



Full wwPDB EM Validation Report ⓘ

Mar 22, 2025 – 03:13 PM EDT

PDB ID : 6U5V
EMDB ID : EMD-20657
Title : Electron cryomicroscopy Structure of C. albicans FAS in the Apo state
Authors : Lou, J.W.; Mazhab-Jafari, M.T.
Deposited on : 2019-08-28
Resolution : 2.80 Å (reported)
Based on initial model : 2UV8

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.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

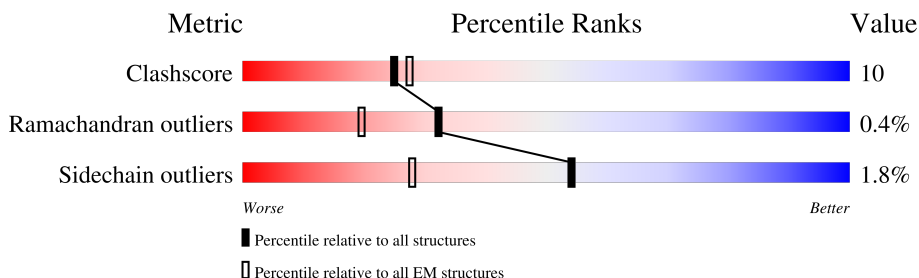
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1885	<div> <div>28%</div> <div>69%</div> <div>15%</div> <div>15%</div> </div>
2	B	2037	<div> <div>48%</div> <div>78%</div> <div>20%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FMN	B	2101	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28187 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 Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1596	Total	C	N	O	S	0	0
			12096	7645	2057	2349	45		

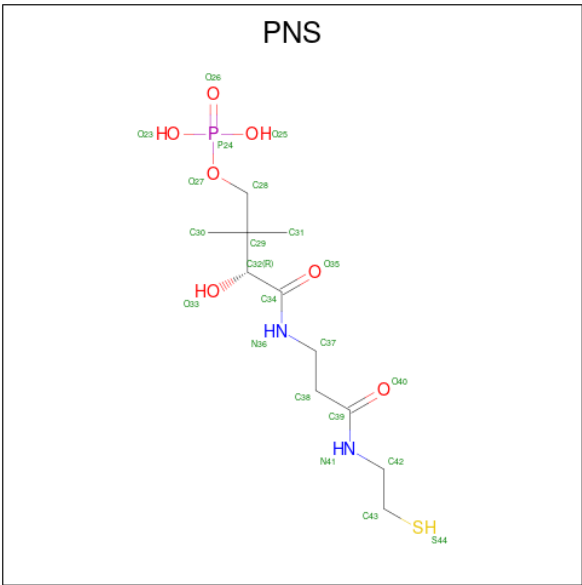
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	350	VAL	SER	conflict	UNP P43098
A	351	ASP	ARG	conflict	UNP P43098
A	353	ASN	LYS	conflict	UNP P43098
A	354	LYS	GLN	conflict	UNP P43098
A	357	ALA	LEU	conflict	UNP P43098
A	814	THR	PRO	conflict	UNP P43098
A	1067	LYS	GLN	conflict	UNP P43098
A	1124	VAL	ILE	conflict	UNP P43098
A	1445	GLU	LYS	conflict	UNP P43098
A	1743	SER	ASN	conflict	UNP P43098

- Molecule 2 is a protein called Fatty acid synthase subunit beta.

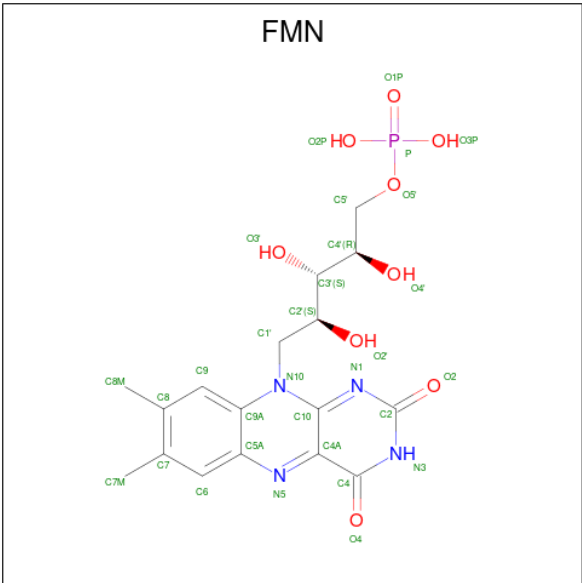
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	2033	Total	C	N	O	S	1	0
			16054	10290	2665	3045	54		

- Molecule 3 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: C₁₁H₂₃N₂O₇PS).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			6	2	3	1	

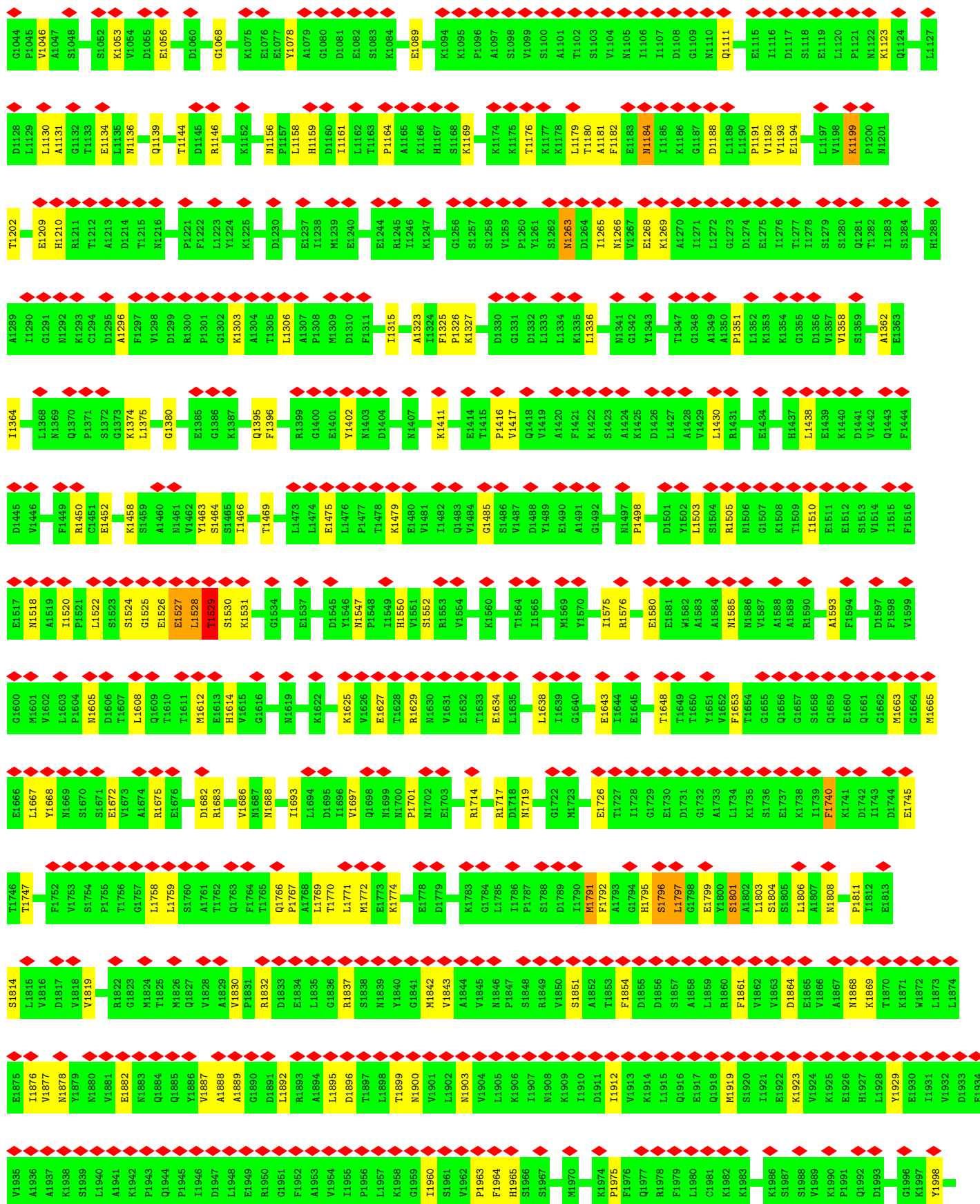
- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			31	17	4	9	1	







N2001	L2002	T2003	A2004	K2005	F2006	F2007	E2008	L2009	T2010	K2011	E2012	Y2013	F2014	Q2015	D2019	L2020	T2021	K2022	S2023	E2024	K2025	S2028	T2029	L2030	D2031	N2032	K2033	E2034	Q2035	Y2036	E2037
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	92958	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTFFIND4 within cryoSPARC2	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.505	Depositor
Minimum map value	-1.098	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.142	Depositor
Recommended contour level	0.744	Depositor
Map size (\AA)	373.12, 373.12, 373.12	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.49	1/12322 (0.0%)	0.61	2/16684 (0.0%)
2	B	0.42	0/16423	0.62	12/22279 (0.1%)
All	All	0.45	1/28745 (0.0%)	0.62	14/38963 (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	A	0	1
2	B	0	3
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	VAL	CB-CG1	-5.10	1.42	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1529	THR	CB-CA-C	-6.29	94.61	111.60
2	B	1430	LEU	CA-CB-CG	6.26	129.71	115.30
2	B	1667	LEU	CA-CB-CG	6.15	129.44	115.30
2	B	2009	LEU	CA-CB-CG	5.85	128.76	115.30
2	B	1529	THR	N-CA-C	5.52	125.91	111.00
2	B	1430	LEU	CB-CG-CD2	-5.51	101.64	111.00
2	B	326	LEU	CA-CB-CG	5.45	127.83	115.30
2	B	1791	MET	CB-CG-SD	5.40	128.60	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	137	LEU	CA-CB-CG	5.37	127.66	115.30
1	A	370	LEU	CA-CB-CG	5.22	127.32	115.30
2	B	1022	LEU	CB-CG-CD2	-5.09	102.35	111.00
2	B	727[A]	HIS	CB-CA-C	5.06	120.52	110.40
2	B	727[B]	HIS	CB-CA-C	5.06	120.52	110.40
1	A	1327	LEU	CB-CG-CD2	-5.04	102.43	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1588	PRO	Peptide
2	B	1111	GLN	Peptide
2	B	1199	LYS	Peptide
2	B	481	HIS	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	A	12096	0	11589	197	0
2	B	16054	0	16016	406	0
3	A	6	0	2	0	0
4	B	31	0	19	32	0
All	All	28187	0	27626	576	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 10.

All (576) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1007:PRO:HD2	2:B:1016:PHE:CE2	1.08	1.59
2:B:886:PHE:CE2	2:B:1017:PHE:CE1	1.83	1.58
2:B:886:PHE:CE2	2:B:1017:PHE:HE1	0.92	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:886:PHE:CZ	2:B:1017:PHE:CE1	1.93	1.54
2:B:1007:PRO:CD	2:B:1016:PHE:HE2	0.89	1.52
2:B:584:MET:HB3	4:B:2101:FMN:C5A	1.43	1.47
2:B:1032:VAL:CG2	2:B:1038:ARG:HD2	1.42	1.46
2:B:1032:VAL:CG2	2:B:1038:ARG:HH11	1.16	1.37
2:B:251:ARG:NH2	2:B:274:ASP:OD1	1.62	1.30
1:A:252:GLU:HA	1:A:257:LEU:CA	1.57	1.28
2:B:1036:VAL:O	2:B:1039:THR:HG22	1.20	1.24
1:A:252:GLU:HA	1:A:257:LEU:N	1.49	1.23
2:B:1007:PRO:CD	2:B:1016:PHE:CE2	1.82	1.21
2:B:886:PHE:CZ	2:B:1017:PHE:HE1	1.39	1.21
2:B:1036:VAL:O	2:B:1039:THR:CG2	1.90	1.18
2:B:1032:VAL:HG23	2:B:1038:ARG:CD	1.75	1.16
1:A:214:PHE:CB	1:A:218:PHE:CB	2.22	1.16
2:B:1032:VAL:CG2	2:B:1038:ARG:CD	2.23	1.16
1:A:216:ASP:CB	1:A:1067:LYS:C	2.16	1.14
2:B:1524:SER:O	2:B:1527:GLU:OE2	1.65	1.12
2:B:887:GLN:HB3	2:B:1038:ARG:O	1.50	1.11
1:A:252:GLU:CA	1:A:257:LEU:H	1.65	1.10
2:B:793:MET:SD	4:B:2101:FMN:HM71	1.91	1.10
2:B:886:PHE:CD2	2:B:1017:PHE:HE1	1.70	1.09
2:B:727[A]:HIS:HB2	2:B:841:ILE:HD13	1.35	1.07
2:B:1032:VAL:HG22	2:B:1038:ARG:HH11	1.11	1.06
2:B:590:ASN:O	2:B:592:ASP:N	1.88	1.05
2:B:588:THR:O	2:B:607:ALA:HB3	1.54	1.05
2:B:1032:VAL:HG22	2:B:1038:ARG:NH1	1.62	1.05
2:B:1007:PRO:HD3	2:B:1016:PHE:CE2	1.87	1.04
2:B:1032:VAL:CG2	2:B:1038:ARG:NH1	1.98	1.03
1:A:205:THR:CB	1:A:209:GLU:CB	2.40	1.00
2:B:584:MET:HB3	4:B:2101:FMN:C6	1.91	1.00
2:B:727[A]:HIS:HB2	2:B:841:ILE:CD1	1.93	0.99
2:B:1032:VAL:HG23	2:B:1038:ARG:HD2	1.31	0.99
2:B:584:MET:CB	4:B:2101:FMN:C5A	2.40	0.98
2:B:886:PHE:CD2	2:B:1017:PHE:CE1	2.48	0.98
2:B:1529:THR:HG22	2:B:1530:SER:N	1.75	0.98
2:B:756:SER:HA	4:B:2101:FMN:O5'	1.65	0.96
1:A:252:GLU:HA	1:A:257:LEU:H	1.15	0.95
2:B:1032:VAL:HG22	2:B:1038:ARG:HD2	1.46	0.94
2:B:757:GLY:N	4:B:2101:FMN:P	2.41	0.93
2:B:790:SER:OG	4:B:2101:FMN:HM81	1.68	0.93
2:B:584:MET:HB3	4:B:2101:FMN:N5	1.82	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ASP:CB	1:A:1067:LYS:O	2.17	0.93
1:A:1137:LYS:NZ	1:A:1141:GLU:OE2	2.02	0.93
2:B:757:GLY:H	4:B:2101:FMN:P	1.91	0.93
1:A:177:VAL:O	1:A:178:ASN:CB	2.17	0.92
2:B:1032:VAL:HG21	2:B:1038:ARG:HD2	1.51	0.91
1:A:252:GLU:C	1:A:257:LEU:H	1.74	0.91
2:B:1007:PRO:HD2	2:B:1016:PHE:CZ	2.03	0.90
2:B:919:VAL:CG2	2:B:1030:SER:HB2	2.01	0.90
2:B:585:THR:HB	2:B:586:PRO:HD3	1.53	0.90
1:A:501:LYS:NZ	1:A:509:GLU:OE2	2.06	0.89
2:B:886:PHE:CZ	2:B:1017:PHE:CZ	2.60	0.89
2:B:886:PHE:CE1	2:B:1017:PHE:CZ	2.61	0.89
2:B:1527:GLU:N	2:B:1527:GLU:OE1	2.06	0.88
1:A:27:ARG:NH1	1:A:30:GLU:OE2	2.07	0.88
2:B:919:VAL:HG22	2:B:1030:SER:HB2	1.55	0.87
2:B:886:PHE:CE1	2:B:1017:PHE:CE1	2.63	0.87
2:B:1526:GLU:N	2:B:1527:GLU:OE1	2.08	0.86
1:A:189:GLY:HA2	2:B:643:PRO:CB	2.05	0.85
2:B:790:SER:OG	4:B:2101:FMN:C8M	2.24	0.84
1:A:767:ASP:O	1:A:818:ARG:NH1	2.11	0.84
2:B:847:ARG:NH1	2:B:885:ASP:OD1	2.10	0.83
2:B:1774:LYS:NZ	2:B:1804:SER:OG	2.11	0.83
2:B:1525:GLY:C	2:B:1527:GLU:OE1	2.17	0.83
2:B:757:GLY:HA2	4:B:2101:FMN:O1P	1.77	0.83
2:B:847:ARG:H	2:B:1037:GLN:HG3	1.43	0.83
2:B:248:GLY:N	2:B:274:ASP:O	2.13	0.82
2:B:587:THR:OG1	4:B:2101:FMN:HM73	1.80	0.82
2:B:793:MET:SD	4:B:2101:FMN:C7M	2.67	0.82
2:B:846:THR:HB	2:B:1037:GLN:HA	1.61	0.81
2:B:756:SER:HA	4:B:2101:FMN:C5'	2.11	0.81
2:B:1022:LEU:HD23	2:B:1022:LEU:O	1.81	0.80
2:B:590:ASN:C	2:B:592:ASP:H	1.85	0.80
1:A:459:GLU:O	1:A:466:LYS:NZ	2.14	0.80
2:B:584:MET:HA	4:B:2101:FMN:C4A	2.11	0.80
2:B:886:PHE:CE2	2:B:1017:PHE:CD1	2.68	0.79
2:B:1797:LEU:HD22	2:B:1797:LEU:O	1.83	0.78
1:A:512:GLU:OE2	1:A:873:ARG:NH1	2.16	0.78
2:B:757:GLY:CA	4:B:2101:FMN:O1P	2.32	0.78
2:B:588:THR:HB	2:B:607:ALA:HB2	1.66	0.78
1:A:144:GLU:O	1:A:260:GLY:O	2.00	0.77
2:B:1032:VAL:HG22	2:B:1038:ARG:CZ	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:GLU:HA	1:A:257:LEU:CB	2.15	0.77
2:B:585:THR:HB	2:B:586:PRO:CD	2.14	0.77
2:B:757:GLY:N	4:B:2101:FMN:O2P	2.15	0.76
1:A:338:LYS:NZ	1:A:342:GLU:OE2	2.18	0.76
2:B:251:ARG:NH1	2:B:271:ALA:O	2.18	0.76
2:B:586:PRO:HB3	2:B:1022:LEU:CD2	2.15	0.76
1:A:217:SER:O	1:A:219:SER:N	2.19	0.75
2:B:584:MET:HA	4:B:2101:FMN:N5	2.02	0.75
2:B:887:GLN:NE2	2:B:1021:SER:CB	2.50	0.75
1:A:894:ARG:NH1	1:A:895:THR:O	2.21	0.74
2:B:757:GLY:N	4:B:2101:FMN:O1P	2.20	0.74
1:A:26:VAL:HG21	2:B:1795:HIS:HD2	1.52	0.74
2:B:584:MET:CB	4:B:2101:FMN:N5	2.51	0.74
2:B:1672:GLU:OE1	2:B:1675:ARG:NH1	2.21	0.74
2:B:506:GLU:OE2	2:B:746:ARG:NH2	2.21	0.74
2:B:588:THR:O	2:B:607:ALA:CB	2.34	0.73
2:B:330:ASP:O	2:B:362:ARG:NH1	2.22	0.73
2:B:966:GLN:NE2	2:B:970:ASP:OD2	2.22	0.73
2:B:1032:VAL:HG23	2:B:1038:ARG:HH11	1.45	0.72
2:B:584:MET:CB	4:B:2101:FMN:C6	2.65	0.72
2:B:584:MET:CA	4:B:2101:FMN:N5	2.53	0.72
2:B:1134:GLU:OE2	2:B:1136:ASN:ND2	2.23	0.72
2:B:183:GLU:OE2	2:B:187:GLN:NE2	2.23	0.71
2:B:296:ARG:HH11	2:B:425:LEU:HB3	1.56	0.70
1:A:252:GLU:CA	1:A:257:LEU:CA	2.52	0.70
2:B:727[A]:HIS:CB	2:B:841:ILE:HD13	2.03	0.70
2:B:1032:VAL:HG23	2:B:1038:ARG:HD3	1.70	0.70
1:A:214:PHE:CA	1:A:218:PHE:CB	2.68	0.70
2:B:1529:THR:HG22	2:B:1530:SER:H	1.54	0.70
1:A:21:GLN:NE2	2:B:1796:SER:HA	2.07	0.70
1:A:252:GLU:CA	1:A:257:LEU:N	2.29	0.70
2:B:887:GLN:NE2	2:B:1021:SER:HB2	2.06	0.70
2:B:1032:VAL:CG2	2:B:1038:ARG:CZ	2.70	0.69
2:B:563:LYS:HZ2	2:B:565:TYR:HE1	1.40	0.69
2:B:727[A]:HIS:HA	2:B:841:ILE:HD13	1.75	0.69
2:B:1452:GLU:OE2	2:B:1469:THR:OG1	2.11	0.69
1:A:33:ASP:OD2	1:A:64:LYS:NZ	2.26	0.69
2:B:584:MET:HB2	2:B:587:THR:HB	1.74	0.68
2:B:888:LYS:NZ	2:B:1019:LYS:O	2.25	0.67
2:B:1663:MET:HB3	2:B:1772:MET:HG3	1.77	0.67
2:B:378:LEU:HD23	2:B:381:ARG:HH12	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:887:GLN:HE22	2:B:1021:SER:CB	2.07	0.67
2:B:887:GLN:CB	2:B:1038:ARG:O	2.35	0.67
1:A:983:GLU:OE2	1:A:1086:LYS:NZ	2.27	0.66
1:A:216:ASP:CB	1:A:1068:GLY:N	2.57	0.66
2:B:799:HIS:CB	2:B:1026:GLU:HG3	2.25	0.66
2:B:1792:PHE:CZ	2:B:1998:TYR:HB2	2.31	0.66
2:B:902:GLN:NE2	2:B:988:CYS:SG	2.68	0.66
2:B:1683:ARG:HA	2:B:1686:VAL:HG12	1.78	0.65
1:A:215:GLN:C	1:A:217:SER:H	1.99	0.65
2:B:1007:PRO:CD	2:B:1016:PHE:CD2	2.72	0.65
2:B:1527:GLU:H	2:B:1527:GLU:CD	1.96	0.65
1:A:1270:GLN:HB3	1:A:1273:ILE:HG23	1.79	0.65
2:B:52:PRO:HG3	2:B:61:LYS:HZ2	1.60	0.65
1:A:215:GLN:O	1:A:217:SER:N	2.28	0.65
2:B:344:ASN:HB3	2:B:349:ARG:HH12	1.62	0.65
2:B:571:SER:HB3	2:B:578:PRO:HG3	1.78	0.65
2:B:1529:THR:CG2	2:B:1530:SER:N	2.48	0.64
2:B:164:ARG:NH1	2:B:205:TRP:O	2.31	0.64
1:A:1188:ILE:H	1:A:1379:GLN:HE21	1.43	0.64
1:A:1007:GLU:O	1:A:1448:LYS:NZ	2.27	0.64
1:A:674:LEU:HD21	1:A:910:THR:HG22	1.79	0.64
2:B:1024:GLN:N	2:B:1024:GLN:OE1	2.29	0.64
2:B:1006:VAL:HA	2:B:1016:PHE:HD2	1.62	0.64
1:A:189:GLY:CA	2:B:643:PRO:CB	2.76	0.63
2:B:887:GLN:NE2	2:B:1021:SER:OG	2.31	0.63
1:A:26:VAL:HG21	2:B:1795:HIS:CD2	2.33	0.63
1:A:1060:LYS:HZ2	1:A:1077:ALA:HA	1.64	0.63
2:B:728:HIS:ND1	2:B:842:HIS:N	2.43	0.63
1:A:1366:ARG:NH1	1:A:1371:THR:O	2.30	0.62
2:B:590:ASN:C	2:B:592:ASP:N	2.44	0.62
2:B:1792:PHE:HB3	2:B:1806:LEU:HD22	1.79	0.62
1:A:824:LEU:HD23	1:A:846:LEU:HB3	1.81	0.62
2:B:906:TYR:OH	2:B:987:ASP:OD2	2.14	0.62
2:B:919:VAL:HG21	2:B:1030:SER:HB2	1.78	0.62
1:A:658:LEU:HD22	1:A:916:LEU:HD11	1.81	0.62
2:B:1263:ASN:ND2	2:B:1325:PHE:O	2.31	0.62
2:B:357:LEU:HB2	2:B:365:VAL:HB	1.82	0.62
1:A:251:LEU:O	1:A:257:LEU:CB	2.48	0.62
1:A:1188:ILE:HG12	1:A:1379:GLN:HG3	1.82	0.62
2:B:799:HIS:O	2:B:1026:GLU:HA	2.00	0.61
2:B:887:GLN:HE21	2:B:1021:SER:HB2	1.62	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LEU:O	1:A:76:ARG:NH2	2.34	0.61
1:A:700:ILE:HG13	1:A:735:LEU:HD12	1.82	0.61
1:A:985:ARG:HG2	2:B:943:GLU:HG2	1.81	0.61
2:B:1306:LEU:HD11	2:B:1351:PRO:HB2	1.82	0.61
1:A:148:ALA:HB2	1:A:214:PHE:CB	2.30	0.61
1:A:483:LEU:HD23	1:A:484:THR:HG23	1.82	0.61
2:B:886:PHE:CD1	2:B:1017:PHE:CZ	2.89	0.61
2:B:1006:VAL:HG12	2:B:1016:PHE:HB3	1.83	0.61
1:A:742:GLN:O	1:A:801:ASN:ND2	2.34	0.61
1:A:1369:THR:O	1:A:1372:ARG:NH1	2.33	0.61
2:B:268:VAL:HG21	2:B:460:ILE:HG21	1.82	0.61
1:A:824:LEU:HD21	1:A:849:LEU:HD12	1.82	0.61
2:B:1796:SER:HB2	2:B:1965:HIS:CE1	2.36	0.61
1:A:296:ALA:HB1	1:A:302:SER:HA	1.82	0.61
2:B:727[A]:HIS:CB	2:B:841:ILE:CD1	2.66	0.61
2:B:756:SER:HA	4:B:2101:FMN:H5'2	1.83	0.61
2:B:344:ASN:O	2:B:349:ARG:NH1	2.34	0.61
2:B:1799:GLU:OE1	2:B:2001:ASN:ND2	2.33	0.61
2:B:1006:VAL:HA	2:B:1016:PHE:CD2	2.35	0.60
2:B:886:PHE:CD1	2:B:1017:PHE:HZ	2.19	0.60
2:B:1416:PRO:HB3	2:B:1450:ARG:HG2	1.84	0.60
2:B:790:SER:HG	4:B:2101:FMN:HM81	1.65	0.60
1:A:1499:ARG:NH1	1:A:1746:TYR:OH	2.35	0.60
2:B:296:ARG:NH1	2:B:425:LEU:HB3	2.15	0.60
2:B:586:PRO:HB3	2:B:1022:LEU:HD21	1.83	0.59
1:A:1026:VAL:HG12	1:A:1188:ILE:HD12	1.84	0.59
1:A:1194:ALA:HB1	1:A:1199:ILE:HD12	1.84	0.59
1:A:984:PRO:HD2	1:A:1086:LYS:HZ1	1.66	0.59
2:B:1336:LEU:HD11	2:B:1396:PHE:HB3	1.84	0.59
2:B:1522:LEU:HD12	2:B:1612:MET:HG2	1.85	0.59
2:B:1576:ARG:NH1	2:B:1580:GLU:OE1	2.35	0.59
2:B:1717:ARG:NH1	2:B:1747:THR:O	2.35	0.59
1:A:1300:PRO:HG3	1:A:1313:ILE:HD12	1.85	0.58
2:B:583:GLY:O	2:B:637:ASN:ND2	2.36	0.58
2:B:337:GLU:HA	2:B:340:ILE:HG12	1.84	0.58
2:B:1028:LEU:O	2:B:1028:LEU:HG	2.04	0.58
2:B:1131:ALA:HB1	2:B:1139:GLN:HG2	1.84	0.58
1:A:17:LEU:HD23	2:B:2002:LEU:HD23	1.84	0.58
1:A:1374:GLY:HA2	1:A:1550:THR:HG22	1.85	0.58
2:B:13:SER:H	2:B:46:PHE:HZ	1.51	0.58
2:B:1416:PRO:HB2	2:B:1510:ILE:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1375:LEU:HD11	2:B:1395:GLN:HE21	1.68	0.58
1:A:648:THR:OG1	1:A:650:ASP:OD1	2.22	0.58
2:B:728:HIS:HD1	2:B:842:HIS:N	2.02	0.58
2:B:1184:ASN:ND2	2:B:1188:ASP:O	2.37	0.58
1:A:984:PRO:HD2	1:A:1086:LYS:NZ	2.19	0.58
2:B:399:ARG:HH22	2:B:731:GLU:HG2	1.68	0.58
2:B:885:ASP:O	2:B:1038:ARG:HA	2.05	0.57
1:A:919:GLU:HG3	1:A:920:GLU:HG2	1.85	0.57
2:B:1796:SER:HB2	2:B:1965:HIS:HE1	1.68	0.57
2:B:232:GLN:HG2	2:B:490:GLY:HA2	1.86	0.57
1:A:878:MET:HG3	1:A:881:ASN:HD22	1.70	0.57
2:B:1770:THR:HG22	2:B:1801:SER:OG	2.05	0.57
2:B:905:THR:HA	2:B:982:LEU:HA	1.86	0.57
1:A:1032:SER:O	1:A:1602:GLN:NE2	2.36	0.56
2:B:1036:VAL:O	2:B:1039:THR:HG23	1.96	0.56
2:B:1799:GLU:OE2	2:B:1998:TYR:OH	2.16	0.56
1:A:18:LEU:CD2	2:B:1799:GLU:HG2	2.35	0.56
2:B:727[B]:HIS:HA	2:B:841:ILE:HA	1.87	0.56
2:B:1726:GLU:H	2:B:1975:PRO:HG3	1.70	0.56
1:A:771:ILE:HG22	1:A:773:PRO:HD3	1.87	0.56
2:B:136:LEU:HD21	2:B:538:ALA:HA	1.88	0.56
2:B:1130:LEU:HD23	2:B:1179:LEU:HD11	1.86	0.56
2:B:1529:THR:HG23	2:B:1608:LEU:O	2.05	0.56
1:A:963:ILE:HG21	2:B:1505:ARG:HH12	1.71	0.56
1:A:1304:CYS:HB2	1:A:1649:GLY:HA2	1.87	0.56
1:A:1029:TRP:O	1:A:1034:THR:OG1	2.24	0.56
2:B:587:THR:HG1	4:B:2101:FMN:HM73	1.71	0.56
2:B:1032:VAL:HG23	2:B:1038:ARG:NH1	2.11	0.56
2:B:1136:ASN:ND2	2:B:1176:THR:OG1	2.39	0.56
1:A:767:ASP:OD1	1:A:813:LYS:NZ	2.39	0.56
1:A:1248:SER:HB3	1:A:1279:ILE:HG23	1.86	0.56
2:B:882:LEU:HD13	2:B:1006:VAL:HG21	1.88	0.56
2:B:815:PRO:HD2	2:B:818:GLN:HE21	1.71	0.56
2:B:1458:LYS:HB2	2:B:1464:SER:HB2	1.88	0.56
1:A:18:LEU:HD21	2:B:1803:LEU:HD21	1.88	0.55
1:A:767:ASP:HB3	1:A:818:ARG:NH1	2.21	0.55
1:A:1063:ASN:ND2	1:A:1072:SER:OG	2.38	0.55
1:A:1562:ASN:HD22	1:A:1625:TYR:HD1	1.52	0.55
2:B:1263:ASN:HB3	2:B:1327:LYS:NZ	2.20	0.55
2:B:1851:SER:HB3	2:B:1854:PHE:HB2	1.87	0.55
2:B:293:ILE:HD11	2:B:465:VAL:HG12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:847:ARG:HG3	2:B:1037:GLN:HG2	1.88	0.55
2:B:799:HIS:HB2	2:B:1026:GLU:HG3	1.87	0.55
1:A:1420:PRO:HB2	1:A:1556:ASN:HD22	1.71	0.55
1:A:1118:LYS:NZ	1:A:1336:GLU:OE2	2.31	0.55
2:B:232:GLN:HE21	2:B:491:PRO:HD3	1.72	0.55
1:A:437:GLN:O	1:A:441:ARG:NE	2.35	0.55
1:A:1689:TYR:OH	2:B:981:GLN:NE2	2.34	0.55
2:B:107:TYR:OH	2:B:110:THR:O	2.24	0.55
2:B:590:ASN:OD1	2:B:799:HIS:CE1	2.59	0.55
2:B:52:PRO:HG3	2:B:61:LYS:NZ	2.21	0.55
2:B:1479:LYS:NZ	2:B:1808:ASN:HB2	2.21	0.55
2:B:831:ILE:HD11	2:B:849:VAL:HG12	1.89	0.54
2:B:1022:LEU:HD23	2:B:1022:LEU:C	2.20	0.54
2:B:453:PHE:HD1	2:B:456:LEU:HD11	1.72	0.54
2:B:1156:ASN:HB3	2:B:1159:HIS:HB2	1.89	0.54
2:B:42:PRO:HB3	2:B:46:PHE:HE1	1.72	0.54
1:A:883:ILE:HG13	1:A:884:ILE:HG23	1.90	0.54
1:A:44:ILE:HG23	1:A:78:VAL:HA	1.89	0.54
2:B:586:PRO:HG2	4:B:2101:FMN:H6	1.89	0.54
1:A:215:GLN:C	1:A:217:SER:N	2.61	0.54
2:B:931:ARG:NH1	2:B:962:ASN:OD1	2.40	0.54
1:A:522:GLU:HG2	1:A:671:ILE:HG22	1.89	0.54
2:B:245:LEU:HD12	2:B:249:GLU:HG3	1.90	0.54
1:A:180:LYS:CB	1:A:183:VAL:CB	2.86	0.53
2:B:1792:PHE:CE2	2:B:1998:TYR:HD1	2.27	0.53
2:B:1181:ALA:HB3	2:B:1193:VAL:HB	1.89	0.53
1:A:769:ASP:OD1	1:A:818:ARG:NE	2.41	0.53
2:B:590:ASN:ND2	2:B:799:HIS:CD2	2.77	0.53
1:A:21:GLN:HE21	2:B:1796:SER:HA	1.73	0.53
1:A:269:ALA:O	1:A:273:GLU:N	2.42	0.53
1:A:46:GLU:OE1	1:A:54:ALA:N	2.40	0.53
2:B:708:LYS:NZ	2:B:747:CYS:SG	2.76	0.53
2:B:919:VAL:HG21	2:B:1030:SER:CB	2.37	0.53
2:B:1688:ASN:O	2:B:1719:ASN:ND2	2.41	0.53
1:A:1456:GLU:HA	1:A:1459:LYS:HG2	1.90	0.53
2:B:1593:ALA:HB3	2:B:1643:GLU:HB2	1.91	0.53
2:B:727[B]:HIS:HD2	2:B:841:ILE:HG23	1.73	0.53
1:A:412:VAL:HG11	1:A:450:MET:HG2	1.90	0.52
2:B:727[A]:HIS:HD2	2:B:727[A]:HIS:O	1.93	0.52
2:B:1037:GLN:C	2:B:1039:THR:H	2.12	0.52
2:B:1830:VAL:HB	2:B:1832:ARG:HH12	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:PRO:HA	2:B:1965:HIS:HB3	1.92	0.52
1:A:676:PHE:HD2	1:A:702:GLY:HA3	1.74	0.52
2:B:219:LEU:HD21	2:B:409:PRO:HB3	1.91	0.52
2:B:1032:VAL:HG22	2:B:1038:ARG:CD	2.17	0.52
1:A:1472:GLU:OE1	1:A:1493:ARG:NH1	2.42	0.52
2:B:57:GLU:OE2	2:B:113:LYS:HB3	2.09	0.52
2:B:726:GLY:HA2	2:B:1042:LEU:HD23	1.92	0.52
2:B:1529:THR:HG22	2:B:1530:SER:O	2.10	0.52
1:A:16:GLU:OE2	2:B:2025:LYS:HE2	2.10	0.52
2:B:1919:MET:HE2	2:B:1923:LYS:HE2	1.92	0.52
1:A:1565:MET:HB3	1:A:1570:ARG:HG3	1.91	0.51
2:B:1036:VAL:C	2:B:1039:THR:HG22	2.18	0.51
2:B:1811:PRO:HD2	2:B:1814:SER:HB2	1.92	0.51
2:B:871:LEU:HD22	2:B:1009:LEU:HD12	1.92	0.51
2:B:1876:ILE:HA	2:B:1888:ALA:HA	1.93	0.51
1:A:856:GLU:OE1	1:A:858:TRP:NE1	2.35	0.51
2:B:563:LYS:NZ	2:B:565:TYR:HE1	2.07	0.51
2:B:87:LEU:HB3	2:B:91:ASN:HA	1.92	0.51
2:B:727[A]:HIS:HA	2:B:841:ILE:HA	1.91	0.51
2:B:886:PHE:CE1	2:B:1017:PHE:HZ	2.21	0.51
1:A:1305:ALA:HB1	1:A:1647:SER:OG	2.11	0.51
1:A:1588:PRO:HB2	1:A:1591:ALA:HB3	1.93	0.51
2:B:1037:GLN:N	2:B:1037:GLN:OE1	2.43	0.51
2:B:1037:GLN:C	2:B:1039:THR:N	2.64	0.51
2:B:1191:PRO:O	2:B:1210:HIS:NE2	2.41	0.51
1:A:251:LEU:C	1:A:257:LEU:CB	2.79	0.51
2:B:843:LYS:HZ2	2:B:849:VAL:HG13	1.75	0.51
1:A:1279:ILE:HG21	1:A:1301:VAL:HG22	1.92	0.50
1:A:815:THR:HG22	1:A:817:THR:H	1.76	0.50
2:B:727[A]:HIS:C	2:B:727[A]:HIS:CD2	2.85	0.50
2:B:93:ASN:HD21	2:B:536:THR:HG23	1.75	0.50
2:B:894:ASN:ND2	2:B:903:GLU:O	2.44	0.50
2:B:984:SER:OG	2:B:986:GLU:OE1	2.30	0.50
1:A:325:ALA:O	1:A:326:LEU:C	2.48	0.50
2:B:1896:ASP:O	2:B:1900:ASN:ND2	2.45	0.50
1:A:1366:ARG:NH1	1:A:1371:THR:HG23	2.27	0.50
2:B:1015:PHE:C	2:B:1015:PHE:CD2	2.84	0.50
2:B:1672:GLU:CD	2:B:1675:ARG:HH12	2.14	0.50
1:A:868:VAL:HB	1:A:925:ASP:HA	1.92	0.50
2:B:518:LEU:HD13	2:B:530:LYS:HB3	1.93	0.50
2:B:1899:THR:O	2:B:1903:ASN:ND2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1529:THR:CG2	2:B:1530:SER:H	2.21	0.49
2:B:1869:LYS:HG3	2:B:1929:TYR:HE1	1.77	0.49
2:B:723:ARG:HD2	2:B:1046:VAL:HG11	1.93	0.49
2:B:1877:VAL:HB	2:B:1965:HIS:HB2	1.93	0.49
2:B:585:THR:N	4:B:2101:FMN:O4	2.45	0.49
2:B:1842:MET:HB2	2:B:1960:ILE:HG21	1.94	0.49
1:A:723:ASN:OD1	1:A:727:ARG:NH2	2.45	0.49
2:B:1180:THR:HG23	2:B:1194:GLU:HG2	1.94	0.49
1:A:1649:GLY:N	1:A:1653:LYS:O	2.44	0.49
2:B:756:SER:H	4:B:2101:FMN:H5'2	1.77	0.49
1:A:686:ALA:O	1:A:721:TYR:OH	2.29	0.49
2:B:1209:GLU:OE1	2:B:1552:SER:OG	2.25	0.49
2:B:1774:LYS:HZ1	2:B:1804:SER:CB	2.23	0.49
2:B:1169:LYS:HZ2	2:B:1182:PHE:HD2	1.58	0.49
1:A:252:GLU:CA	1:A:257:LEU:CB	2.89	0.49
1:A:984:PRO:HB3	2:B:946:THR:HG23	1.95	0.49
2:B:344:ASN:HB3	2:B:349:ARG:NH1	2.27	0.49
1:A:1104:LEU:HA	1:A:1184:VAL:HA	1.95	0.49
1:A:58:ASN:HD21	1:A:78:VAL:HG11	1.78	0.49
2:B:1682:ASP:HB3	2:B:1693:ILE:HG22	1.95	0.49
1:A:91:LYS:NZ	2:B:1518:ASN:HB2	2.27	0.48
1:A:1354:GLU:OE1	1:A:1366:ARG:NH2	2.46	0.48
1:A:1549:SER:O	1:A:1549:SER:OG	2.30	0.48
2:B:590:ASN:CG	2:B:799:HIS:CE1	2.86	0.48
1:A:14:LEU:HD21	2:B:1803:LEU:HD22	1.95	0.48
2:B:556:LEU:HB2	2:B:1078:TYR:HE2	1.78	0.48
2:B:1878:ASN:HB2	2:B:1887:VAL:HB	1.95	0.48
1:A:234:MET:O	1:A:238:MET:CB	2.61	0.48
2:B:79:LEU:HD21	2:B:126:VAL:HG23	1.94	0.48
2:B:1266:ASN:HD22	2:B:1269:LYS:HE3	1.77	0.48
1:A:1018:VAL:HG11	1:A:1315:ILE:HG12	1.95	0.48
2:B:584:MET:O	2:B:607:ALA:HB2	2.14	0.48
1:A:888:ILE:HD13	1:A:930:LEU:HD21	1.96	0.48
2:B:222:PRO:HG3	2:B:295:SER:HA	1.96	0.48
1:A:148:ALA:CB	1:A:214:PHE:CB	2.92	0.48
1:A:411:ASP:HA	1:A:414:SER:HB3	1.96	0.48
1:A:871:TRP:HB2	1:A:930:LEU:HD11	1.95	0.48
1:A:1234:TYR:OH	1:A:1291:LEU:O	2.22	0.47
2:B:693:LYS:HG2	2:B:718:GLN:HB2	1.96	0.47
1:A:1248:SER:OG	1:A:1249:GLY:N	2.47	0.47
2:B:146:LEU:HD23	2:B:485:HIS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1192:VAL:HG23	2:B:1193:VAL:HG23	1.96	0.47
2:B:1032:VAL:CG2	2:B:1038:ARG:NE	2.75	0.47
2:B:1717:ARG:NH2	2:B:1745:GLU:O	2.47	0.47
2:B:522:PRO:HD3	2:B:529:PHE:HE2	1.80	0.47
2:B:590:ASN:O	2:B:593:ILE:N	2.45	0.47
2:B:481:HIS:HD2	2:B:505:LYS:NZ	2.12	0.47
1:A:984:PRO:HG2	1:A:1086:LYS:HD3	1.96	0.47
1:A:1304:CYS:HA	1:A:1589:LYS:O	2.15	0.47
2:B:246:THR:HG22	2:B:248:GLY:H	1.79	0.47
2:B:831:ILE:HD13	2:B:853:LYS:HE2	1.96	0.47
2:B:1524:SER:C	2:B:1527:GLU:OE2	2.47	0.47
2:B:1531:LYS:NZ	2:B:1605:ASN:O	2.46	0.47
2:B:1792:PHE:O	2:B:1792:PHE:CD2	2.67	0.47
1:A:1035:ARG:NH1	1:A:1039:GLU:OE1	2.47	0.47
2:B:761:ASP:OD2	2:B:1068:GLY:HA3	2.15	0.47
2:B:790:SER:HA	4:B:2101:FMN:HM83	1.97	0.47
2:B:1374:LYS:HB2	2:B:1402:TYR:HD2	1.80	0.47
2:B:440:LEU:HB3	2:B:454:GLN:HG2	1.96	0.46
2:B:1053:LYS:HE3	2:B:1056:GLU:HB3	1.97	0.46
2:B:1792:PHE:O	2:B:1792:PHE:CG	2.69	0.46
1:A:494:ARG:HD3	1:A:514:GLN:HG2	1.97	0.46
1:A:1367:PRO:O	1:A:1369:THR:OG1	2.30	0.46
2:B:728:HIS:HD1	2:B:842:HIS:H	1.63	0.46
2:B:799:HIS:O	2:B:1026:GLU:CA	2.40	0.46
1:A:1220:GLU:HA	1:A:1223:LEU:HB2	1.98	0.46
2:B:1032:VAL:HG22	2:B:1038:ARG:NE	2.30	0.46
1:A:214:PHE:HA	1:A:218:PHE:CB	2.45	0.46
1:A:1008:LEU:HG	1:A:1668:VAL:HG12	1.97	0.46
2:B:1767:PRO:HG3	2:B:1819:VAL:HG13	1.98	0.46
2:B:42:PRO:HA	2:B:51:GLU:OE2	2.16	0.46
2:B:233:LEU:HD13	2:B:283:SER:HB2	1.97	0.46
1:A:939:PHE:HD1	1:A:942:LYS:HZ3	1.60	0.46
1:A:1118:LYS:HG3	1:A:1336:GLU:OE2	2.16	0.46
1:A:1401:ALA:HB2	1:A:1601:ILE:HG12	1.98	0.46
1:A:1510:LYS:HA	1:A:1514:ASN:HB2	1.97	0.46
2:B:192:PHE:HE1	2:B:296:ARG:HE	1.63	0.46
2:B:1026:GLU:HA	2:B:1026:GLU:OE1	2.16	0.46
2:B:1792:PHE:CE2	2:B:1998:TYR:CD1	3.03	0.46
2:B:1795:HIS:CE1	2:B:1878:ASN:ND2	2.84	0.46
2:B:1795:HIS:NE2	2:B:1878:ASN:ND2	2.63	0.46
1:A:985:ARG:HB2	2:B:944:ARG:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:560:SER:HB2	2:B:1089:GLU:HA	1.98	0.45
1:A:963:ILE:HG21	2:B:1505:ARG:NH1	2.30	0.45
1:A:1230:PRO:HB3	1:A:1291:LEU:HD23	1.98	0.45
2:B:727[A]:HIS:HB2	2:B:841:ILE:HD11	1.88	0.45
1:A:1495:GLU:OE1	1:A:1499:ARG:NH2	2.49	0.45
2:B:94:ILE:HA	2:B:97:PHE:HB3	1.97	0.45
2:B:273:SER:HB2	2:B:279:PHE:HA	1.98	0.45
2:B:313:ASP:OD1	2:B:317:ASN:ND2	2.49	0.45
2:B:381:ARG:HA	2:B:384:LYS:HG2	1.98	0.45
1:A:893:VAL:HG21	1:A:933:ILE:HD11	1.99	0.45
1:A:1060:LYS:NZ	1:A:1077:ALA:HA	2.31	0.45
1:A:91:LYS:NZ	2:B:1518:ASN:HD22	2.15	0.45
1:A:1276:GLU:HA	1:A:1281:THR:HG21	1.98	0.45
2:B:727[A]:HIS:O	2:B:727[A]:HIS:CD2	2.70	0.45
2:B:1665:MET:HA	2:B:1668:TYR:HB3	1.98	0.45
1:A:752:VAL:HG21	1:A:808:ALA:HB1	1.99	0.45
1:A:1258:GLY:HA2	1:A:1262:ASP:HB2	1.98	0.45
2:B:1864:ASP:O	2:B:1868:ASN:ND2	2.50	0.45
2:B:102:LEU:HD11	2:B:111:ILE:HD13	1.99	0.45
2:B:584:MET:O	2:B:607:ALA:CB	2.65	0.45
2:B:723:ARG:HH11	2:B:1046:VAL:HG11	1.82	0.45
2:B:236:TYR:CG	2:B:270:ILE:HD11	2.52	0.45
2:B:389:LEU:HD23	2:B:391:GLN:HE21	1.82	0.45
2:B:847:ARG:N	2:B:1037:GLN:HG3	2.23	0.45
2:B:1022:LEU:CD2	2:B:1022:LEU:C	2.85	0.45
1:A:41:THR:HG22	2:B:1648:THR:HG22	1.99	0.44
1:A:47:ILE:HD12	2:B:1653:PHE:HE1	1.83	0.44
1:A:1721:ASP:OD2	1:A:1724:ALA:HB2	2.17	0.44
2:B:502:HIS:HB2	2:B:512:ILE:HG13	1.98	0.44
2:B:1529:THR:CG2	2:B:1608:LEU:O	2.65	0.44
2:B:63:ILE:HD11	2:B:79:LEU:HA	1.99	0.44
2:B:1017:PHE:CD1	2:B:1017:PHE:C	2.84	0.44
2:B:590:ASN:O	2:B:591:THR:C	2.48	0.44
1:A:182:THR:CB	2:B:672:VAL:O	2.66	0.44
1:A:459:GLU:OE2	1:A:469:LYS:HD2	2.18	0.44
2:B:727[B]:HIS:HA	2:B:841:ILE:HD13	1.75	0.44
2:B:847:ARG:H	2:B:1037:GLN:CG	2.24	0.44
2:B:1031:VAL:HG13	2:B:1032:VAL:HG22	1.98	0.44
2:B:1268:GLU:OE2	2:B:1411:LYS:NZ	2.45	0.44
2:B:1315:ILE:HD13	2:B:1358:VAL:HG11	1.99	0.44
2:B:1547:ASN:HB3	2:B:1550:HIS:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1187:GLN:H	1:A:1187:GLN:HG2	1.53	0.44
2:B:251:ARG:NH1	2:B:441:LYS:HB2	2.33	0.44
2:B:1013:PHE:O	2:B:1017:PHE:N	2.51	0.44
2:B:1158:LEU:HA	2:B:1161:ILE:HG12	2.00	0.44
1:A:2:LYS:HE2	1:A:5:ILE:HD12	2.00	0.43
1:A:1259:MET:HB3	1:A:1273:ILE:HD13	2.00	0.43
1:A:700:ILE:HG22	1:A:729:GLY:HA2	2.00	0.43
2:B:846:THR:CB	2:B:1037:GLN:HA	2.42	0.43
2:B:1463:TYR:HD2	2:B:1466:ILE:HD11	1.83	0.43
2:B:1629:ARG:NH2	2:B:1634:GLU:OE1	2.50	0.43
1:A:691:ILE:HD11	1:A:872:THR:HG21	2.00	0.43
1:A:709:THR:HG23	1:A:740:PHE:HB3	1.99	0.43
1:A:741:ASN:HB3	1:A:747:ASP:OD2	2.18	0.43
1:A:1210:ILE:HD11	1:A:1331:TYR:HD2	1.84	0.43
2:B:1701:PRO:HD2	2:B:1758:LEU:HD12	2.00	0.43
2:B:1792:PHE:HZ	2:B:1998:TYR:HB2	1.81	0.43
2:B:1889:ALA:HB1	2:B:1963:PRO:HB3	2.00	0.43
2:B:1960:ILE:HD11	2:B:1964:PHE:HE1	1.83	0.43
1:A:1229:ASP:OD1	1:A:1229:ASP:N	2.52	0.43
2:B:727[B]:HIS:HD2	2:B:841:ILE:CG2	2.25	0.43
2:B:1037:GLN:O	2:B:1039:THR:N	2.52	0.43
2:B:1861:PHE:HD2	2:B:1912:ILE:HD13	1.83	0.43
1:A:222:LEU:O	1:A:226:SER:CB	2.67	0.43
2:B:1266:ASN:HB3	2:B:1269:LYS:NZ	2.33	0.43
2:B:221:VAL:HG21	2:B:412:ALA:HB2	1.99	0.43
2:B:221:VAL:HG12	2:B:294:GLY:HA2	2.00	0.43
2:B:1362:ALA:HA	2:B:1380:GLY:HA2	2.01	0.43
2:B:1438:LEU:HA	2:B:1485:GLY:HA3	2.01	0.43
2:B:586:PRO:HD2	4:B:2101:FMN:H6	2.01	0.43
2:B:1528:LEU:HA	2:B:1528:LEU:HD22	1.64	0.43
1:A:18:LEU:HD23	2:B:1799:GLU:HG2	2.00	0.42
2:B:590:ASN:ND2	2:B:592:ASP:HB3	2.33	0.42
2:B:919:VAL:HG11	2:B:1029:GLU:OE1	2.19	0.42
1:A:788:ASP:O	1:A:791:SER:OG	2.30	0.42
1:A:1006:PRO:O	1:A:1008:LEU:N	2.51	0.42
2:B:260:HIS:CG	2:B:261:SER:H	2.37	0.42
2:B:1843:VAL:O	2:B:1888:ALA:N	2.47	0.42
1:A:823:ILE:HD13	1:A:865:CYS:HB3	2.01	0.42
1:A:998:TYR:CZ	1:A:1002:LYS:NZ	2.87	0.42
2:B:333:ILE:HG13	2:B:364:LEU:HD21	2.01	0.42
2:B:1266:ASN:HB3	2:B:1269:LYS:HZ2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1366:ARG:HH11	1:A:1371:THR:HG23	1.85	0.42
2:B:585:THR:N	4:B:2101:FMN:N5	2.67	0.42
1:A:216:ASP:CB	1:A:1067:LYS:CA	2.97	0.42
2:B:756:SER:CA	4:B:2101:FMN:H5'2	2.48	0.42
2:B:879:ILE:O	2:B:883:ASN:ND2	2.53	0.42
2:B:1520:ILE:HG13	2:B:1614:HIS:HB3	2.01	0.42
1:A:30:GLU:HA	1:A:33:ASP:HB2	2.02	0.42
1:A:1028:PRO:HD3	1:A:1595:TRP:CH2	2.55	0.42
2:B:428:ASP:OD1	2:B:431:LYS:NZ	2.53	0.42
2:B:481:HIS:HD2	2:B:505:LYS:HZ2	1.68	0.42
1:A:451:GLN:HE22	1:A:473:GLN:HE22	1.68	0.42
1:A:904:ASN:HB3	1:A:926:LEU:HD13	2.02	0.42
1:A:964:GLU:HG2	2:B:1498:PRO:HB3	2.01	0.42
1:A:1017:VAL:O	1:A:1389:ALA:N	2.52	0.42
1:A:1375:PHE:HB3	1:A:1548:THR:O	2.20	0.42
2:B:185:LEU:O	2:B:189:HIS:N	2.53	0.42
2:B:822:THR:HG22	2:B:832:THR:H	1.85	0.42
1:A:51:PRO:HB3	1:A:54:ALA:HB3	2.02	0.42
1:A:495:ILE:HG23	1:A:900:GLU:OE2	2.19	0.42
2:B:276:TRP:CE3	2:B:276:TRP:HA	2.54	0.42
2:B:306:LEU:HD23	2:B:311:LEU:HB3	2.01	0.42
2:B:1475:GLU:OE2	2:B:1479:LYS:HA	2.19	0.42
1:A:521:PHE:HA	1:A:524:TYR:HB3	2.01	0.41
2:B:61:LYS:NZ	2:B:117:ASN:OD1	2.31	0.41
2:B:1265:ILE:HB	2:B:1326:PRO:HG3	2.00	0.41
1:A:1132:PRO:HG3	1:A:1165:ARG:HB2	2.02	0.41
2:B:307:PRO:HA	2:B:308:PRO:HD3	1.87	0.41
1:A:1305:ALA:HB2	1:A:1647:SER:C	2.40	0.41
2:B:218:LEU:O	2:B:224:SER:OG	2.38	0.41
2:B:1017:PHE:CD1	2:B:1017:PHE:O	2.74	0.41
2:B:1771:LEU:HD23	2:B:1771:LEU:HA	1.89	0.41
1:A:296:ALA:O	1:A:300:GLY:N	2.53	0.41
1:A:1557:GLU:OE2	1:A:1646:THR:OG1	2.21	0.41
2:B:461:ILE:HA	2:B:464:VAL:HG12	2.02	0.41
2:B:486:ILE:HB	2:B:512:ILE:HD13	2.01	0.41
2:B:568:THR:N	2:B:571:SER:OG	2.44	0.41
2:B:1575:ILE:HG13	2:B:1638:LEU:HD12	2.01	0.41
2:B:262:GLN:HE21	2:B:290:LEU:HD23	1.84	0.41
2:B:744:ILE:HG21	2:B:752:LEU:HD12	2.01	0.41
2:B:73:GLN:HA	2:B:76:GLU:OE2	2.21	0.41
2:B:319:GLU:OE2	2:B:381:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1417:VAL:HG11	2:B:1503:LEU:HB3	2.03	0.41
2:B:1697:VAL:HA	2:B:1759:LEU:HD22	2.03	0.41
1:A:1116:LYS:HD3	1:A:1183:LEU:HD21	2.02	0.41
2:B:1199:LYS:O	2:B:1202:THR:OG1	2.30	0.41
2:B:181:ILE:HG23	2:B:287:VAL:HG21	2.03	0.41
2:B:833:VAL:HG11	2:B:843:LYS:HZ3	1.85	0.41
2:B:1296:ALA:HA	2:B:1303:LYS:NZ	2.35	0.41
2:B:1525:GLY:CA	2:B:1527:GLU:OE1	2.68	0.41
1:A:497:GLY:HA3	1:A:515:LYS:HD3	2.02	0.41
1:A:1050:ILE:HG22	1:A:1088:ILE:HG21	2.02	0.41
1:A:1375:PHE:HA	1:A:1549:SER:HB3	2.02	0.41
2:B:471:LEU:HA	2:B:472:PRO:HD3	1.94	0.41
2:B:1144:THR:HG22	2:B:1146:ARG:H	1.85	0.41
1:A:417:PHE:HD2	1:A:1635:ILE:HD11	1.85	0.41
1:A:930:LEU:HD23	1:A:933:ILE:HD12	2.03	0.41
1:A:1020:VAL:HG22	1:A:1386:ILE:HG22	2.03	0.41
2:B:1144:THR:O	2:B:1156:ASN:ND2	2.54	0.41
1:A:7:GLN:O	1:A:11:HIS:N	2.46	0.40
1:A:1312:ASP:HA	1:A:1406:THR:HG21	2.02	0.40
2:B:332:SER:H	2:B:335:GLN:HE21	1.68	0.40
2:B:1766:GLN:HG3	2:B:1819:VAL:HG22	2.02	0.40
1:A:29:ILE:HG21	2:B:1882:GLU:OE2	2.21	0.40
1:A:983:GLU:O	2:B:943:GLU:HG3	2.22	0.40
1:A:1046:LEU:HD23	1:A:1089:LYS:HE2	2.03	0.40
2:B:150:PHE:HE1	2:B:489:PHE:HB2	1.85	0.40
2:B:843:LYS:NZ	2:B:849:VAL:HG13	2.35	0.40
2:B:1769:LEU:HD23	2:B:1769:LEU:HA	1.95	0.40
1:A:1208:ASP:N	1:A:1208:ASP:OD1	2.55	0.40
1:A:1742:SER:HB3	1:A:1744:GLN:HG2	2.03	0.40
2:B:322:PRO:HA	2:B:407:PHE:CG	2.56	0.40
2:B:1323:ALA:HB1	2:B:1364:ILE:HD12	2.04	0.40
2:B:1740:PHE:HD1	2:B:1740:PHE:HA	1.75	0.40
2:B:145:LYS:HZ3	2:B:482:LYS:HG3	1.87	0.40
2:B:852:TRP:CH2	2:B:1018:LYS:HA	2.56	0.40
2:B:955:LEU:HD12	2:B:955:LEU:HA	1.92	0.40
1:A:627:ILE:HD12	1:A:628:GLN:HG2	2.04	0.40
2:B:846:THR:HB	2:B:1037:GLN:CA	2.42	0.40
2:B:1123:LYS:HA	2:B:1164:PRO:HG2	2.03	0.40
2:B:1625:LYS:HD3	2:B:1627:GLU:OE2	2.21	0.40
2:B:1892:LEU:HD23	2:B:1895:LEU:HD22	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	1586/1885 (84%)	1513 (95%)	64 (4%)	9 (1%)	22	51
2	B	2032/2037 (100%)	1924 (95%)	103 (5%)	5 (0%)	44	73
All	All	3618/3922 (92%)	3437 (95%)	167 (5%)	14 (0%)	32	61

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	PHE
2	B	591	THR
2	B	1032	VAL
1	A	178	ASN
2	B	1038	ARG
2	B	1796	SER
1	A	206	PRO
1	A	207	LEU
1	A	216	ASP
1	A	1301	VAL
1	A	215	GLN
1	A	1007	GLU
2	B	1022	LEU
1	A	1006	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1221/1579 (77%)	1204 (99%)	17 (1%)	62	87
2	B	1780/1784 (100%)	1742 (98%)	38 (2%)	48	80
All	All	3001/3363 (89%)	2946 (98%)	55 (2%)	54	83

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	406	ASN
1	A	580	LYS
1	A	712	ARG
1	A	786	ASN
1	A	799	LEU
1	A	987	ASN
1	A	1063	ASN
1	A	1179	ARG
1	A	1383	ILE
1	A	1429	ARG
1	A	1449	ARG
1	A	1503	ARG
1	A	1553	ASN
1	A	1589	LYS
1	A	1690	ARG
1	A	1707	LYS
1	A	1738	LYS
2	B	5	ARG
2	B	252	ASN
2	B	277	ASP
2	B	334	LYS
2	B	363	ASN
2	B	480	ASN
2	B	584	MET
2	B	589	VAL
2	B	727[A]	HIS
2	B	727[B]	HIS
2	B	864	LYS
2	B	957	ASN
2	B	1015	PHE
2	B	1016	PHE
2	B	1021	SER
2	B	1022	LEU
2	B	1025	SER
2	B	1026	GLU

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Mol	Chain	Res	Type
2	B	1028	LEU
2	B	1029	GLU
2	B	1032	VAL
2	B	1033	ASP
2	B	1034	GLU
2	B	1037	GLN
2	B	1039	THR
2	B	1040	CYS
2	B	1184	ASN
2	B	1263	ASN
2	B	1527	GLU
2	B	1528	LEU
2	B	1529	THR
2	B	1585	ASN
2	B	1714	ARG
2	B	1740	PHE
2	B	1791	MET
2	B	1797	LEU
2	B	1801	SER
2	B	1837	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	451	GLN
1	A	478	ASN
1	A	786	ASN
1	A	881	ASN
1	A	987	ASN
1	A	1016	ASN
1	A	1062	HIS
1	A	1063	ASN
1	A	1238	HIS
1	A	1379	GLN
1	A	1546	HIS
1	A	1553	ASN
2	B	187	GLN
2	B	252	ASN
2	B	262	GLN
2	B	282	ASN
2	B	335	GLN

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Mol	Chain	Res	Type
2	B	363	ASN
2	B	391	GLN
2	B	415	HIS
2	B	480	ASN
2	B	481	HIS
2	B	572	GLN
2	B	590	ASN
2	B	734	HIS
2	B	799	HIS
2	B	818	GLN
2	B	872	ASN
2	B	887	GLN
2	B	902	GLN
2	B	957	ASN
2	B	981	GLN
2	B	1069	HIS
2	B	1136	ASN
2	B	1153	HIS
2	B	1184	ASN
2	B	1338	HIS
2	B	1518	ASN
2	B	1550	HIS
2	B	1567	HIS
2	B	1585	ASN
2	B	1614	HIS
2	B	1684	HIS
2	B	1868	ASN
2	B	1900	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

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FMN	B	2101	-	33,33,33	6.45	22 (66%)	48,50,50	1.35	6 (12%)
3	PNS	A	1901	1	2,5,21	0.59	0	1,5,29	0.16	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FMN	B	2101	-	-	5/18/18/18	0/3/3/3
3	PNS	A	1901	1	-	1/1/3/27	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2101	FMN	C6-C7	13.49	1.58	1.39
4	B	2101	FMN	C6-C5A	12.40	1.58	1.40
4	B	2101	FMN	C9-C9A	12.37	1.59	1.39
4	B	2101	FMN	C9-C8	11.90	1.55	1.39
4	B	2101	FMN	O4-C4	9.96	1.42	1.23
4	B	2101	FMN	C4A-N5	9.56	1.51	1.30
4	B	2101	FMN	C9A-C5A	8.70	1.55	1.41
4	B	2101	FMN	O2-C2	8.20	1.40	1.24
4	B	2101	FMN	C2-N1	7.47	1.53	1.36
4	B	2101	FMN	C10-N1	7.19	1.47	1.33
4	B	2101	FMN	C8-C7	7.09	1.58	1.40
4	B	2101	FMN	C10-N10	6.61	1.51	1.37
4	B	2101	FMN	C5A-N5	6.53	1.51	1.39
4	B	2101	FMN	C2-N3	6.16	1.52	1.39
4	B	2101	FMN	C4-N3	6.15	1.50	1.38
4	B	2101	FMN	C9A-N10	5.22	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2101	FMN	C4A-C10	3.64	1.54	1.44
4	B	2101	FMN	C1'-C2'	3.06	1.56	1.52
4	B	2101	FMN	P-O2P	3.03	1.66	1.54
4	B	2101	FMN	P-O3P	2.73	1.64	1.54
4	B	2101	FMN	C4A-C4	2.43	1.53	1.44
4	B	2101	FMN	C7M-C7	2.03	1.54	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2101	FMN	C4'-C3'-C2'	-3.56	107.64	113.57
4	B	2101	FMN	C4A-C10-N10	3.07	120.87	116.48
4	B	2101	FMN	C10-C4A-N5	-2.77	119.16	124.81
4	B	2101	FMN	C4-N3-C2	-2.44	121.31	125.64
4	B	2101	FMN	C5A-C9A-N10	2.03	119.81	117.97
4	B	2101	FMN	O2-C2-N1	-2.01	118.45	121.80

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1901	PNS	C29-C28-O27-P24
4	B	2101	FMN	C2'-C3'-C4'-C5'
4	B	2101	FMN	O3'-C3'-C4'-C5'
4	B	2101	FMN	C2'-C3'-C4'-O4'
4	B	2101	FMN	O3'-C3'-C4'-O4'
4	B	2101	FMN	C4'-C5'-O5'-P

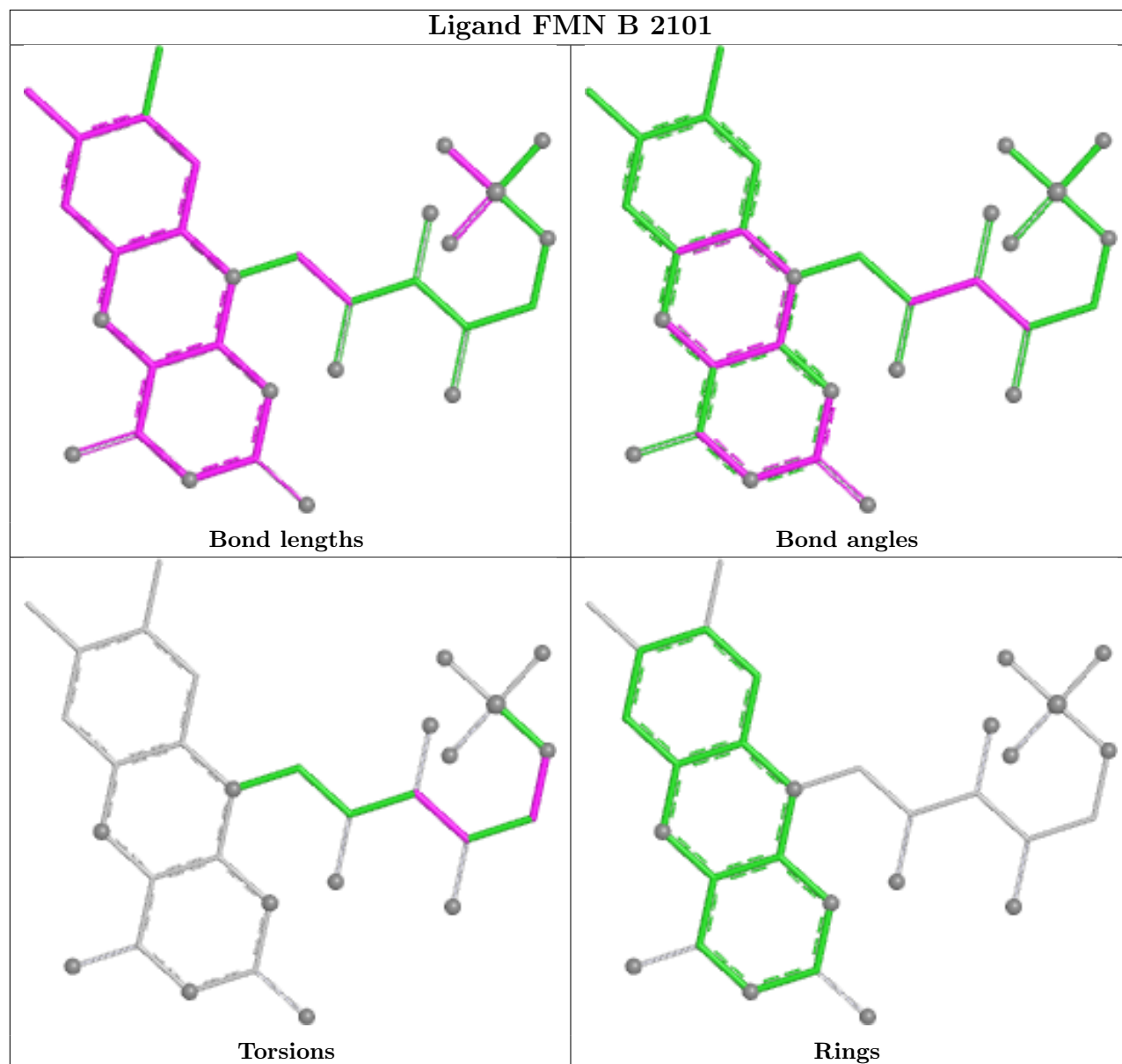
There are no ring outliers.

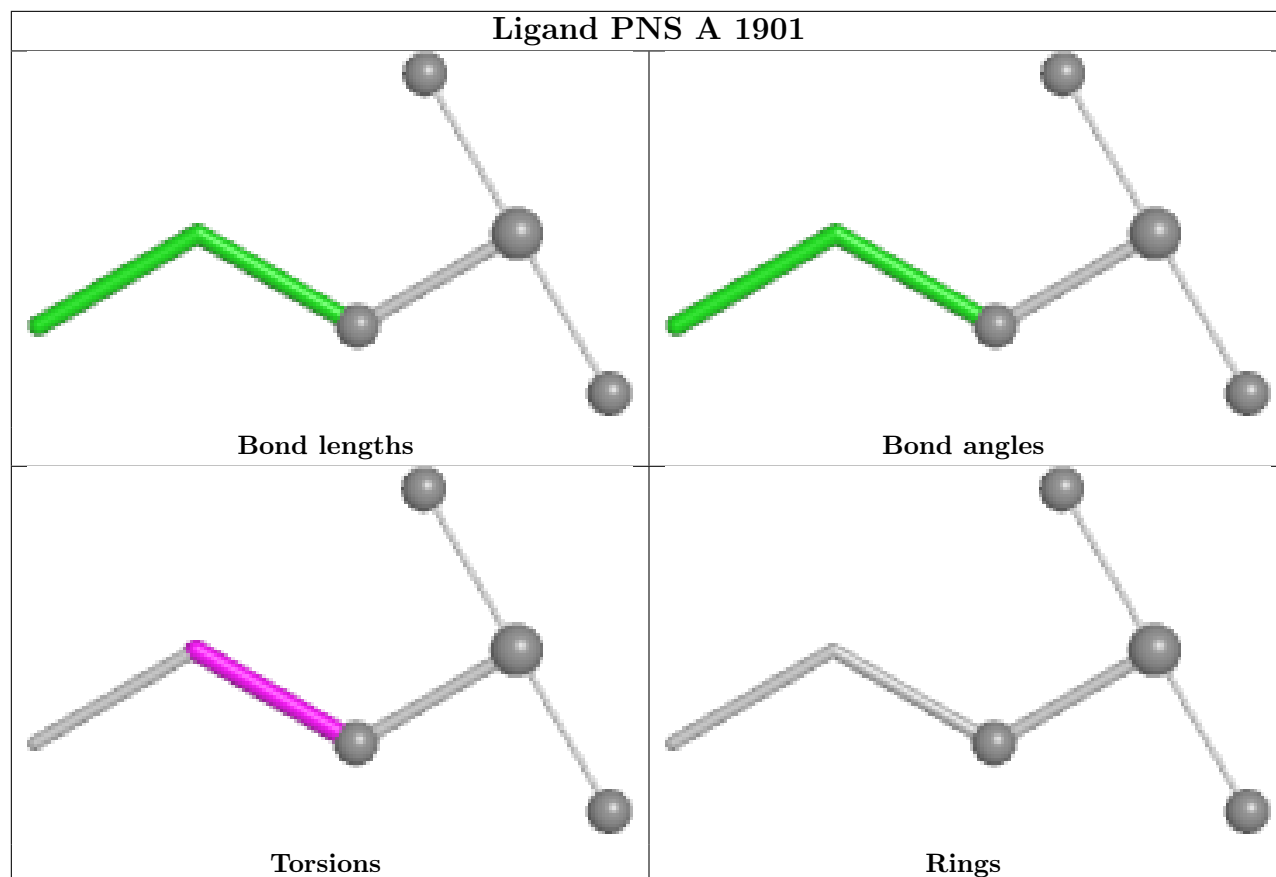
1 monomer is involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2101	FMN	32	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

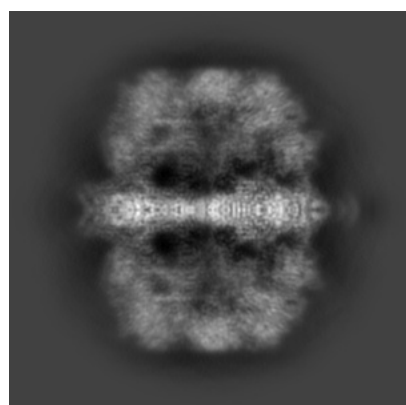
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20657. These allow visual inspection of the internal detail of the map and identification of artifacts.

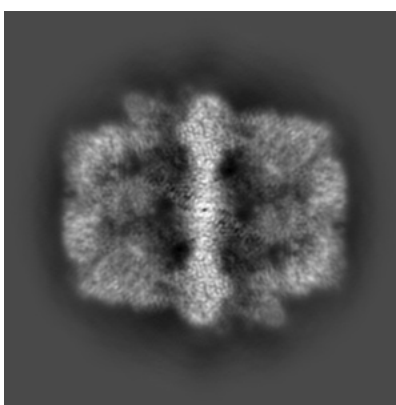
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

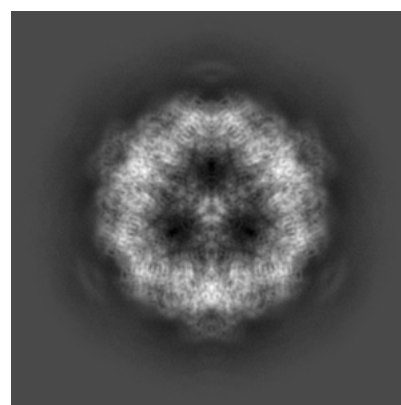
6.1.1 Primary map



X



Y

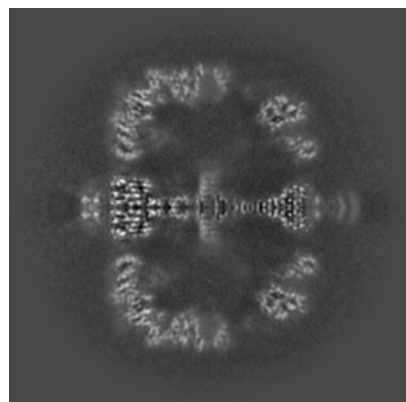


Z

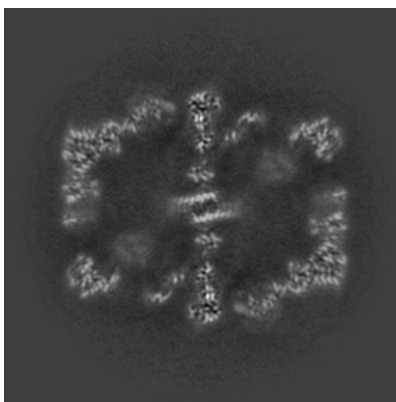
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

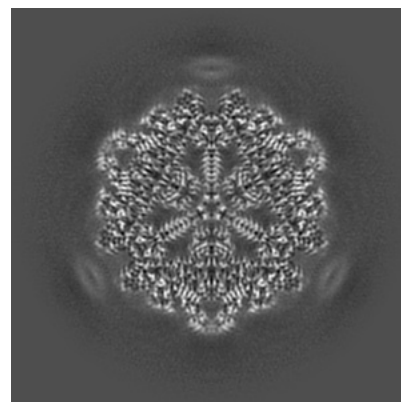
6.2.1 Primary map



X Index: 176



Y Index: 176

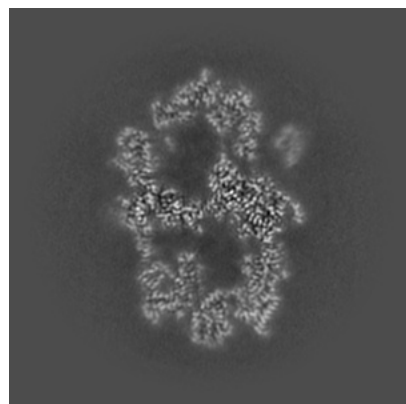


Z Index: 176

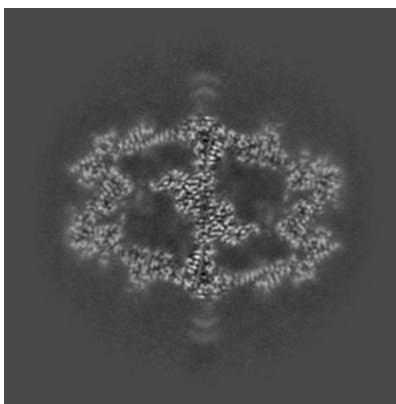
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

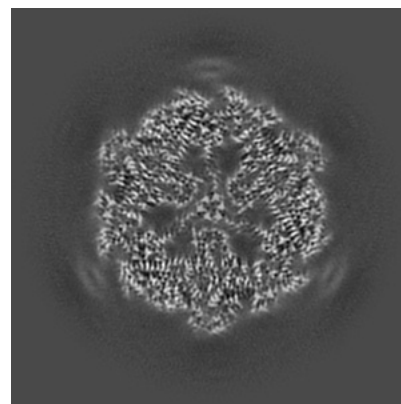
6.3.1 Primary map



X Index: 237



Y Index: 120

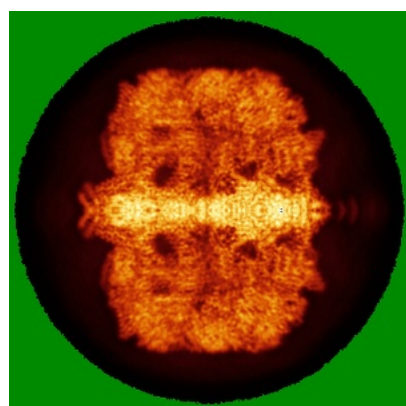


Z Index: 172

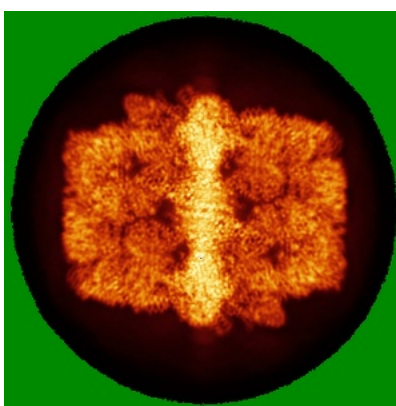
The images above show the largest variance slices of the map in three orthogonal directions.

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

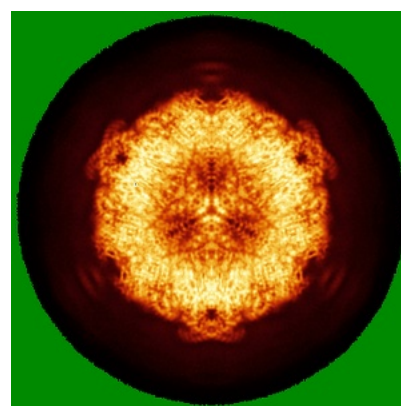
6.4.1 Primary map



X



Y

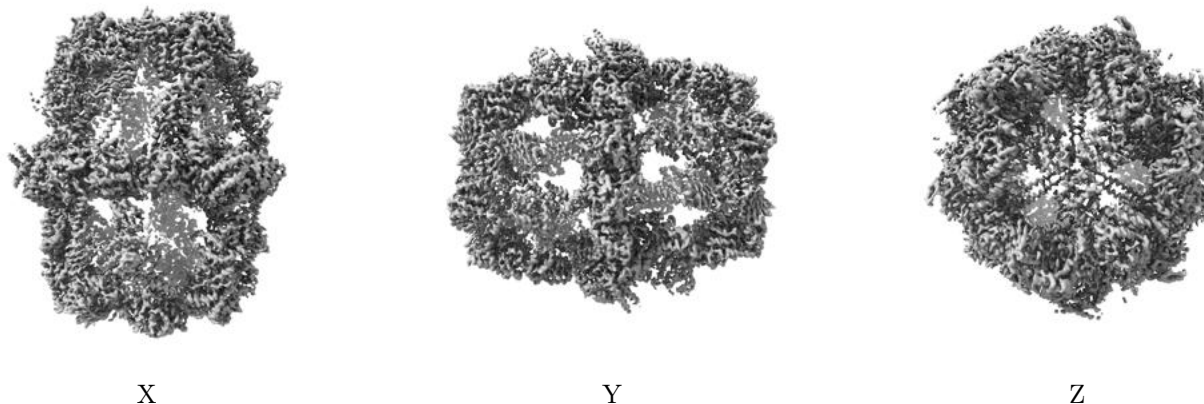


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.744. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

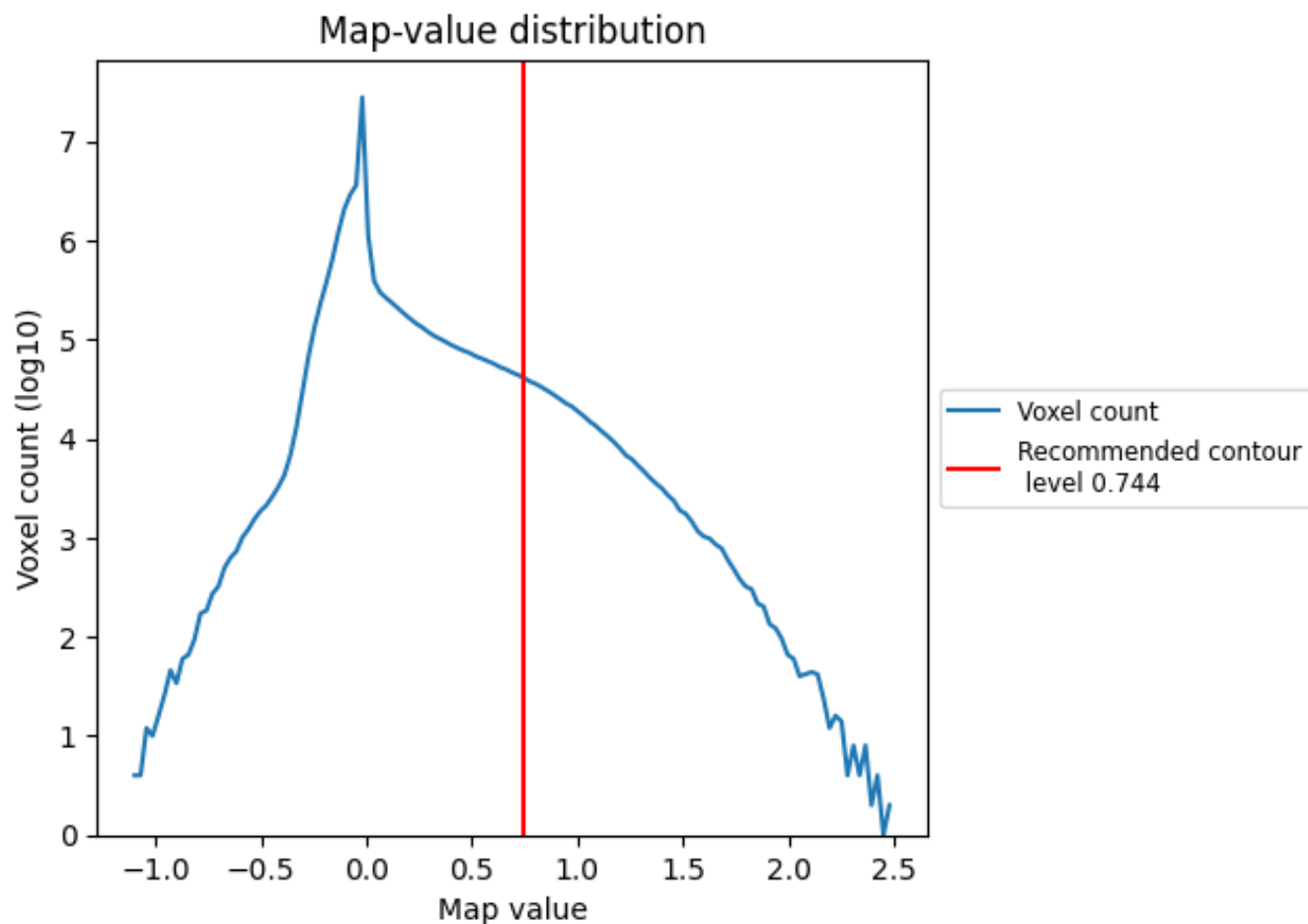
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

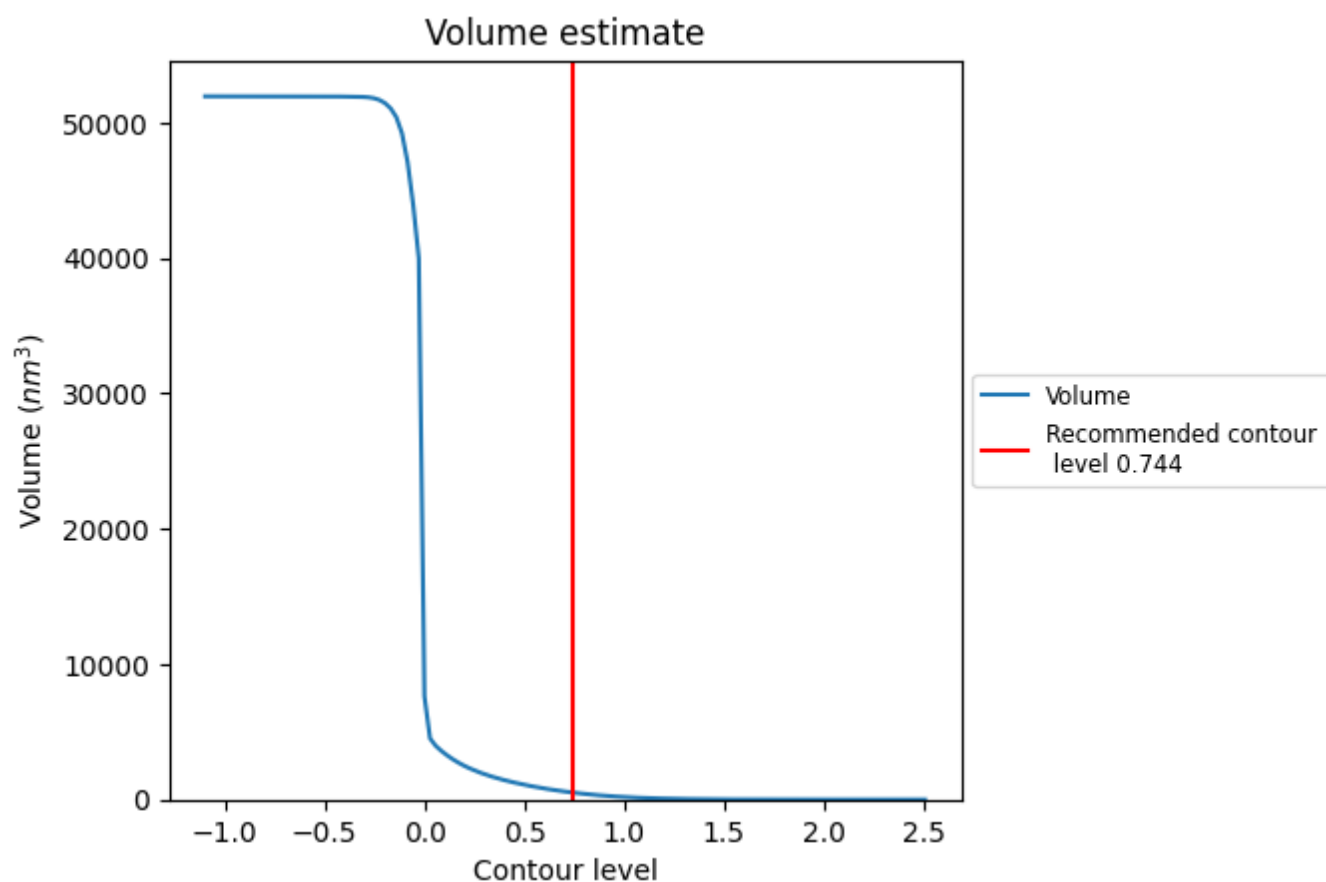
This section contains the results of statistical analysis of the map.

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.

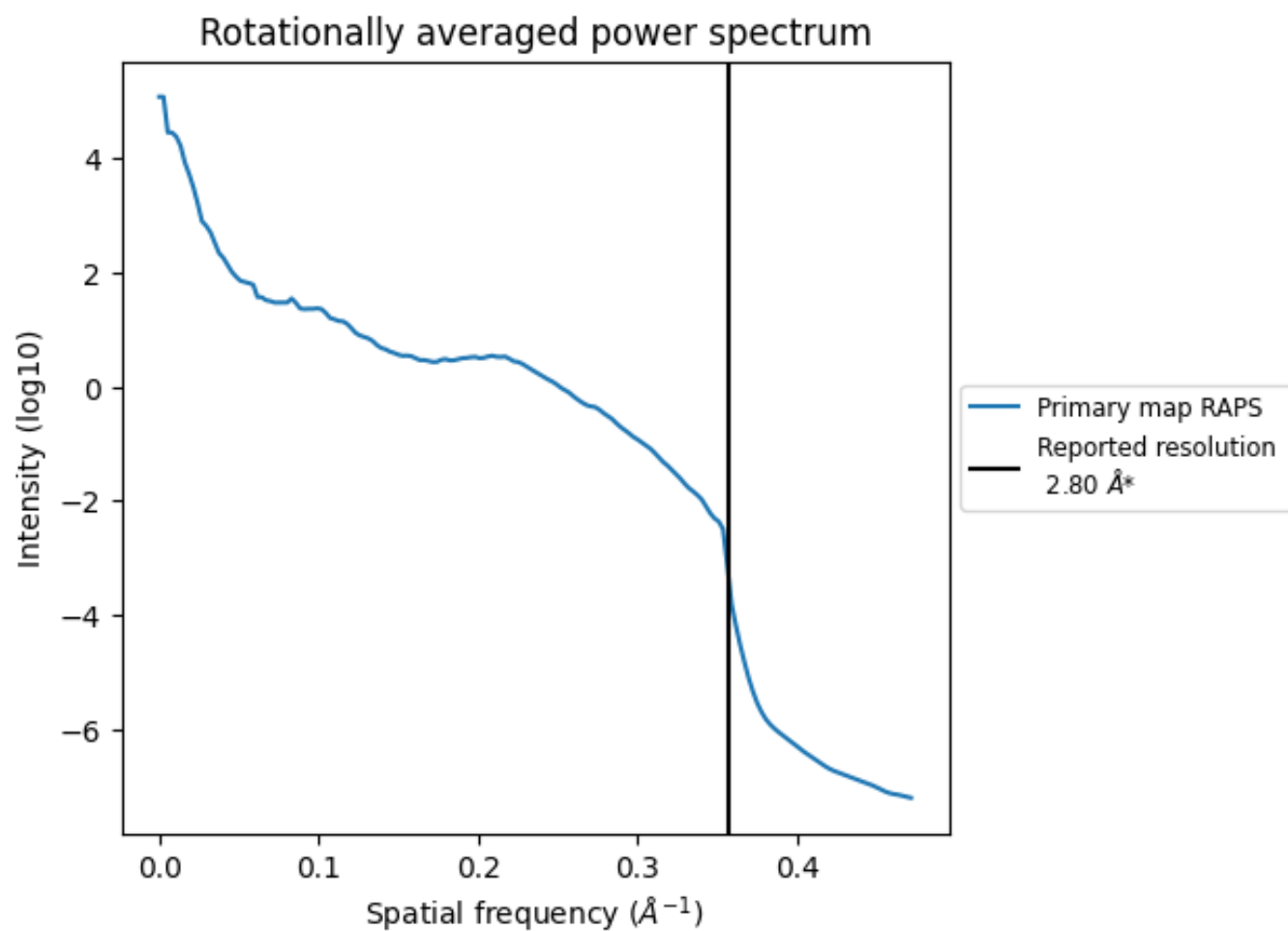
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 515 nm³; this corresponds to an approximate mass of 465 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 0.357 Å⁻¹

8 Fourier-Shell correlation ⓘ

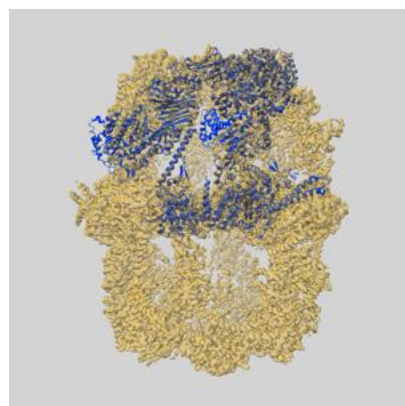
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

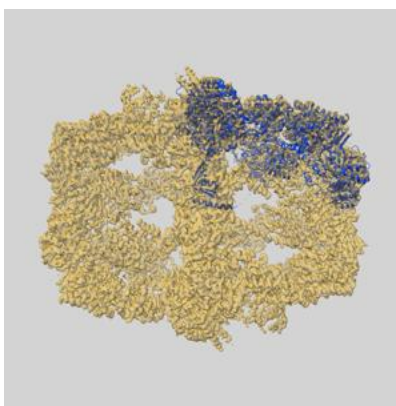
This section contains information regarding the fit between EMDB map EMD-20657 and PDB model 6U5V. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

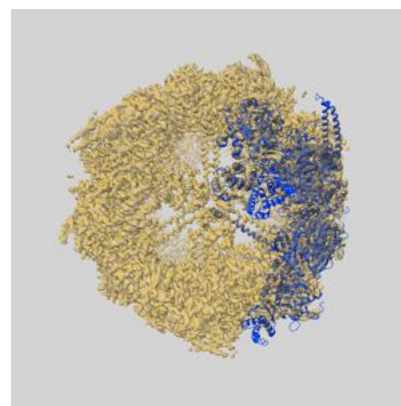
9.1.1 Map-model overlay [i](#)



X

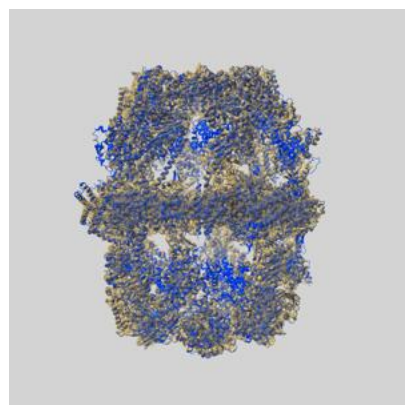


Y

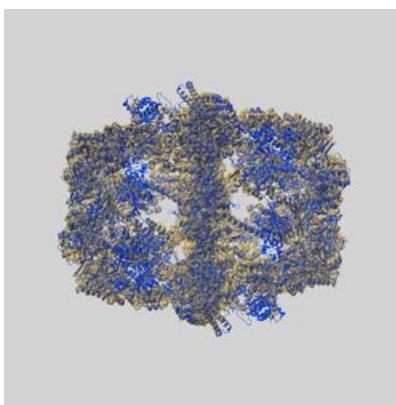


Z

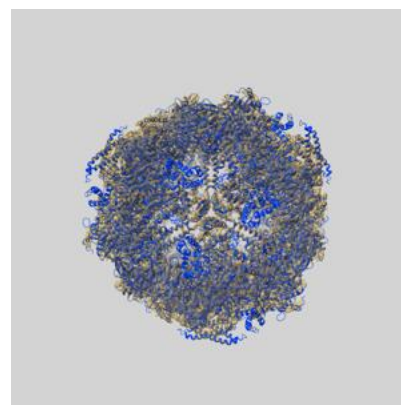
9.1.2 Map-model assembly overlay [i](#)



X



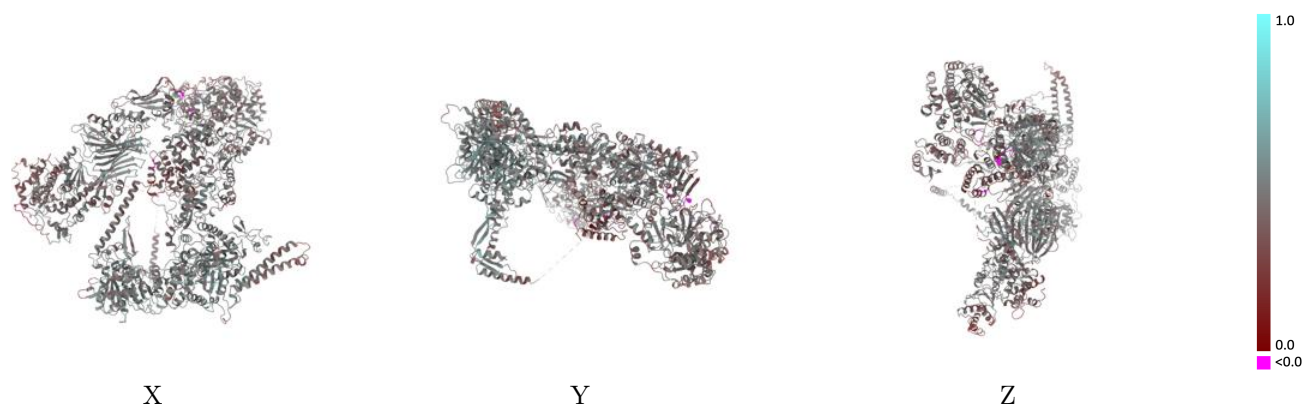
Y



Z

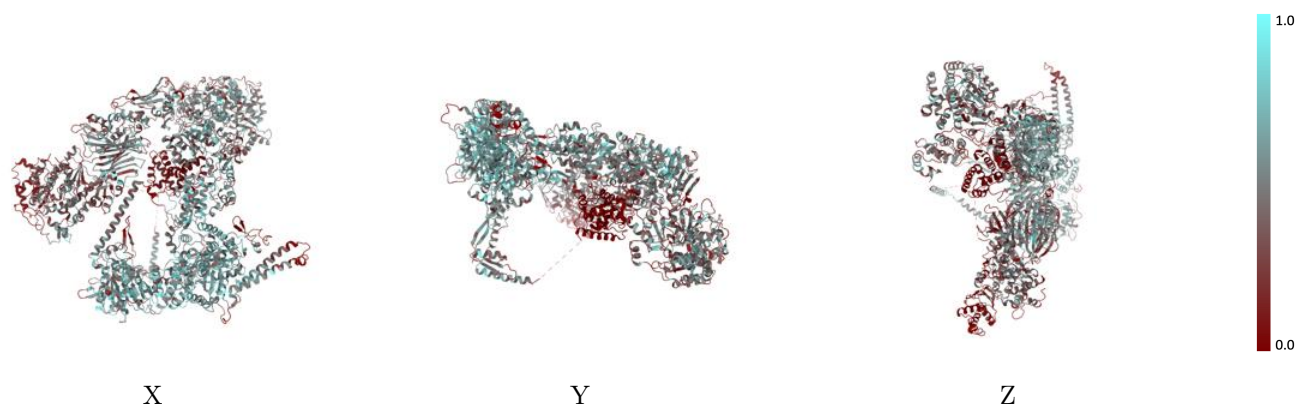
The images above show the 3D surface view of the map at the recommended contour level 0.744 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



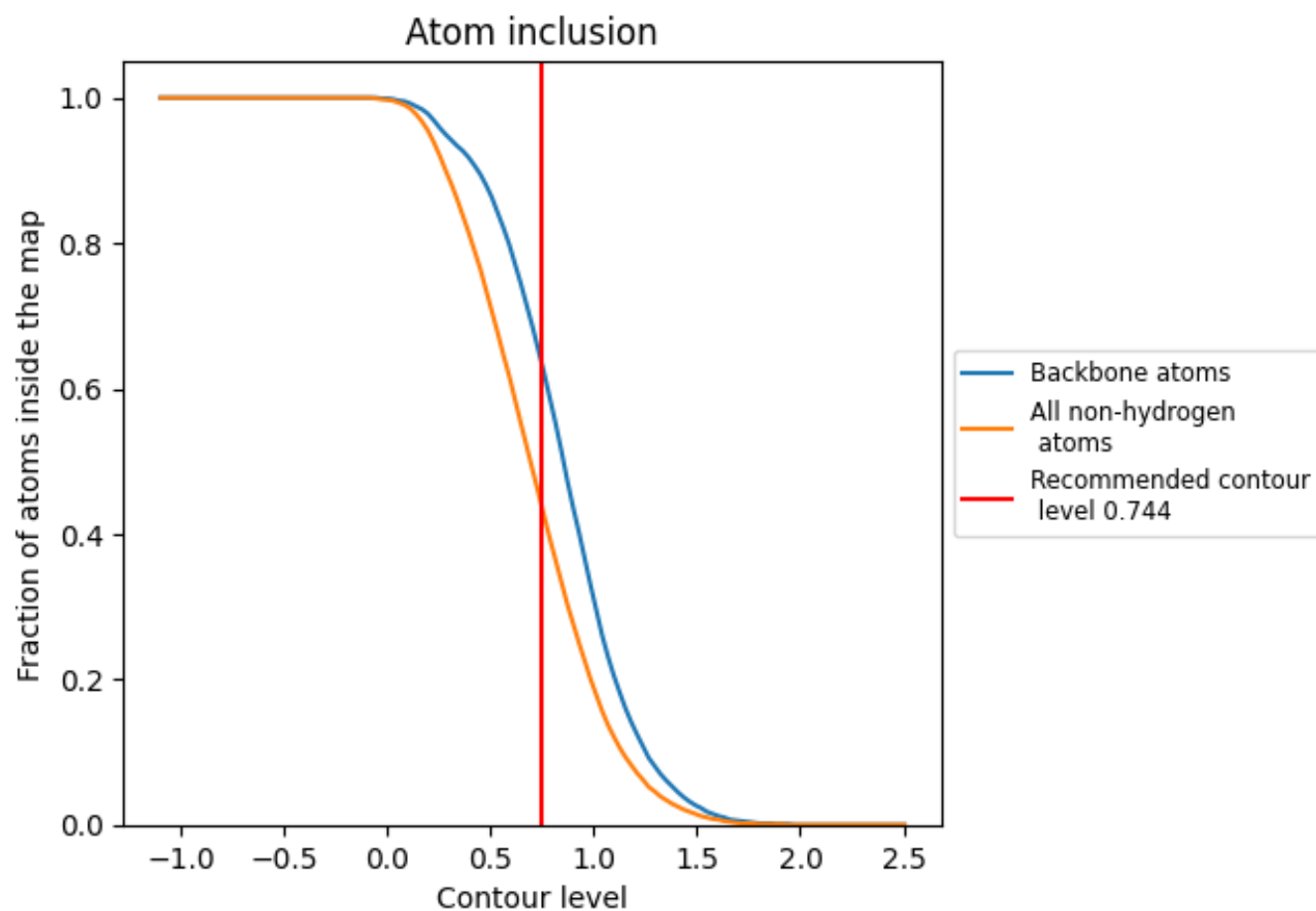
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.744).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 44% 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 (0.744) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4420	<div></div> 0.4530
A	<div></div> 0.4990	<div></div> 0.4750
B	<div></div> 0.4000	<div></div> 0.4360

