0.44
1:A:572:LEU:HD12	1:A:572:LEU:N	2.33	0.44
1:A:325:MET:HE3	1:A:328:HIS:HD2	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:LEU:HD21	1:A:435:PHE:CB	2.49	0.43
1:A:261:ASN:O	1:A:264:THR:HG22	2.19	0.43
1:A:552:PHE:CD1	1:A:608:ARG:CG	3.02	0.43
1:A:591:LEU:C	1:A:592:LYS:HG3	2.44	0.43
1:A:521:MET:HE3	1:A:521:MET:HB3	1.83	0.43
1:A:670:ASN:C	1:A:671:ILE:CG1	2.90	0.43
1:A:239:TRP:CZ2	1:A:256:LEU:CD2	3.02	0.43
1:A:336:LYS:HA	1:A:458:ILE:O	2.18	0.43
1:A:502:LEU:HD23	1:A:502:LEU:HA	1.70	0.43
1:A:625:GLU:OE1	1:A:625:GLU:N	2.51	0.43
1:A:672:ASP:CG	1:A:672:ASP:O	2.61	0.43
1:A:390:MET:CG	1:A:402:ALA:HB2	2.47	0.43
1:A:477:LEU:O	1:A:478:VAL:HG23	2.17	0.43
1:A:644:PHE:HB3	1:A:645:PRO:HD3	2.01	0.42
1:A:646:ASP:O	1:A:647:ILE:C	2.61	0.42
1:A:154:MET:O	1:A:157:GLU:HB3	2.19	0.42
1:A:203:TYR:O	1:A:205:MET:N	2.52	0.42
1:A:212:GLU:O	1:A:216:LYS:HB2	2.19	0.42
1:A:172:PHE:CD1	1:A:172:PHE:C	2.93	0.42
1:A:167:GLN:HA	1:A:206:LEU:HD21	2.00	0.42
1:A:575:ASP:N	1:A:575:ASP:OD1	2.52	0.42
1:A:363:LEU:CD1	1:A:366:LYS:HD3	2.50	0.42
1:A:617:VAL:CG1	1:A:628:PHE:CE1	3.02	0.42
1:A:282:GLU:O	1:A:285:GLN:N	2.53	0.42
1:A:537:ILE:HD12	1:A:537:ILE:H	1.84	0.42
1:A:559:GLU:C	1:A:559:GLU:OE1	2.63	0.42
1:A:177:LEU:O	1:A:177:LEU:HD23	2.20	0.42
1:A:652:LYS:HB2	1:A:709:VAL:HG22	2.00	0.42
1:A:207:ASP:OD1	1:A:289:TYR:OH	2.35	0.42
1:A:481:PRO:O	1:A:483:ASN:N	2.53	0.42
1:A:483:ASN:O	1:A:485:SER:N	2.53	0.41
1:A:498:LEU:C	1:A:498:LEU:HD23	2.46	0.41
1:A:378:ARG:HE	1:A:427:THR:HG22	1.85	0.41
1:A:453:LEU:O	1:A:454:PRO:C	2.62	0.41
1:A:601:LEU:HD23	1:A:601:LEU:N	2.35	0.41
1:A:670:ASN:O	1:A:671:ILE:HG12	2.19	0.41
1:A:570:LEU:HD23	1:A:570:LEU:HA	1.76	0.41
1:A:638:GLU:OE1	1:A:638:GLU:N	2.40	0.41
1:A:145:LYS:O	1:A:149:VAL:HG23	2.20	0.41
1:A:262:TRP:O	1:A:263:PHE:C	2.63	0.41
1:A:288:THR:O	1:A:289:TYR:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:ASN:O	1:A:659:ILE:C	2.62	0.41
1:A:172:PHE:HD1	1:A:175:LYS:NZ	2.19	0.41
1:A:561:ILE:O	1:A:565:ILE:HG13	2.20	0.41
1:A:265:ILE:H	1:A:265:ILE:HG13	1.71	0.41
1:A:284:GLU:HB2	1:A:294:ILE:CD1	2.50	0.41
1:A:537:ILE:N	1:A:537:ILE:CD1	2.83	0.41
1:A:665:LYS:HB3	1:A:666:TYR:CD2	2.56	0.40
1:A:447:ASP:OD1	1:A:447:ASP:C	2.64	0.40
1:A:349:VAL:HG12	1:A:351:LEU:HG	2.04	0.40
1:A:499:SER:HB2	1:A:519:LEU:HD22	2.04	0.40
1:A:534:ASP:O	1:A:535:GLY:C	2.65	0.40
1:A:632:GLU:OE1	1:A:633:PRO:HD2	2.21	0.40
1:A:682:SER:O	1:A:684:PRO:HD2	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	546/776 (70%)	422 (77%)	86 (16%)	38 (7%)	1 5

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	GLU
1	A	202	MET
1	A	423	PRO
1	A	480	GLU
1	A	481	PRO
1	A	482	ARG
1	A	545	GLU
1	A	548	ASN

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Mol	Chain	Res	Type
1	A	596	PRO
1	A	683	ARG
1	A	384	GLY
1	A	445	VAL
1	A	159	GLU
1	A	197	LEU
1	A	333	LEU
1	A	386	HIS
1	A	394	GLU
1	A	399	SER
1	A	475	ASN
1	A	667	LEU
1	A	668	TYR
1	A	669	PRO
1	A	293	PRO
1	A	332	PRO
1	A	393	GLU
1	A	589	ALA
1	A	597	GLY
1	A	653	VAL
1	A	196	GLN
1	A	367	ASP
1	A	449	GLU
1	A	628	PHE
1	A	580	GLY
1	A	610	GLY
1	A	442	PRO
1	A	465	PRO
1	A	248	ILE
1	A	426	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	A	506/719 (70%)	449 (89%)	57 (11%)	5 22

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	A	160	ILE
1	A	168	ASP
1	A	172	PHE
1	A	196	GLN
1	A	206	LEU
1	A	215	HIS
1	A	224	THR
1	A	225	GLU
1	A	226	LEU
1	A	236	LEU
1	A	243	GLN
1	A	245	SER
1	A	264	THR
1	A	291	HIS
1	A	295	THR
1	A	321	ARG
1	A	332	PRO
1	A	382	ILE
1	A	386	HIS
1	A	399	SER
1	A	405	ARG
1	A	409	LEU
1	A	423	PRO
1	A	430	LEU
1	A	436	GLU
1	A	445	VAL
1	A	447	ASP
1	A	450	THR
1	A	452	SER
1	A	455	VAL
1	A	476	MET
1	A	478	VAL
1	A	498	LEU
1	A	509	VAL
1	A	541	ARG
1	A	558	ILE
1	A	559	GLU
1	A	562	LEU
1	A	575	ASP
1	A	578	ILE
1	A	583	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	587	GLU
1	A	596	PRO
1	A	598	THR
1	A	613	THR
1	A	617	VAL
1	A	625	GLU
1	A	643	THR
1	A	649	ARG
1	A	660	PRO
1	A	667	LEU
1	A	670	ASN
1	A	671	ILE
1	A	684	PRO
1	A	702	ILE
1	A	707	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
1	A	244	GLN
1	A	260	GLN
1	A	271	GLN
1	A	276	GLN
1	A	297	ASN
1	A	357	ASN
1	A	381	ASN
1	A	386	HIS
1	A	408	GLN
1	A	475	ASN
1	A	594	GLN
1	A	670	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	PTR	A	701	1	15,16,17	0.88	1 (6%)	17,22,24	1.21	1 (5%)

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	PTR	A	701	1	-	1/10/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	701	PTR	P-O3P	-2.30	1.46	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	701	PTR	O2P-P-OH	3.36	115.27	105.32

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	701	PTR	CZ-OH-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

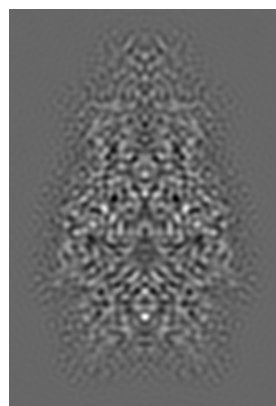
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39680. These allow visual inspection of the internal detail of the map and identification of artifacts.

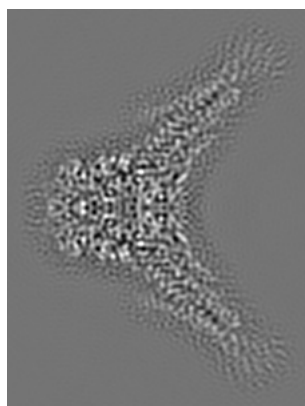
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

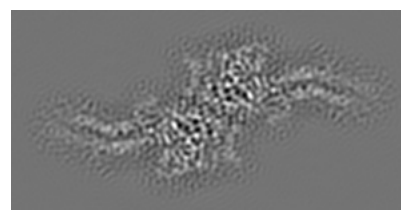
6.1.1 Primary map



X

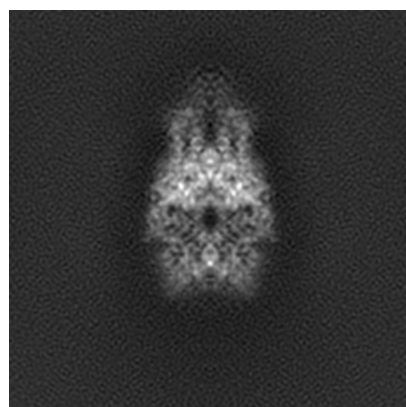


Y

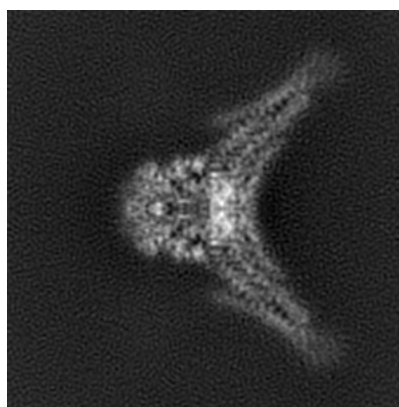


Z

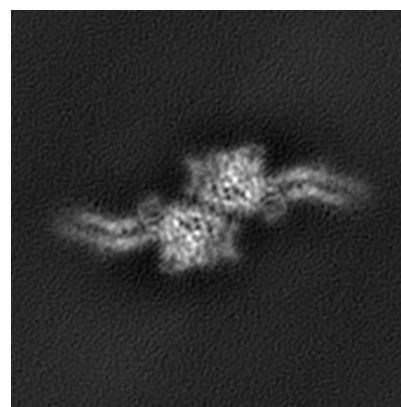
6.1.2 Raw map



X



Y

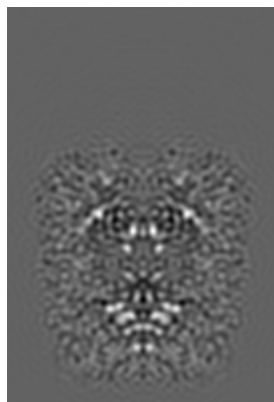


Z

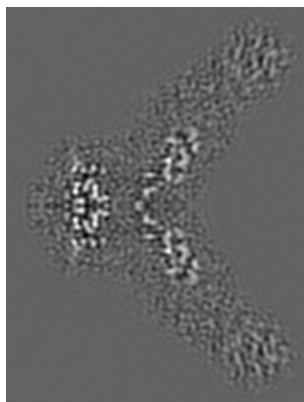
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

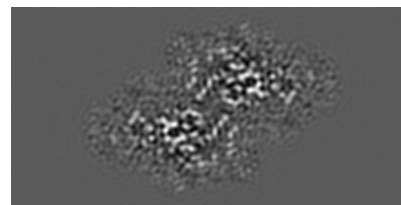
6.2.1 Primary map



X Index: 81

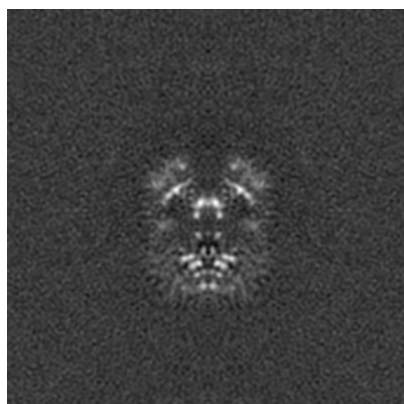


Y Index: 41

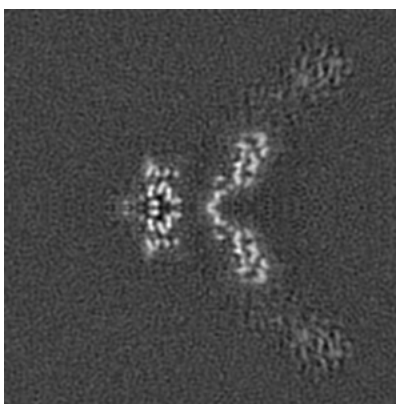


Z Index: 61

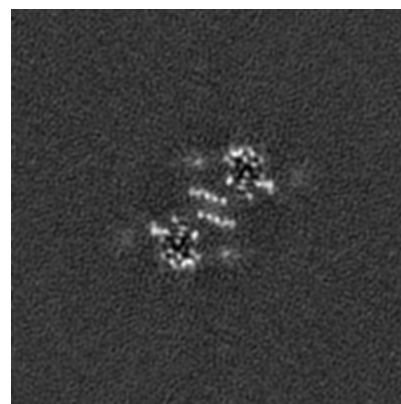
6.2.2 Raw map



X Index: 85



Y Index: 85

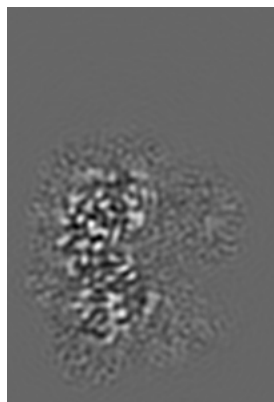


Z Index: 85

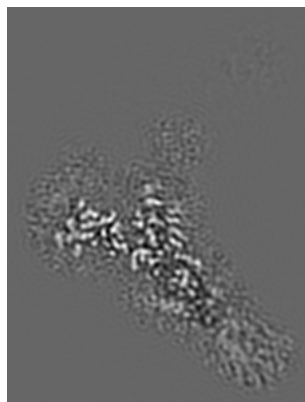
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

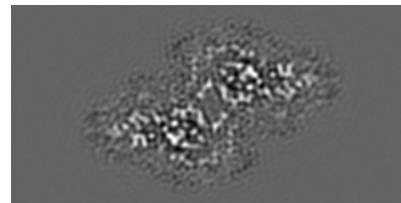
6.3.1 Primary map



X Index: 69

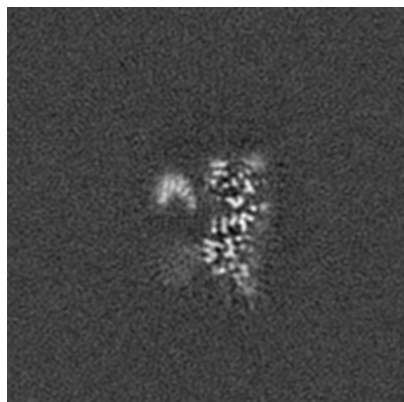


Y Index: 31

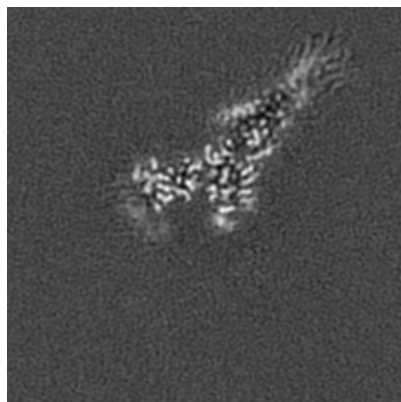


Z Index: 62

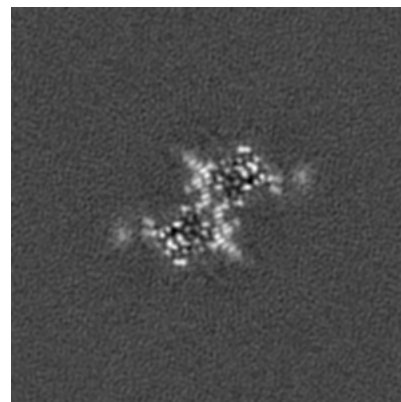
6.3.2 Raw map



X Index: 93



Y Index: 95

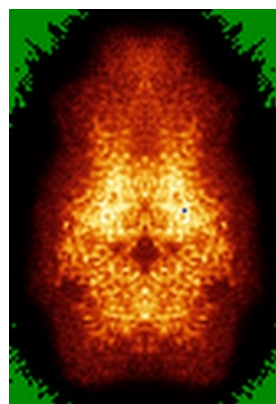


Z Index: 90

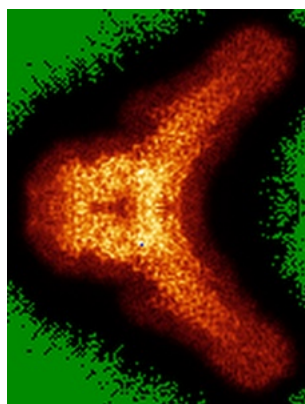
The images above show the largest variance slices of the map in three orthogonal directions.

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

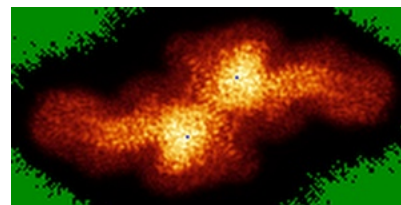
6.4.1 Primary map



X

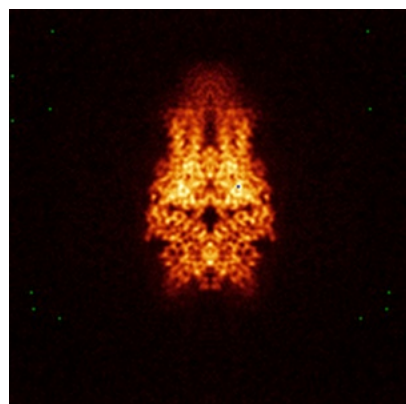


Y

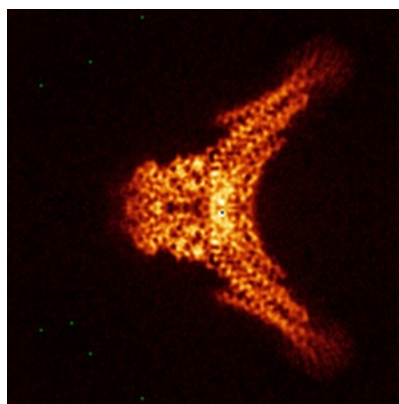


Z

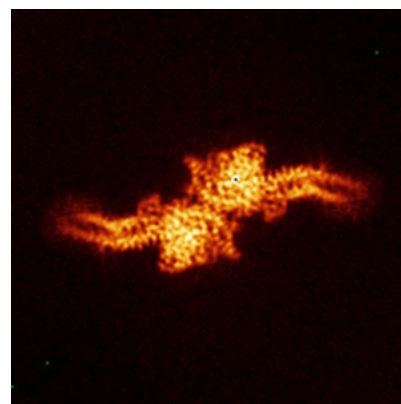
6.4.2 Raw map



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

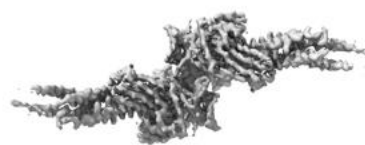
6.5.2 Raw map



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.

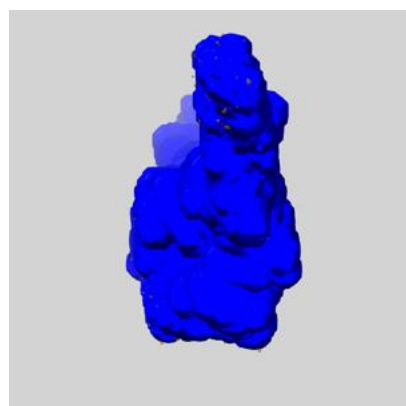
6.6 Mask visualisation [i](#)

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

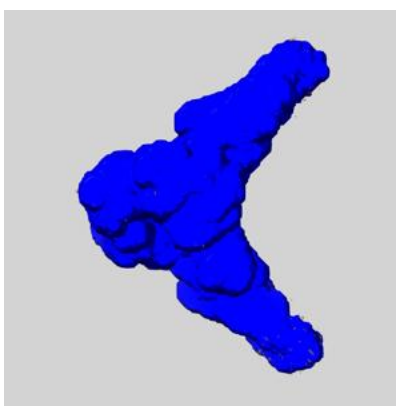
A mask typically either:

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

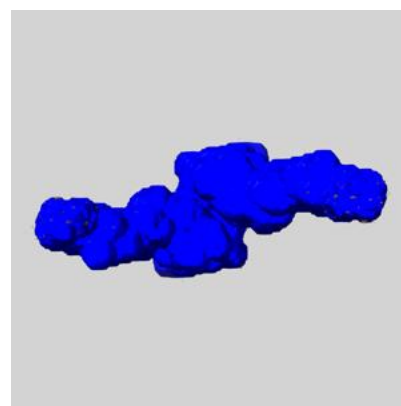
6.6.1 emd_39680_msk_1.map [i](#)



X



Y

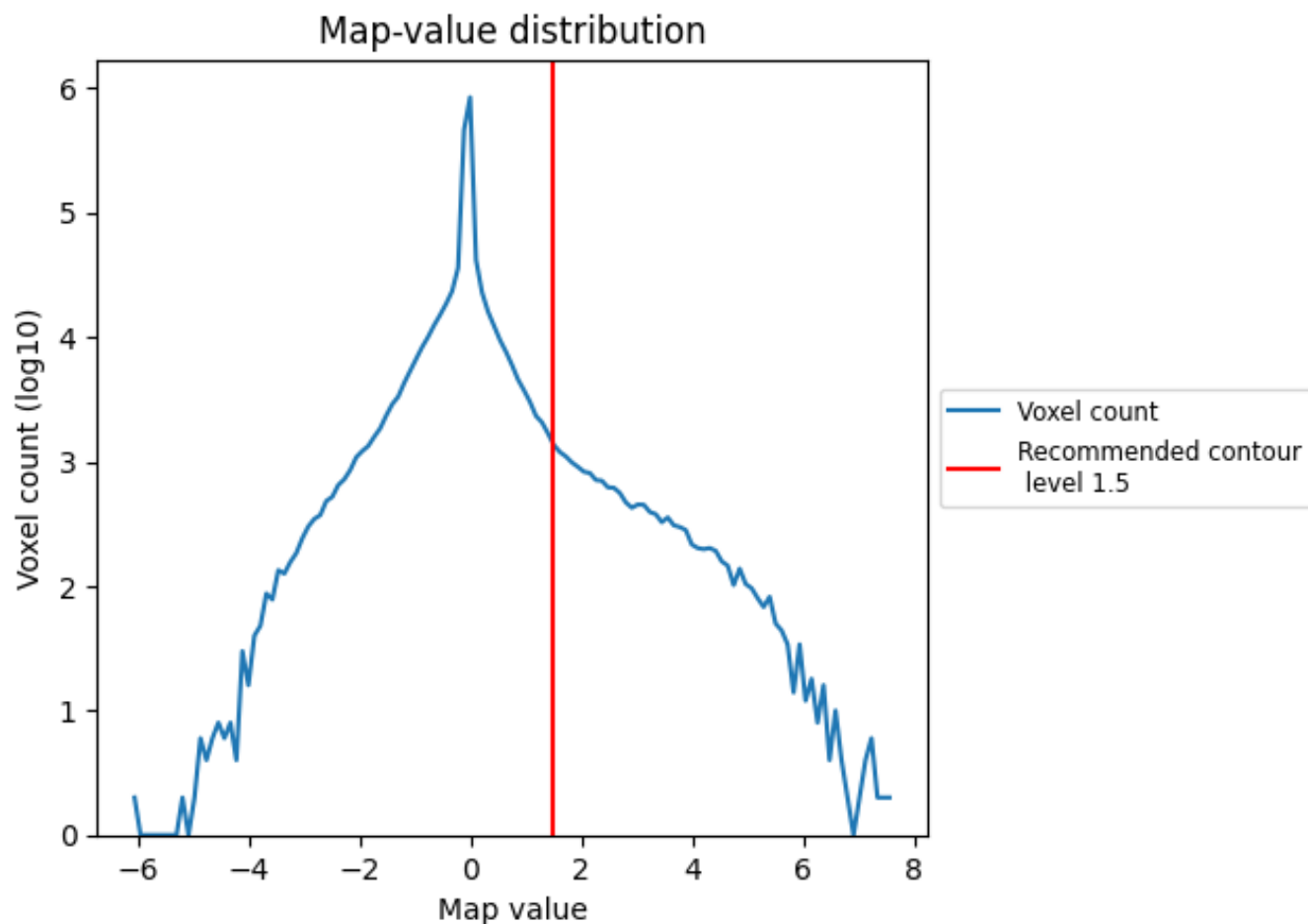


Z

7 Map analysis [i](#)

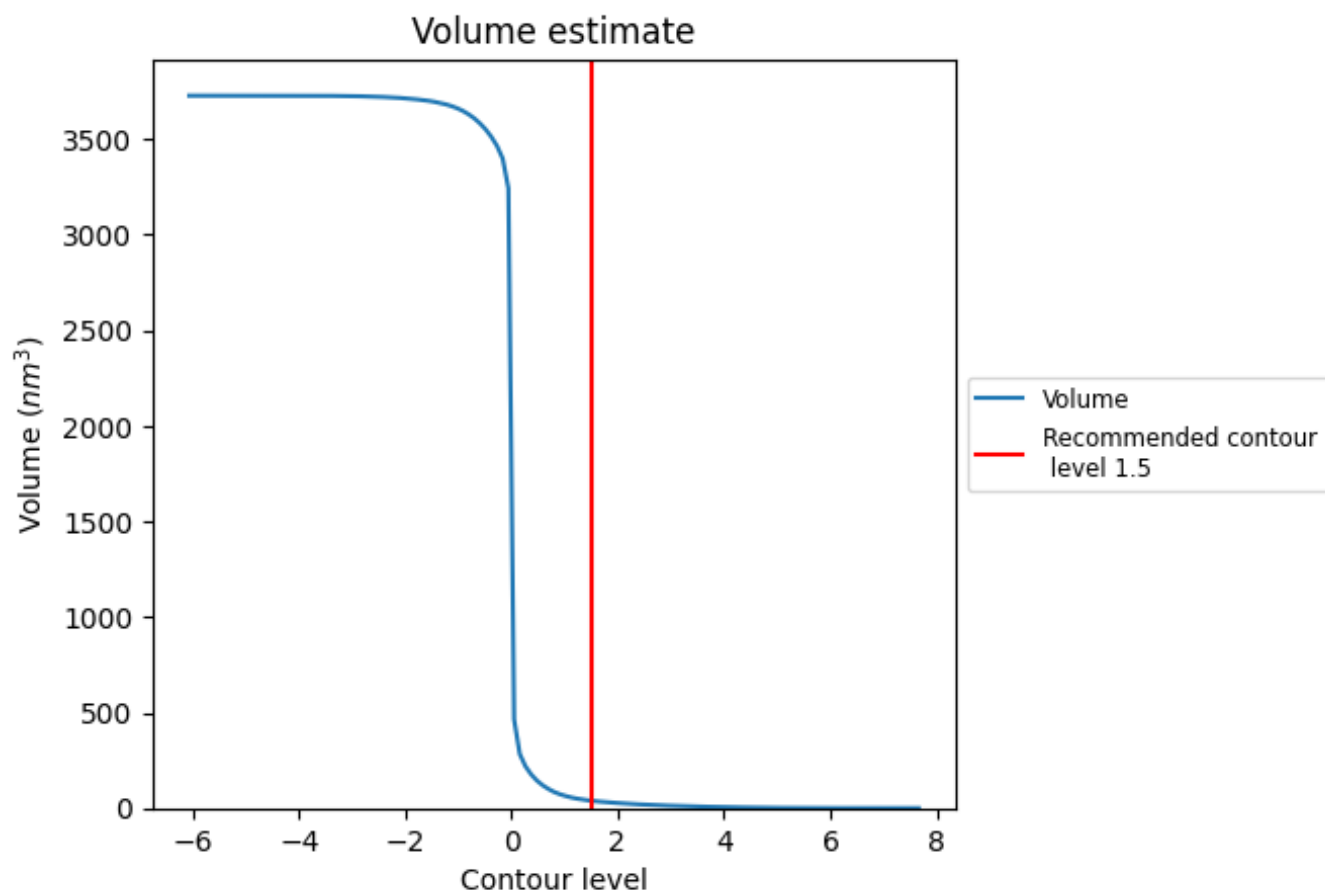
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 39 nm³; this corresponds to an approximate mass of 35 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.

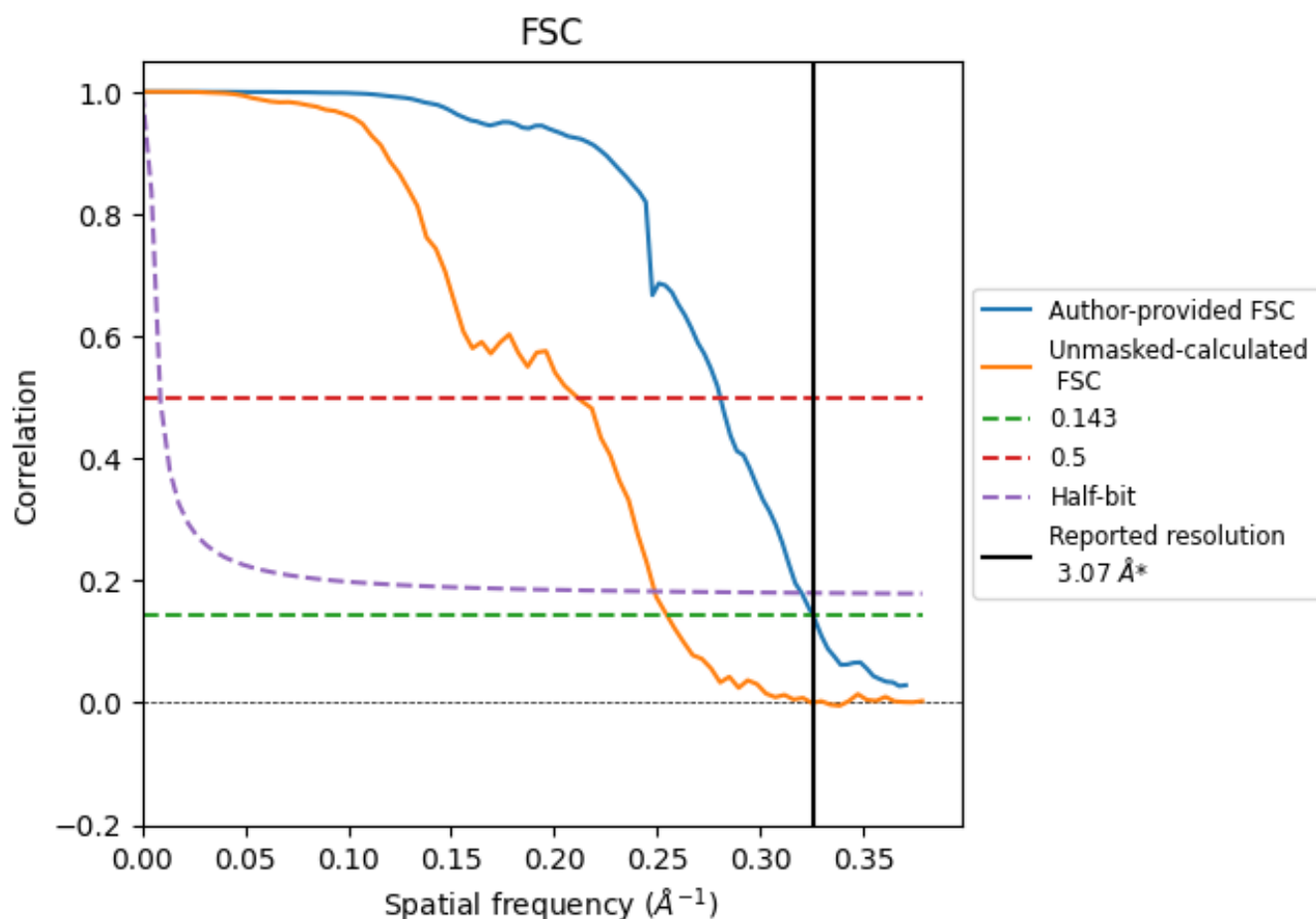
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.326 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.07	-	-
Author-provided FSC curve	3.07	3.56	3.12
Unmasked-calculated*	3.92	4.73	4.02

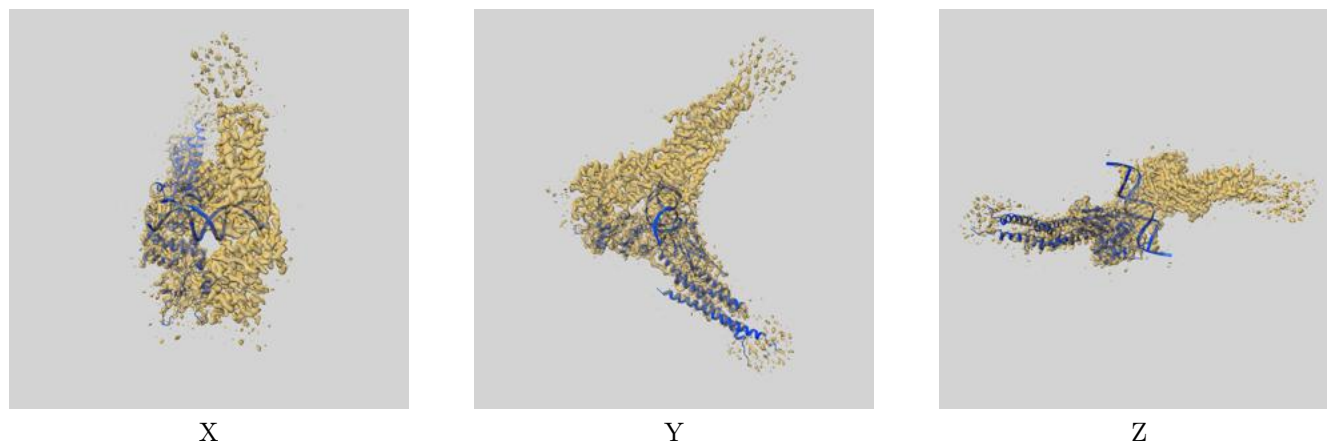
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.92 differs from the reported value 3.07 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39680 and PDB model 8YYV. Per-residue inclusion information can be found in section [3](#) on page [5](#).

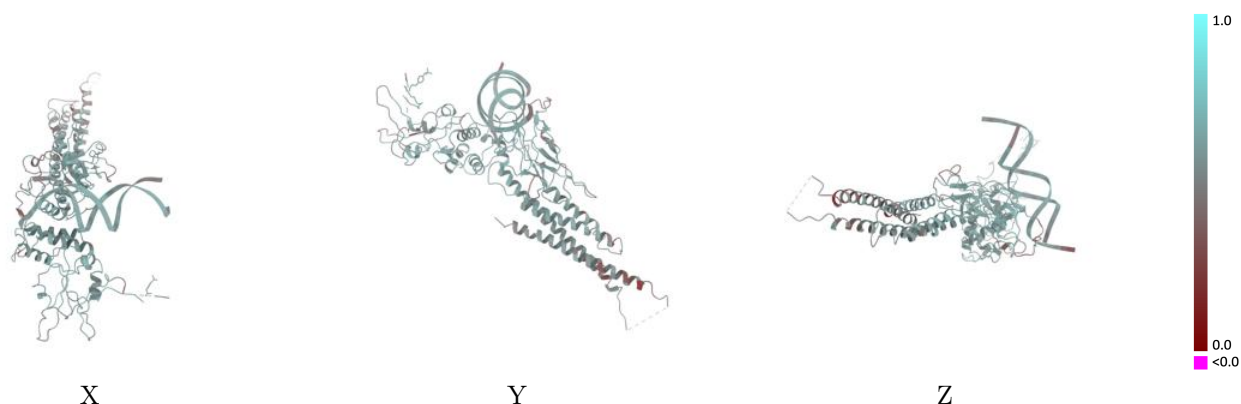
9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)



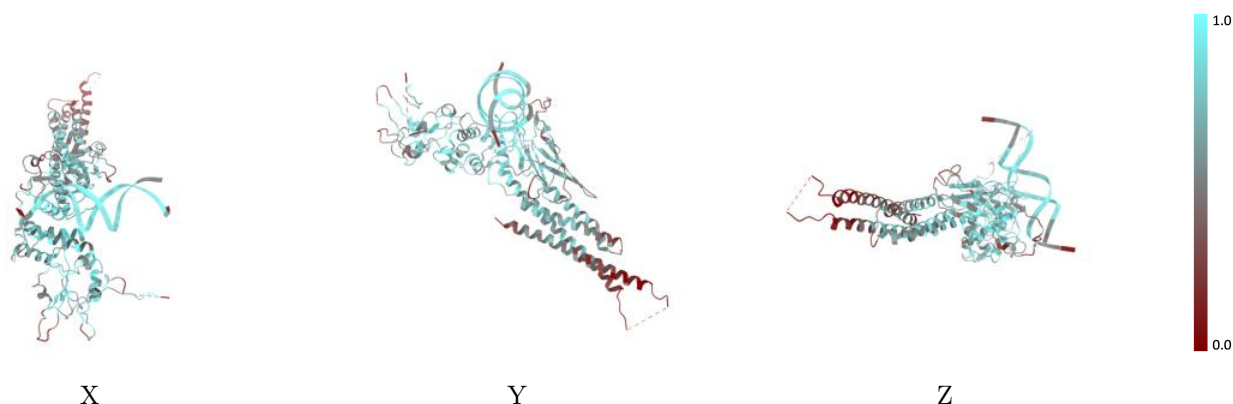
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



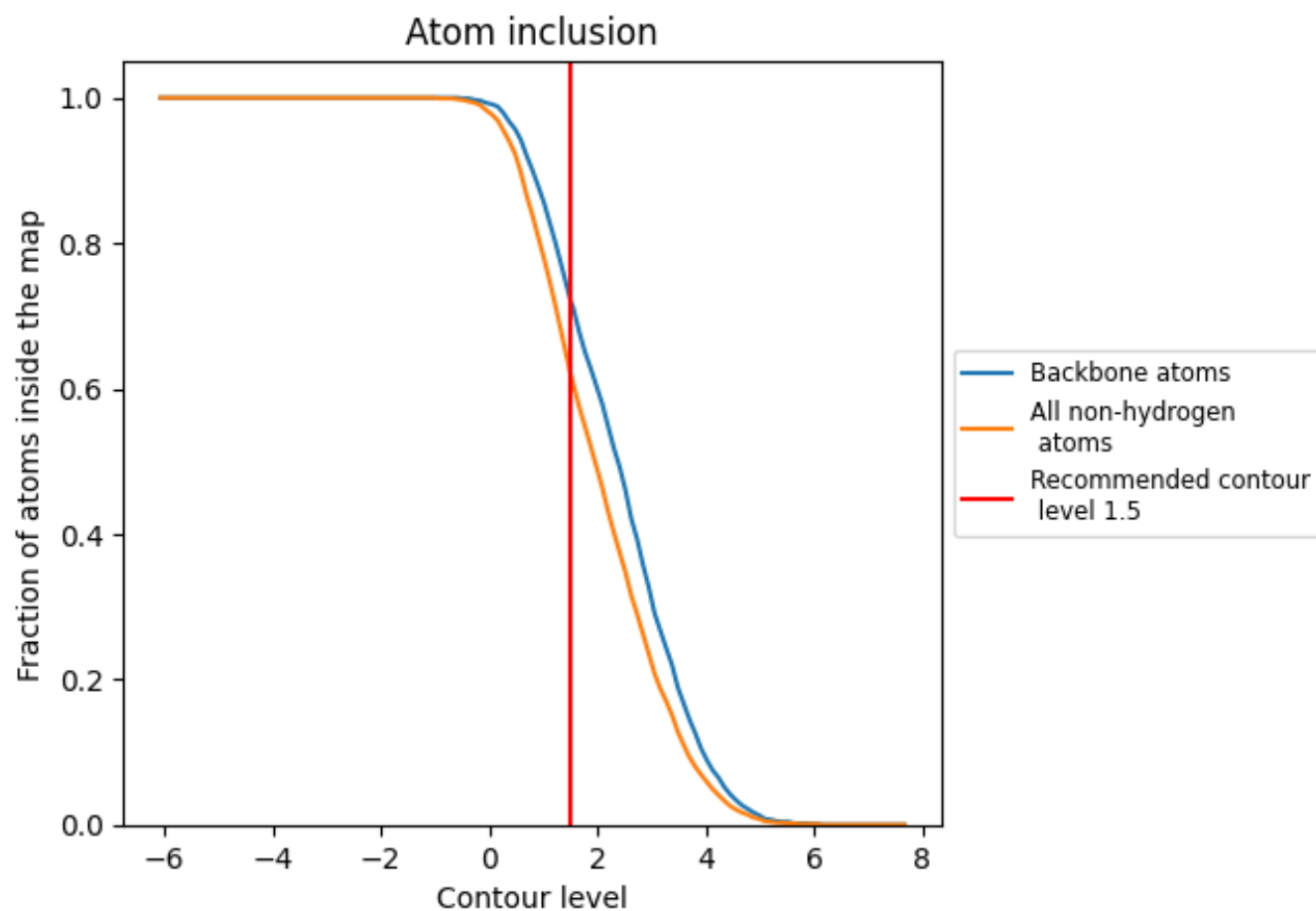
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 62% 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 (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6210	0.5480
A	0.6070	0.5480
B	0.6910	0.5430
C	0.7210	0.5550

