



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:11 PM UTC

PDB ID : 8ILM / pdb_00008ilm
EMDB ID : EMD-35536
Title : The cryo-EM structure of eight Rubisco large subunits (RbcL), two Arabidopsis thaliana Rubisco accumulation factors 1 (AtRaf1), and seven Arabidopsis thaliana Bundle Sheath Defective 2 (AtBSD2)
Authors : Wang, R.; Song, H.; Zhang, W.; Wang, N.; Zhang, S.; Shao, R.
Deposited on : 2023-03-03
Resolution : 3.30 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:

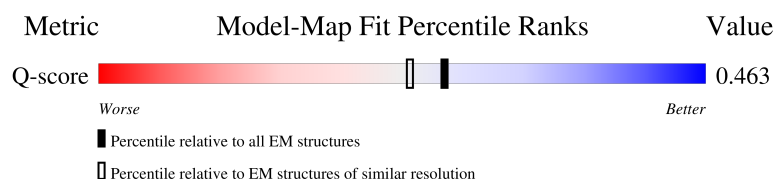
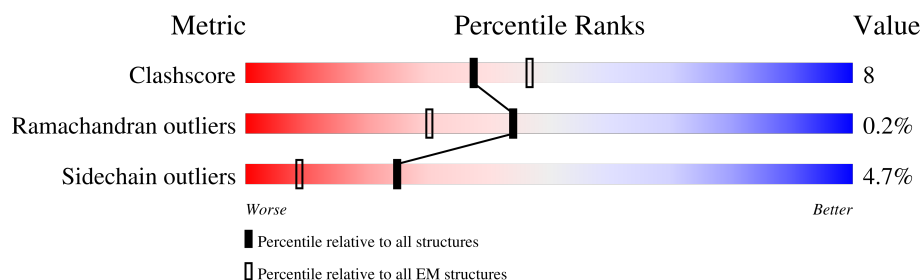
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	472	
1	B	472	
1	F	472	
1	G	472	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	472	
1	I	472	
1	J	472	
1	K	472	
2	C	81	
2	L	81	
2	M	81	
2	N	81	
2	O	81	
2	P	81	
2	Q	81	
3	D	389	
3	E	389	
3	R	389	
3	S	389	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 37908 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 Ribulose biphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	456	Total	C	N	O	S	0	0
			3581	2279	626	658	18		
1	B	453	Total	C	N	O	S	0	0
			3557	2265	623	652	17		
1	F	456	Total	C	N	O	S	0	0
			3581	2279	626	658	18		
1	G	456	Total	C	N	O	S	0	0
			3581	2279	626	658	18		
1	H	456	Total	C	N	O	S	0	0
			3581	2279	626	658	18		
1	I	453	Total	C	N	O	S	0	0
			3557	2265	623	652	17		
1	J	453	Total	C	N	O	S	0	0
			3557	2265	623	652	17		
1	K	453	Total	C	N	O	S	0	0
			3557	2265	623	652	17		

- Molecule 2 is a protein called Protein BUNDLE SHEATH DEFECTIVE 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	73	Total	C	N	O	S	0	0
			515	316	93	97	9		
2	L	79	Total	C	N	O	S	0	0
			564	345	101	109	9		
2	M	79	Total	C	N	O	S	0	0
			564	345	101	109	9		
2	N	73	Total	C	N	O	S	0	0
			519	320	92	98	9		
2	O	80	Total	C	N	O	S	0	0
			569	348	102	110	9		
2	P	80	Total	C	N	O	S	0	0
			569	348	102	110	9		
2	Q	73	Total	C	N	O	S	0	0
			519	320	92	98	9		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP Q9SN73
L	0	MET	-	initiating methionine	UNP Q9SN73
M	0	MET	-	initiating methionine	UNP Q9SN73
N	0	MET	-	initiating methionine	UNP Q9SN73
O	0	MET	-	initiating methionine	UNP Q9SN73
P	0	MET	-	initiating methionine	UNP Q9SN73
Q	0	MET	-	initiating methionine	UNP Q9SN73

- Molecule 3 is a protein called Rubisco accumulation factor 1.2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	207	Total	C	N	O	S	0	0
			1640	1035	282	319	4		
3	E	207	Total	C	N	O	S	0	0
			1640	1035	282	319	4		
3	R	149	Total	C	N	O	S	0	0
			1133	730	192	208	3		
3	S	150	Total	C	N	O	S	0	0
			1124	723	193	205	3		

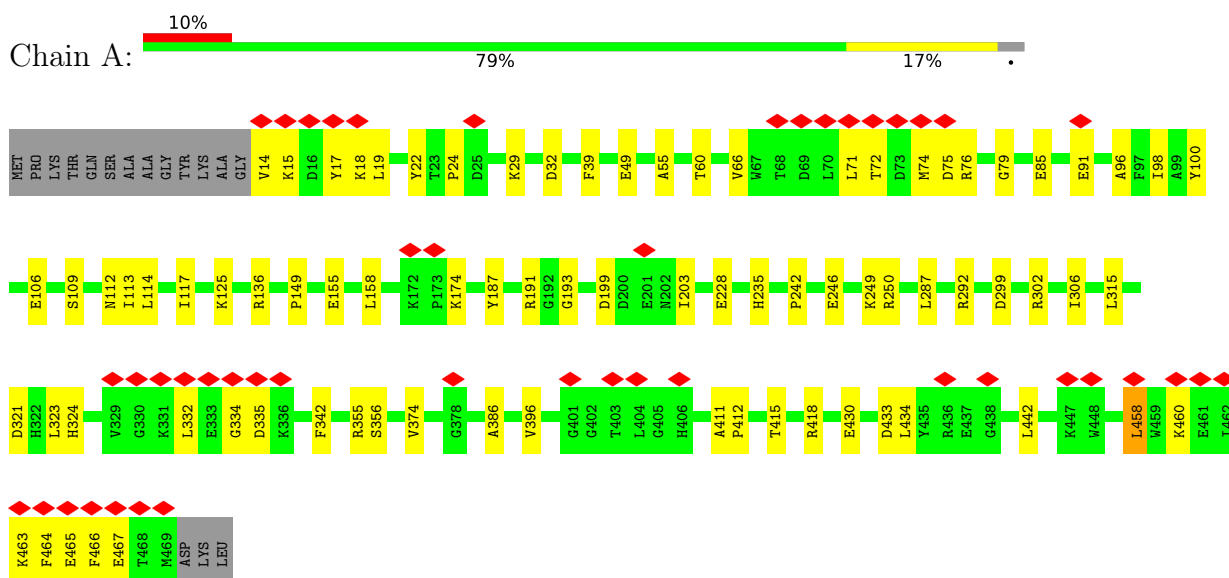
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP Q9SR19
E	1	MET	-	initiating methionine	UNP Q9SR19
R	61	MET	-	initiating methionine	UNP Q9SR19
S	61	MET	-	initiating methionine	UNP Q9SR19

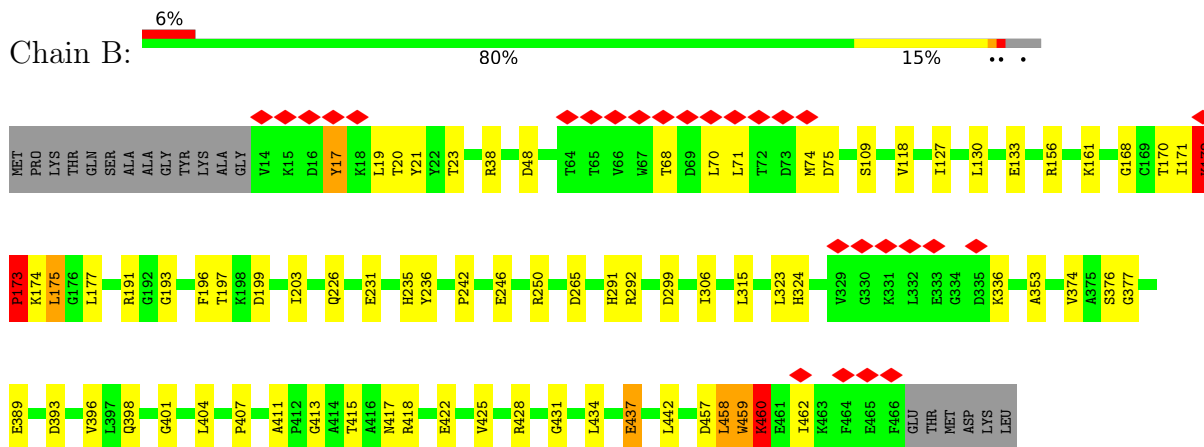
3 Residue-property plots

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.

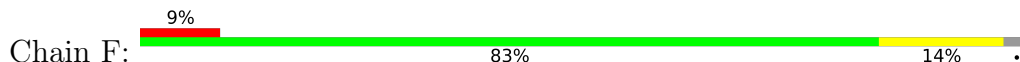
- Molecule 1: Ribulose biphosphate carboxylase large chain

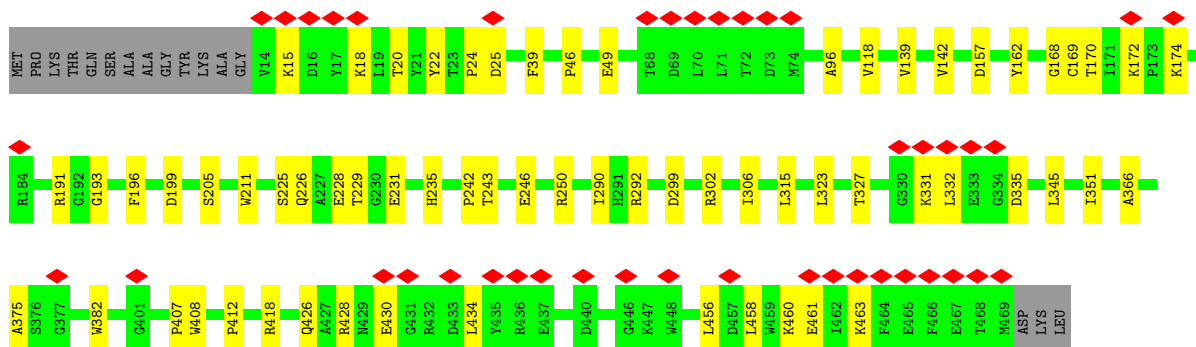


- Molecule 1: Ribulose biphosphate carboxylase large chain

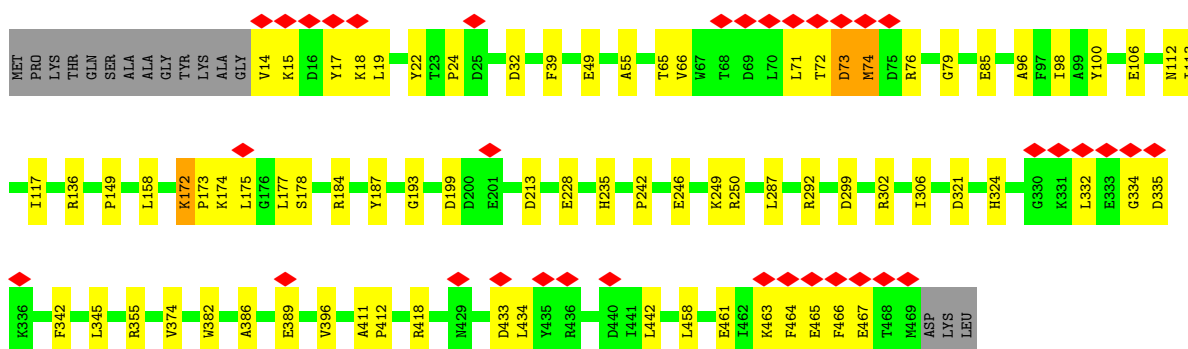
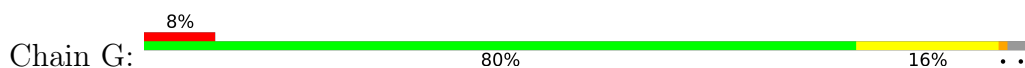


- Molecule 1: Ribulose biphosphate carboxylase large chain

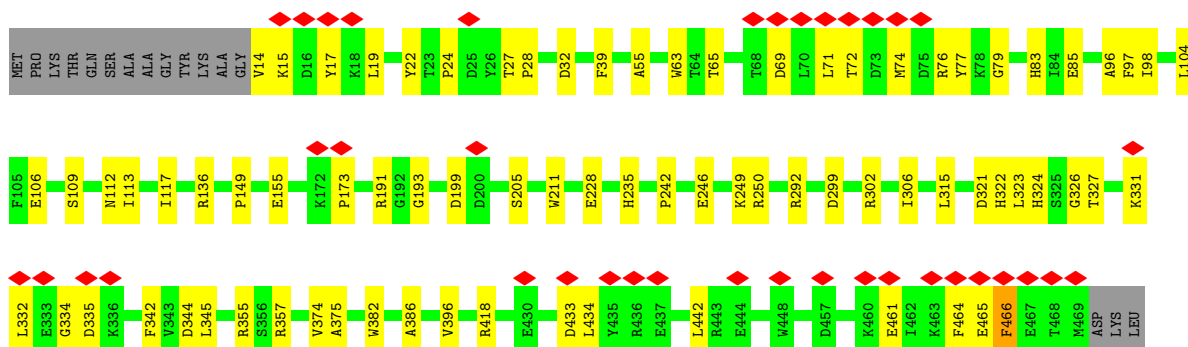
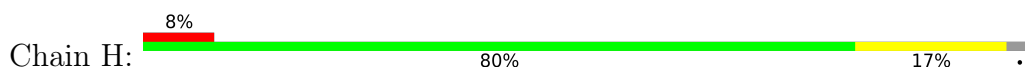




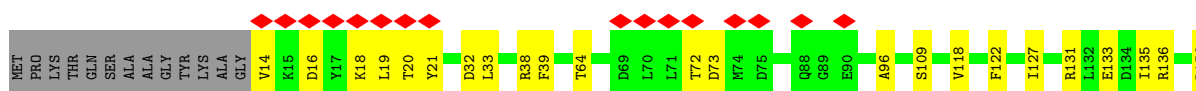
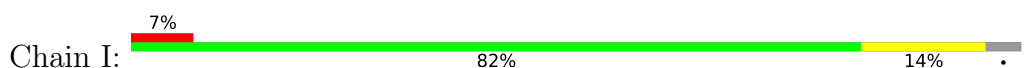
- Molecule 1: Ribulose biphosphate carboxylase large chain

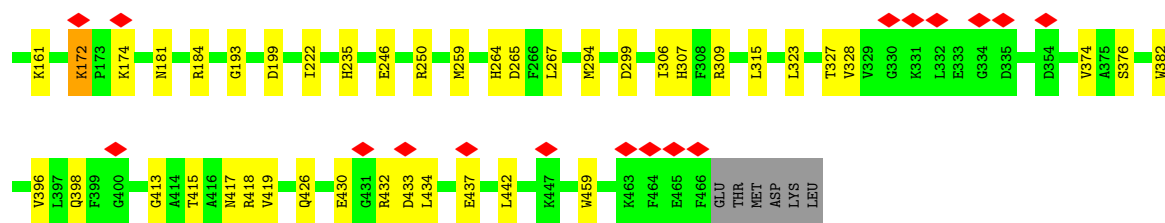


- Molecule 1: Ribulose biphosphate carboxylase large chain

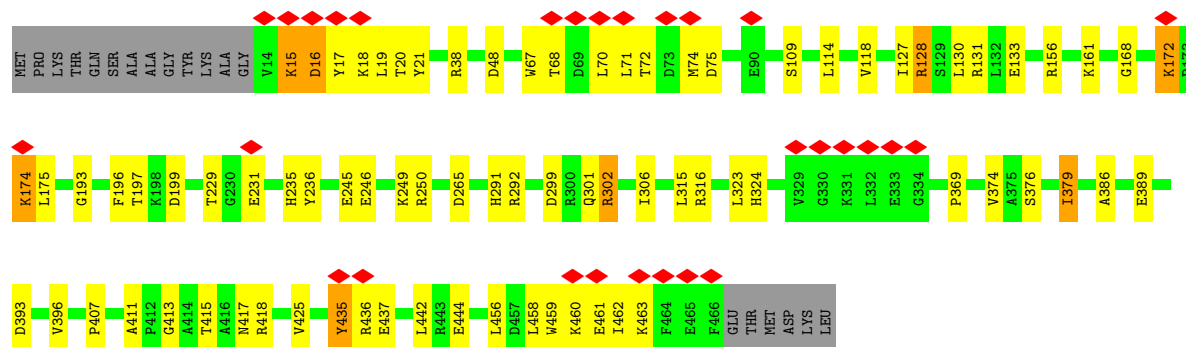
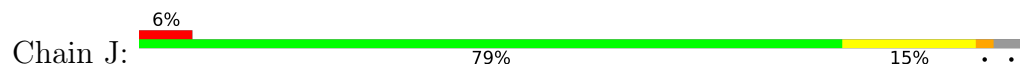


- Molecule 1: Ribulose biphosphate carboxylase large chain

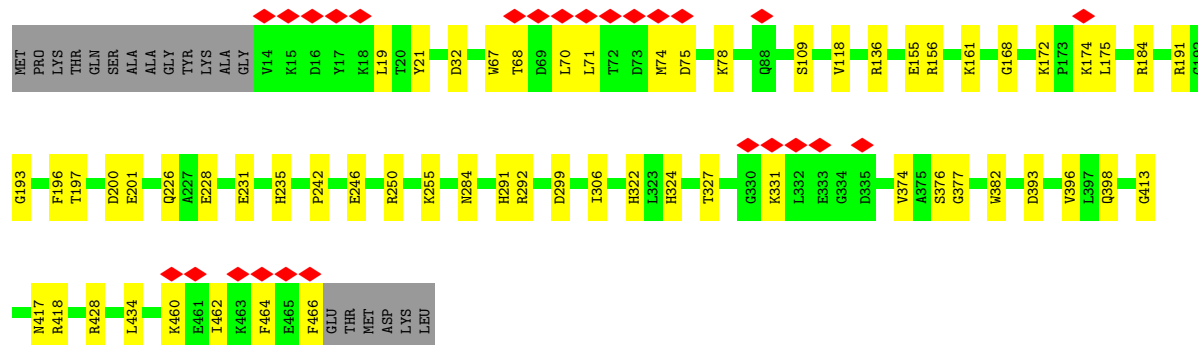
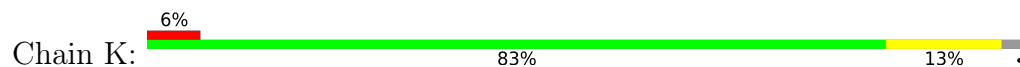




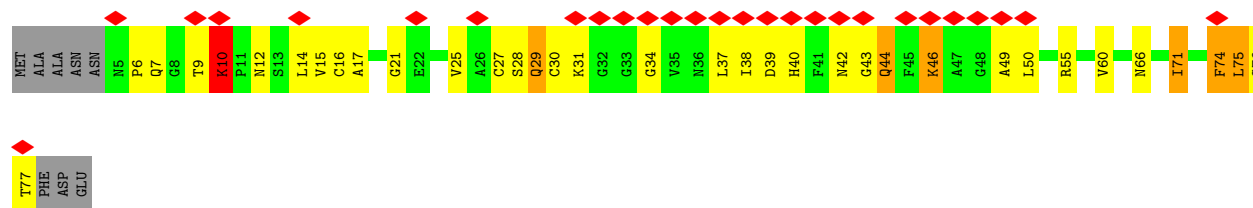
- Molecule 1: Ribulose biphosphate carboxylase large chain



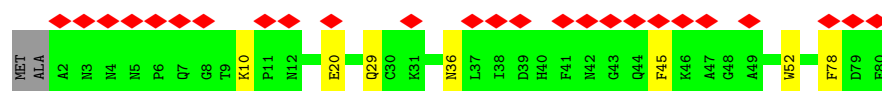
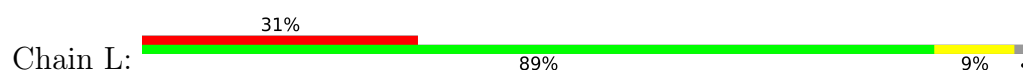
- Molecule 1: Ribulose biphosphate carboxylase large chain



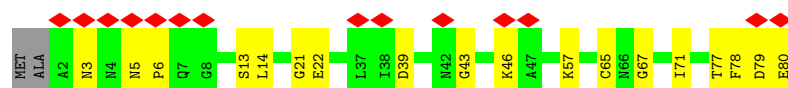
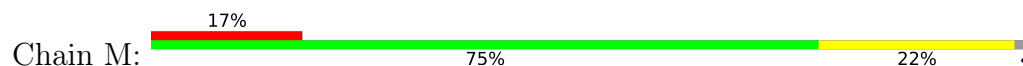
- Molecule 2: Protein BUNDLE SHEATH DEFECTIVE 2, chloroplastic



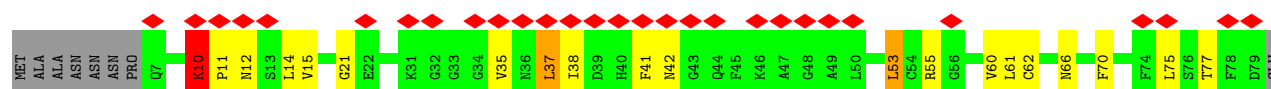
- Molecule 2: Protein BUNDLE SHEATH DEFECTIVE 2, chloroplastic



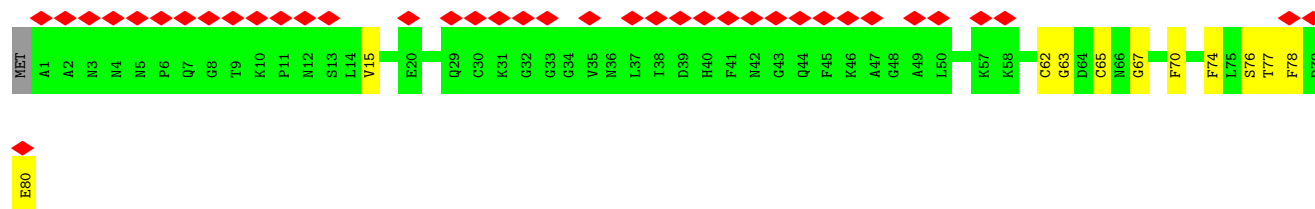
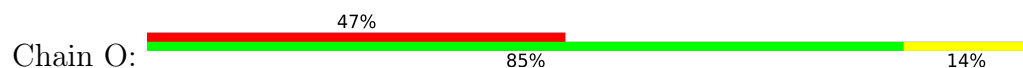
- Molecule 2: Protein BUNDLE SHEATH DEFECTIVE 2, chloroplastic



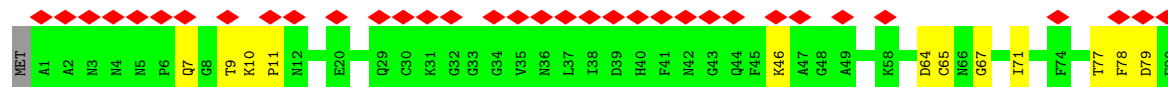
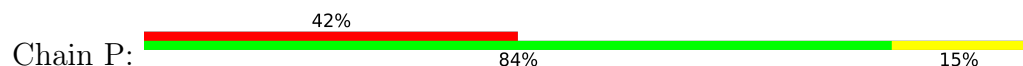
- Molecule 2: Protein BUNDLE SHEATH DEFECTIVE 2, chloroplastic



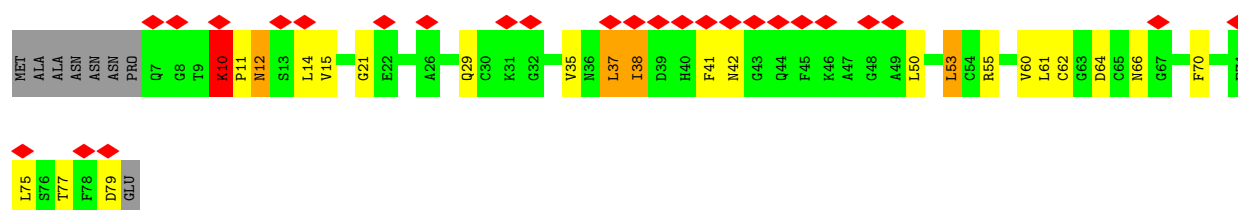
- Molecule 2: Protein BUNDLE SHEATH DEFECTIVE 2, chloroplastic



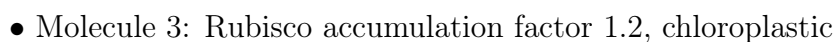
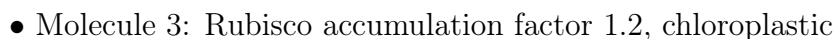
- Molecule 2: Protein BUNDLE SHEATH DEFECTIVE 2, chloroplastic

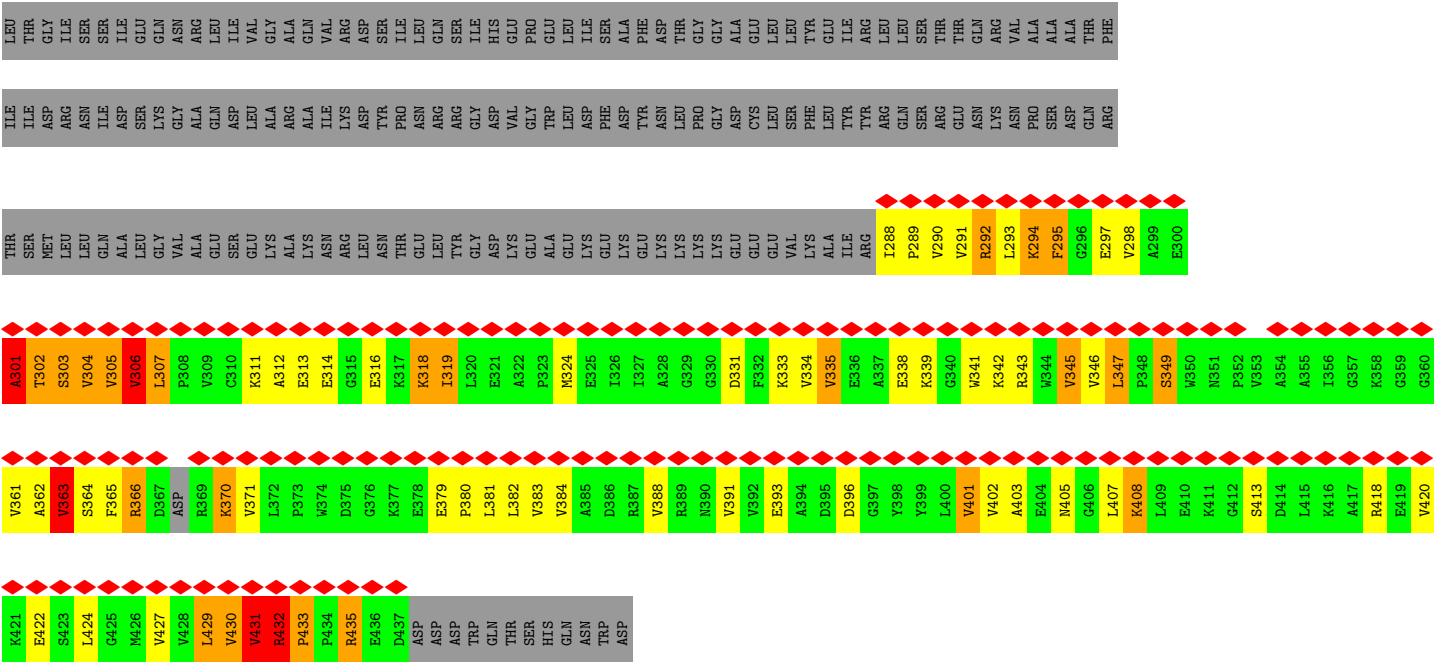


- Molecule 2: Protein BUNDLE SHEATH DEFECTIVE 2, chloroplastic

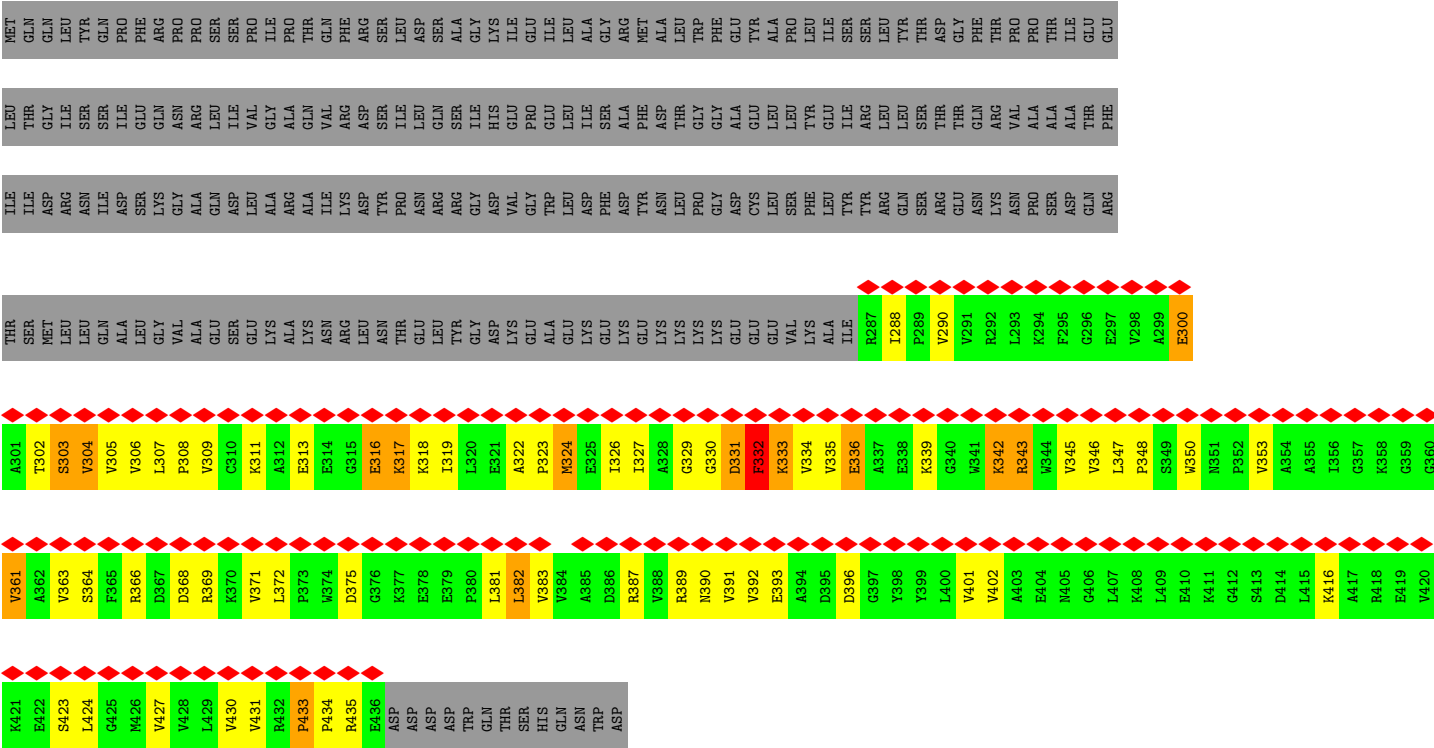


- Chain D:





• Molecule 3: Rubisco accumulation factor 1.2, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99991	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.127	Depositor
Minimum map value	-0.071	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0183	Depositor
Map size ($\text{\AA}$)	344.32, 344.32, 344.32	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.076, 1.076, 1.076	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	A	0.50	0/3672	0.54	1/4975 (0.0%)
1	B	0.53	1/3648 (0.0%)	0.65	9/4943 (0.2%)
1	F	0.39	0/3672	0.43	0/4975
1	G	0.51	0/3672	0.55	1/4975 (0.0%)
1	H	0.39	0/3672	0.45	0/4975
1	I	0.37	0/3648	0.43	0/4943
1	J	0.50	0/3648	0.58	4/4943 (0.1%)
1	K	0.38	0/3648	0.44	0/4943
2	C	0.70	0/523	1.35	9/701 (1.3%)
2	L	0.21	0/573	0.37	0/769
2	M	0.22	0/573	0.42	0/769
2	N	0.78	0/527	1.00	0/705
2	O	0.25	0/578	0.49	0/776
2	P	0.25	0/578	0.37	0/776
2	Q	0.78	0/527	1.00	0/705
3	D	0.21	0/1673	0.41	0/2269
3	E	0.21	0/1673	0.41	0/2269
3	R	0.67	1/1153 (0.1%)	1.54	18/1565 (1.2%)
3	S	0.54	0/1145	1.17	10/1560 (0.6%)
All	All	0.45	2/38803 (0.0%)	0.62	52/52536 (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	I	0	1
3	D	0	1
3	E	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	459	TRP	N-CA	-6.17	1.38	1.46
3	R	433	PRO	CA-C	6.16	1.57	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	431	VAL	N-CA-C	30.80	138.77	110.74
2	C	15	VAL	N-CA-C	-14.27	91.47	109.30
1	B	17	TYR	N-CA-C	-11.16	99.06	112.89
3	R	433	PRO	N-CA-C	10.67	123.72	110.70
3	R	303	SER	N-CA-C	10.10	123.35	108.60
3	R	331	ASP	N-CA-C	-9.92	102.25	114.75
2	C	75	LEU	N-CA-C	-9.80	100.45	111.82
3	R	304	VAL	N-CA-C	9.67	122.42	109.37
3	S	330	GLY	N-CA-C	9.30	122.63	111.93
3	R	431	VAL	CB-CA-C	-8.91	100.18	111.94
3	R	301	ALA	N-CA-C	8.53	128.97	110.80
1	B	460	LYS	N-CA-C	7.73	119.71	111.28
1	B	459	TRP	N-CA-CB	-7.56	100.36	110.57
3	S	433	PRO	N-CA-C	7.46	118.57	110.58
1	B	175	LEU	N-CA-C	7.41	122.21	112.72
1	J	172	LYS	CA-C-N	-7.32	114.26	121.65
1	J	172	LYS	C-N-CA	-7.32	114.26	121.65
1	B	171	ILE	N-CA-C	-6.73	97.81	107.37
3	S	332	PHE	N-CA-CB	6.69	120.33	110.56
3	R	293	LEU	N-CA-C	-6.69	98.30	108.67
1	B	172	LYS	N-CA-C	-6.69	100.57	110.20
1	B	458	LEU	O-C-N	6.57	128.84	122.07
2	C	28	SER	N-CA-C	6.51	118.37	111.28
3	S	329	GLY	N-CA-C	-6.33	98.17	113.18
3	R	380	PRO	CA-C-O	-6.26	114.07	122.08
2	C	49	ALA	N-CA-C	6.22	118.06	111.28
2	C	74	PHE	N-CA-C	6.15	119.23	110.68
1	B	173	PRO	N-CA-C	6.13	125.11	112.47
3	R	432	ARG	N-CA-C	5.96	122.99	109.81
2	C	34	GLY	N-CA-C	-5.82	105.31	114.10
3	S	372	LEU	CA-C-N	-5.79	112.92	119.28
3	S	372	LEU	C-N-CA	-5.79	112.92	119.28
3	R	429	LEU	CA-CB-CG	5.76	136.46	116.30
3	R	324	MET	N-CA-C	5.73	117.60	111.36
2	C	10	LYS	CA-C-N	-5.56	114.04	119.76
2	C	10	LYS	C-N-CA	-5.56	114.04	119.76
3	S	342	LYS	N-CA-C	5.54	117.32	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	459	TRP	N-CA-C	-5.48	99.02	108.56
3	R	363	VAL	N-CA-C	5.47	115.97	107.28
2	C	29	GLN	N-CA-C	5.46	118.74	112.57
1	J	17	TYR	N-CA-C	-5.37	105.83	112.38
3	R	306	VAL	N-CA-C	5.37	116.40	108.45
3	S	350	TRP	N-CA-C	-5.36	102.95	110.50
3	R	432	ARG	CA-C-N	5.32	125.86	120.38
3	R	432	ARG	C-N-CA	5.32	125.86	120.38
1	A	76	ARG	N-CA-C	-5.30	105.93	112.72
3	R	304	VAL	CB-CA-C	-5.25	103.02	111.59
3	R	334	VAL	N-CA-C	-5.10	102.92	109.30
1	G	172	LYS	N-CA-C	5.10	121.08	109.81
3	S	307	LEU	CA-C-N	-5.04	115.04	120.03
3	S	307	LEU	C-N-CA	-5.04	115.04	120.03
1	J	174	LYS	N-CA-C	5.02	116.75	111.28

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	175	ASN	Peptide
3	E	175	ASN	Peptide
1	I	172	LYS	Peptide

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	3581	0	3496	66	0
1	B	3557	0	3472	56	0
1	F	3581	0	3497	41	0
1	G	3581	0	3497	53	0
1	H	3581	0	3497	49	0
1	I	3557	0	3475	41	0
1	J	3557	0	3475	63	0
1	K	3557	0	3475	49	0
2	C	515	0	495	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	564	0	529	5	0
2	M	564	0	529	14	0
2	N	519	0	495	11	0
2	O	569	0	537	7	0
2	P	569	0	537	8	0
2	Q	519	0	495	23	0
3	D	1640	0	1620	40	0
3	E	1640	0	1620	34	0
3	R	1133	0	1160	42	0
3	S	1124	0	1133	35	0
All	All	37908	0	37034	563	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 8.

All (563) 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)
3:D:65:SER:HB3	1:K:184:ARG:CZ	1.47	1.41
1:J:459:TRP:CZ3	2:N:66:ASN:OD1	1.79	1.34
3:D:65:SER:CB	1:K:184:ARG:CZ	2.05	1.33
1:B:460:LYS:NZ	2:Q:64:ASP:OD1	1.66	1.25
1:G:66:VAL:HG11	2:N:61:LEU:CD2	1.67	1.24
1:J:459:TRP:HZ3	2:N:66:ASN:OD1	0.93	1.24
1:A:66:VAL:HG11	2:Q:61:LEU:CD2	1.67	1.22
3:D:65:SER:HB3	1:K:184:ARG:NE	1.59	1.17
1:G:66:VAL:HG11	2:N:61:LEU:HD21	1.24	1.16
1:J:386:ALA:HA	1:J:435:TYR:CE1	1.82	1.15
1:G:66:VAL:CG1	2:N:61:LEU:HD21	1.78	1.14
1:A:66:VAL:CG1	2:Q:61:LEU:HD21	1.79	1.11
1:A:66:VAL:HG11	2:Q:61:LEU:HD21	1.24	1.10
3:D:65:SER:HB2	1:K:184:ARG:NH2	1.65	1.10
1:J:386:ALA:CB	1:J:435:TYR:HE1	1.63	1.08
1:J:386:ALA:CB	1:J:435:TYR:CE1	2.37	1.07
1:J:386:ALA:CA	1:J:435:TYR:HE1	1.65	1.07
1:B:460:LYS:HZ1	2:Q:64:ASP:CG	1.65	1.03
1:J:386:ALA:HB2	1:J:435:TYR:CE1	1.93	1.03
1:J:386:ALA:CA	1:J:435:TYR:CE1	2.38	1.02
1:J:386:ALA:HB1	1:J:435:TYR:OH	1.62	0.97
1:B:459:TRP:CZ3	2:Q:66:ASN:OD1	2.19	0.95
1:B:457:ASP:OD2	2:Q:29:GLN:NE2	2.00	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:38:ARG:HD3	1:J:302:ARG:NH1	1.82	0.94
3:E:59:GLU:OE2	1:G:184:ARG:NH1	2.03	0.91
3:D:65:SER:CB	1:K:184:ARG:NH2	2.29	0.88
1:J:386:ALA:HB2	1:J:435:TYR:HE1	1.27	0.88
1:J:38:ARG:HD3	1:J:302:ARG:HH12	1.44	0.82
1:A:66:VAL:HG11	2:Q:61:LEU:HD22	1.62	0.81
3:D:65:SER:HB2	1:K:184:ARG:CZ	1.93	0.81
1:J:197:THR:HG1	1:J:235:HIS:HD1	1.28	0.80
1:F:199:ASP:OD1	1:F:235:HIS:NE2	2.13	0.80
1:B:460:LYS:NZ	2:Q:64:ASP:CG	2.31	0.80
1:K:197:THR:HG1	1:K:235:HIS:HD1	1.27	0.80
2:C:40:HIS:CE1	2:C:44:GLN:HE21	2.01	0.79
1:B:197:THR:HG1	1:B:235:HIS:HD1	1.31	0.78
1:F:243:THR:OG1	1:F:246:GLU:OE1	2.01	0.78
1:G:66:VAL:HG11	2:N:61:LEU:HD22	1.62	0.77
1:A:85:GLU:OE2	1:A:355:ARG:NH2	2.18	0.77
1:I:199:ASP:OD1	1:I:235:HIS:NE2	2.17	0.76
1:G:85:GLU:OE2	1:G:355:ARG:NH2	2.18	0.75
1:B:193:GLY:O	1:B:418:ARG:NH1	2.19	0.75
3:D:65:SER:CB	1:K:184:ARG:NH1	2.49	0.75
1:J:193:GLY:O	1:J:418:ARG:NH1	2.19	0.75
2:O:65:CYS:O	2:O:67:GLY:N	2.20	0.74
3:R:304:VAL:HG13	3:S:346:VAL:HB	1.70	0.74
2:M:71:ILE:O	2:M:77:THR:OG1	2.07	0.73
1:H:85:GLU:OE2	1:H:355:ARG:NH2	2.22	0.73
1:B:377:GLY:O	2:Q:79:ASP:N	2.22	0.72
2:C:40:HIS:HE1	2:C:44:GLN:HE21	1.36	0.72
3:R:365:PHE:HB2	3:R:381:LEU:HB2	1.72	0.72
3:E:157:LEU:HD23	3:E:192:GLU:HG3	1.72	0.71
1:J:197:THR:OG1	1:J:235:HIS:ND1	2.18	0.71
1:K:193:GLY:O	1:K:418:ARG:NH1	2.23	0.71
2:C:43:GLY:HA2	2:C:46:LYS:HB3	1.72	0.71
3:D:157:LEU:HD23	3:D:192:GLU:HG3	1.72	0.71
1:J:386:ALA:CB	1:J:435:TYR:CZ	2.74	0.70
1:G:242:PRO:HG3	1:J:109:SER:HB2	1.72	0.70
1:J:386:ALA:CB	1:J:435:TYR:OH	2.37	0.70
2:C:40:HIS:CE1	2:C:44:GLN:NE2	2.60	0.70
1:A:74:MET:HG3	1:A:75:ASP:H	1.57	0.69
1:A:332:LEU:HG	1:A:334:GLY:H	1.58	0.69
1:K:155:GLU:OE2	1:K:322:HIS:NE2	2.25	0.69
1:G:332:LEU:HG	1:G:334:GLY:H	1.58	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:197:THR:OG1	1:K:235:HIS:ND1	2.21	0.69
1:F:426:GLN:NE2	1:F:430:GLU:OE2	2.27	0.68
3:D:173:ASN:ND2	3:D:179:GLN:OE1	2.27	0.68
1:A:242:PRO:HG3	1:B:109:SER:HB2	1.74	0.67
1:H:242:PRO:HG3	1:K:109:SER:HB2	1.75	0.67
1:H:71:LEU:HG	1:H:72:THR:HG22	1.76	0.67
1:B:197:THR:OG1	1:B:235:HIS:ND1	2.18	0.67
3:E:173:ASN:ND2	3:E:179:GLN:OE1	2.27	0.67
1:K:191:ARG:NE	1:K:228:GLU:OE2	2.28	0.66
1:B:156:ARG:NH1	1:B:161:LYS:O	2.28	0.66
1:J:156:ARG:NH1	1:J:161:LYS:O	2.28	0.66
1:K:156:ARG:NH1	1:K:161:LYS:O	2.30	0.65
1:F:461:GLU:HG2	1:F:463:LYS:HE3	1.77	0.65
1:B:460:LYS:CE	2:Q:64:ASP:OD1	2.43	0.64
2:P:7:GLN:HG3	2:P:64:ASP:HB2	1.78	0.64
1:I:16:ASP:HB3	2:O:15:VAL:HG11	1.78	0.64
2:P:65:CYS:O	2:P:67:GLY:N	2.29	0.64
1:F:302:ARG:NH2	1:F:335:ASP:OD2	2.30	0.64
2:C:27:CYS:HB2	2:C:60:VAL:HG13	1.80	0.64
3:R:345:VAL:HG21	3:S:334:VAL:HA	1.80	0.64
1:J:461:GLU:HB3	1:J:463:LYS:HE3	1.79	0.64
1:J:74:MET:SD	1:J:75:ASP:N	2.65	0.64
1:F:172:LYS:O	1:F:172:LYS:NZ	2.25	0.63
1:H:332:LEU:HG	1:H:334:GLY:H	1.63	0.63
2:C:40:HIS:H	2:C:46:LYS:HB2	1.64	0.63
2:O:74:PHE:HA	2:O:78:PHE:HB2	1.80	0.62
1:H:77:TYR:HB3	1:H:104:LEU:HD21	1.80	0.62
3:R:362:ALA:HB1	3:R:382:LEU:HD11	1.81	0.62
3:R:433:PRO:HA	3:S:331:ASP:HA	1.81	0.62
1:G:463:LYS:NZ	1:G:465:GLU:O	2.34	0.61
1:B:413:GLY:O	1:B:417:ASN:ND2	2.34	0.61
1:H:155:GLU:OE1	1:H:322:HIS:NE2	2.32	0.61
1:J:413:GLY:O	1:J:417:ASN:ND2	2.34	0.61
2:M:65:CYS:O	2:M:67:GLY:N	2.34	0.61
1:I:426:GLN:NE2	1:I:430:GLU:OE2	2.33	0.61
3:D:174:LYS:HG2	3:D:175:ASN:H	1.65	0.61
1:B:74:MET:SD	1:B:75:ASP:N	2.65	0.61
1:K:377:GLY:HA3	2:M:78:PHE:HB3	1.83	0.60
1:A:463:LYS:NZ	1:A:465:GLU:O	2.34	0.60
1:B:431:GLY:O	3:D:111:THR:HG23	2.01	0.60
1:F:193:GLY:O	1:F:418:ARG:NH1	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:306:VAL:HG22	3:S:346:VAL:HG21	1.82	0.60
3:E:174:LYS:HG2	3:E:175:ASN:H	1.65	0.60
1:I:374:VAL:HG22	1:I:396:VAL:HB	1.83	0.60
1:H:106:GLU:HB2	1:H:112:ASN:HD22	1.67	0.59
2:P:9:THR:HG22	2:P:71:ILE:HG13	1.84	0.59
2:L:10:LYS:NZ	2:L:20:GLU:OE1	2.30	0.59
1:A:49:GLU:OE1	2:Q:12:ASN:HB3	2.02	0.59
3:E:85:SER:O	3:E:87:HIS:ND1	2.32	0.59
1:K:413:GLY:O	1:K:417:ASN:ND2	2.35	0.59
3:R:401:VAL:HG23	3:R:408:LYS:HG3	1.84	0.59
1:B:68:THR:HB	1:B:74:MET:HG3	1.85	0.58
1:B:459:TRP:HZ3	2:Q:66:ASN:OD1	1.78	0.58
1:K:74:MET:HE3	1:K:75:ASP:H	1.67	0.58
1:J:68:THR:HB	1:J:74:MET:HG3	1.85	0.58
1:A:191:ARG:NH2	3:E:4:LEU:HB3	2.18	0.58
1:A:49:GLU:CD	2:Q:12:ASN:HB3	2.28	0.58
1:G:65:THR:HG22	1:G:74:MET:HE2	1.85	0.58
1:I:39:PHE:HB2	1:I:127:ILE:HD11	1.85	0.58
1:K:172:LYS:C	1:K:174:LYS:H	2.12	0.58
1:I:156:ARG:NH1	1:I:161:LYS:O	2.37	0.58
1:G:374:VAL:HG22	1:G:396:VAL:HB	1.86	0.58
3:D:85:SER:O	3:D:87:HIS:ND1	2.31	0.57
1:K:331:LYS:NZ	2:M:80:GLU:O	2.36	0.57
1:F:428:ARG:HB2	1:F:434:LEU:HD11	1.86	0.57
1:A:199:ASP:OD1	1:A:235:HIS:NE2	2.34	0.57
3:D:105:GLU:HG2	3:D:132:GLN:HG3	1.85	0.57
1:H:14:VAL:HG22	1:H:63:TRP:HB3	1.87	0.57
3:R:302:THR:HB	3:S:348:PRO:CB	2.34	0.57
1:G:292:ARG:HG2	1:G:324:HIS:HB2	1.86	0.57
1:H:15:LYS:HZ1	2:M:22:GLU:HA	1.70	0.57
1:B:415:THR:HG21	3:D:7:PRO:HG2	1.85	0.57
1:K:376:SER:HB3	1:K:398:GLN:HB2	1.87	0.56
1:I:193:GLY:O	1:I:418:ARG:NH1	2.37	0.56
1:A:292:ARG:HG2	1:A:324:HIS:HB2	1.86	0.56
1:G:199:ASP:OD1	1:G:235:HIS:NE2	2.34	0.56
1:H:173:PRO:HB2	1:K:67:TRP:CD1	2.41	0.56
1:K:174:LYS:HG3	1:K:175:LEU:HD23	1.87	0.56
3:E:105:GLU:HG2	3:E:132:GLN:HG3	1.85	0.56
1:I:222:ILE:HG13	1:I:259:MET:HE1	1.88	0.56
3:S:311:LYS:HB3	3:S:366:ARG:HH12	1.71	0.55
1:B:393:ASP:OD1	1:B:393:ASP:N	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:393:ASP:OD1	1:J:393:ASP:N	2.40	0.55
1:H:246:GLU:O	1:H:250:ARG:HG3	2.07	0.55
1:K:255:LYS:HE2	1:K:284:ASN:HB3	1.89	0.55
1:A:17:TYR:O	1:A:19:LEU:N	2.39	0.55
1:G:98:ILE:HD11	1:G:100:TYR:OH	2.06	0.55
1:A:98:ILE:HD11	1:A:100:TYR:OH	2.06	0.55
1:I:133:GLU:O	1:I:309:ARG:NH1	2.40	0.55
1:A:299:ASP:HB3	1:A:306:ILE:O	2.07	0.55
3:R:302:THR:HB	3:S:348:PRO:HB3	1.88	0.55
1:G:299:ASP:HB3	1:G:306:ILE:O	2.07	0.54
1:I:172:LYS:HB3	1:I:174:LYS:HE3	1.89	0.54
1:J:411:ALA:O	1:J:415:THR:HG23	2.07	0.54
2:P:10:LYS:HB3	2:P:11:PRO:HD2	1.89	0.54
2:C:21:GLY:HA3	1:J:16:ASP:HB2	1.89	0.54
1:H:292:ARG:HG2	1:H:324:HIS:HB2	1.88	0.54
1:F:327:THR:HG22	1:F:375:ALA:HB1	1.89	0.54
1:H:433:ASP:OD1	1:H:434:LEU:N	2.40	0.54
1:B:246:GLU:O	1:B:250:ARG:HG3	2.07	0.54
1:I:181:ASN:OD1	1:I:184:ARG:NH2	2.40	0.54
1:B:411:ALA:O	1:B:415:THR:HG23	2.08	0.54
1:H:299:ASP:HB3	1:H:306:ILE:O	2.08	0.54
3:R:403:ALA:HB2	3:R:408:LYS:HB3	1.89	0.54
1:F:408:TRP:CD1	1:F:412:PRO:HG2	2.42	0.53
1:J:246:GLU:O	1:J:250:ARG:HG3	2.07	0.53
3:R:289:PRO:HD2	3:R:429:LEU:HD12	1.89	0.53
1:A:74:MET:CG	1:A:75:ASP:H	2.20	0.53
3:R:295:PHE:HA	3:S:303:SER:HB2	1.90	0.53
2:O:76:SER:OG	2:O:77:THR:N	2.40	0.53
3:R:305:VAL:H	3:S:346:VAL:HG11	1.74	0.53
3:S:332:PHE:O	3:S:333:LYS:HB2	2.07	0.53
1:B:374:VAL:HG22	1:B:396:VAL:HB	1.91	0.53
3:R:431:VAL:HG12	3:S:331:ASP:HB2	1.91	0.53
1:F:172:LYS:O	1:F:174:LYS:N	2.42	0.53
1:F:225:SER:O	1:F:229:THR:HG22	2.08	0.53
3:R:347:LEU:HG	3:R:384:VAL:HG21	1.89	0.53
1:F:246:GLU:O	1:F:250:ARG:HG3	2.09	0.52
1:H:65:THR:HB	1:H:69:ASP:OD2	2.09	0.52
1:I:415:THR:O	1:I:419:VAL:HG23	2.09	0.52
1:A:113:ILE:O	1:A:117:ILE:HG12	2.09	0.52
1:A:433:ASP:OD1	1:A:434:LEU:N	2.43	0.52
1:G:15:LYS:HG3	1:G:17:TYR:H	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:246:GLU:O	1:I:250:ARG:HG3	2.09	0.52
3:R:290:VAL:HG13	3:R:430:VAL:HB	1.92	0.52
1:A:60:THR:HG21	1:A:74:MET:HE1	1.90	0.52
1:G:113:ILE:O	1:G:117:ILE:HG12	2.09	0.52
1:K:374:VAL:HG22	1:K:396:VAL:HB	1.90	0.52
1:I:432:ARG:NH2	1:I:437:GLU:OE1	2.42	0.52
1:K:156:ARG:NH2	1:K:393:ASP:O	2.43	0.52
2:M:5:ASN:HB2	2:M:6:PRO:HD3	1.91	0.52
1:J:460:LYS:O	1:J:462:ILE:HD12	2.09	0.52
1:K:174:LYS:HD2	1:K:200:ASP:OD1	2.10	0.52
1:J:19:LEU:O	1:J:21:TYR:N	2.43	0.52
1:A:15:LYS:HG3	1:A:17:TYR:H	1.74	0.51
1:A:55:ALA:HB1	1:A:79:GLY:O	2.10	0.51
1:I:315:LEU:HD22	1:I:323:LEU:HD13	1.93	0.51
1:G:55:ALA:HB1	1:G:79:GLY:O	2.10	0.51
1:A:109:SER:HB2	1:B:242:PRO:HB3	1.93	0.51
1:B:175:LEU:HD12	1:B:203:ILE:HD11	1.93	0.51
3:E:151:LEU:HD23	3:E:151:LEU:H	1.76	0.51
1:G:433:ASP:OD1	1:G:434:LEU:N	2.43	0.51
1:B:19:LEU:O	1:B:21:TYR:N	2.43	0.51
3:D:151:LEU:HD23	3:D:151:LEU:H	1.76	0.51
1:G:17:TYR:O	1:G:19:LEU:N	2.39	0.51
1:F:157:ASP:OD2	1:F:162:TYR:OH	2.24	0.51
3:D:19:PHE:HB3	3:D:22:LEU:HD12	1.92	0.51
1:F:408:TRP:HD1	1:F:412:PRO:HG2	1.74	0.51
1:J:374:VAL:HG22	1:J:396:VAL:HB	1.91	0.51
1:H:193:GLY:O	1:H:418:ARG:NH1	2.43	0.51
1:B:407:PRO:HD3	1:B:458:LEU:HD22	1.93	0.51
1:F:22:TYR:CE2	1:F:24:PRO:HG3	2.46	0.51
1:I:413:GLY:O	1:I:417:ASN:ND2	2.44	0.51
1:J:38:ARG:NH1	1:J:133:GLU:OE2	2.44	0.51
3:R:346:VAL:HG11	3:S:346:VAL:HG22	1.93	0.51
1:B:376:SER:HB3	1:B:398:GLN:HB2	1.93	0.50
1:H:32:ASP:O	1:H:136:ARG:NH1	2.43	0.50
1:B:38:ARG:NH1	1:B:133:GLU:OE2	2.44	0.50
1:J:156:ARG:NH2	1:J:393:ASP:O	2.44	0.50
1:F:315:LEU:HD22	1:F:323:LEU:HD13	1.92	0.50
3:R:290:VAL:HG22	3:R:430:VAL:HB	1.92	0.50
1:I:376:SER:HB3	1:I:398:GLN:HB2	1.93	0.50
3:E:19:PHE:HB3	3:E:22:LEU:HD12	1.92	0.50
1:F:191:ARG:NH2	1:F:228:GLU:OE2	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:38:ARG:HG3	1:I:133:GLU:HG3	1.94	0.50
1:B:299:ASP:HB3	1:B:306:ILE:O	2.12	0.49
3:R:383:VAL:HG13	3:R:427:VAL:HG13	1.94	0.49
2:C:77:THR:HB	1:G:173:PRO:HG3	1.93	0.49
3:D:141:TYR:OH	3:D:153:PHE:O	2.29	0.49
1:K:168:GLY:HA2	1:K:196:PHE:O	2.12	0.49
1:F:25:ASP:OD2	1:F:25:ASP:N	2.40	0.49
1:H:106:GLU:H	1:H:112:ASN:HD22	1.60	0.49
3:R:307:LEU:HD11	3:R:347:LEU:HB2	1.94	0.49
1:A:106:GLU:HB2	1:A:112:ASN:HD22	1.78	0.49
1:F:242:PRO:HB3	1:I:109:SER:HB2	1.95	0.49
1:G:14:VAL:N	1:G:19:LEU:HA	2.28	0.49
2:M:13:SER:OG	2:M:14:LEU:N	2.45	0.49
1:J:299:ASP:HB3	1:J:306:ILE:O	2.12	0.49
1:J:407:PRO:HD3	1:J:458:LEU:HD22	1.94	0.49
1:K:393:ASP:OD1	1:K:393:ASP:N	2.42	0.49
1:A:71:LEU:HD12	1:A:72:THR:N	2.28	0.49
3:S:309:VAL:HB	3:S:343:ARG:HB2	1.95	0.49
3:S:290:VAL:HG22	3:S:430:VAL:HB	1.93	0.49
3:D:109:LEU:O	3:D:114:ARG:NH2	2.40	0.49
1:F:18:LYS:C	1:F:20:THR:H	2.21	0.49
3:R:292:ARG:HD3	3:R:432:ARG:HB3	1.95	0.49
1:A:14:VAL:N	1:A:19:LEU:HA	2.28	0.49
1:F:139:VAL:HA	1:F:142:VAL:HG22	1.95	0.49
1:B:156:ARG:NH2	1:B:393:ASP:O	2.44	0.48
1:H:113:ILE:O	1:H:117:ILE:HG12	2.13	0.48
1:G:32:ASP:O	1:G:136:ARG:NH1	2.46	0.48
1:G:193:GLY:O	1:G:418:ARG:NH1	2.46	0.48
1:B:422:GLU:HA	1:B:425:VAL:HG12	1.95	0.48
1:H:55:ALA:HB1	1:H:79:GLY:O	2.13	0.48
1:G:106:GLU:HB2	1:G:112:ASN:HD22	1.78	0.48
1:H:302:ARG:NH2	1:H:335:ASP:OD2	2.45	0.48
1:J:118:VAL:HG23	1:J:118:VAL:O	2.13	0.48
1:F:299:ASP:HB3	1:F:306:ILE:O	2.14	0.48
1:I:327:THR:CG2	2:L:78:PHE:HB3	2.44	0.48
3:E:127:ASP:HB2	1:J:72:THR:HB	1.95	0.48
3:E:141:TYR:OH	3:E:153:PHE:O	2.29	0.48
1:G:71:LEU:HD12	1:G:72:THR:N	2.28	0.48
1:A:32:ASP:O	1:A:136:ARG:NH1	2.46	0.48
1:B:460:LYS:NZ	2:Q:64:ASP:OD2	2.47	0.48
3:E:109:LEU:O	3:E:114:ARG:NH2	2.40	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:152:ASP:OD2	3:D:199:ARG:NH2	2.41	0.48
1:B:460:LYS:H	1:B:460:LYS:HG3	1.40	0.48
3:D:109:LEU:HB3	3:D:113:GLN:HG3	1.95	0.48
1:H:465:GLU:HG2	1:H:466:PHE:CD1	2.49	0.48
1:K:246:GLU:O	1:K:250:ARG:HG3	2.13	0.48
3:R:306:VAL:HG13	3:R:346:VAL:HG12	1.95	0.48
1:H:205:SER:HB2	1:H:211:TRP:HD1	1.78	0.48
1:I:72:THR:OG1	1:I:73:ASP:N	2.47	0.48
1:K:118:VAL:O	1:K:118:VAL:HG23	2.14	0.48
3:E:175:ASN:HB2	3:E:176:PRO:HD3	1.96	0.47
3:E:109:LEU:HB3	3:E:113:GLN:HG3	1.95	0.47
1:G:158:LEU:HD12	1:G:287:LEU:HD21	1.95	0.47
1:K:428:ARG:HB2	1:K:434:LEU:HD11	1.95	0.47
1:A:74:MET:HG3	1:A:75:ASP:N	2.28	0.47
1:A:106:GLU:H	1:A:112:ASN:HD22	1.62	0.47
1:A:158:LEU:HD12	1:A:287:LEU:HD21	1.95	0.47
1:B:118:VAL:HG23	1:B:118:VAL:O	2.13	0.47
1:H:327:THR:OG1	2:P:78:PHE:HB3	2.13	0.47
1:G:187:TYR:OH	1:G:228:GLU:OE2	2.26	0.47
1:K:19:LEU:O	1:K:21:TYR:N	2.48	0.47
1:A:193:GLY:O	1:A:418:ARG:NH1	2.46	0.47
3:S:304:VAL:HG22	3:S:348:PRO:HA	1.96	0.47
1:G:106:GLU:H	1:G:112:ASN:HD22	1.62	0.47
1:H:17:TYR:O	1:H:19:LEU:N	2.42	0.47
1:H:327:THR:HG22	1:H:375:ALA:HB1	1.95	0.47
1:K:327:THR:O	1:K:331:LYS:NZ	2.34	0.47
3:R:306:VAL:HG21	3:R:335:VAL:HG11	1.95	0.47
2:C:6:PRO:HB2	2:C:17:ALA:H	1.80	0.47
1:H:14:VAL:O	2:M:21:GLY:HA3	2.15	0.47
3:D:175:ASN:HB2	3:D:176:PRO:HD3	1.96	0.47
1:G:249:LYS:HB2	1:G:249:LYS:HE3	1.64	0.47
1:A:418:ARG:HG2	3:E:8:PHE:CG	2.50	0.47
1:B:353:ALA:O	3:D:172:GLU:HG2	2.15	0.47
1:G:466:PHE:CG	1:G:467:GLU:N	2.83	0.47
1:I:19:LEU:C	1:I:21:TYR:H	2.23	0.47
3:S:308:PRO:HG2	3:S:361:VAL:HG23	1.97	0.46
1:J:16:ASP:C	1:J:18:LYS:N	2.71	0.46
1:J:38:ARG:HD3	1:J:302:ARG:HH11	1.72	0.46
2:O:62:CYS:SG	2:O:63:GLY:N	2.88	0.46
3:E:9:ARG:HD3	3:E:10:PRO:HD2	1.98	0.46
1:F:407:PRO:HG3	1:F:458:LEU:HD12	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:109:SER:HB2	1:K:242:PRO:HB3	1.97	0.46
1:A:246:GLU:O	1:A:250:ARG:HG3	2.15	0.46
1:G:246:GLU:O	1:G:250:ARG:HG3	2.15	0.46
1:H:292:ARG:O	1:H:292:ARG:HG3	2.15	0.46
1:I:264:HIS:CG	1:I:265:ASP:H	2.34	0.46
1:A:466:PHE:CG	1:A:467:GLU:N	2.83	0.46
1:B:265:ASP:OD1	1:B:291:HIS:HB3	2.15	0.46
1:A:386:ALA:HB2	1:A:464:PHE:CZ	2.51	0.46
3:D:9:ARG:HD3	3:D:10:PRO:HD2	1.98	0.46
1:A:191:ARG:HH22	3:E:5:TYR:HB2	1.71	0.46
1:B:199:ASP:HB2	1:B:236:TYR:O	2.15	0.46
1:K:32:ASP:O	1:K:136:ARG:NH1	2.48	0.46
2:N:37:LEU:H	2:N:37:LEU:HG	1.51	0.46
1:F:169:CYS:SG	1:F:170:THR:N	2.89	0.46
1:J:265:ASP:OD1	1:J:291:HIS:HB3	2.15	0.46
3:S:327:ILE:HB	3:S:336:GLU:HG2	1.97	0.46
1:A:374:VAL:HG22	1:A:396:VAL:HB	1.97	0.45
1:I:172:LYS:HD2	1:I:174:LYS:HD2	1.98	0.45
3:S:316:GLU:H	3:S:316:GLU:HG3	1.47	0.45
1:F:15:LYS:HA	1:F:15:LYS:HD2	1.79	0.45
1:H:39:PHE:HE2	1:H:96:ALA:HB2	1.81	0.45
1:B:437:GLU:H	1:B:437:GLU:HG3	1.62	0.45
1:F:290:ILE:HD12	1:F:315:LEU:HD21	1.99	0.45
1:G:72:THR:O	1:G:74:MET:N	2.49	0.45
1:K:68:THR:O	1:K:70:LEU:N	2.47	0.45
1:I:327:THR:OG1	1:I:328:VAL:N	2.49	0.45
1:J:461:GLU:OE2	1:J:461:GLU:N	2.47	0.45
2:L:29:GLN:HE21	2:L:52:TRP:HE1	1.64	0.45
3:E:49:TYR:OH	3:E:69:GLN:OE1	2.27	0.45
1:G:386:ALA:HB2	1:G:464:PHE:CZ	2.51	0.45
1:J:131:ARG:HD2	1:J:302:ARG:O	2.17	0.45
1:J:172:LYS:HD3	1:J:172:LYS:C	2.42	0.45
2:M:43:GLY:O	2:M:46:LYS:HE2	2.17	0.45
2:Q:37:LEU:H	2:Q:37:LEU:HG	1.51	0.45
3:R:312:ALA:HA	3:R:407:LEU:HD12	1.97	0.45
1:J:442:LEU:HD23	1:J:442:LEU:HA	1.80	0.45
3:D:169:GLN:HB3	3:D:183:MET:HE1	1.99	0.45
1:I:16:ASP:OD1	1:I:16:ASP:N	2.36	0.45
1:J:15:LYS:HB2	1:J:15:LYS:HE2	1.73	0.45
1:B:175:LEU:C	1:B:177:LEU:H	2.24	0.45
1:G:98:ILE:HD13	1:G:98:ILE:HG21	1.74	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:83:HIS:HB3	1:H:97:PHE:HB2	1.99	0.45
1:I:32:ASP:O	1:I:136:ARG:NH1	2.50	0.45
1:J:48:ASP:OD1	1:J:48:ASP:N	2.49	0.45
1:J:199:ASP:HB2	1:J:236:TYR:O	2.15	0.45
1:H:374:VAL:HG22	1:H:396:VAL:HB	1.99	0.45
3:S:323:PRO:HG3	3:S:339:LYS:HB2	1.99	0.45
3:D:97:THR:CG2	2:M:57:LYS:HE3	2.47	0.44
3:R:431:VAL:CG1	3:S:331:ASP:HB2	2.47	0.44
3:S:382:LEU:HB3	3:S:431:VAL:HB	1.99	0.44
2:C:10:LYS:H	2:C:10:LYS:HG3	1.56	0.44
3:R:347:LEU:HD22	3:R:347:LEU:HA	1.83	0.44
1:A:249:LYS:HB2	1:A:249:LYS:HE3	1.64	0.44
3:R:363:VAL:O	3:R:382:LEU:HA	2.17	0.44
3:E:19:PHE:CD2	3:E:44:LEU:HD11	2.53	0.44
3:E:169:GLN:HB3	3:E:183:MET:HE1	1.99	0.44
1:I:327:THR:HG21	2:L:78:PHE:HB3	1.98	0.44
3:S:324:MET:HE3	3:S:324:MET:HB3	1.66	0.44
1:J:38:ARG:CD	1:J:302:ARG:NH1	2.68	0.44
1:B:48:ASP:OD1	1:B:48:ASP:N	2.49	0.44
3:D:49:TYR:OH	3:D:69:GLN:OE1	2.27	0.44
1:F:290:ILE:HD13	1:F:315:LEU:HD11	1.99	0.44
1:I:14:VAL:N	1:I:64:THR:HA	2.33	0.44
1:J:316:ARG:NH2	1:J:369:PRO:O	2.43	0.44
3:R:349:SER:O	3:S:300:GLU:HA	2.18	0.44
1:B:175:LEU:C	1:B:177:LEU:N	2.75	0.44
3:D:19:PHE:CD2	3:D:44:LEU:HD11	2.53	0.44
1:F:331:LYS:O	1:F:332:LEU:HD23	2.17	0.44
1:G:39:PHE:HE2	1:G:96:ALA:HB2	1.82	0.44
1:H:326:GLY:HA2	2:P:79:ASP:CG	2.42	0.44
1:J:172:LYS:HD3	1:J:172:LYS:O	2.18	0.44
3:R:347:LEU:HD21	3:S:332:PHE:CD2	2.53	0.44
1:A:39:PHE:HE2	1:A:96:ALA:HB2	1.82	0.44
1:H:344:ASP:OD2	1:H:357:ARG:NH2	2.41	0.44
3:E:15:ILE:HG13	3:E:16:PRO:HD2	2.00	0.44
1:H:106:GLU:H	1:H:112:ASN:ND2	2.16	0.44
1:K:464:PHE:CZ	1:K:466:PHE:HA	2.53	0.44
2:M:39:ASP:OD1	2:M:46:LYS:HA	2.18	0.44
3:R:366:ARG:HD2	3:R:366:ARG:HA	1.46	0.44
1:G:14:VAL:O	2:N:21:GLY:HA3	2.18	0.43
3:D:15:ILE:HG13	3:D:16:PRO:HD2	2.00	0.43
1:G:442:LEU:HD23	1:G:442:LEU:HA	1.80	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:77:THR:OG1	2:P:78:PHE:N	2.50	0.43
1:B:226:GLN:HG3	1:B:231:GLU:O	2.19	0.43
1:B:415:THR:CG2	3:D:7:PRO:HG2	2.48	0.43
1:I:433:ASP:OD1	1:I:434:LEU:N	2.51	0.43
3:S:317:LYS:H	3:S:317:LYS:HG3	1.52	0.43
1:B:168:GLY:HA2	1:B:196:PHE:O	2.18	0.43
1:J:459:TRP:CE3	2:N:66:ASN:OD1	2.57	0.43
2:L:36:ASN:ND2	2:L:45:PHE:O	2.51	0.43
3:R:382:LEU:H	3:R:431:VAL:HG21	1.84	0.43
1:A:91:GLU:OE1	1:A:91:GLU:N	2.44	0.43
1:A:415:THR:HG21	3:E:7:PRO:HB2	2.01	0.43
1:G:177:LEU:HD23	1:G:177:LEU:HA	1.81	0.43
1:K:172:LYS:O	1:K:174:LYS:NZ	2.49	0.43
1:A:106:GLU:H	1:A:112:ASN:ND2	2.17	0.43
1:H:386:ALA:HB2	1:H:464:PHE:CE1	2.53	0.43
1:J:128:ARG:HE	1:J:128:ARG:HB2	1.57	0.43
2:Q:50:LEU:HD23	2:Q:50:LEU:HA	1.84	0.43
1:B:127:ILE:HD12	1:B:130:LEU:HB2	2.01	0.43
3:E:71:ARG:NH1	1:J:71:LEU:HD21	2.33	0.43
1:J:168:GLY:HA2	1:J:196:PHE:O	2.18	0.43
1:K:201:GLU:HG2	1:K:291:HIS:CE1	2.53	0.43
3:R:347:LEU:HD21	3:S:332:PHE:CE2	2.54	0.43
3:D:41:TYR:HA	3:D:44:LEU:HD13	2.00	0.43
1:G:18:LYS:HE2	1:G:18:LYS:HA	2.01	0.43
1:H:22:TYR:CZ	1:H:24:PRO:HG3	2.54	0.43
1:H:331:LYS:HE2	1:H:335:ASP:HB3	2.01	0.43
3:R:435:ARG:HD2	3:R:435:ARG:HA	1.58	0.43
1:A:18:LYS:HE2	1:A:18:LYS:HA	2.01	0.43
1:G:302:ARG:NH2	1:G:335:ASP:OD2	2.52	0.43
1:A:149:PRO:HD2	1:A:321:ASP:OD1	2.19	0.43
1:B:172:LYS:HB2	1:B:172:LYS:HE2	1.63	0.43
3:E:41:TYR:HA	3:E:44:LEU:HD13	2.00	0.43
3:E:78:VAL:HG13	3:E:114:ARG:HD3	2.01	0.43
1:G:106:GLU:H	1:G:112:ASN:ND2	2.17	0.43
1:G:342:PHE:HA	1:G:345:LEU:HB2	2.01	0.43
1:H:191:ARG:NE	1:H:228:GLU:OE2	2.37	0.43
1:A:14:VAL:O	2:Q:21:GLY:HA3	2.19	0.42
1:A:292:ARG:O	1:A:292:ARG:HG3	2.19	0.42
1:A:332:LEU:H	1:A:332:LEU:HD23	1.84	0.42
1:A:356:SER:OG	3:E:144:ARG:NH1	2.50	0.42
1:J:127:ILE:HD12	1:J:130:LEU:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:70:LEU:HG	1:K:71:LEU:HD13	2.00	0.42
1:F:118:VAL:HG23	1:I:294:MET:HG3	2.02	0.42
1:G:22:TYR:CZ	1:G:24:PRO:HG3	2.54	0.42
1:H:74:MET:C	1:H:76:ARG:H	2.26	0.42
2:O:70:PHE:O	2:O:70:PHE:CG	2.72	0.42
3:S:368:ASP:HB3	3:S:381:LEU:HD13	2.01	0.42
1:A:49:GLU:OE1	2:Q:12:ASN:CB	2.67	0.42
1:F:172:LYS:HA	1:F:174:LYS:NZ	2.34	0.42
1:F:460:LYS:HD2	1:F:460:LYS:HA	1.82	0.42
1:H:199:ASP:OD1	1:H:235:HIS:NE2	2.40	0.42
1:H:342:PHE:HA	1:H:345:LEU:HB2	2.02	0.42
1:K:75:ASP:HA	1:K:78:LYS:HE3	2.02	0.42
1:K:226:GLN:HG3	1:K:231:GLU:O	2.19	0.42
1:G:149:PRO:HD2	1:G:321:ASP:OD1	2.19	0.42
1:I:19:LEU:O	1:I:21:TYR:N	2.52	0.42
3:R:297:GLU:HB2	3:S:302:THR:HG21	2.02	0.42
3:R:318:LYS:HG3	3:R:341:TRP:HZ2	1.84	0.42
3:E:118:ALA:HA	3:E:121:ILE:HG12	2.02	0.42
1:H:249:LYS:HB2	1:H:249:LYS:HE3	1.71	0.42
1:J:315:LEU:HD23	1:J:323:LEU:HD22	2.01	0.42
1:B:177:LEU:HD12	1:B:177:LEU:HA	1.85	0.42
2:C:40:HIS:HE1	2:C:44:GLN:NE2	2.08	0.42
3:E:165:LEU:HD12	3:E:168:ARG:HH21	1.85	0.42
1:I:39:PHE:HE2	1:I:96:ALA:HB2	1.84	0.42
1:K:299:ASP:HB3	1:K:306:ILE:O	2.20	0.42
1:A:174:LYS:HE2	1:A:174:LYS:HB2	1.86	0.42
1:B:70:LEU:HG	1:B:71:LEU:N	2.35	0.42
1:K:70:LEU:HD23	1:K:71:LEU:H	1.84	0.42
1:A:203:ILE:HD13	1:A:203:ILE:HA	1.83	0.42
1:F:39:PHE:HE2	1:F:96:ALA:HB2	1.83	0.42
1:I:118:VAL:HG13	1:I:122:PHE:CE1	2.55	0.42
1:A:22:TYR:CZ	1:A:24:PRO:HG3	2.54	0.42
1:B:172:LYS:HD2	1:B:401:GLY:HA2	2.02	0.42
1:H:315:LEU:HD22	1:H:323:LEU:HD13	2.02	0.42
1:I:382:TRP:NE1	1:I:459:TRP:O	2.53	0.42
1:A:66:VAL:CG1	2:Q:61:LEU:CD2	2.51	0.42
1:A:302:ARG:NH2	1:A:335:ASP:OD2	2.52	0.42
1:B:315:LEU:HD23	1:B:323:LEU:HD22	2.01	0.42
3:D:78:VAL:HG13	3:D:114:ARG:HD3	2.01	0.42
1:H:98:ILE:HD13	1:H:98:ILE:HG21	1.81	0.42
2:Q:10:LYS:HB3	2:Q:11:PRO:HD3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:LEU:HD23	1:A:442:LEU:HA	1.80	0.41
1:B:172:LYS:O	1:B:173:PRO:C	2.64	0.41
1:B:315:LEU:HD12	1:B:315:LEU:HA	1.88	0.41
2:C:66:ASN:O	1:J:67:TRP:CH2	2.73	0.41
3:D:165:LEU:HD12	3:D:168:ARG:HH21	1.85	0.41
1:K:460:LYS:HD3	2:M:3:ASN:HA	2.02	0.41
3:R:370:LYS:HZ3	3:R:370:LYS:HG2	1.70	0.41
3:D:16:PRO:HD3	3:D:43:PRO:HB2	2.02	0.41
3:E:49:TYR:CE1	3:E:58:ILE:HD12	2.55	0.41
1:F:205:SER:HB2	1:F:211:TRP:HD1	1.85	0.41
1:F:345:LEU:HD23	1:F:351:ILE:HD13	2.01	0.41
1:G:292:ARG:O	1:G:292:ARG:HG3	2.19	0.41
1:G:332:LEU:HD23	1:G:332:LEU:H	1.84	0.41
1:H:442:LEU:HA	1:H:442:LEU:HD23	1.80	0.41
1:J:292:ARG:HG2	1:J:324:HIS:HB2	2.02	0.41
1:K:382:TRP:CZ3	1:K:462:ILE:HG23	2.55	0.41
1:A:98:ILE:HG21	1:A:98:ILE:HD13	1.74	0.41
2:M:77:THR:O	2:M:79:ASP:N	2.46	0.41
3:E:16:PRO:HD3	3:E:43:PRO:HB2	2.02	0.41
1:F:382:TRP:CZ2	1:F:456:LEU:HD22	2.55	0.41
2:N:53:LEU:HD23	2:N:60:VAL:HG11	2.02	0.41
1:A:71:LEU:HD12	1:A:72:THR:H	1.85	0.41
1:I:267:LEU:HD23	1:I:267:LEU:HA	1.92	0.41
1:J:249:LYS:HE2	1:J:249:LYS:HB3	1.67	0.41
3:S:316:GLU:HA	3:S:319:ILE:HD12	2.03	0.41
3:E:74:VAL:HG11	3:E:107:ARG:HD2	2.03	0.41
3:E:152:ASP:OD2	3:E:199:ARG:NH2	2.41	0.41
1:F:139:VAL:HG13	1:F:366:ALA:HB2	2.01	0.41
1:G:71:LEU:HD12	1:G:72:THR:H	1.85	0.41
3:R:294:LYS:HD2	3:R:294:LYS:HA	1.33	0.41
2:N:10:LYS:HB3	2:N:11:PRO:HD3	2.02	0.41
3:S:322:ALA:HA	3:S:323:PRO:HD3	1.98	0.41
1:A:187:TYR:OH	1:A:228:GLU:OE2	2.26	0.41
3:D:65:SER:OG	1:K:184:ARG:NH1	2.53	0.41
3:D:118:ALA:HA	3:D:121:ILE:HG12	2.02	0.41
3:E:104:TYR:O	3:E:107:ARG:HD3	2.21	0.41
1:F:226:GLN:HG3	1:F:231:GLU:O	2.21	0.41
1:K:292:ARG:HG2	1:K:324:HIS:HB2	2.03	0.41
3:R:301:ALA:HB1	3:R:302:THR:H	1.76	0.41
3:R:382:LEU:N	3:R:431:VAL:HG11	2.35	0.41
1:A:114:LEU:HD23	1:A:114:LEU:HA	1.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:LEU:HD22	1:A:323:LEU:HD13	2.03	0.41
1:A:434:LEU:HD23	1:A:434:LEU:HA	1.78	0.41
1:A:458:LEU:H	1:A:458:LEU:HG	1.43	0.41
1:B:292:ARG:HG2	1:B:324:HIS:HB2	2.02	0.41
3:D:19:PHE:HD2	3:D:44:LEU:HD11	1.86	0.41
3:D:49:TYR:CE1	3:D:58:ILE:HD12	2.55	0.41
3:D:74:VAL:HG11	3:D:107:ARG:HD2	2.03	0.41
3:D:104:TYR:O	3:D:107:ARG:HD3	2.21	0.41
1:F:168:GLY:HA2	1:F:196:PHE:O	2.21	0.41
1:G:465:GLU:HG3	1:G:466:PHE:H	1.85	0.41
1:H:27:THR:HA	1:H:28:PRO:HD3	1.94	0.41
1:I:18:LYS:C	1:I:20:THR:H	2.29	0.41
1:J:379:ILE:H	1:J:379:ILE:HG12	1.32	0.41
3:R:384:VAL:HG23	3:S:332:PHE:CZ	2.56	0.41
1:G:458:LEU:HD12	1:G:458:LEU:HA	1.87	0.41
1:I:131:ARG:HH21	1:I:307:HIS:CD2	2.39	0.41
1:I:299:ASP:HB3	1:I:306:ILE:O	2.21	0.41
1:J:315:LEU:HA	1:J:315:LEU:HD12	1.88	0.41
1:J:386:ALA:O	1:J:389:GLU:HG3	2.21	0.41
2:P:46:LYS:HE3	2:P:46:LYS:HB3	1.89	0.41
3:R:290:VAL:HG22	3:R:430:VAL:CG2	2.51	0.41
3:S:383:VAL:HG13	3:S:427:VAL:HG13	2.02	0.41
3:S:433:PRO:HA	3:S:434:PRO:HD3	1.99	0.41
1:G:411:ALA:HB3	1:G:412:PRO:HD3	2.03	0.40
2:Q:38:ILE:H	2:Q:38:ILE:HG13	1.79	0.40
3:S:390:ASN:HB2	3:S:423:SER:O	2.21	0.40
3:S:392:VAL:HG12	3:S:416:LYS:HE2	2.02	0.40
1:A:465:GLU:HG3	1:A:466:PHE:H	1.85	0.40
3:E:19:PHE:HD2	3:E:44:LEU:HD11	1.86	0.40
1:H:382:TRP:CE3	1:H:461:GLU:HG3	2.56	0.40
1:B:428:ARG:HB2	1:B:434:LEU:HD11	2.02	0.40
1:B:442:LEU:HD23	1:B:442:LEU:HA	1.88	0.40
1:F:46:PRO:HG2	1:F:49:GLU:HG3	2.02	0.40
1:H:149:PRO:HD2	1:H:321:ASP:OD1	2.22	0.40
1:I:33:LEU:HD21	1:I:135:ILE:HD11	2.03	0.40
1:J:70:LEU:HG	1:J:71:LEU:N	2.35	0.40
2:M:77:THR:C	2:M:79:ASP:H	2.29	0.40
1:A:411:ALA:HB3	1:A:412:PRO:HD3	2.03	0.40
1:F:292:ARG:HH21	2:O:80:GLU:CD	2.29	0.40
1:G:382:TRP:CE3	1:G:461:GLU:HG3	2.56	0.40
1:K:74:MET:CE	1:K:75:ASP:H	2.34	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:319:ILE:HG21	3:R:424:LEU:HB3	2.04	0.40
1:A:155:GLU:HG2	1:A:287:LEU:HD13	2.03	0.40
1:B:431:GLY:HA2	3:D:114:ARG:NH2	2.36	0.40
1:G:386:ALA:HB2	1:G:464:PHE:CE1	2.56	0.40
1:I:442:LEU:HD23	1:I:442:LEU:HA	1.90	0.40
1:J:114:LEU:HD23	1:J:114:LEU:HA	1.90	0.40
2:Q:53:LEU:HD23	2:Q:60:VAL:HG11	2.02	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	454/472 (96%)	414 (91%)	40 (9%)	0	100	100
1	B	451/472 (96%)	409 (91%)	40 (9%)	2 (0%)	30	60
1	F	454/472 (96%)	414 (91%)	40 (9%)	0	100	100
1	G	454/472 (96%)	414 (91%)	39 (9%)	1 (0%)	43	71
1	H	454/472 (96%)	412 (91%)	41 (9%)	1 (0%)	43	71
1	I	451/472 (96%)	414 (92%)	37 (8%)	0	100	100
1	J	451/472 (96%)	412 (91%)	38 (8%)	1 (0%)	43	71
1	K	451/472 (96%)	410 (91%)	41 (9%)	0	100	100
2	C	71/81 (88%)	64 (90%)	6 (8%)	1 (1%)	9	33
2	L	77/81 (95%)	71 (92%)	6 (8%)	0	100	100
2	M	77/81 (95%)	64 (83%)	13 (17%)	0	100	100
2	N	71/81 (88%)	68 (96%)	2 (3%)	1 (1%)	9	33
2	O	78/81 (96%)	61 (78%)	17 (22%)	0	100	100
2	P	78/81 (96%)	65 (83%)	13 (17%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Q	71/81 (88%)	68 (96%)	2 (3%)	1 (1%)	9	33
3	D	205/389 (53%)	186 (91%)	19 (9%)	0	100	100
3	E	205/389 (53%)	185 (90%)	20 (10%)	0	100	100
3	R	145/389 (37%)	137 (94%)	6 (4%)	2 (1%)	9	33
3	S	148/389 (38%)	142 (96%)	5 (3%)	1 (1%)	18	49
All	All	4846/5899 (82%)	4410 (91%)	425 (9%)	11 (0%)	44	71

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	73	ASP
2	N	10	LYS
2	Q	10	LYS
3	S	333	LYS
1	B	20	THR
1	B	173	PRO
1	J	20	THR
1	H	466	PHE
3	R	301	ALA
2	C	71	ILE
3	R	432	ARG

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	372/383 (97%)	366 (98%)	6 (2%)	55	72
1	B	369/383 (96%)	356 (96%)	13 (4%)	32	58
1	F	372/383 (97%)	372 (100%)	0	100	100
1	G	372/383 (97%)	362 (97%)	10 (3%)	39	63
1	H	372/383 (97%)	372 (100%)	0	100	100
1	I	369/383 (96%)	369 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	369/383 (96%)	351 (95%)	18 (5%)	22	51
1	K	369/383 (96%)	369 (100%)	0	100	100
2	C	54/60 (90%)	32 (59%)	22 (41%)	0	0
2	L	59/60 (98%)	59 (100%)	0	100	100
2	M	59/60 (98%)	59 (100%)	0	100	100
2	N	54/60 (90%)	39 (72%)	15 (28%)	0	2
2	O	59/60 (98%)	59 (100%)	0	100	100
2	P	59/60 (98%)	59 (100%)	0	100	100
2	Q	54/60 (90%)	39 (72%)	15 (28%)	0	2
3	D	178/332 (54%)	178 (100%)	0	100	100
3	E	178/332 (54%)	178 (100%)	0	100	100
3	R	119/332 (36%)	71 (60%)	48 (40%)	0	0
3	S	115/332 (35%)	78 (68%)	37 (32%)	0	1
All	All	3952/4812 (82%)	3768 (95%)	184 (5%)	25	52

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	125	LYS
1	A	342	PHE
1	A	430	GLU
1	A	458	LEU
1	A	460	LYS
1	B	17	TYR
1	B	23	THR
1	B	170	THR
1	B	172	LYS
1	B	173	PRO
1	B	174	LYS
1	B	191	ARG
1	B	336	LYS
1	B	389	GLU
1	B	404	LEU
1	B	437	GLU
1	B	460	LYS
1	B	462	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	7	GLN
2	C	9	THR
2	C	10	LYS
2	C	12	ASN
2	C	14	LEU
2	C	16	CYS
2	C	25	VAL
2	C	29	GLN
2	C	30	CYS
2	C	31	LYS
2	C	37	LEU
2	C	38	ILE
2	C	39	ASP
2	C	42	ASN
2	C	44	GLN
2	C	46	LYS
2	C	50	LEU
2	C	55	ARG
2	C	71	ILE
2	C	74	PHE
2	C	75	LEU
2	C	76	SER
1	G	49	GLU
1	G	73	ASP
1	G	74	MET
1	G	76	ARG
1	G	172	LYS
1	G	174	LYS
1	G	175	LEU
1	G	178	SER
1	G	213	ASP
1	G	389	GLU
1	J	15	LYS
1	J	16	ASP
1	J	128	ARG
1	J	174	LYS
1	J	175	LEU
1	J	229	THR
1	J	231	GLU
1	J	245	GLU
1	J	301	GLN
1	J	302	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	376	SER
1	J	379	ILE
1	J	425	VAL
1	J	435	TYR
1	J	436	ARG
1	J	437	GLU
1	J	444	GLU
1	J	456	LEU
2	N	10	LYS
2	N	12	ASN
2	N	14	LEU
2	N	15	VAL
2	N	35	VAL
2	N	37	LEU
2	N	38	ILE
2	N	41	PHE
2	N	42	ASN
2	N	53	LEU
2	N	55	ARG
2	N	62	CYS
2	N	70	PHE
2	N	75	LEU
2	N	77	THR
2	Q	10	LYS
2	Q	12	ASN
2	Q	14	LEU
2	Q	15	VAL
2	Q	35	VAL
2	Q	37	LEU
2	Q	38	ILE
2	Q	41	PHE
2	Q	42	ASN
2	Q	53	LEU
2	Q	55	ARG
2	Q	62	CYS
2	Q	70	PHE
2	Q	75	LEU
2	Q	77	THR
3	R	288	ILE
3	R	291	VAL
3	R	292	ARG
3	R	294	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	R	295	PHE
3	R	298	VAL
3	R	302	THR
3	R	303	SER
3	R	305	VAL
3	R	306	VAL
3	R	307	LEU
3	R	311	LYS
3	R	313	GLU
3	R	314	GLU
3	R	316	GLU
3	R	318	LYS
3	R	319	ILE
3	R	333	LYS
3	R	335	VAL
3	R	338	GLU
3	R	339	LYS
3	R	342	LYS
3	R	343	ARG
3	R	345	VAL
3	R	347	LEU
3	R	349	SER
3	R	361	VAL
3	R	363	VAL
3	R	364	SER
3	R	366	ARG
3	R	370	LYS
3	R	371	VAL
3	R	379	GLU
3	R	388	VAL
3	R	391	VAL
3	R	393	GLU
3	R	396	ASP
3	R	401	VAL
3	R	402	VAL
3	R	405	ASN
3	R	408	LYS
3	R	413	SER
3	R	418	ARG
3	R	420	VAL
3	R	422	GLU
3	R	430	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	R	431	VAL
3	R	435	ARG
3	S	288	ILE
3	S	300	GLU
3	S	303	SER
3	S	304	VAL
3	S	305	VAL
3	S	306	VAL
3	S	313	GLU
3	S	316	GLU
3	S	317	LYS
3	S	318	LYS
3	S	324	MET
3	S	326	ILE
3	S	331	ASP
3	S	332	PHE
3	S	335	VAL
3	S	336	GLU
3	S	342	LYS
3	S	343	ARG
3	S	345	VAL
3	S	347	LEU
3	S	353	VAL
3	S	361	VAL
3	S	363	VAL
3	S	364	SER
3	S	369	ARG
3	S	371	VAL
3	S	375	ASP
3	S	382	LEU
3	S	387	ARG
3	S	389	ARG
3	S	391	VAL
3	S	393	GLU
3	S	396	ASP
3	S	401	VAL
3	S	402	VAL
3	S	424	LEU
3	S	435	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	209	GLN
1	A	291	HIS
1	A	304	HIS
1	A	322	HIS
1	A	350	HIS
1	A	380	HIS
1	A	410	ASN
1	A	417	ASN
1	A	426	GLN
1	B	92	ASN
1	B	181	ASN
1	B	291	HIS
1	B	322	HIS
2	C	7	GLN
2	C	29	GLN
2	C	40	HIS
3	D	6	GLN
3	D	77	GLN
3	D	173	ASN
3	D	179	GLN
3	E	6	GLN
3	E	77	GLN
3	E	173	ASN
3	E	179	GLN
1	F	274	ASN
1	F	322	HIS
1	F	383	HIS
1	F	410	ASN
1	G	112	ASN
1	G	181	ASN
1	G	209	GLN
1	G	291	HIS
1	G	307	HIS
1	G	322	HIS
1	G	350	HIS
1	G	410	ASN
1	G	417	ASN
1	H	112	ASN
1	H	209	GLN
1	H	304	HIS
1	I	289	HIS
1	I	304	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	120	ASN
1	J	181	ASN
1	J	291	HIS
1	J	322	HIS
1	K	112	ASN
1	K	181	ASN
1	K	291	HIS
2	L	5	ASN
2	L	29	GLN
2	M	5	ASN
2	M	7	GLN
2	M	40	HIS
2	N	66	ASN
2	O	18	ASN
2	P	3	ASN
2	P	7	GLN
2	P	12	ASN
2	P	18	ASN
2	P	44	GLN
3	S	405	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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.

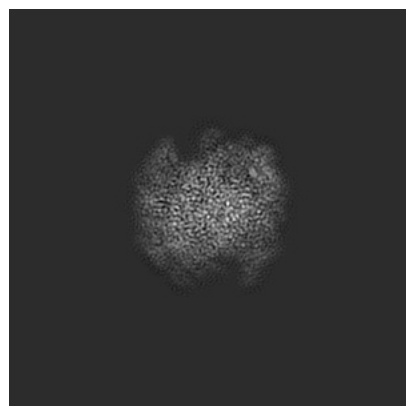
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35536. These allow visual inspection of the internal detail of the map and identification of artifacts.

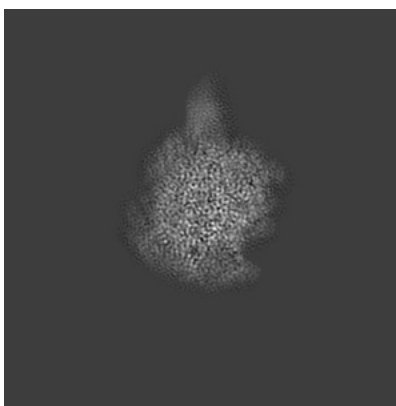
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

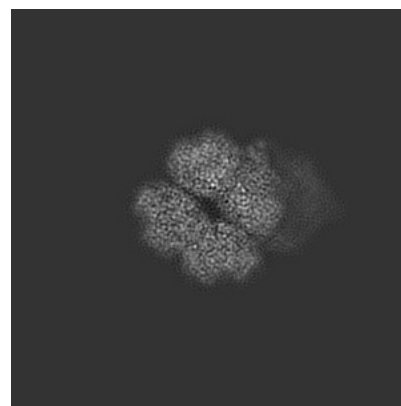
6.1.1 Primary map



X

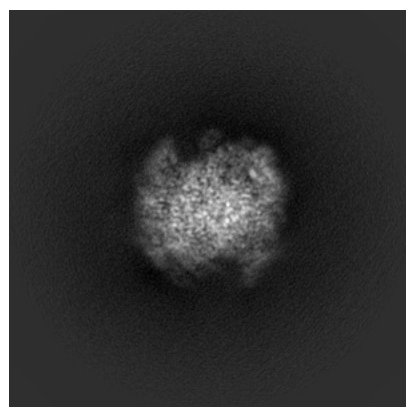


Y

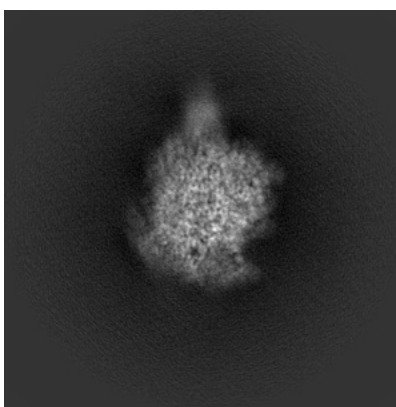


Z

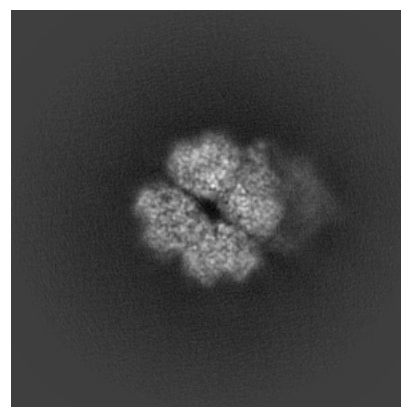
6.1.2 Raw map



X



Y

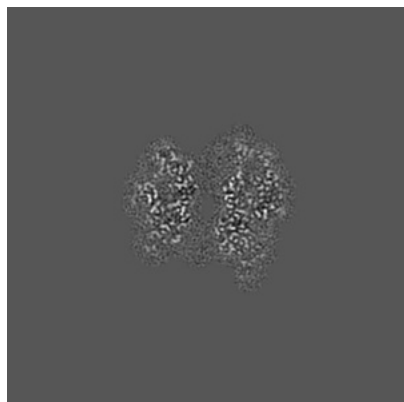


Z

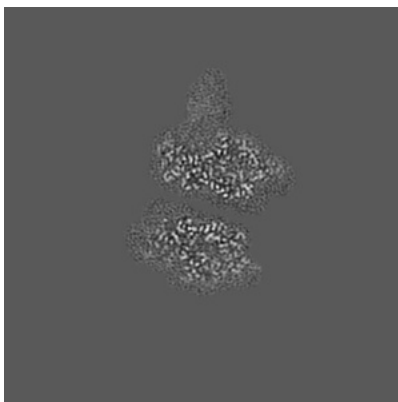
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

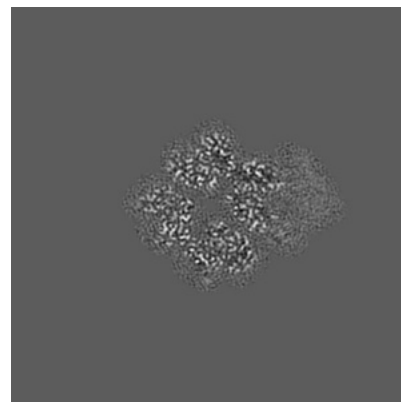
6.2.1 Primary map



X Index: 160

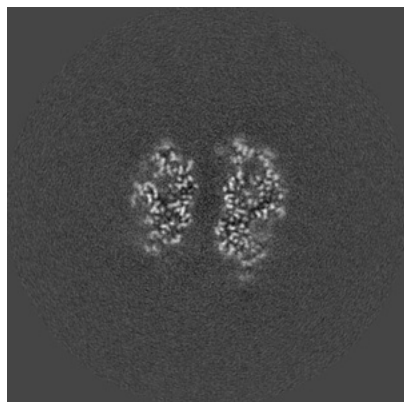


Y Index: 160

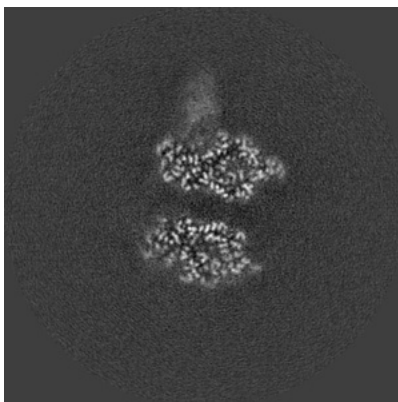


Z Index: 160

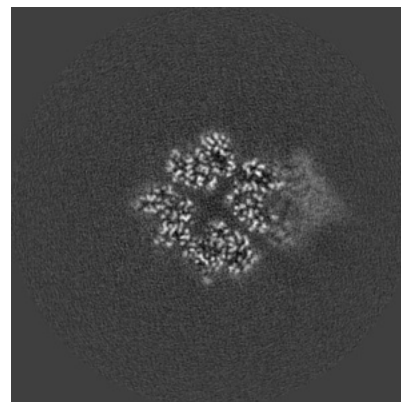
6.2.2 Raw map



X Index: 160



Y Index: 160

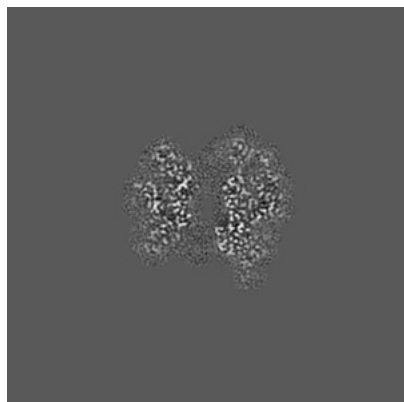


Z Index: 160

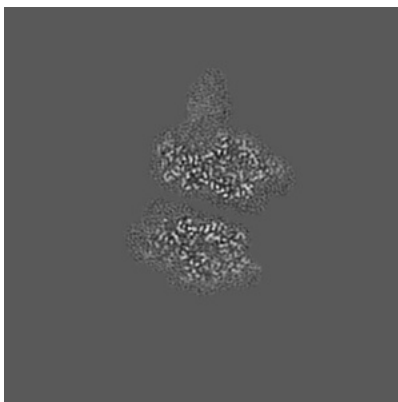
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

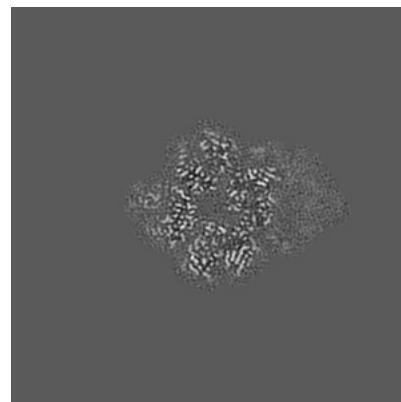
6.3.1 Primary map



X Index: 161

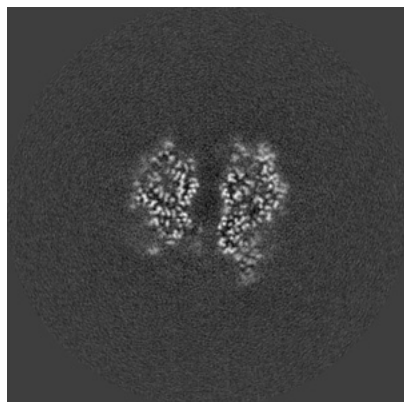


Y Index: 160

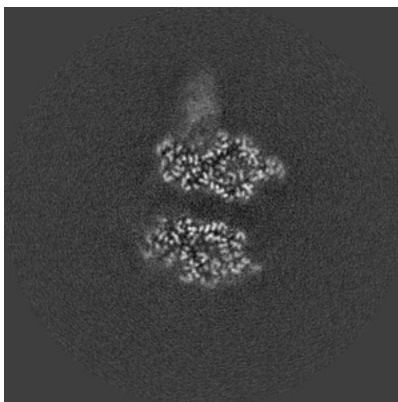


Z Index: 167

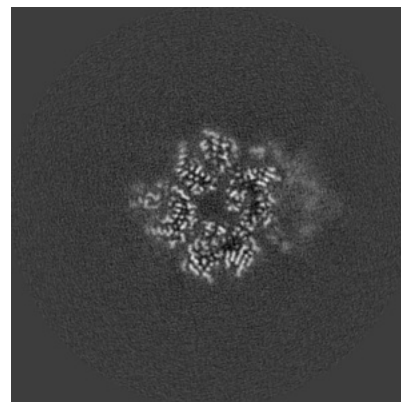
6.3.2 Raw map



X Index: 157



Y Index: 160

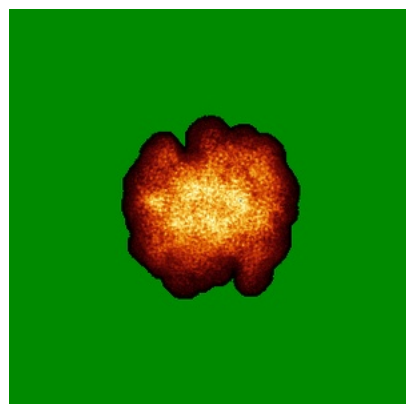


Z Index: 167

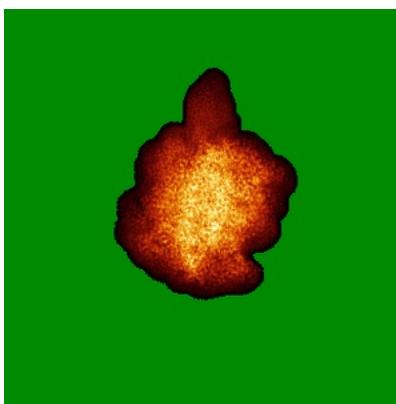
The images above show the largest variance slices of the map in three orthogonal directions.

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

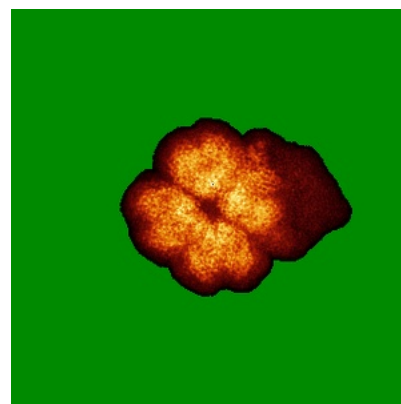
6.4.1 Primary map



X

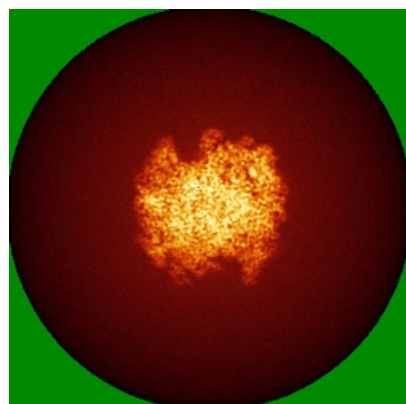


Y

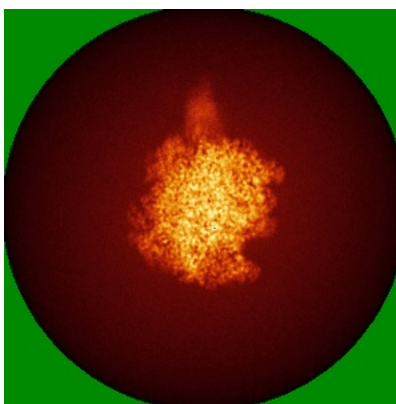


Z

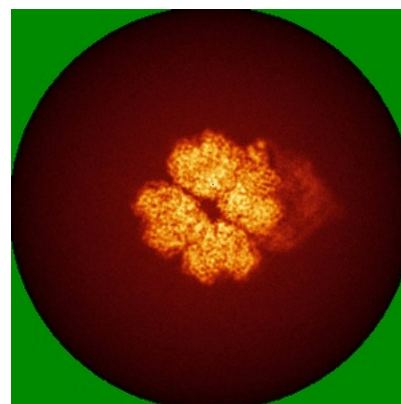
6.4.2 Raw map



X



Y

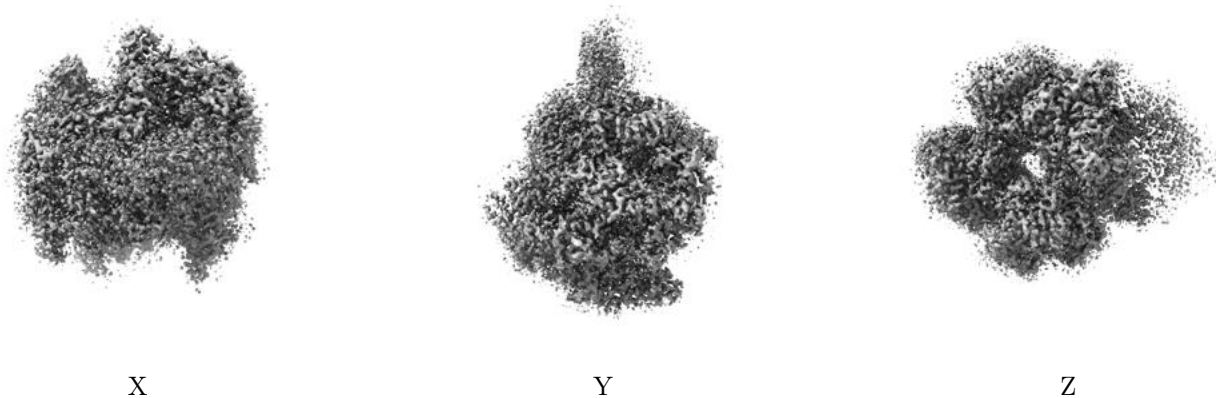


Z

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.

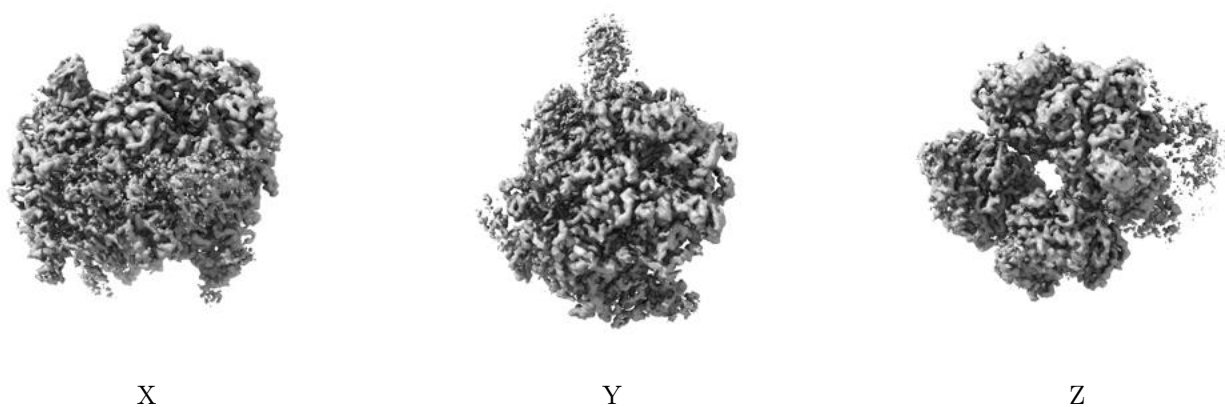
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

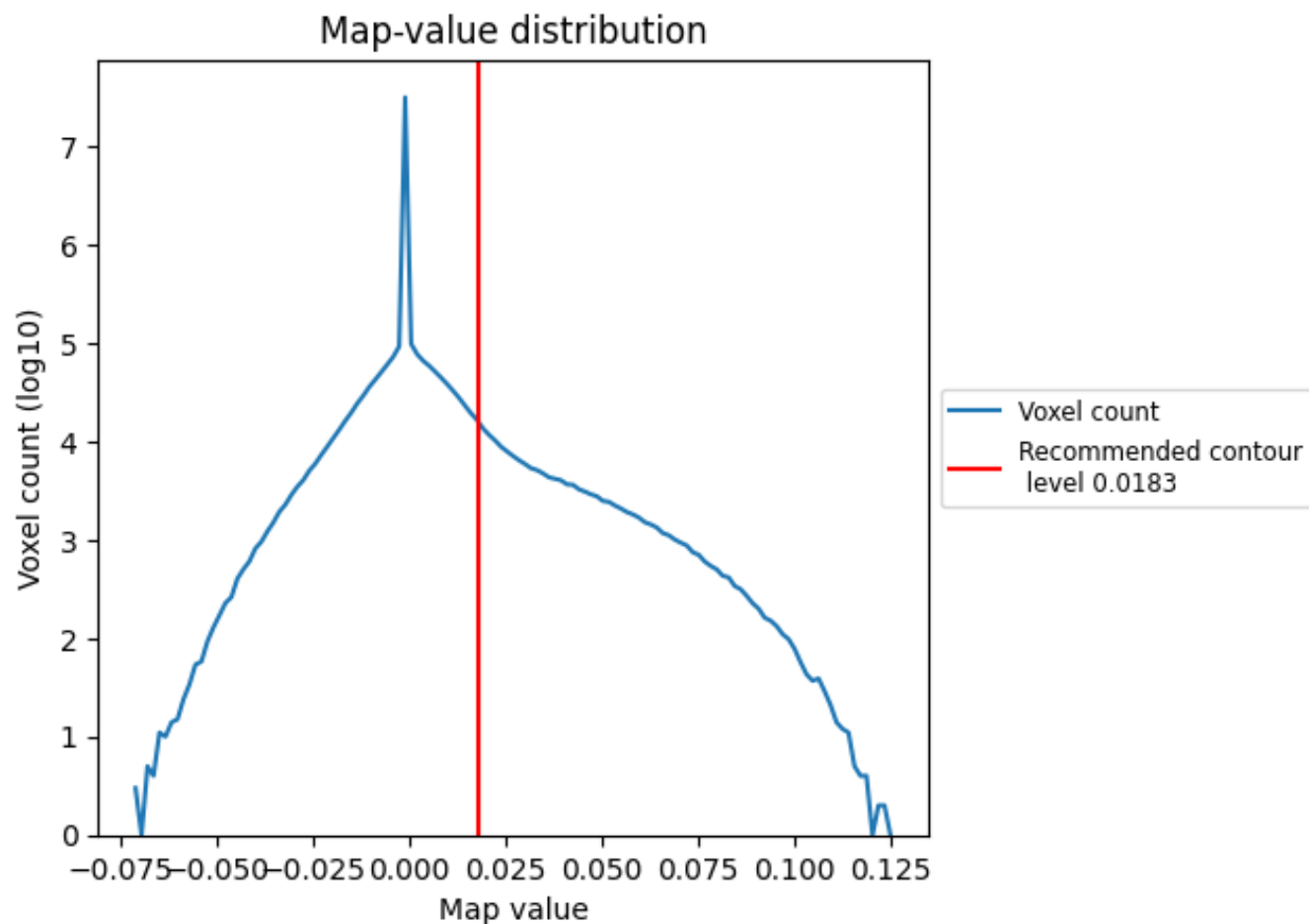
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

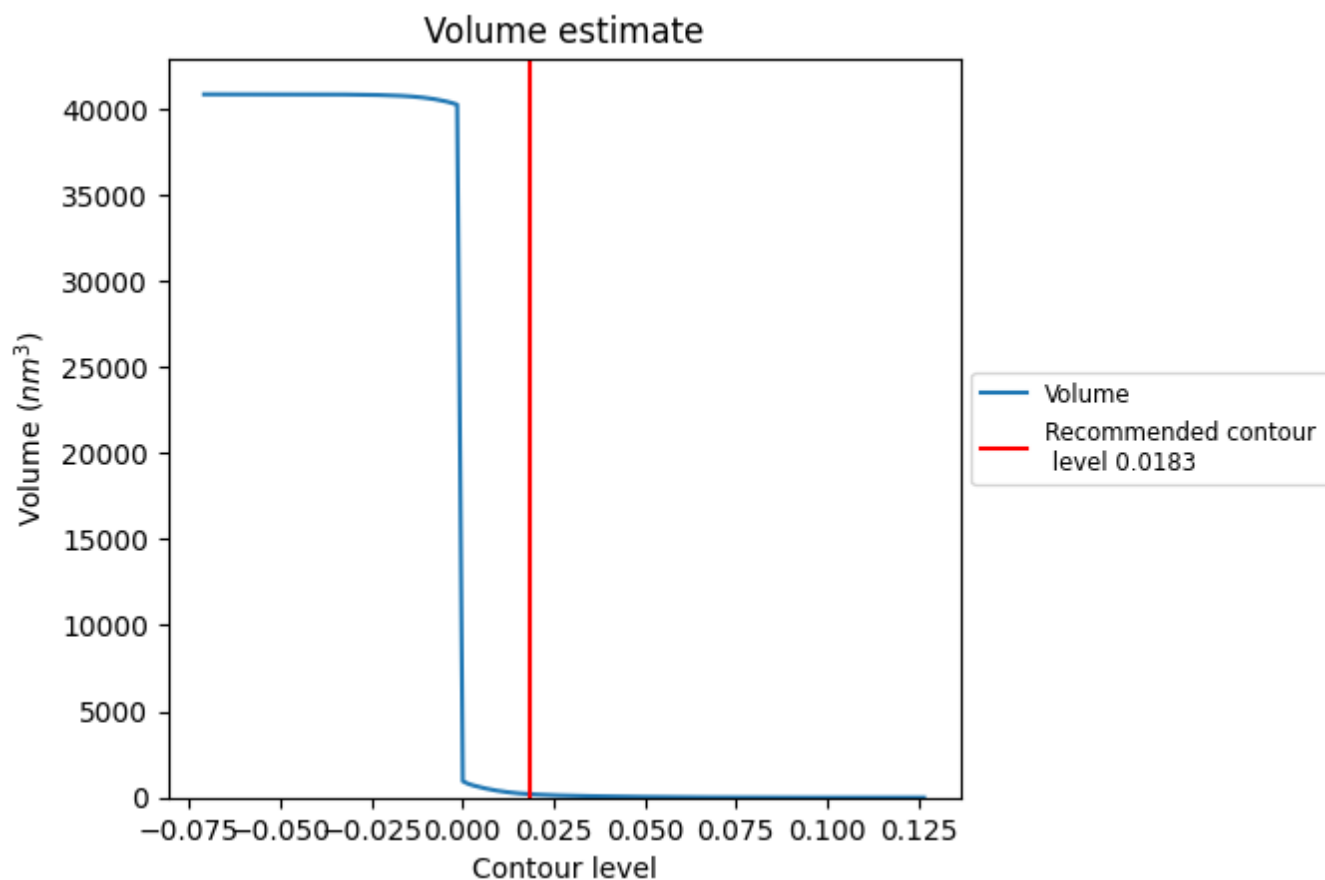
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

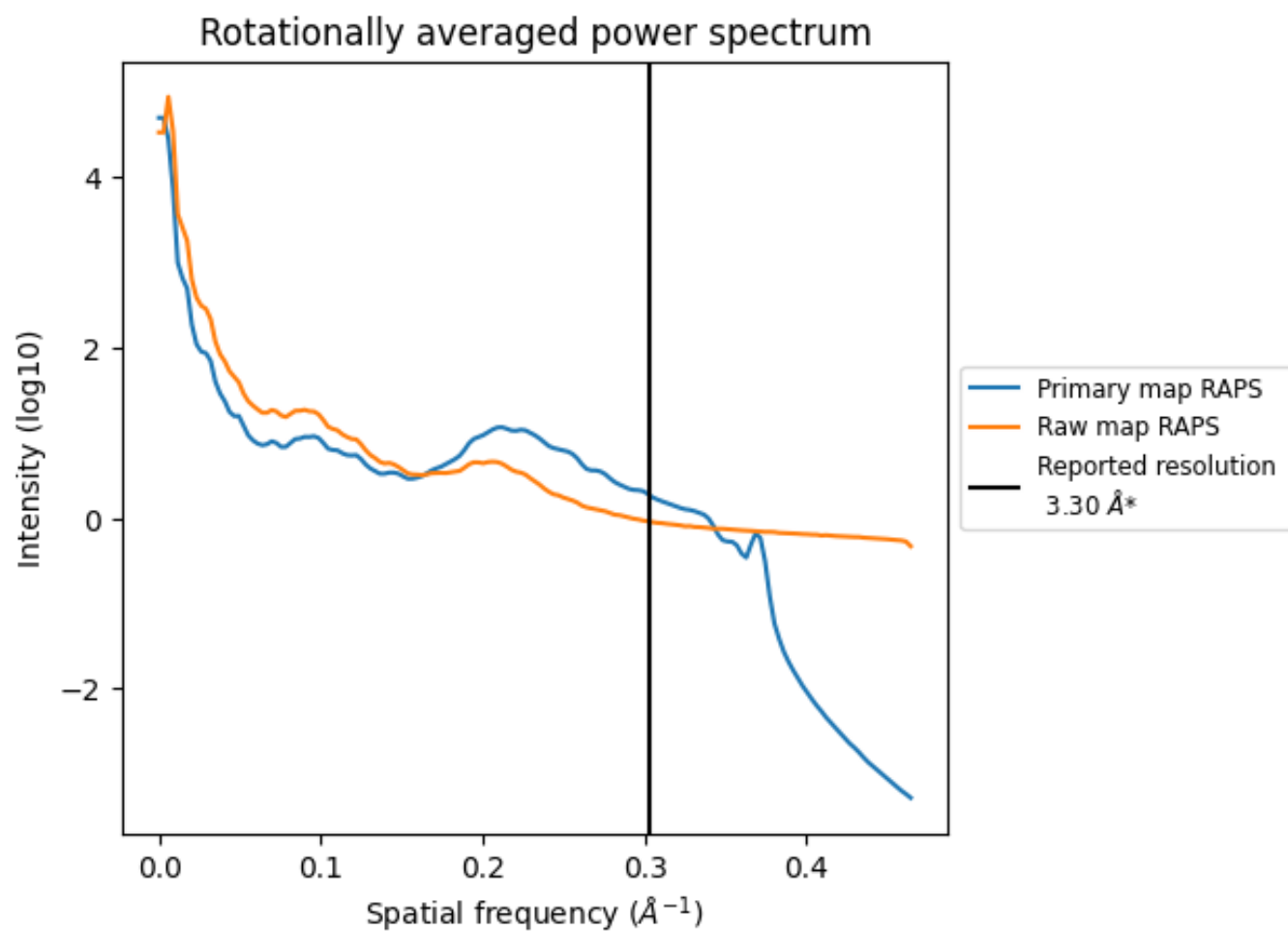
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 199 nm^3 ; this corresponds to an approximate mass of 180 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

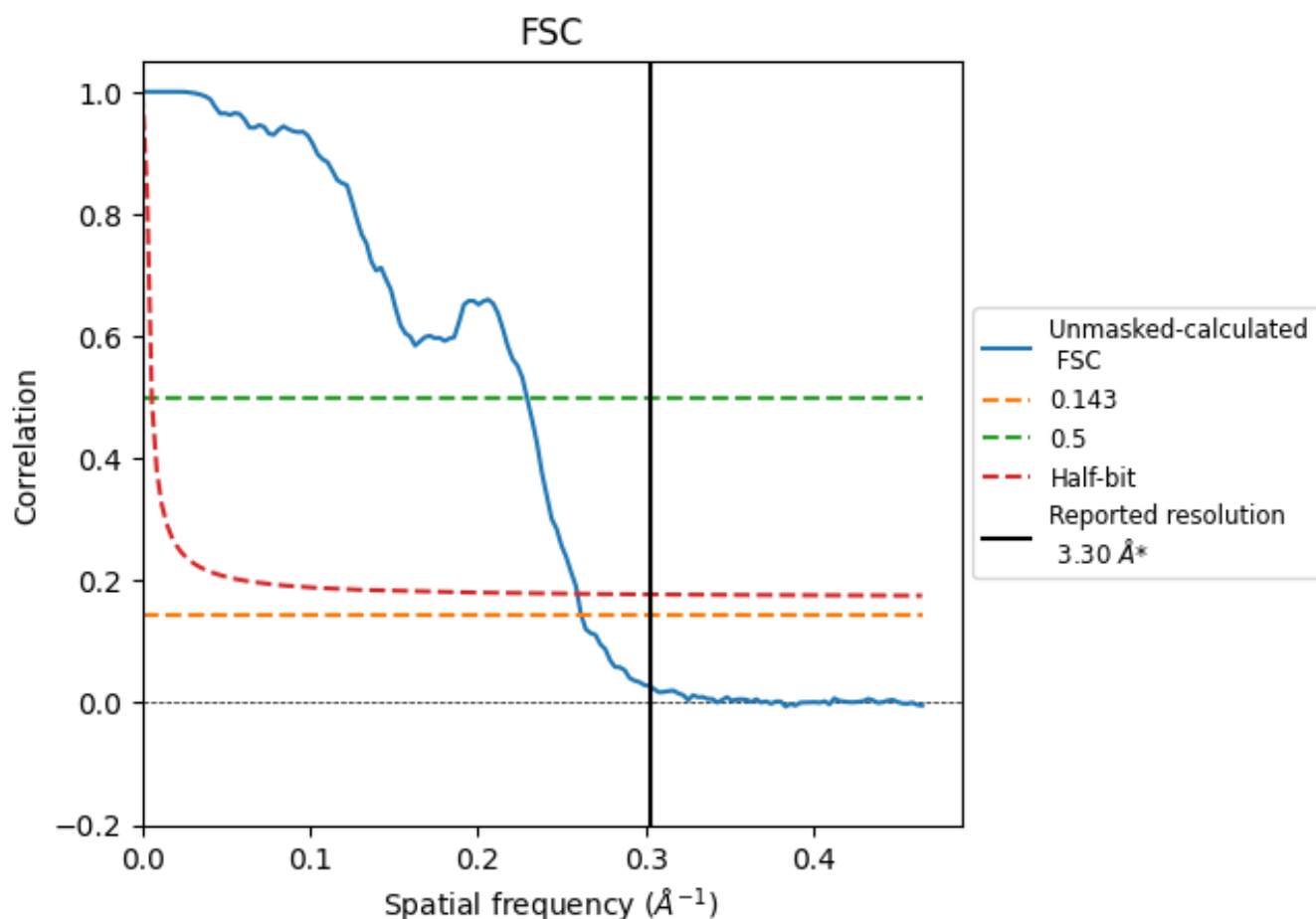


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

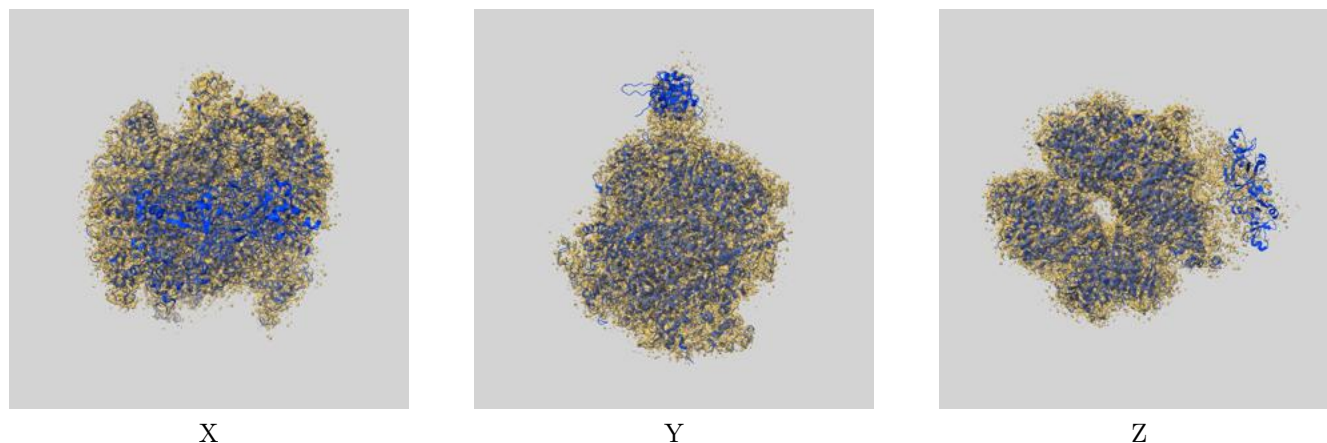
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.82	4.36	3.86

*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 3.82 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

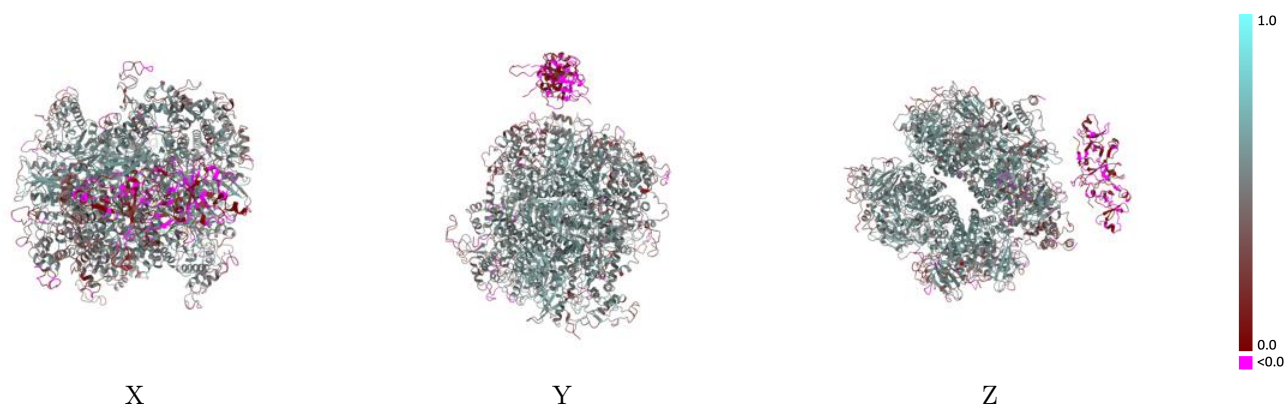
This section contains information regarding the fit between EMDB map EMD-35536 and PDB model 8ILM. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



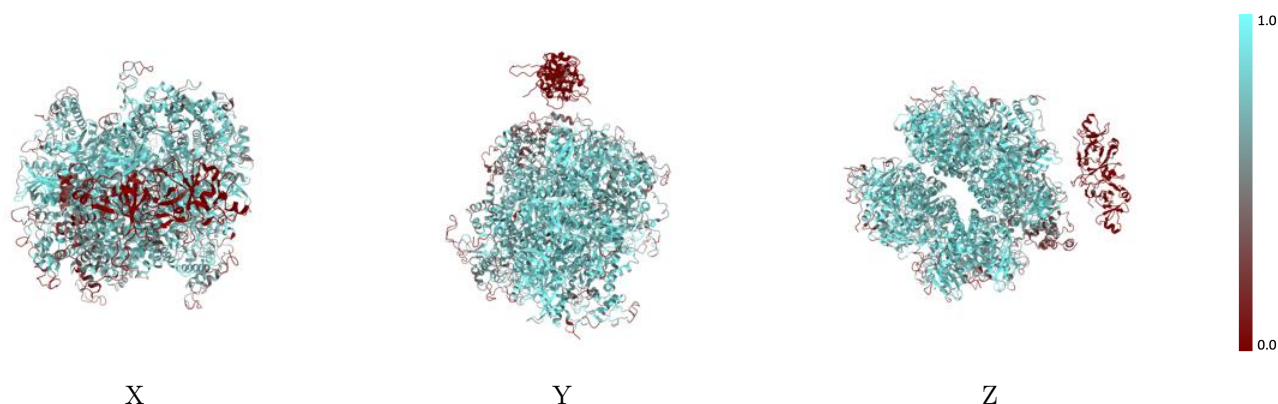
The images above show the 3D surface view of the map at the recommended contour level 0.0183 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



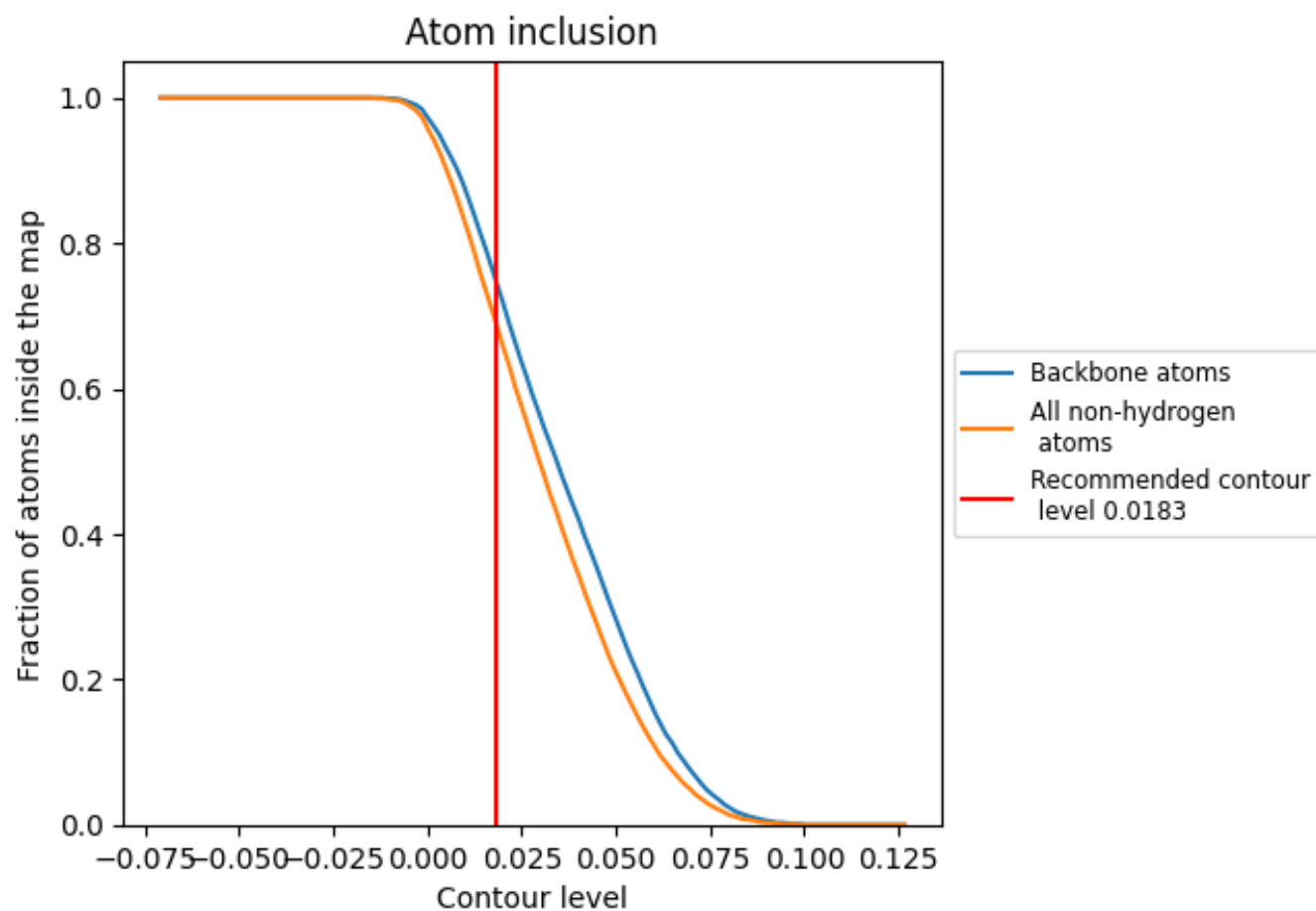
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0183).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0183) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6880	 0.4630
A	 0.7680	 0.5070
B	 0.7970	 0.5250
C	 0.4770	 0.2740
D	 0.6990	 0.4500
E	 0.3680	 0.3450
F	 0.7570	 0.5120
G	 0.7790	 0.5200
H	 0.7800	 0.5190
I	 0.7810	 0.5280
J	 0.7910	 0.5210
K	 0.8060	 0.5250
L	 0.5420	 0.4140
M	 0.6560	 0.4130
N	 0.4790	 0.2990
O	 0.4120	 0.3430
P	 0.4520	 0.3730
Q	 0.5150	 0.2820
R	 0.0210	 0.0380
S	 0.0300	 0.0290

