Full wwPDB EM Validation Report

Jul 31, 2024 – 05:14 pm BST

PDB ID	:	8QRI
EMDB ID	:	EMD-18619
Title	:	TRRAP and EP400 in the human Tip60 complex
Authors	:	Li, C.; Smirnova, E.; Schnitzler, C.; Crucifix, C.; Concordet, J.P.; Brion, A.; Poterszman, A.; SChultz, P.; Papai, G.; Ben-Shem, A.
Deposited on	:	2023-10-09
Resolution	:	3.50 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:

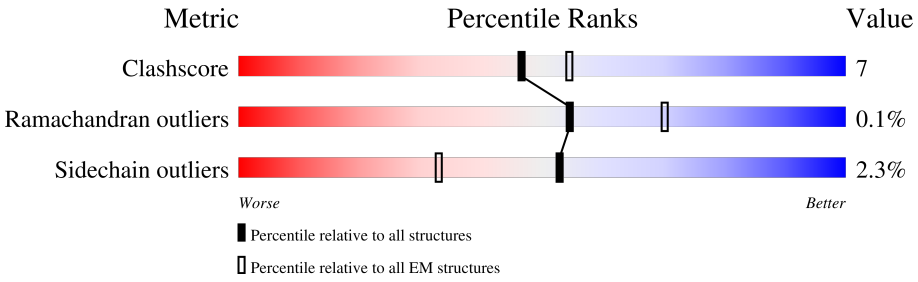
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

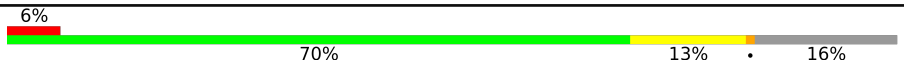
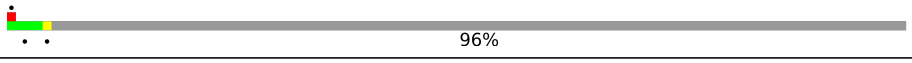
The reported resolution of this entry is 3.50 Å.

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	C	3859	
2	A	3159	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 55049 atoms, of which 27845 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 Transformation/transcription domain-associated protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	C	3246	52887	16810	26759	4496	4634	188	0	0

- Molecule 2 is a protein called E1A-binding protein p400.

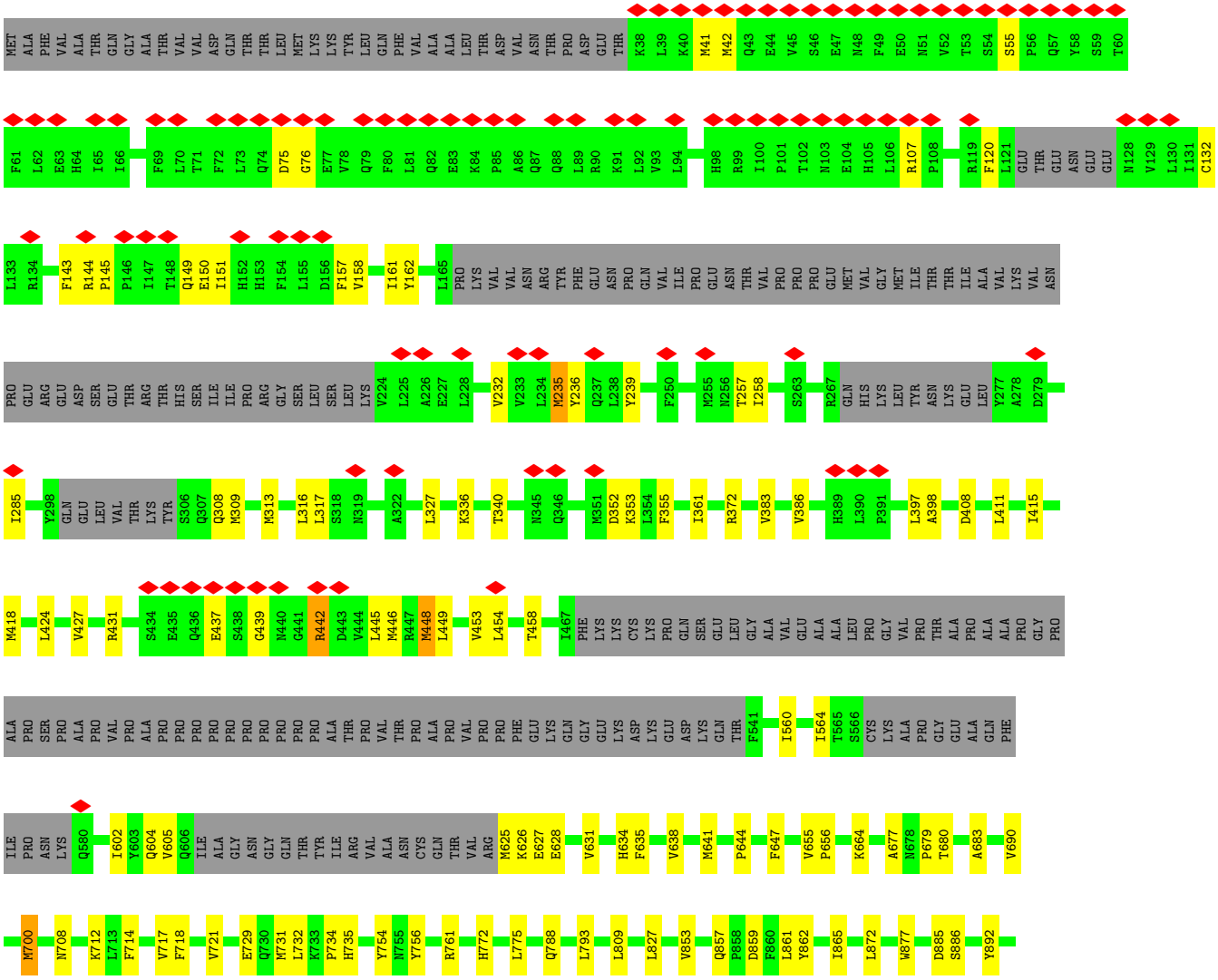
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	A	134	2162	674	1086	197	201	4	0	0

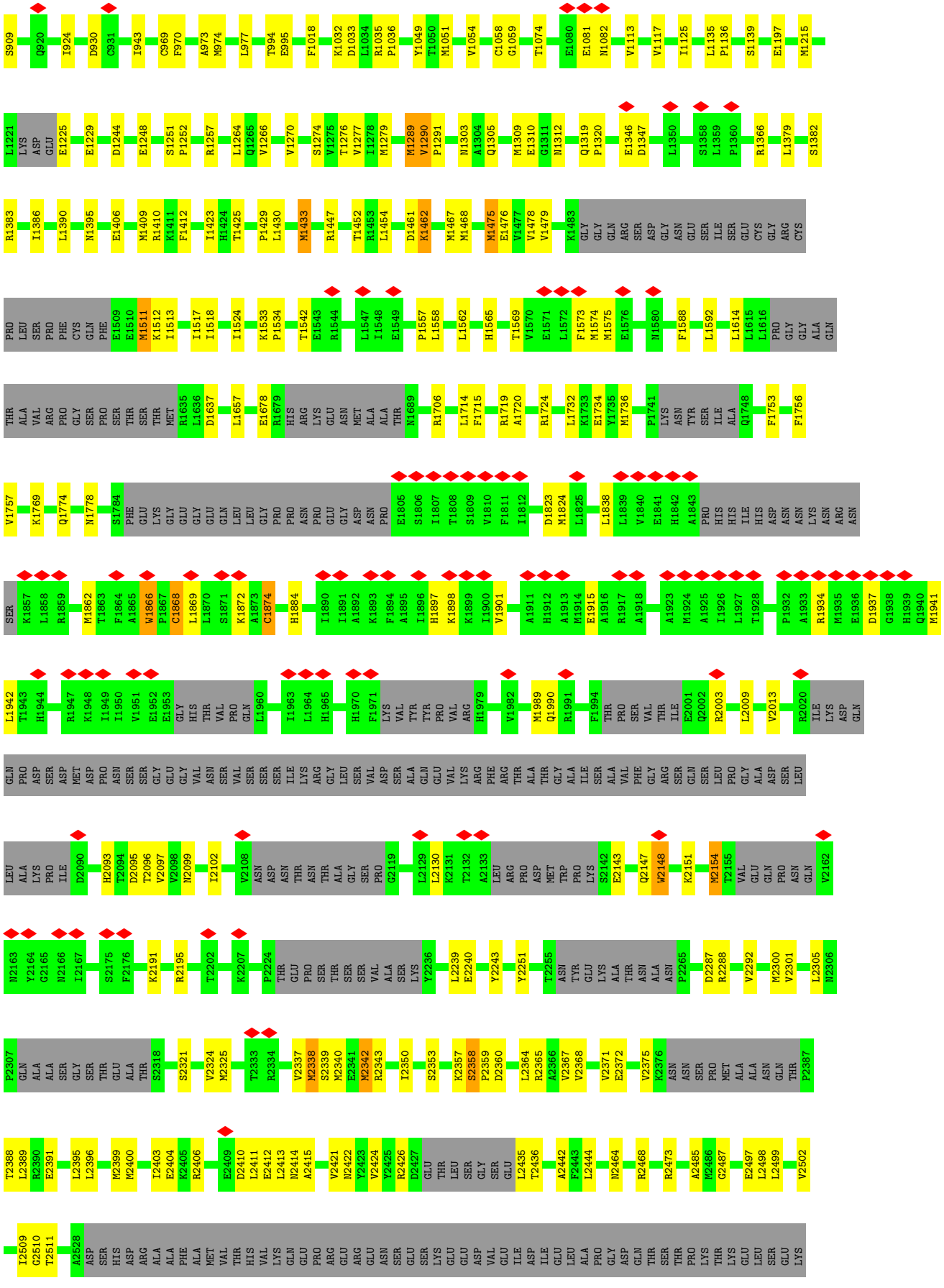
3 Residue-property plots (i)

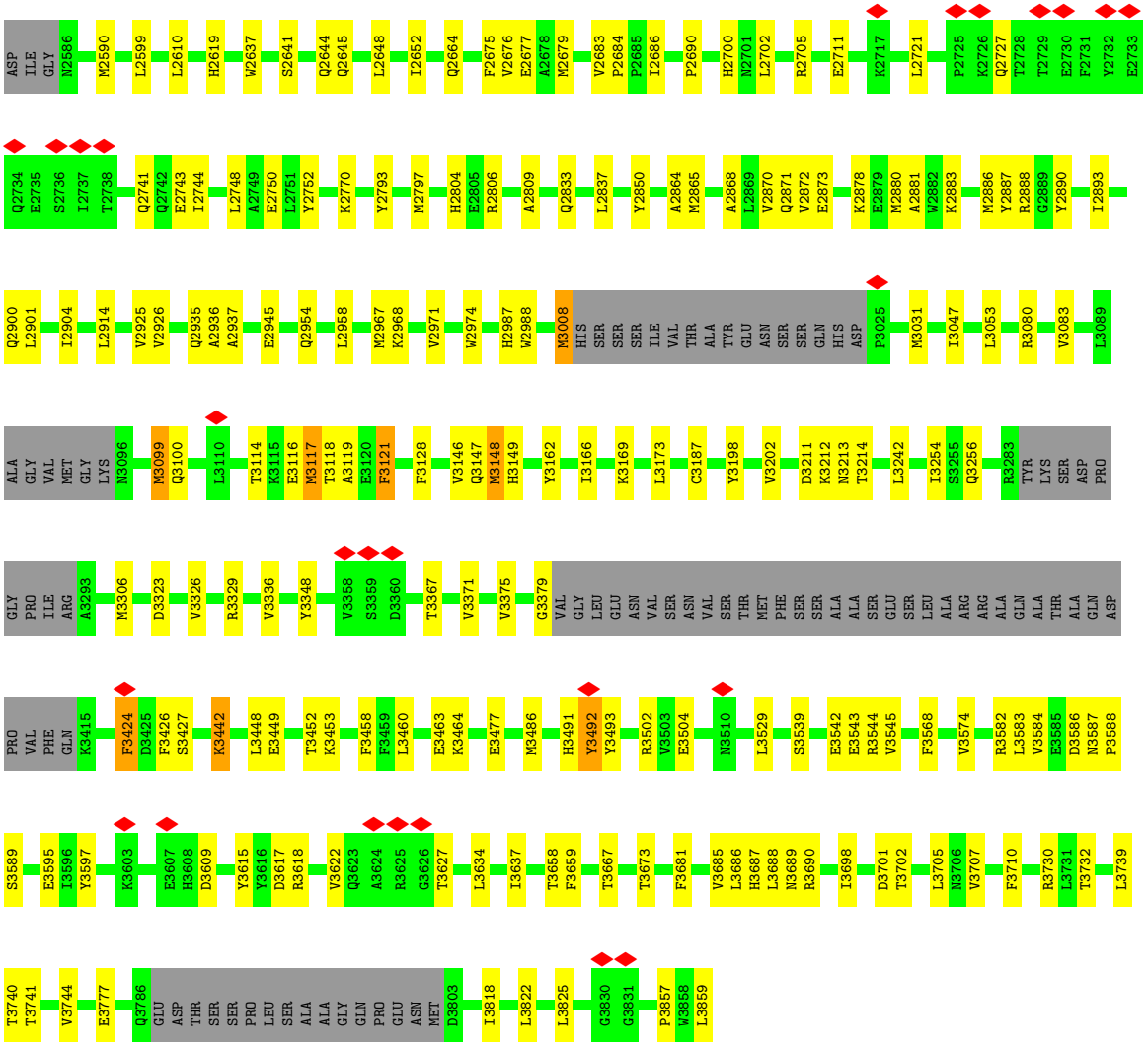
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain C:

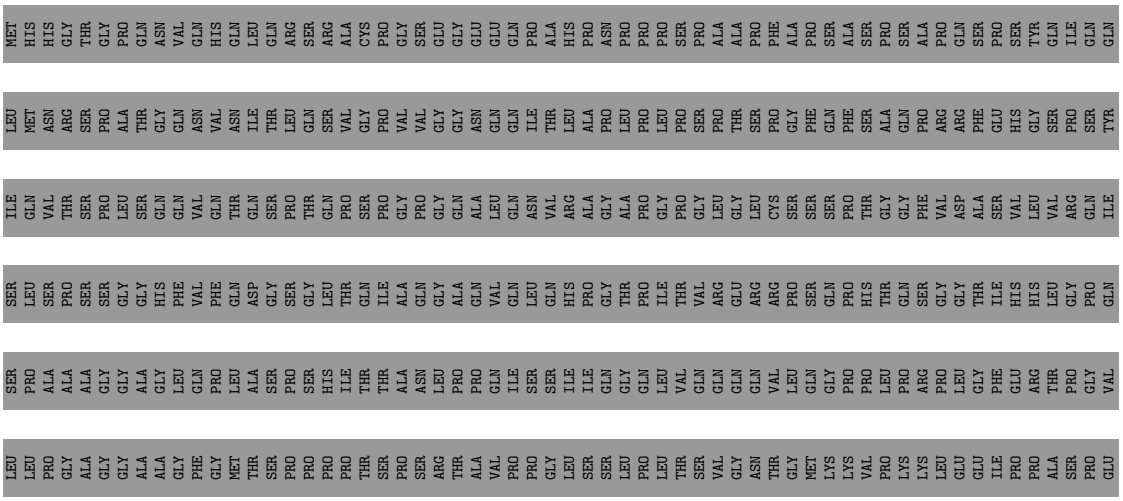


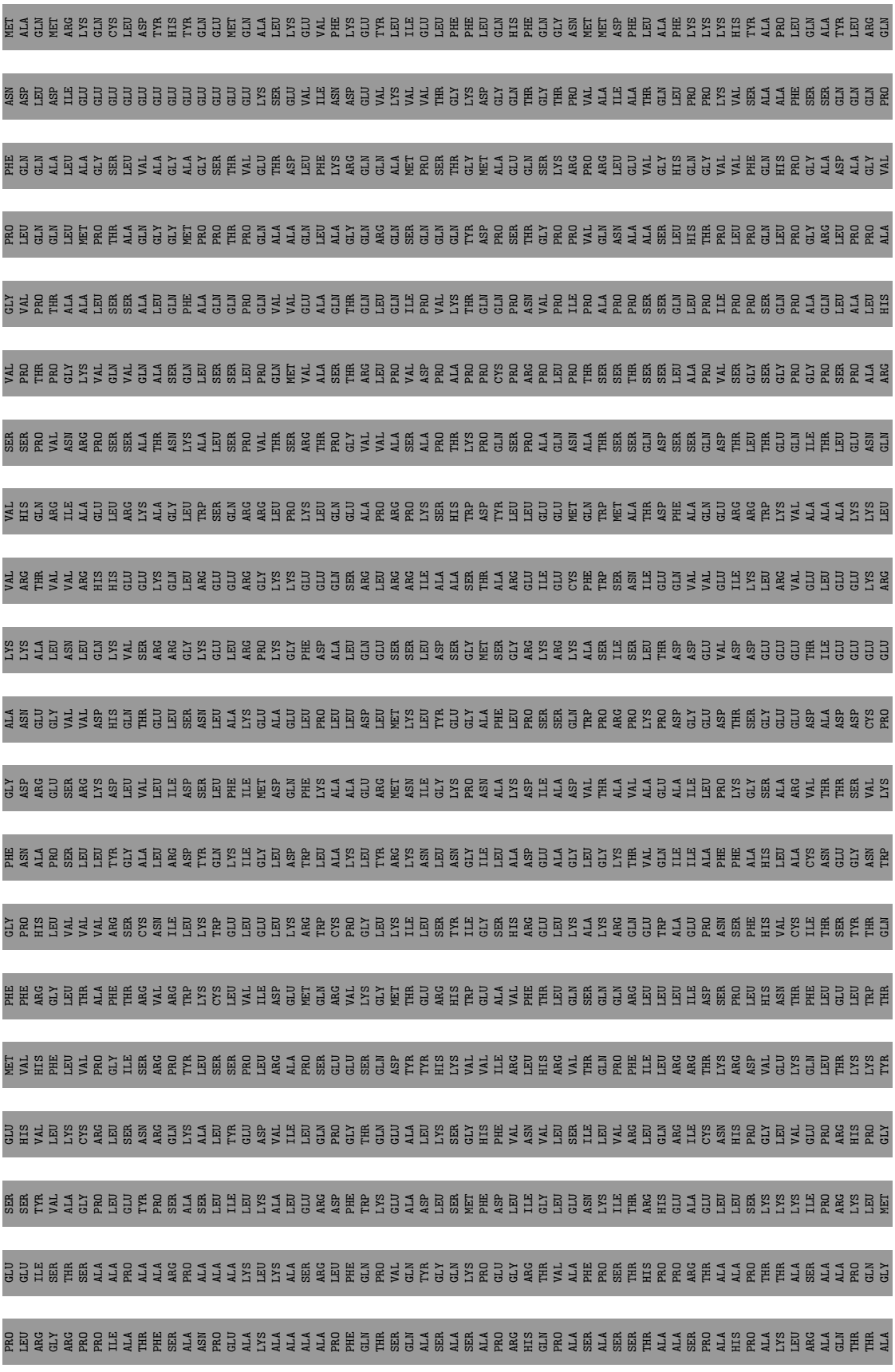


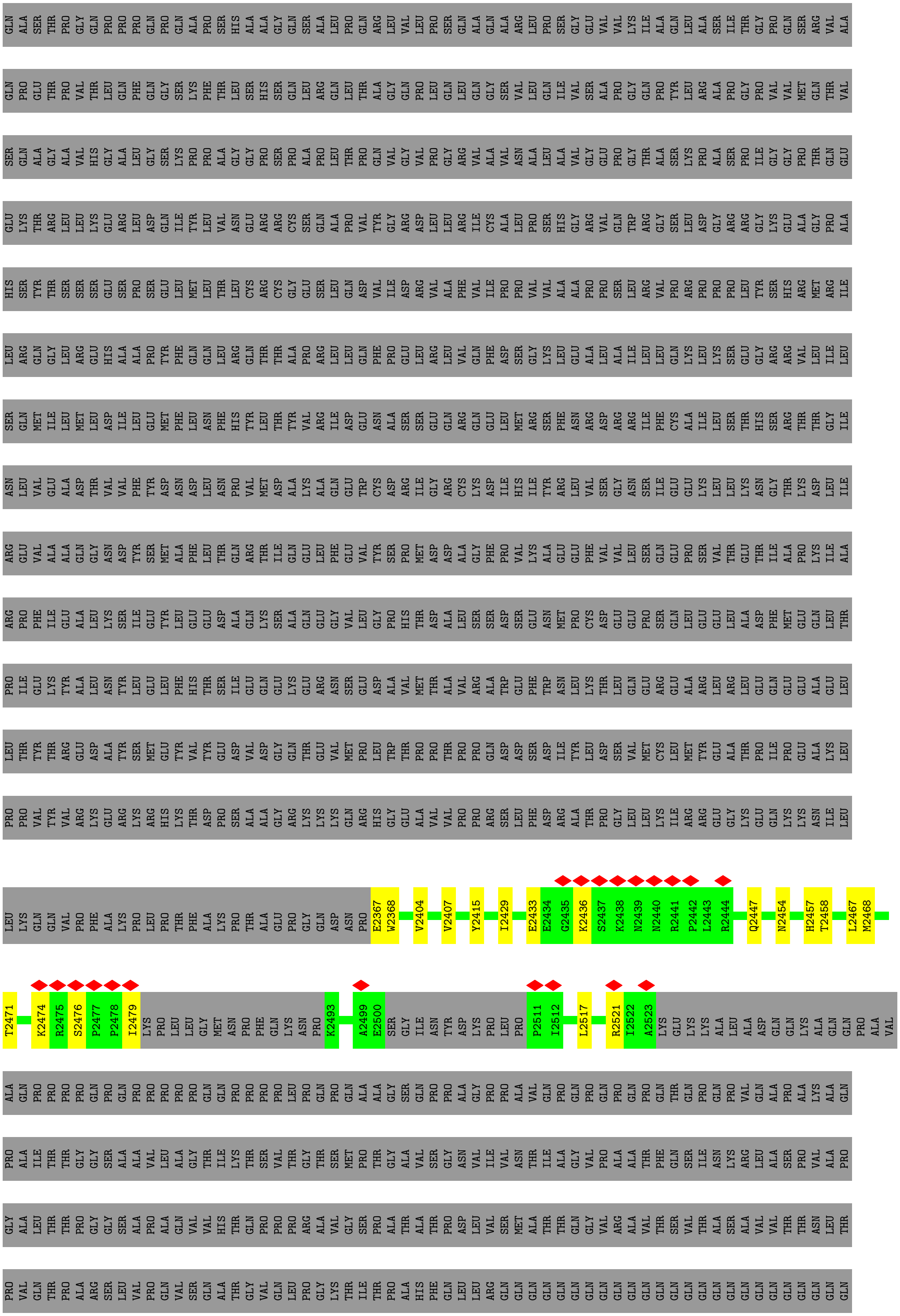


• Molecule 2: E1A-binding protein p400

Chain A: 96%




MET ALA GLN MET ARG LYS GLN CYS LEU ASP TYR HIS TYR GLN GLU MET GLN ALA LEU LYS GLU VAL PHE LYS GLU TYR LEU ILE GLU LEU PHE PHE LEU GLN HIS PHE GLN GLY ASN MET MET ASP PHE LEU ALA PHE LYS LYS LYS HIS TYR ALA PRO LEU GLN ARG GLN
ASN ASP LEU ASP ILE GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU LYS SER GLU VAL ILE ASN ASP GLU VAL LYS VAL VAL THR GLY LYS ASP GLY GLN THR GLY THR PRO VAL ALA ILE ALA THR GLN LEU PRO PRO LYS VAL SER ALA ALA PHE SER SER GLN GLN PRO
PHE GLN GLN ALA LEU ALA GLY SER LEU VAL ALA GLY ALA GLY SER THR VAL GLU THR ASP LEU PHE LYS ARG GLN GLN SER LEU GLU GLN GLN THR GLY MET ALA GLU GLN SER THR GLY ASP GLY GLN HIS PRO GLY ALA ASP ALA GLY GLY VAL
PRO LEU GLN GLN LEU MET PRO THR ALA GLN GLY GLY MET PRO PRO THR PRO GLN GLN ALA ALA GLN LEU ALA GLY GLN ARG GLN SER SER GLN GLN GLN GLN TYR ASP PRO SER THR GLY PRO ARG LEU GLU VAL GLY HIS GLN GLY VAL VAL PRO GLY ARG LEU PRO ALA
GLY VAL PRO THR ALA ALA LEU SER SER ALA LEU GLN GLN GLN GLN VAL VAL GLU ALA GLN THR GLN LEU GLN LEU ILE PRO ALA PRO PRO SER GLN LEU PRO ILE PRO ALA LEU HIS
VAL PRO THR PRO GLY LYS VAL GLN VAL ALA GLN LEU PRO GLN MET MET VAL ALA SER THR ARG LEU PRO VAL ASP PRO ALA PRO PRO ALA ARG PRO LEU LEU PRO THR SER SER SER THR SER SER LEU ALA PRO VAL SER GLY SER GLY PRO ALA GLN LEU PRO ARG
SER SER PRO VAL ASN ARG PRO SER SER ALA THR ASN LYS ALA LEU SER PRO VAL THR SER ARG THR PRO GLY VAL VAL ALA SER ALA PRO THR LYS PRO GLN SER PRO ALA GLN ASN ALA THR SER SER GLN ASP SER SER GLN ASP THR LEU THR GLU GLN ILE THR LEU GLU ASN GLN
VAL HIS GLN ARG ILE ALA GLU LEU ARG LYS ALA GLY LEU TRP SER GLN ARG ARG LEU PRO LYS LEU GLN GLU ALA PRO ARG PRO LYS SER HIS TRP ASP TYR LEU LEU GLU GLU MET GLN TRP MET ALA THR ASP PHE ALA GLN GLU ARG ARG TRP LYS VAL ALA ALA LYS LYS LEU
VAL ARG THR VAL VAL ARG HIS HIS GLU GLU LYS GLN LEU ARG GLU GLU ARG ARG GLY LYS LYS GLU GLU GLN SER ARG LEU ARG ILE ALA ALA SER THR ALA ARG GLU ILE GLU CYS PHE TRP SER ASN ILE GLU GLN VAL VAL GLU ILE LYS LEU ARG VAL GLU LEU GLU GLU LYS ARG
LYS LYS ALA LEU ASN LEU GLN LYS VAL SER ARG ARG GLY LYS GLU LEU ARG PRO LYS GLY PHE ASP ALA LEU GLN GLU SER SER LEU ASP SER GLY MET SER GLY ARG LYS ARG LYS ALA SER ILE SER LEU THR ASP ASP ASP GLU VAL ASP ASP GLU GLU GLU THR ILE GLU GLU GLU GLU
ALA ASN GLU GLY VAL VAL HIS GLN THR GLU LEU SER ASN LEU ALA LYS GLU LEU ASP LEU MET LYS LEU TYR GLU GLY GLY ALA PHE LEU PRO SER SER GLN TRP PRO ARG PRO LYS PRO ASP GLY GLU ASP THR SER ILE SER LEU THR ASP GLY GLU ASP ALA ASP ASP CYS PRO
GLY ASP ARG GLU SER ARG ASP LEU VAL LEU ILE ASP SER LEU PHE ILE MET ASP GLN PHE LYS ALA ALA GLU ARG MET ASN ILE GLY LYS PRO ASN ALA LYS ALA ILE ILE GLU ALA ASP VAL THR ALA VAL ALA GLU ALA ILE LEU PRO LYS ARG LYS ALA SER VAL THR THR SER VAL LYS
PHE ASN ALA PRO SER LEU LEU TYR GLY ALA LEU ARG ASP TYR GLN LYS ILE GLY LEU ASP TRP LEU ALA LYS LEU TYR ARG LYS ASN LEU ASN GLY GLY ILE LEU LEU SER TYR ILE GLY SER HIS ARG GLU LEU LYS ARG GLY GLN GLU TRP ALA ILE ILE ILE ALA PHE PHE HIS LEU ALA GLU PRO ASN SER PHE HIS VAL CYS ILE THR SER TYR THR GLN
PHE PHE ARG GLY LEU THR ARG VAL ARG TRP LYS CYS LEU VAL ILE ASP GLU MET GLN ARG VAL LYS GLY MET THR GLU ARG HIS TRP GLU ALA VAL PHE THR LEU GLN SER GLN ARG LEU LEU LEU ILE ASP SER PRO LEU HIS ASN THR PHE LEU GLU TRP LEU
MET VAL HIS PHE LEU VAL PRO GLY ILE SER ARG PRO TYR LEU SER SER PRO LEU ARG ALA PRO SER GLU GLU SER GLN ASP TYR TYR HIS LYS VAL VAL ILE ARG ARG LEU HIS ARG VAL THR GLN PRO PHE ILE LEU LEU ARG THR LYS ARG ASP VAL GLU LYS GLN LEU THR LYS TYR
GLU HIS VAL LEU LYS CYS ARG LEU TYR GLU ASP VAL ILE LEU LEU GLN PRO GLY THR GLN GLU ALA LEU LYS SER GLY HIS PHE VAL ASN VAL LEU SER ILE LEU VAL ARG LEU GLN ARG ILE CYS ASN HIS PRO GLY LEU VAL GLU PRO ARG HIS PRO GLY
SER SER TYR VAL ALA GLY PRO LEU GLU TYR PRO SER ILE LEU GLU ALA LEU ILE LEU GLU ARG ASP PHE TRP LYS GLU ALA ASP LEU SER MET PHE ASP LEU ILE GLY LEU GLU ASN LYS ILE THR ARG HIS GLU ALA GLU LEU LEU SER LYS LYS LYS ILE PRO ARG LYS LEU MET
GLU GLU ILE SER THR SER THR ALA ALA PRO ALA ALA ALA ARG PRO ALA ALA ALA LYS LEU GLU ALA ALA LYS LEU LYS ALA ALA ALA ALA ALA PRO PHE GLN THR SER GLN ALA ALA SER ALA LEU PRO GLN THR HIS PRO PRO ARG THR ALA ALA ALA PRO THR THR THR PRO GLN GLY
PRO LEU ARG GLY ARG PRO PRO ILE ALA THR PHE SER ALA ASN PRO GLU ALA ALA ALA ALA PHE GLN THR SER ALA SER SER THR ALA ALA SER PRO ALA HIS PRO ALA LYS LEU ARG ALA GLN THR THR ALA


E2367
W2368
V2404
V2407
Y2415
I2429
E2433
E2434
G2435
K2436
S2437
K2438
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N2440
R2441
P2442
L2443
R2444
Q2447
N2454
H2457
T2458
L2467
M2468
T2471
K2474
R2475
S2476
P2477
P2478
I2479
K2493
A2499
E2500
P2511
I2512
L2517
R2521
I2522
A2523

GLN GLN GLN GLN THR THR THR THR SER GLN VAL GLN VAL PRO GLN ILE GLN GLY GLN ALA GLN SER PRO ALA GLN ILE LYS ALA VAL GLY LYS LEU THR PRO GLU HIS LEU ILE LYS MET GLN LYS GLN LYS LEU GLN MET PRO PRO GLN PRO PRO PRO PRO GLN ALA GLN SER ALA PRO

PRO GLN PRO THR ALA GLN VAL GLN VAL GLN THR SER GLN PRO PRO GLN GLN GLN SER PRO GLN LEU THR THR VAL THR ALA PRO ARG PRO GLY ALA LEU LEU THR GLY THR THR VAL ALA ASN LEU GLN VAL ALA ALA ARG LEU THR ARG VAL PRO THR SER GLN LEU GLN ALA GLN GLY GLN

MET GLN THR GLN ALA PRO GLN PRO ALA GLN VAL ALA LEU ALA LYS PRO PRO VAL VAL SER VAL PRO ALA ALA VAL VAL SER SER PRO GLY VAL THR THR LEU PRO MET ASN VAL ALA GLY ILE SER VAL ALA ILE GLY GLN PRO GLN LYS ALA ALA GLY GLN THR VAL VAL ALA GLN PRO

VAL HIS MET GLN GLN LEU LEU LYS LEU LYS GLN GLN ALA VAL GLN GLN LYS ALA ILE GLN PRO GLN ALA ALA GLN GLY PRO ALA ALA VAL GLN GLN LYS ILE THR ALA GLN GLN ILE THR THR PRO GLY ALA GLN GLN LYS VAL ALA TYR ALA ALA GLN PRO ALA LEU LYS THR GLN

PHE LEU THR THR PRO ILE SER GLN ALA GLN LYS LEU ALA GLY ALA GLN GLN VAL GLN THR ILE GLN VAL ALA LYS LEU PRO GLN VAL VAL GLN GLN GLN GLN THR PRO VAL ALA SER ILE GLN GLN GLY VAL ALA SER ALA SER GLN GLN ALA SER PRO GLN THR VAL ALA LEU THR GLN ALA

THR ALA ALA GLY GLN GLN VAL GLN MET ILE PRO ALA VAL THR ALA THR ALA GLN VAL VAL GLN GLN LYS LEU ILE GLN GLN GLN VAL VAL THR THR ALA SER ALA PRO LEU GLN THR PRO GLY ALA PRO ASN PRO ALA GLN VAL PRO ALA SER SER ASP SER PRO SER GLN GLN PRO LYS

LEU GLN MET ARG VAL PRO ALA VAL ARG LEU LYS THR PRO THR LYS PRO PRO CYS GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	181210	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 ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	42.128	Depositor
Minimum map value	-11.918	Depositor
Average map value	0.003	Depositor
Map value standard deviation	1.005	Depositor
Recommended contour level	9.5	Depositor
Map size (Å)	482.72, 482.72, 482.72	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.862, 0.862, 0.862	Depositor

5 Model quality

5.1 Standard geometry

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	C	0.27	0/26668	0.49	1/36065 (0.0%)
2	A	0.25	0/1096	0.49	0/1485
All	All	0.27	0/27764	0.49	1/37550 (0.0%)

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	C	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1868	CYS	CA-CB-SG	5.62	124.12	114.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1290	VAL	Peptide
1	C	1866	TRP	Peptide

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	C	26128	26759	26729	349	0
2	A	1076	1086	1084	17	0
All	All	27204	27845	27813	360	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 7.

All (360) 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:C:1248:GLU:OE2	1:C:1248:GLU:N	2.01	0.94
1:C:2641:SER:OG	1:C:2644:GLN:OE1	1.97	0.82
1:C:2711:GLU:OE2	1:C:2752:TYR:OH	1.99	0.80
1:C:3543:GLU:OE2	1:C:3582:ARG:NH1	2.17	0.78
1:C:3146:VAL:O	2:A:2521:ARG:NH1	2.17	0.77
1:C:700:MET:O	1:C:756:TYR:OH	2.00	0.77
1:C:2925:VAL:HG21	1:C:3667:THR:HG21	1.65	0.76
1:C:3574:VAL:HG22	1:C:3584:VAL:HG23	1.68	0.75
1:C:3617:ASP:OD1	1:C:3618:ARG:N	2.20	0.74
1:C:2677:GLU:OE1	1:C:2705:ARG:NH1	2.22	0.72
1:C:627:GLU:N	1:C:627:GLU:OE1	2.21	0.72
1:C:2143:GLU:O	1:C:2147:GLN:NE2	2.23	0.72
1:C:2338:MET:SD	1:C:2339:SER:N	2.63	0.71
1:C:2251:TYR:OH	1:C:2292:VAL:O	2.07	0.71
2:A:2429:ILE:HG22	2:A:2433:GLU:OE2	1.92	0.70
1:C:2410:ASP:OD2	1:C:2414:ASN:N	2.24	0.70
1:C:3701:ASP:OD2	1:C:3702:THR:N	2.25	0.70
1:C:3689:ASN:OD1	1:C:3690:ARG:N	2.24	0.69
1:C:1934:ARG:NH1	1:C:1937:ASP:OD2	2.23	0.69
1:C:3730:ARG:NH2	1:C:3859:LEU:OXT	2.25	0.69
1:C:1511:MET:SD	1:C:1512:LYS:N	2.67	0.68
1:C:3083:VAL:HG22	1:C:3128:PHE:HE2	1.60	0.67
1:C:634:HIS:O	1:C:638:VAL:HG13	1.95	0.67
1:C:2338:MET:SD	1:C:2343:ARG:NH2	2.68	0.67
1:C:3739:LEU:O	1:C:3740:THR:OG1	2.10	0.66
1:C:1229:GLU:N	1:C:1229:GLU:OE1	2.28	0.66
1:C:107:ARG:NH1	1:C:150:GLU:OE1	2.27	0.65
1:C:3502:ARG:NH1	1:C:3504:GLU:OE2	2.28	0.65
1:C:1081:GLU:OE1	1:C:1082:ASN:ND2	2.30	0.65
1:C:2239:LEU:HD12	1:C:2240:GLU:N	2.12	0.64
1:C:2743:GLU:OE1	1:C:2743:GLU:N	2.30	0.64
1:C:2410:ASP:OD1	1:C:2411:LEU:N	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2300:MET:SD	1:C:2301:VAL:HG23	2.39	0.63
1:C:2421:VAL:O	1:C:2424:VAL:HG12	1.99	0.63
1:C:2404:GLU:OE1	1:C:2404:GLU:N	2.31	0.63
1:C:2388:THR:OG1	1:C:2391:GLU:OE1	2.10	0.62
1:C:3449:GLU:OE2	1:C:3453:LYS:NZ	2.32	0.62
1:C:454:LEU:O	1:C:458:THR:HG23	1.99	0.62
1:C:625:MET:SD	1:C:626:LYS:N	2.70	0.62
1:C:2435:LEU:O	1:C:2436:THR:OG1	2.14	0.62
1:C:3698:ILE:HG22	1:C:3705:LEU:CD2	2.30	0.61
1:C:1289:MET:SD	1:C:1290:VAL:N	2.73	0.61
1:C:313:MET:HE3	1:C:316:LEU:HD11	1.82	0.61
1:C:2637:TRP:CZ3	1:C:2686:ILE:HD11	2.36	0.60
1:C:2410:ASP:OD1	1:C:2412:GLU:N	2.32	0.60
1:C:285:ILE:HG23	1:C:327:LEU:HD13	1.82	0.60
1:C:120:PHE:HD2	1:C:132:CYS:HG	1.50	0.59
1:C:2396:LEU:HD12	1:C:2399:MET:SD	2.43	0.59
1:C:2945:GLU:OE1	1:C:2974:TRP:NE1	2.35	0.59
1:C:3162:TYR:CZ	1:C:3166:ILE:HD11	2.38	0.59
1:C:2300:MET:SD	1:C:2301:VAL:N	2.75	0.58
1:C:446:MET:SD	1:C:446:MET:N	2.76	0.58
1:C:1753:PHE:CE2	1:C:1757:VAL:HG21	2.38	0.58
2:A:2367:GLU:N	2:A:2367:GLU:OE1	2.36	0.58
1:C:974:MET:HE1	1:C:2511:THR:HG21	1.85	0.58
1:C:2690:PRO:CB	1:C:2744:ILE:HG22	2.34	0.58
1:C:2865:MET:SD	1:C:2865:MET:N	2.76	0.58
1:C:635:PHE:O	1:C:638:VAL:HG22	2.04	0.58
1:C:677:ALA:O	1:C:680:THR:OG1	2.15	0.57
1:C:2403:ILE:HD11	1:C:2413:LEU:HD21	1.86	0.57
1:C:3162:TYR:CE1	1:C:3166:ILE:HD11	2.40	0.57
1:C:865:ILE:HD11	1:C:872:LEU:CD2	2.35	0.57
1:C:2988:TRP:CD2	1:C:3047:ILE:HD13	2.39	0.57
1:C:2750:GLU:HA	1:C:2750:GLU:OE1	2.03	0.57
1:C:1475:MET:SD	1:C:1542:THR:HG21	2.45	0.56
1:C:3477:GLU:N	1:C:3477:GLU:OE2	2.36	0.56
1:C:316:LEU:HD12	1:C:317:LEU:N	2.21	0.56
1:C:397:LEU:HD12	1:C:398:ALA:N	2.20	0.56
1:C:2499:LEU:O	1:C:2502:VAL:HG22	2.05	0.56
2:A:2474:LYS:O	2:A:2476:SER:N	2.39	0.56
1:C:1736:MET:SD	1:C:1736:MET:N	2.79	0.56
1:C:641:MET:SD	1:C:641:MET:N	2.76	0.55
1:C:974:MET:CE	1:C:2511:THR:HG21	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2954:GLN:O	1:C:2958:LEU:N	2.36	0.55
1:C:2009:LEU:O	1:C:2013:VAL:HG23	2.07	0.55
1:C:3544:ARG:NH1	1:C:3777:GLU:OE1	2.40	0.55
1:C:3681:PHE:CE1	1:C:3685:VAL:HG21	2.42	0.55
1:C:1054:VAL:HG21	1:C:1125:ILE:HD11	1.89	0.55
1:C:729:GLU:OE1	1:C:775:LEU:N	2.38	0.54
1:C:1588:PHE:CZ	1:C:1592:LEU:HD11	2.42	0.54
1:C:3242:LEU:HD12	1:C:3254:ILE:HD13	1.89	0.54
1:C:2097:VAL:HG21	1:C:2130:LEU:HD22	1.89	0.54
1:C:2360:ASP:OD1	1:C:2360:ASP:N	2.37	0.54
1:C:1423:ILE:HG22	1:C:1425:THR:H	1.71	0.54
1:C:2340:MET:SD	1:C:2343:ARG:NH2	2.80	0.54
2:A:2479:ILE:H	2:A:2479:ILE:HD12	1.73	0.54
1:C:2683:VAL:HG13	1:C:2684:PRO:HD3	1.88	0.54
1:C:3448:LEU:O	1:C:3452:THR:HG23	2.08	0.54
1:C:1461:ASP:OD2	1:C:1462:LYS:N	2.40	0.54
1:C:3732:THR:HG21	1:C:3859:LEU:OXT	2.07	0.54
1:C:3529:LEU:HD23	1:C:3586:ASP:CB	2.38	0.53
1:C:924:ILE:HD13	1:C:2511:THR:HG22	1.90	0.53
1:C:2342:MET:H	1:C:2342:MET:CE	2.22	0.53
1:C:313:MET:CE	1:C:316:LEU:HD11	2.38	0.53
1:C:604:GLN:O	1:C:604:GLN:NE2	2.41	0.53
1:C:3687:HIS:CE1	1:C:3818:ILE:HD13	2.43	0.53
1:C:2683:VAL:CG1	1:C:2684:PRO:HD3	2.39	0.53
1:C:3211:ASP:OD1	1:C:3212:LYS:N	2.40	0.53
1:C:3211:ASP:O	1:C:3213:ASN:ND2	2.41	0.53
1:C:718:PHE:O	1:C:721:VAL:HG12	2.09	0.52
1:C:442:ARG:HA	1:C:445:LEU:HD12	1.91	0.52
1:C:1382:SER:OG	1:C:1386:ILE:HD12	2.09	0.52
1:C:2410:ASP:OD2	1:C:2413:LEU:HB3	2.09	0.52
1:C:2372:GLU:O	1:C:2375:VAL:HG22	2.09	0.52
1:C:2095:ASP:OD1	1:C:2096:THR:N	2.43	0.51
1:C:1915:GLU:OE1	1:C:1915:GLU:N	2.40	0.51
1:C:3491:HIS:CG	1:C:3492:TYR:N	2.78	0.51
1:C:628:GLU:HA	1:C:631:VAL:HG12	1.91	0.51
1:C:3053:LEU:HD12	1:C:3053:LEU:N	2.25	0.51
1:C:445:LEU:HA	1:C:448:MET:HG2	1.93	0.51
1:C:3597:TYR:HB2	1:C:3859:LEU:HD21	1.92	0.51
1:C:877:TRP:CE3	1:C:2926:VAL:HG21	2.46	0.50
1:C:2422:ASN:OD1	1:C:2426:ARG:NH1	2.43	0.50
1:C:3099:MET:CE	1:C:3099:MET:H	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3587:ASN:ND2	1:C:3588:PRO:O	2.43	0.50
1:C:161:ILE:HG22	1:C:162:TYR:N	2.27	0.50
1:C:1058:CYS:SG	1:C:1059:GLY:N	2.84	0.50
1:C:2727:GLN:OE1	1:C:2770:LYS:NZ	2.34	0.50
1:C:1054:VAL:HG21	1:C:1125:ILE:CD1	2.41	0.50
1:C:3491:HIS:CG	1:C:3492:TYR:H	2.29	0.50
1:C:2793:TYR:O	1:C:2797:MET:HG3	2.11	0.50
1:C:2873:GLU:OE2	1:C:2888:ARG:NE	2.43	0.50
1:C:1018:PHE:HE1	1:C:1049:TYR:HH	1.58	0.49
1:C:602:ILE:HA	1:C:605:VAL:HG23	1.93	0.49
1:C:1264:LEU:HD13	1:C:1279:MET:HE2	1.94	0.49
1:C:352:ASP:OD1	1:C:353:LYS:N	2.46	0.49
1:C:1756:PHE:CD1	1:C:1757:VAL:HG23	2.47	0.49
1:C:2148:TRP:HA	1:C:2151:LYS:HB3	1.93	0.49
1:C:2287:ASP:OD1	1:C:2288:ARG:N	2.45	0.49
1:C:2967:MET:SD	1:C:2968:LYS:N	2.85	0.49
1:C:3622:VAL:O	1:C:3627:THR:OG1	2.25	0.49
1:C:1454:LEU:H	1:C:1454:LEU:HD23	1.77	0.49
1:C:3148:MET:SD	1:C:3148:MET:N	2.80	0.49
1:C:3673:THR:HG22	1:C:3739:LEU:HD22	1.93	0.49
1:C:862:TYR:HA	1:C:865:ILE:HG22	1.95	0.48
1:C:2721:LEU:H	1:C:2721:LEU:HD22	1.77	0.48
1:C:3323:ASP:O	1:C:3326:VAL:HG22	2.13	0.48
1:C:383:VAL:HA	1:C:386:VAL:HG22	1.94	0.48
1:C:2748:LEU:HD21	1:C:2752:TYR:CE2	2.49	0.48
1:C:3686:LEU:HB2	1:C:3688:LEU:HD13	1.96	0.48
1:C:2389:LEU:HD22	1:C:2389:LEU:H	1.77	0.48
2:A:2467:LEU:O	2:A:2471:THR:HG23	2.13	0.48
2:A:2447:GLN:N	2:A:2447:GLN:OE1	2.45	0.48
1:C:75:ASP:OD1	1:C:76:GLY:N	2.42	0.48
1:C:2337:VAL:HG12	1:C:2337:VAL:O	2.14	0.48
1:C:336:LYS:O	1:C:340:THR:HG23	2.14	0.48
1:C:560:ILE:O	1:C:564:ILE:HG12	2.13	0.48
1:C:2648:LEU:HD11	1:C:2652:ILE:HD11	1.94	0.48
1:C:151:ILE:HG22	1:C:151:ILE:O	2.13	0.48
1:C:1452:THR:OG1	1:C:1524:ILE:HG22	2.14	0.48
1:C:1518:ILE:HG22	1:C:1557:PRO:HB2	1.94	0.47
1:C:1476:GLU:O	1:C:1479:VAL:HG22	2.13	0.47
1:C:1868:CYS:HB2	1:C:1874:CYS:HB2	1.67	0.47
1:C:3732:THR:HG21	1:C:3859:LEU:CA	2.44	0.47
1:C:625:MET:CE	1:C:625:MET:HA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:690:VAL:HG13	1:C:717:VAL:HG21	1.95	0.47
1:C:1395:ASN:OD1	1:C:1447:ARG:NH2	2.42	0.47
1:C:3099:MET:SD	1:C:3100:GLN:OE1	2.72	0.47
1:C:3118:THR:HA	1:C:3121:PHE:CE2	2.50	0.47
2:A:2436:LYS:HD2	2:A:2436:LYS:N	2.29	0.47
1:C:793:LEU:HD11	1:C:1197:GLU:HB2	1.97	0.47
1:C:1274:SER:OG	1:C:1277:VAL:HG23	2.14	0.47
1:C:1518:ILE:HG21	1:C:1558:LEU:CD2	2.45	0.47
1:C:1562:LEU:HD12	1:C:1569:THR:CG2	2.45	0.47
1:C:1732:LEU:O	1:C:1736:MET:SD	2.73	0.47
1:C:3114:THR:OG1	1:C:3116:GLU:OE1	2.15	0.47
1:C:1264:LEU:HD13	1:C:1279:MET:CE	2.44	0.47
1:C:3707:VAL:HG11	1:C:3710:PHE:CE2	2.49	0.47
1:C:3615:TYR:CD2	1:C:3637:ILE:HD12	2.50	0.47
1:C:924:ILE:HA	1:C:2511:THR:HG22	1.96	0.47
1:C:1244:ASP:O	1:C:1248:GLU:OE2	2.33	0.47
1:C:2357:LYS:O	1:C:2358:SER:CB	2.62	0.47
1:C:2676:VAL:HA	1:C:2679:MET:HG2	1.97	0.47
1:C:3254:ILE:HD12	1:C:3254:ILE:H	1.80	0.47
1:C:3545:VAL:HG11	1:C:3710:PHE:O	2.15	0.47
2:A:2404:VAL:HA	2:A:2407:VAL:HG12	1.97	0.47
1:C:2325:MET:O	1:C:2325:MET:SD	2.73	0.46
1:C:3595:GLU:O	1:C:3595:GLU:OE1	2.32	0.46
1:C:924:ILE:HD13	1:C:2511:THR:CG2	2.45	0.46
1:C:885:ASP:OD2	1:C:886:SER:N	2.48	0.46
1:C:994:THR:OG1	1:C:995:GLU:OE1	2.30	0.46
1:C:1035:ARG:N	1:C:1036:PRO:CD	2.79	0.46
1:C:3491:HIS:O	1:C:3493:TYR:N	2.48	0.46
1:C:3083:VAL:HG22	1:C:3128:PHE:CE2	2.45	0.46
1:C:1290:VAL:O	1:C:1312:ASN:ND2	2.45	0.46
1:C:411:LEU:HD23	1:C:415:ILE:HB	1.98	0.46
1:C:1266:VAL:O	1:C:1270:VAL:HG23	2.16	0.46
1:C:3673:THR:CG2	1:C:3739:LEU:HD22	2.46	0.46
1:C:2412:GLU:O	1:C:2415:ALA:N	2.49	0.46
1:C:2648:LEU:O	1:C:2652:ILE:HG12	2.16	0.46
1:C:2690:PRO:HB3	1:C:2744:ILE:HG22	1.97	0.46
1:C:1774:GLN:NE2	1:C:1778:ASN:OD1	2.42	0.46
1:C:2648:LEU:CD1	1:C:2652:ILE:HD11	2.45	0.45
1:C:731:MET:SD	1:C:732:LEU:N	2.90	0.45
1:C:1562:LEU:HD12	1:C:1569:THR:HG21	1.98	0.45
1:C:3080:ARG:O	1:C:3083:VAL:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:655:VAL:N	1:C:656:PRO:HD2	2.32	0.45
1:C:408:ASP:OD2	1:C:1724:ARG:NH1	2.43	0.45
1:C:2395:LEU:O	1:C:2399:MET:HG3	2.17	0.45
1:C:3574:VAL:HG13	1:C:3583:LEU:O	2.17	0.45
1:C:449:LEU:O	1:C:453:VAL:HG23	2.16	0.45
1:C:1390:LEU:HD13	1:C:1409:MET:HE2	1.97	0.45
1:C:1897:HIS:O	1:C:1901:VAL:HG12	2.17	0.45
1:C:2880:MET:SD	1:C:2880:MET:O	2.75	0.45
1:C:1319:GLN:HB2	1:C:1320:PRO:HD3	1.98	0.45
1:C:2652:ILE:HG21	1:C:2679:MET:CE	2.47	0.45
1:C:2700:HIS:HB2	1:C:2702:LEU:HD23	1.98	0.45
1:C:3588:PRO:O	1:C:3589:SER:OG	2.22	0.45
1:C:424:LEU:O	1:C:427:VAL:HG22	2.16	0.45
1:C:969:CYS:SG	1:C:2610:LEU:HB2	2.57	0.44
1:C:1714:LEU:HD12	1:C:1757:VAL:O	2.17	0.44
1:C:3306:MET:SD	1:C:3306:MET:C	2.96	0.44
1:C:3426:PHE:O	1:C:3427:SER:OG	2.29	0.44
1:C:1511:MET:H	1:C:1511:MET:HE3	1.82	0.44
1:C:3732:THR:HG23	1:C:3857:PRO:O	2.17	0.44
1:C:1588:PHE:CE1	1:C:1592:LEU:HD11	2.53	0.44
1:C:2151:LYS:O	1:C:2154:MET:SD	2.76	0.44
1:C:2809:ALA:HB2	2:A:2454:ASN:HA	1.99	0.44
1:C:3375:VAL:O	1:C:3379:GLY:N	2.48	0.44
1:C:679:PRO:O	1:C:683:ALA:N	2.43	0.44
1:C:1756:PHE:CE1	1:C:1757:VAL:HG23	2.52	0.44
1:C:3147:GLN:O	2:A:2521:ARG:NH2	2.50	0.44
1:C:1467:MET:CE	1:C:1517:ILE:HD12	2.47	0.44
1:C:2833:GLN:O	1:C:2837:LEU:HD12	2.17	0.44
1:C:1678:GLU:OE1	1:C:1719:ARG:NH2	2.51	0.44
1:C:2367:VAL:O	1:C:2371:VAL:HG23	2.18	0.44
1:C:2881:ALA:HB3	1:C:2914:LEU:HD21	2.00	0.44
1:C:3008:MET:SD	1:C:3008:MET:N	2.84	0.44
1:C:232:VAL:HA	1:C:235:MET:SD	2.57	0.44
1:C:2509:ILE:HG22	1:C:2510:GLY:N	2.33	0.44
1:C:892:TYR:CZ	1:C:2937:ALA:HB2	2.52	0.43
1:C:3114:THR:O	1:C:3117:MET:SD	2.76	0.43
1:C:361:ILE:O	1:C:372:ARG:NH2	2.46	0.43
1:C:977:LEU:HB3	1:C:2599:LEU:HD11	2.00	0.43
1:C:2399:MET:SD	1:C:2400:MET:N	2.91	0.43
1:C:973:ALA:HB2	1:C:2509:ILE:HG21	2.01	0.43
1:C:2590:MET:SD	1:C:2590:MET:C	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3822:LEU:O	1:C:3825:LEU:HD23	2.18	0.43
1:C:1941:MET:O	1:C:1941:MET:SD	2.76	0.43
1:C:3458:PHE:CE2	1:C:3502:ARG:HD2	2.53	0.43
1:C:853:VAL:HG22	1:C:861:LEU:HD21	2.01	0.43
1:C:1406:GLU:OE2	1:C:1410:ARG:NE	2.49	0.43
1:C:677:ALA:O	1:C:680:THR:HG23	2.19	0.43
1:C:1290:VAL:CG1	1:C:1291:PRO:HD3	2.49	0.43
1:C:1429:PRO:O	1:C:1433:MET:CE	2.67	0.43
1:C:3212:LYS:O	1:C:3214:THR:N	2.47	0.43
1:C:857:GLN:O	1:C:859:ASP:N	2.52	0.43
1:C:1074:THR:O	1:C:1074:THR:HG22	2.19	0.43
1:C:2925:VAL:CG2	1:C:3667:THR:HG21	2.44	0.43
1:C:3529:LEU:HD13	1:C:3529:LEU:HA	1.92	0.43
1:C:257:THR:O	1:C:258:ILE:HG22	2.19	0.43
1:C:1390:LEU:HD13	1:C:1409:MET:CE	2.48	0.43
1:C:2444:LEU:HD13	1:C:2485:ALA:HB3	2.01	0.43
1:C:1409:MET:HG2	1:C:1454:LEU:HD11	2.00	0.42
1:C:2243:TYR:N	1:C:2243:TYR:CD1	2.87	0.42
1:C:2305:LEU:HD12	1:C:2357:LYS:HD3	2.01	0.42
1:C:2870:VAL:HG23	1:C:2871:GLN:N	2.34	0.42
1:C:2358:SER:N	1:C:2359:PRO:CD	2.82	0.42
1:C:2637:TRP:CH2	1:C:2686:ILE:HD11	2.53	0.42
1:C:1346:GLU:OE1	1:C:1366:ARG:NH2	2.51	0.42
1:C:1347:ASP:OD1	1:C:1347:ASP:N	2.49	0.42
1:C:1574:MET:SD	1:C:1588:PHE:CD1	3.12	0.42
1:C:41:MET:HE3	1:C:42:MET:SD	2.59	0.42
1:C:308:GLN:HG2	1:C:309:MET:H	1.85	0.42
1:C:761:ARG:HB2	1:C:809:LEU:HD21	2.02	0.42
1:C:1257:ARG:NE	1:C:1310:GLU:OE1	2.51	0.42
1:C:1305:GLN:O	1:C:1309:MET:HG3	2.19	0.42
1:C:1774:GLN:OE1	1:C:1778:ASN:ND2	2.52	0.42
1:C:1032:LYS:O	1:C:1033:ASP:CG	2.58	0.42
1:C:1215:MET:SD	1:C:1215:MET:C	2.98	0.42
1:C:2365:ARG:O	1:C:2368:VAL:HG22	2.19	0.42
1:C:3634:LEU:O	1:C:3637:ILE:HG12	2.19	0.42
1:C:232:VAL:O	1:C:235:MET:SD	2.77	0.42
1:C:1379:LEU:O	1:C:1383:ARG:NH2	2.52	0.42
1:C:3031:MET:HE3	1:C:3031:MET:HA	2.00	0.42
1:C:158:VAL:HA	1:C:161:ILE:HD12	2.00	0.42
1:C:943:ILE:HD11	1:C:970:PHE:CG	2.53	0.42
1:C:1533:LYS:HB3	1:C:1534:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2364:LEU:O	1:C:2367:VAL:HG22	2.19	0.42
1:C:3187:CYS:SG	1:C:3198:TYR:HB2	2.60	0.42
1:C:308:GLN:HG2	1:C:309:MET:N	2.34	0.42
1:C:827:LEU:HD12	1:C:827:LEU:C	2.40	0.42
1:C:1513:ILE:O	1:C:1517:ILE:HG12	2.19	0.42
1:C:2013:VAL:HG11	1:C:2093:HIS:CD2	2.54	0.42
1:C:2880:MET:SD	1:C:2883:LYS:HB2	2.60	0.42
1:C:161:ILE:HG22	1:C:162:TYR:H	1.82	0.42
1:C:445:LEU:O	1:C:448:MET:HG3	2.20	0.42
1:C:734:PRO:O	1:C:735:HIS:CG	2.73	0.42
1:C:1989:MET:SD	1:C:1990:GLN:N	2.93	0.42
1:C:2797:MET:SD	2:A:2468:MET:SD	3.18	0.42
1:C:2873:GLU:OE2	1:C:2888:ARG:NH2	2.51	0.42
1:C:3687:HIS:ND1	1:C:3818:ILE:HD13	2.35	0.42
1:C:437:GLU:O	1:C:439:GLY:N	2.53	0.41
1:C:2487:GLY:O	1:C:2664:GLN:NE2	2.52	0.41
1:C:2809:ALA:HB2	2:A:2458:THR:HG23	2.02	0.41
1:C:446:MET:O	1:C:449:LEU:HG	2.20	0.41
1:C:772:HIS:HB2	1:C:775:LEU:HB2	2.02	0.41
1:C:1113:VAL:O	1:C:1117:VAL:HG23	2.20	0.41
1:C:418:MET:SD	1:C:418:MET:C	2.98	0.41
1:C:442:ARG:O	1:C:446:MET:SD	2.78	0.41
1:C:788:GLN:C	1:C:788:GLN:OE1	2.59	0.41
1:C:2321:SER:O	1:C:2324:VAL:HG22	2.20	0.41
1:C:2864:ALA:O	1:C:2868:ALA:N	2.48	0.41
1:C:3542:GLU:O	1:C:3545:VAL:HG12	2.21	0.41
1:C:150:GLU:O	1:C:150:GLU:HG3	2.21	0.41
1:C:1478:VAL:HG13	1:C:1479:VAL:N	2.35	0.41
1:C:2412:GLU:O	1:C:2415:ALA:HB3	2.19	0.41
1:C:2637:TRP:NE1	1:C:2645:GLN:OE1	2.53	0.41
1:C:2893:ILE:HD11	1:C:2904:ILE:CD1	2.51	0.41
1:C:3424:PHE:CD1	1:C:3424:PHE:C	2.93	0.41
1:C:3460:LEU:N	1:C:3460:LEU:HD22	2.36	0.41
1:C:1248:GLU:HB2	1:C:1251:SER:HB3	2.02	0.41
1:C:1276:THR:HG21	1:C:1320:PRO:HD2	2.03	0.41
1:C:149:GLN:O	1:C:150:GLU:HG2	2.20	0.41
1:C:1511:MET:H	1:C:1511:MET:CE	2.34	0.41
1:C:1225:GLU:OE1	1:C:1225:GLU:N	2.54	0.41
1:C:1657:LEU:HD22	1:C:1706:ARG:HG3	2.02	0.41
1:C:1824:MET:N	1:C:1824:MET:SD	2.94	0.41
1:C:1866:TRP:O	1:C:1869:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3539:SER:O	1:C:3543:GLU:OE1	2.39	0.41
1:C:161:ILE:CG2	1:C:162:TYR:H	2.34	0.41
1:C:2868:ALA:O	1:C:2872:VAL:HG23	2.20	0.41
1:C:3119:ALA:HB2	1:C:3148:MET:SD	2.60	0.41
1:C:3336:VAL:HG11	1:C:3448:LEU:CD1	2.51	0.41
1:C:3367:THR:O	1:C:3371:VAL:HG23	2.20	0.41
1:C:316:LEU:HD12	1:C:316:LEU:C	2.41	0.41
1:C:1257:ARG:NH2	1:C:1310:GLU:OE1	2.52	0.41
1:C:1386:ILE:HG21	1:C:1412:PHE:CE1	2.55	0.41
1:C:1511:MET:SD	1:C:1512:LYS:HG3	2.60	0.41
1:C:1614:LEU:HD23	1:C:1614:LEU:O	2.20	0.41
1:C:2900:GLN:O	1:C:2901:LEU:HG	2.21	0.41
1:C:2968:LYS:O	1:C:2971:VAL:HG12	2.21	0.41
1:C:3198:TYR:O	1:C:3202:VAL:HG23	2.21	0.41
1:C:3442:LYS:NZ	1:C:3609:ASP:OD2	2.53	0.41
1:C:3463:GLU:O	1:C:3464:LYS:HG2	2.21	0.41
1:C:3658:THR:HG23	1:C:3659:PHE:CD2	2.55	0.41
1:C:3741:THR:O	1:C:3744:VAL:HG22	2.20	0.41
1:C:144:ARG:HB3	1:C:145:PRO:HD3	2.03	0.41
1:C:644:PRO:HA	1:C:647:PHE:HB3	2.02	0.41
1:C:2338:MET:H	1:C:2338:MET:CE	2.34	0.41
1:C:3147:GLN:HB3	1:C:3148:MET:HE3	2.03	0.41
1:C:2676:VAL:O	1:C:2679:MET:HG3	2.21	0.40
1:C:2935:GLN:HG2	1:C:2987:HIS:CD2	2.56	0.40
1:C:2497:GLU:OE2	1:C:2619:HIS:NE2	2.46	0.40
2:A:2479:ILE:HD12	2:A:2479:ILE:N	2.34	0.40
1:C:708:ASN:O	1:C:712:LYS:HG2	2.22	0.40
1:C:1136:PRO:O	1:C:1139:SER:N	2.53	0.40
1:C:1252:PRO:CB	1:C:1303:ASN:OD1	2.70	0.40
1:C:2473:ARG:NH1	1:C:2498:LEU:HD12	2.37	0.40
1:C:2886:MET:HG2	1:C:2890:TYR:HE1	1.86	0.40
1:C:1823:ASP:N	1:C:1824:MET:SD	2.95	0.40
1:C:2099:ASN:O	1:C:2102:ILE:HG22	2.22	0.40
1:C:2400:MET:CG	1:C:2442:ALA:HB2	2.51	0.40
1:C:2936:ALA:O	1:C:2937:ALA:C	2.60	0.40
2:A:2517:LEU:HD21	2:A:2521:ARG:HH12	1.86	0.40
2:A:2517:LEU:HD21	2:A:2521:ARG:NH1	2.36	0.40
1:C:1637:ASP:N	1:C:1637:ASP:OD1	2.54	0.40
1:C:1734:GLU:N	1:C:1734:GLU:OE1	2.55	0.40
1:C:2350:ILE:O	1:C:2353:SER:OG	2.26	0.40
1:C:2850:TYR:CZ	2:A:2415:TYR:CE1	3.10	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	C	3180/3859 (82%)	2966 (93%)	211 (7%)	3 (0%)	51 84
2	A	128/3159 (4%)	114 (89%)	14 (11%)	0	100 100
All	All	3308/7018 (47%)	3080 (93%)	225 (7%)	3 (0%)	54 84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2358	SER
1	C	55	SER
1	C	1720	ALA

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	C	2903/3423 (85%)	2835 (98%)	68 (2%)	50 77
2	A	121/2663 (4%)	119 (98%)	2 (2%)	60 82
All	All	3024/6086 (50%)	2954 (98%)	70 (2%)	53 77

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	143	PHE
1	C	157	PHE
1	C	235	MET
1	C	236	TYR
1	C	239	TYR
1	C	355	PHE
1	C	431	ARG
1	C	442	ARG
1	C	448	MET
1	C	664	LYS
1	C	700	MET
1	C	714	PHE
1	C	754	TYR
1	C	909	SER
1	C	930	ASP
1	C	1051	MET
1	C	1135	LEU
1	C	1289	MET
1	C	1430	LEU
1	C	1433	MET
1	C	1462	LYS
1	C	1468	MET
1	C	1475	MET
1	C	1511	MET
1	C	1565	HIS
1	C	1573	PHE
1	C	1575	MET
1	C	1715	PHE
1	C	1769	LYS
1	C	1838	LEU
1	C	1862	MET
1	C	1872	LYS
1	C	1874	CYS
1	C	1884	HIS
1	C	1898	LYS
1	C	1942	LEU
1	C	2003	ARG
1	C	2148	TRP
1	C	2154	MET
1	C	2191	LYS
1	C	2195	ARG
1	C	2338	MET
1	C	2342	MET

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Mol	Chain	Res	Type
1	C	2406	ARG
1	C	2464	ASN
1	C	2468	ARG
1	C	2675	PHE
1	C	2741	GLN
1	C	2804	HIS
1	C	2806	ARG
1	C	2878	LYS
1	C	2887	TYR
1	C	3008	MET
1	C	3099	MET
1	C	3117	MET
1	C	3121	PHE
1	C	3148	MET
1	C	3149	HIS
1	C	3169	LYS
1	C	3173	LEU
1	C	3256	GLN
1	C	3329	ARG
1	C	3348	TYR
1	C	3424	PHE
1	C	3442	LYS
1	C	3486	MET
1	C	3492	TYR
1	C	3568	PHE
2	A	2368	TRP
2	A	2457	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	160	GLN
1	C	992	ASN
1	C	1082	ASN
1	C	1470	HIS
1	C	1897	HIS
1	C	2414	ASN
1	C	2464	ASN
1	C	2589	HIS
1	C	2593	ASN
1	C	2700	HIS
1	C	2804	HIS

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Mol	Chain	Res	Type
1	C	2846	HIS
1	C	2935	GLN
1	C	2976	ASN
1	C	2987	HIS
1	C	3149	HIS
2	A	2457	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

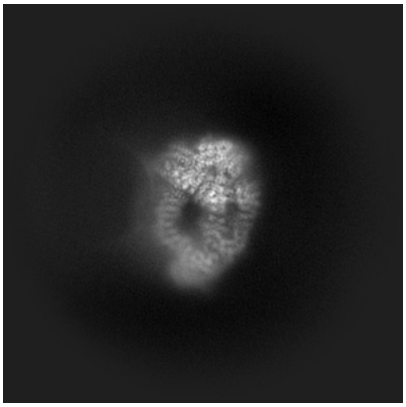
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18619. These allow visual inspection of the internal detail of the map and identification of artifacts.

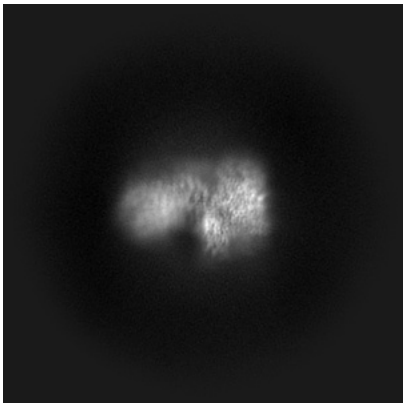
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

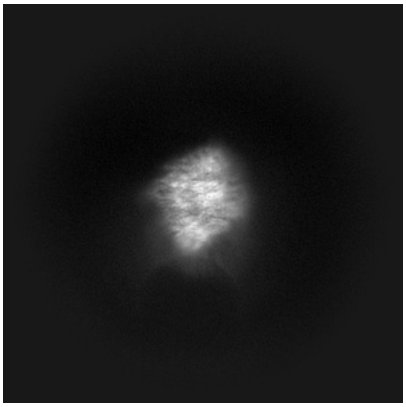
6.1.1 Primary map



X



Y

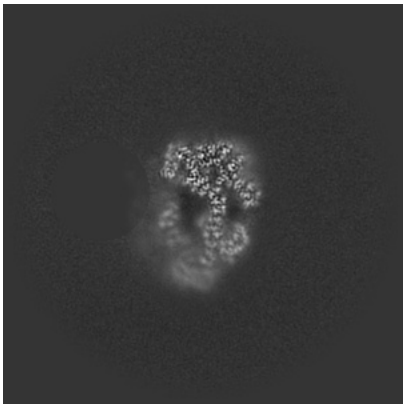


Z

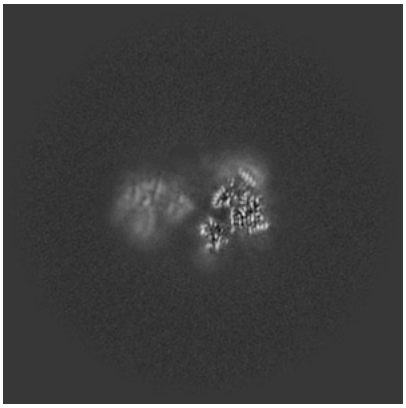
The images above show the map projected in three orthogonal directions.

6.2 Central slices

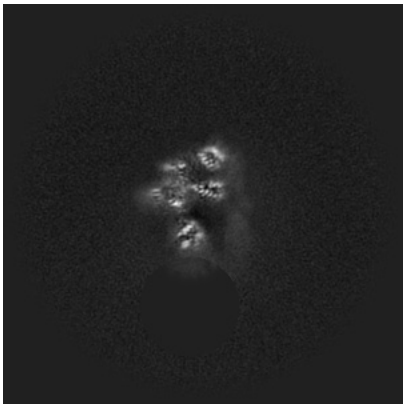
6.2.1 Primary map



X Index: 280



Y Index: 280

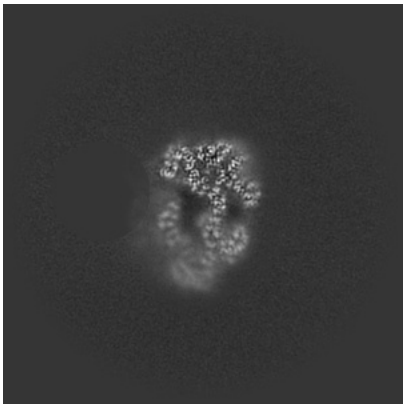


Z Index: 280

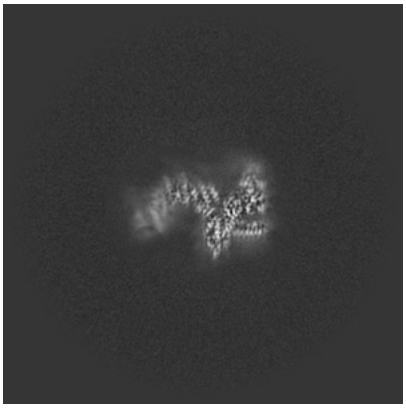
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

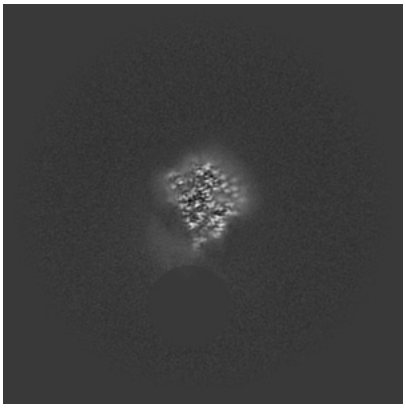
6.3.1 Primary map



X Index: 278



Y Index: 305

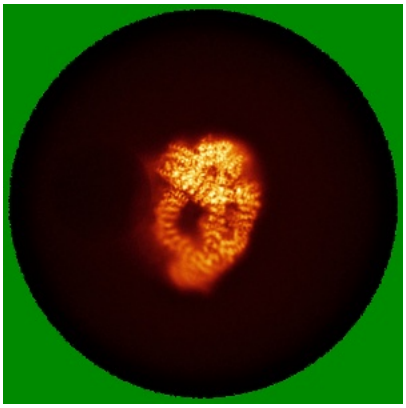


Z Index: 339

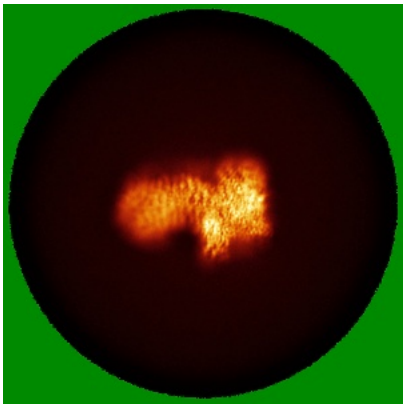
The images above show the largest variance slices of the map in three orthogonal directions.

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

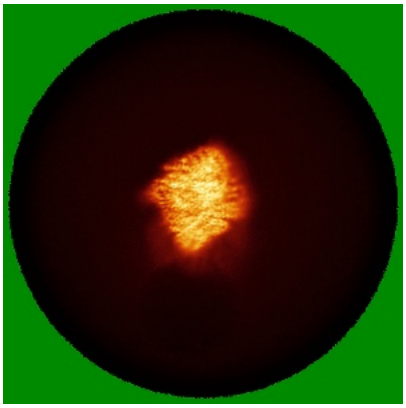
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 9.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

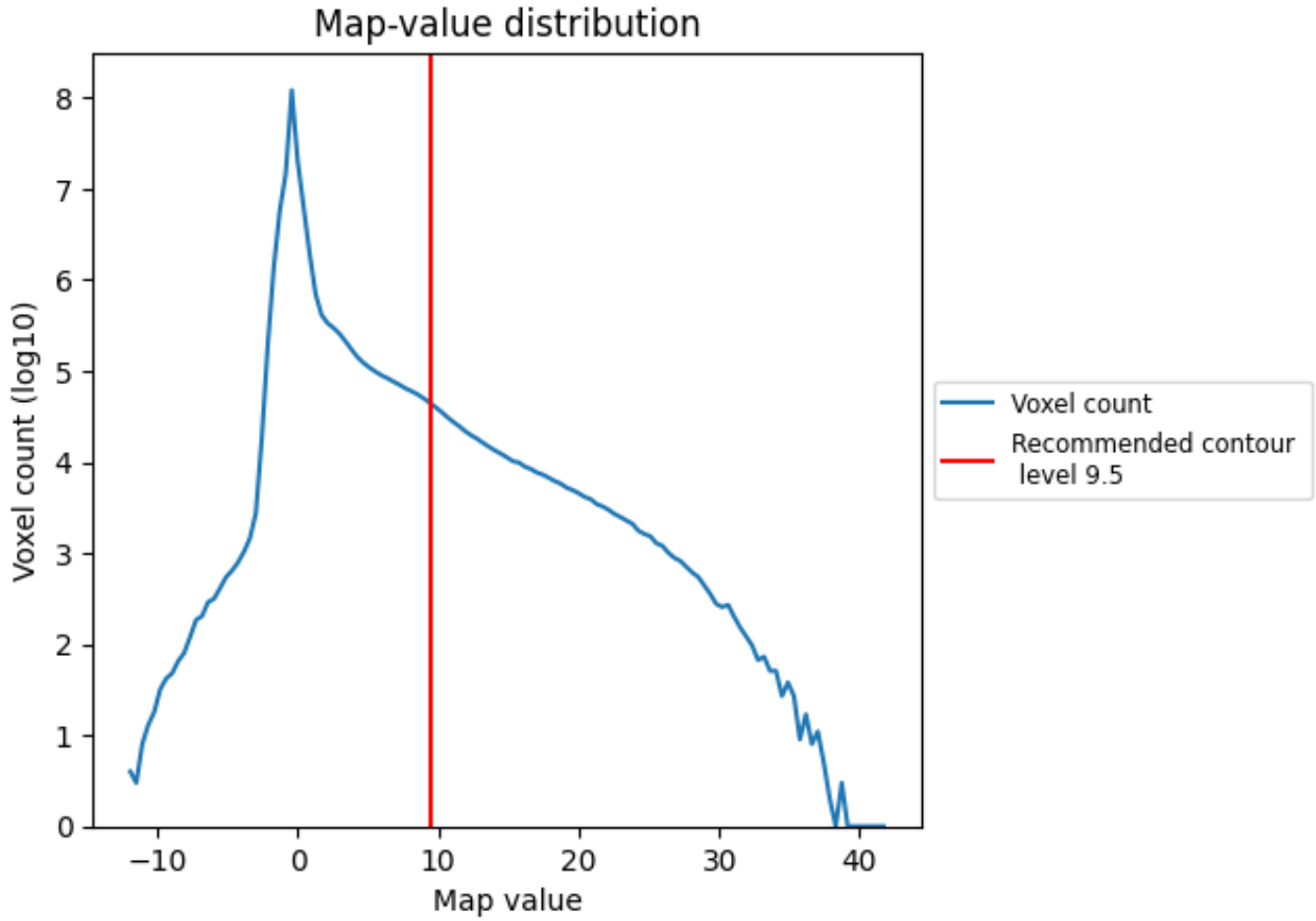
6.6 Mask visualisation (i)

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

7 Map analysis

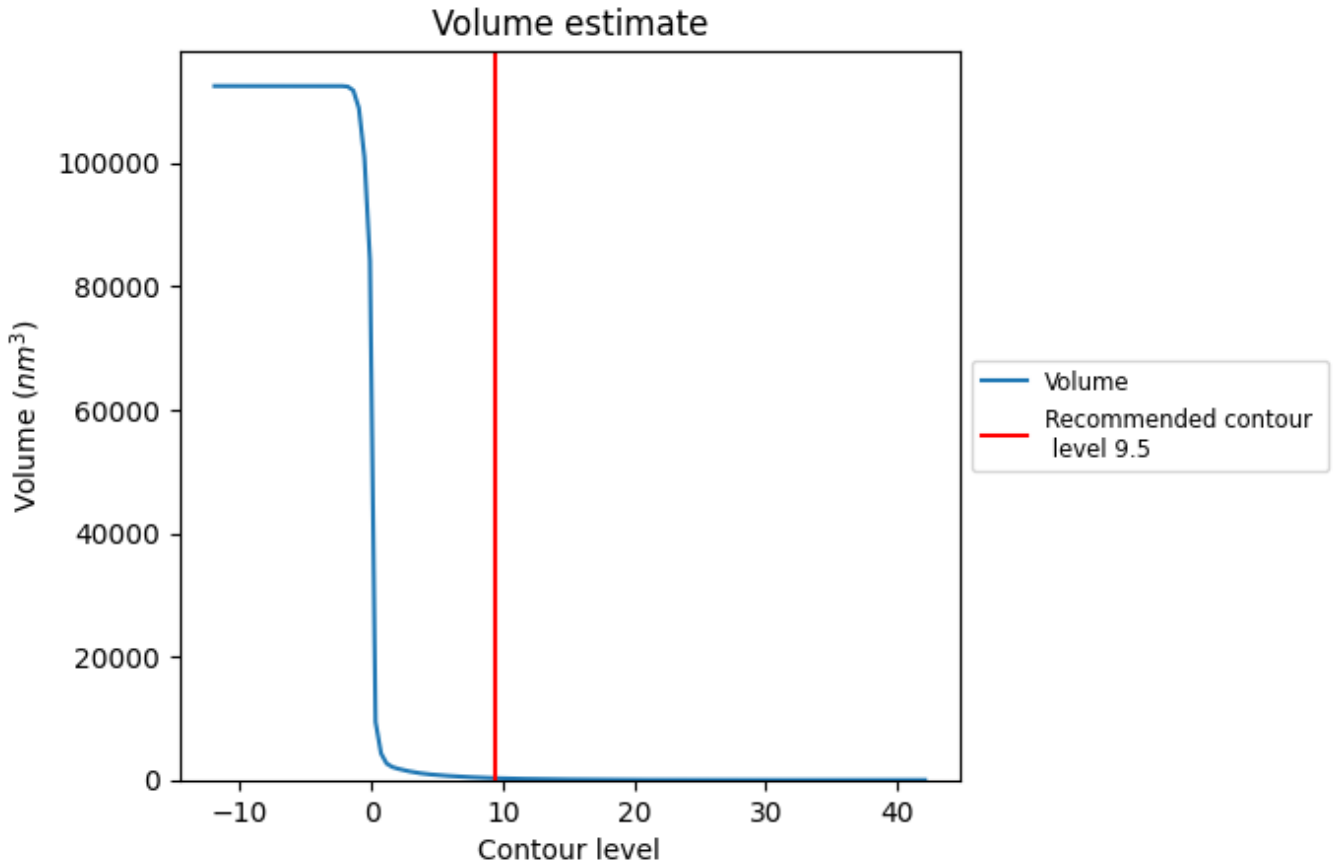
This section contains the results of statistical analysis of the map.

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.

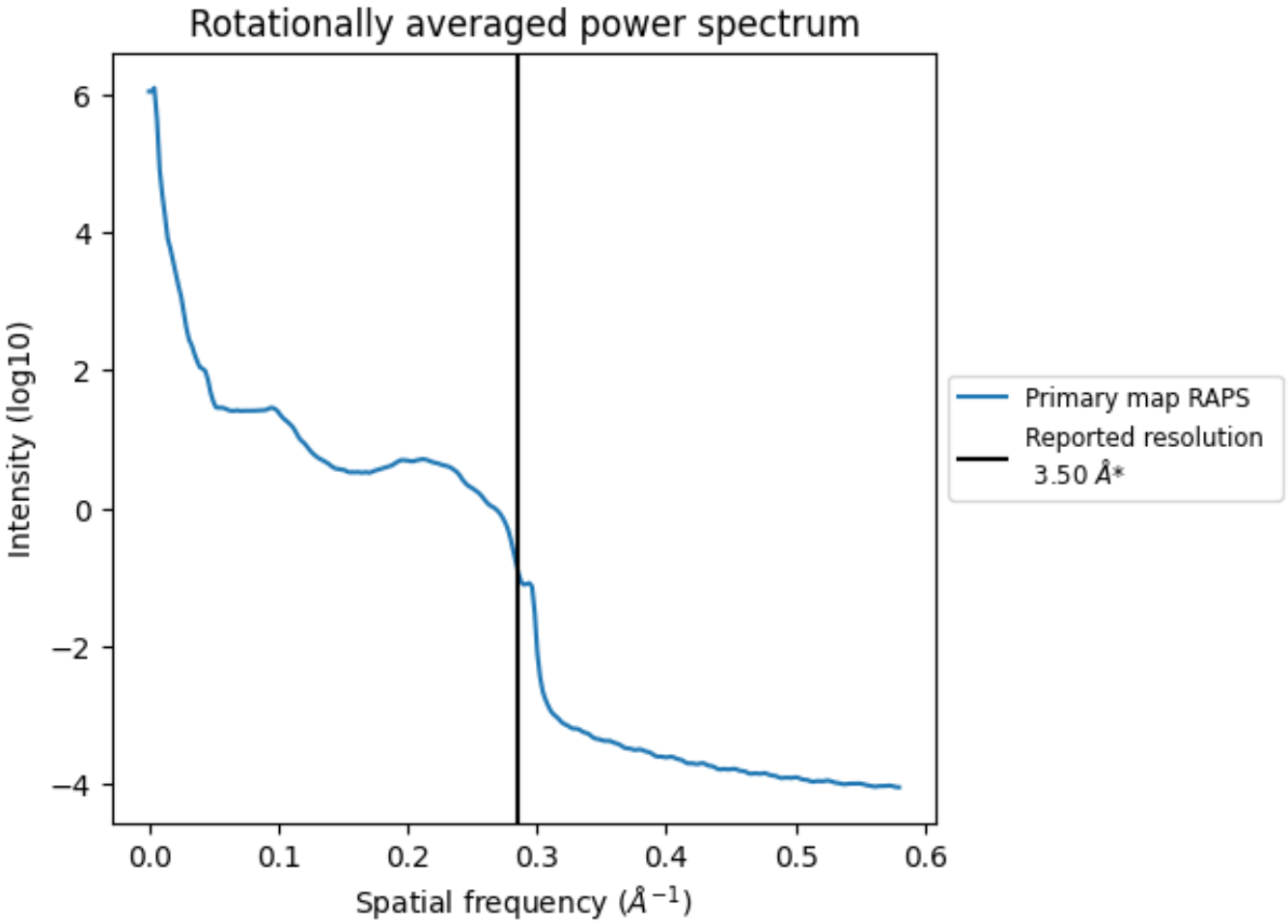
7.2 Volume estimate



The volume at the recommended contour level is 285 nm^3; this corresponds to an approximate mass of 258 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 0.286 Å^{-1}

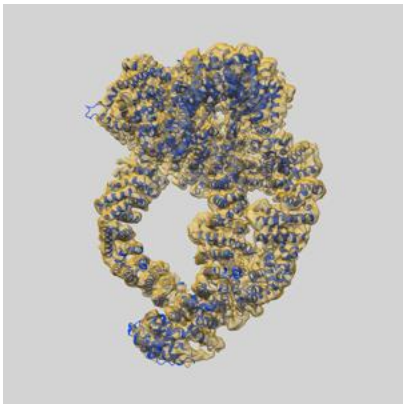
8 Fourier-Shell correlation (i)

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

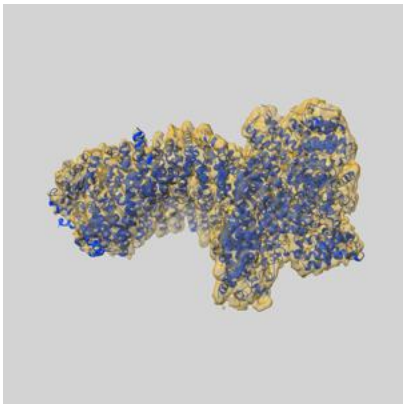
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18619 and PDB model 8QRI. Per-residue inclusion information can be found in section 3 on page 4.

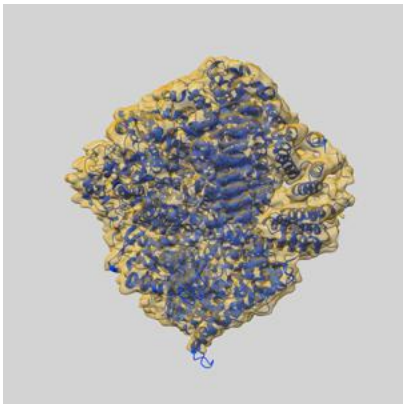
9.1 Map-model overlay



X



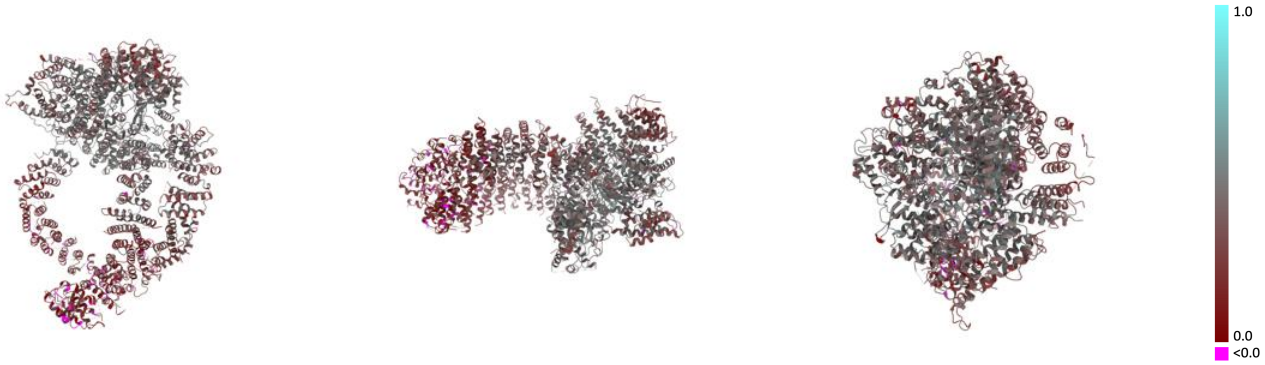
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 9.5 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.

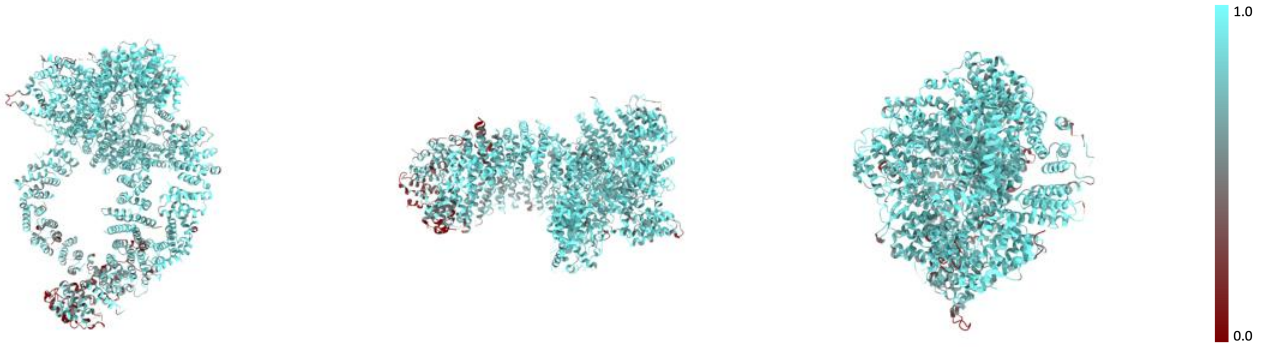
9.2 Q-score mapped to coordinate model (i)



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.

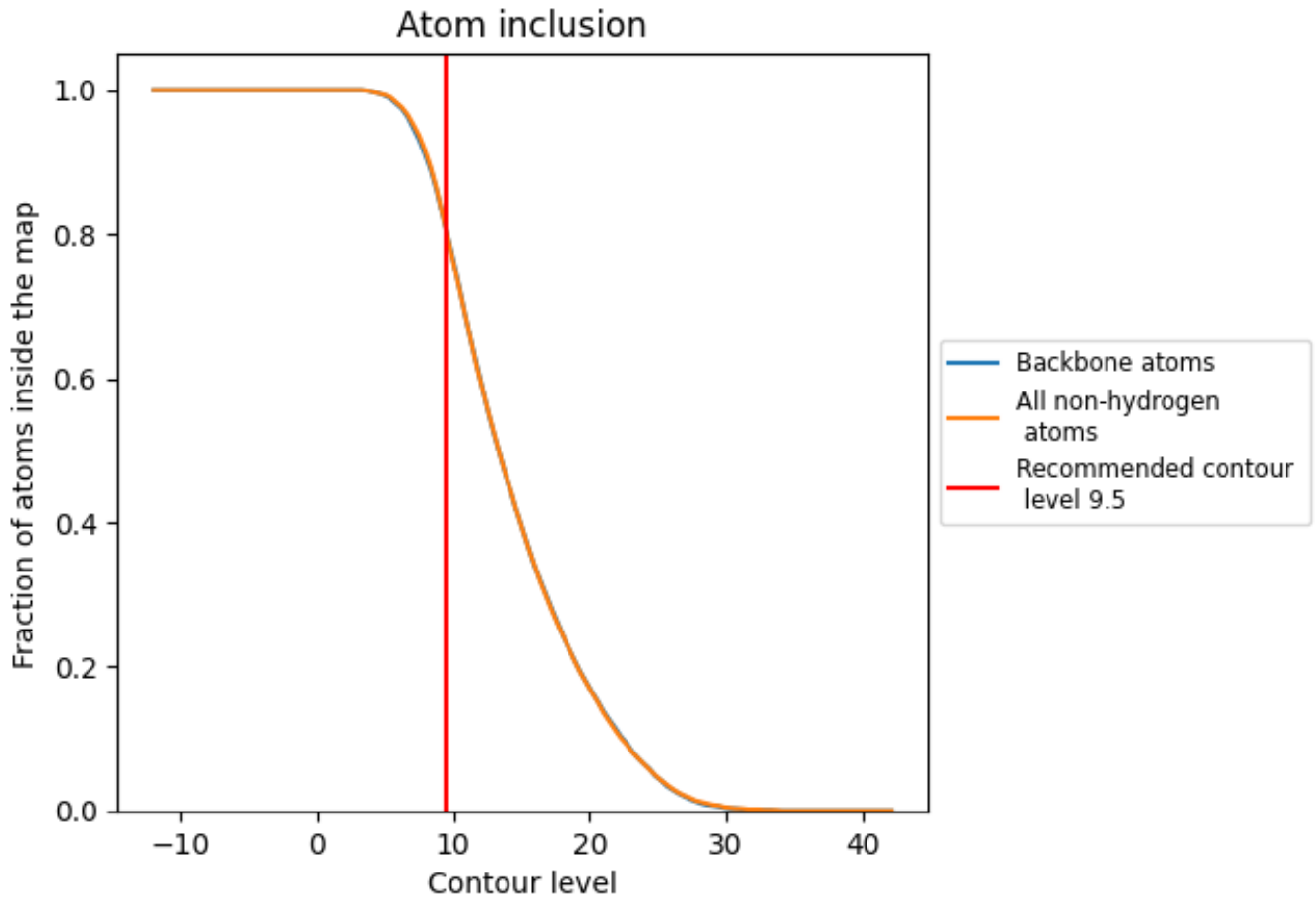
9.3 Atom inclusion mapped to coordinate model (i)



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 (9.5).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (9.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8040	0.3490
A	0.7320	0.3490
C	0.8140	0.3490