



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 10:46 AM UTC

PDB ID : 3JBR / pdb_00003jbr
EMDB ID : EMD-6475
Title : Cryo-EM structure of the rabbit voltage-gated calcium channel Cav1.1 complex at 4.2 angstrom
Authors : Wu, J.P.; Yan, Z.; Yan, N.
Deposited on : 2015-09-29
Resolution : 4.20 Å(reported)
Based on initial model : 1T0J

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

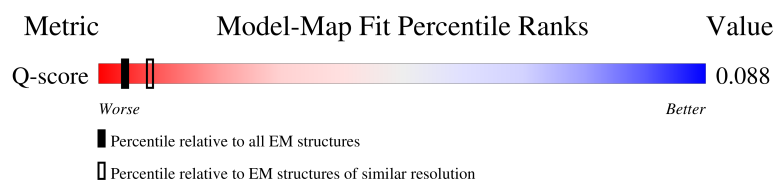
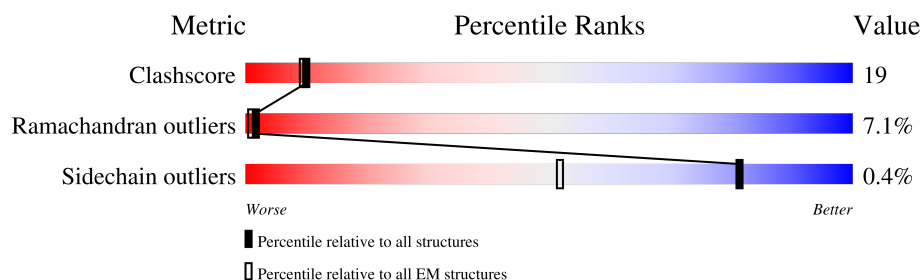
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	531 (5.60 - 6.60)

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	1873	
2	B	356	
3	E	222	
4	F	1106	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16467 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 Voltage-dependent L-type calcium channel subunit alpha-1S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1224	Total	C	N	O	S	0	0
			7601	4843	1330	1400	28		

- Molecule 2 is a protein called Voltage-dependent L-type calcium channel subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	281	Total	C	N	O	S	0	0
			2210	1405	385	411	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	14	GLY	-	expression tag	UNP Q8VGC3
B	15	HIS	-	expression tag	UNP Q8VGC3
B	16	MET	-	expression tag	UNP Q8VGC3
B	201	MET	-	linker	UNP Q8VGC3

- Molecule 3 is a protein called Voltage-dependent calcium channel gamma-1 subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	138	Total	C	N	O	0	0
			688	410	138	140		

- Molecule 4 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	872	Total	C	N	O	S	0	0
			5735	3570	1042	1108	15		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



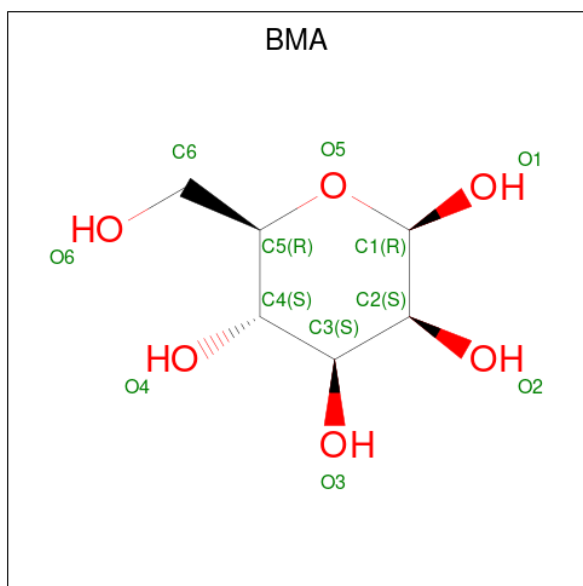
Mol	Chain	Residues	Atoms				AltConf
6	F	1	Total	C	N	O	0
			14	8	1	5	
6	F	1	Total	C	N	O	0
			14	8	1	5	
6	F	1	Total	C	N	O	0
			14	8	1	5	
6	F	1	Total	C	N	O	0
			14	8	1	5	
6	F	1	Total	C	N	O	0
			14	8	1	5	
6	F	1	Total	C	N	O	0
			14	8	1	5	
6	F	1	Total	C	N	O	0
			14	8	1	5	
6	F	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
6	F	1	Total	C	N	O	0
			14	8	1	5	
6	F	1	Total	C	N	O	0
			14	8	1	5	
6	F	1	Total	C	N	O	0
			14	8	1	5	
6	F	1	Total	C	N	O	0
			14	8	1	5	
6	F	1	Total	C	N	O	0
			14	8	1	5	

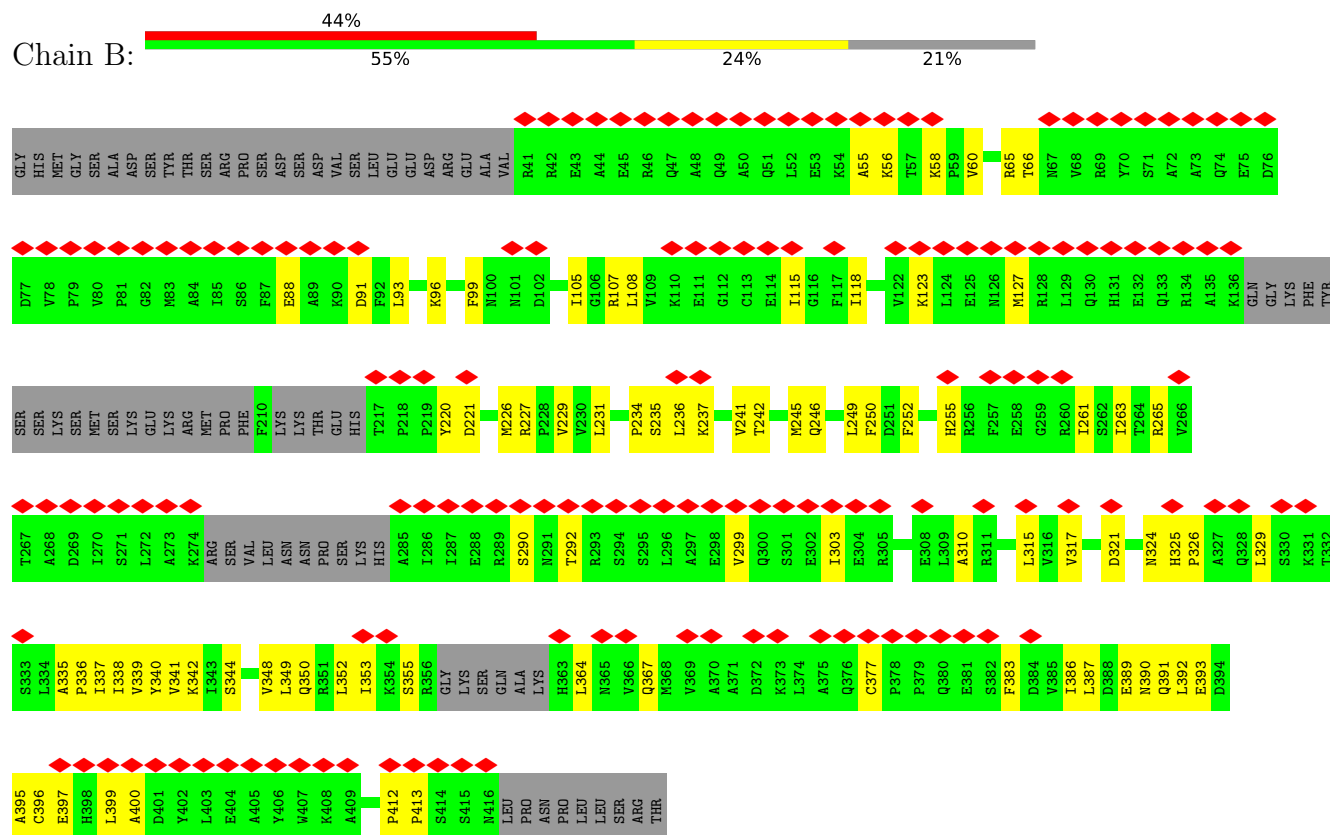
- Molecule 7 is beta-D-mannopyranose (CCD ID: BMA) (formula: C₆H₁₂O₆).



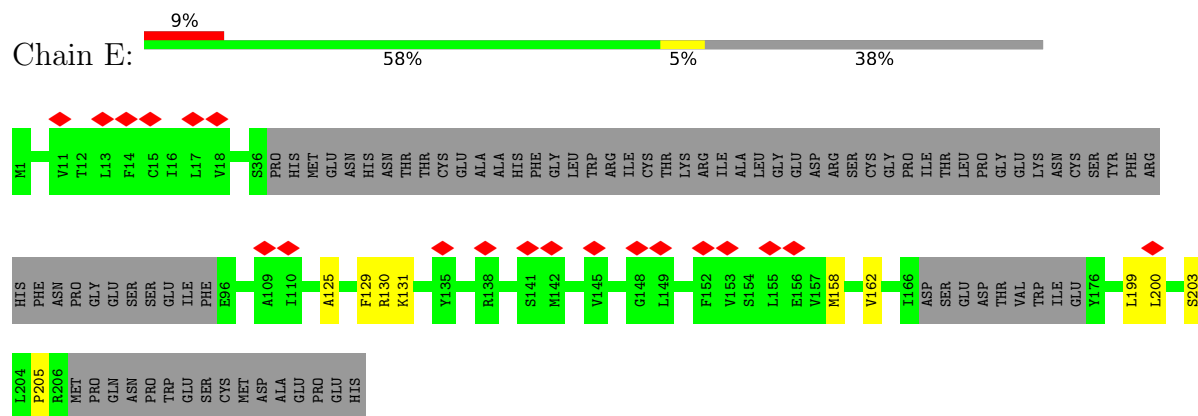
Mol	Chain	Residues	Atoms			AltConf
7	F	1	Total	C	O	0
			11	6	5	
7	F	1	Total	C	O	0
			11	6	5	



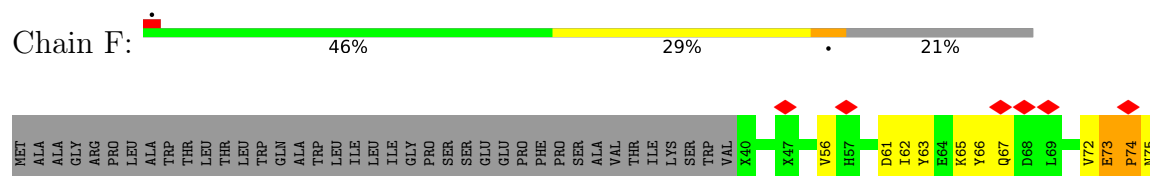
Chain B:



Chain E:



Chain F:





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	353372	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	each micrograph	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	2.0	Depositor
Maximum defocus (nm)	3.3	Depositor
Magnification	Not provided	
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.040	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	Depositor
Map size ($\text{\AA}$)	337.92, 337.92, 337.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.32, 1.32, 1.32	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, BMA

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	0.62	0/7080	0.93	28/9723 (0.3%)
2	B	0.31	0/2252	0.72	0/3051
3	E	0.53	0/685	0.89	0/950
4	F	0.63	1/4603 (0.0%)	1.02	27/6265 (0.4%)
All	All	0.58	1/14620 (0.0%)	0.93	55/19989 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	627	PRO	N-CD	5.11	1.54	1.47

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	987	PRO	N-CA-CB	12.13	110.96	102.35
4	F	509	CYS	CA-C-N	8.25	130.15	119.84
4	F	509	CYS	C-N-CA	8.25	130.15	119.84
4	F	1059	PRO	N-CA-CB	8.02	110.44	103.31
4	F	171	PRO	N-CA-CB	7.96	110.44	103.27
4	F	1044	PRO	N-CA-CB	7.79	110.28	103.27
1	A	521	PRO	N-CA-CB	7.69	110.15	103.31
1	A	904	PRO	N-CA-CB	7.43	110.26	103.20
1	A	1346	PRO	N-CA-CB	7.31	110.92	103.25
1	A	583	GLY	N-CA-C	-7.29	106.66	114.67
1	A	73	PRO	N-CA-CB	7.02	110.62	103.25
1	A	253	PRO	N-CA-CB	7.02	110.62	103.25
1	A	242	PRO	N-CA-CB	7.00	110.60	103.25
1	A	457	PRO	N-CA-CB	6.96	110.91	103.39
1	A	75	PRO	N-CA-CB	6.88	110.48	103.25
4	F	553	PRO	N-CA-CB	6.83	110.51	103.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	821	PRO	N-CA-CB	6.82	110.42	103.25
4	F	142	PRO	N-CA-CB	6.82	110.42	103.25
1	A	1103	PRO	N-CA-CB	6.81	110.49	103.00
4	F	1053	PRO	N-CA-CB	6.80	110.39	103.25
4	F	488	GLY	N-CA-C	-6.74	104.14	112.77
1	A	1340	PRO	N-CA-CB	6.73	110.31	103.25
4	F	1046	PRO	N-CA-CB	6.72	110.30	103.25
4	F	74	PRO	N-CA-CB	6.61	110.19	103.25
4	F	1028	PRO	N-CA-CB	6.60	110.26	103.00
1	A	582	GLY	N-CA-C	-6.59	106.69	115.32
1	A	268	PRO	N-CA-CB	6.55	110.13	103.25
1	A	1106	PRO	N-CA-CB	6.52	110.10	103.25
4	F	653	PRO	N-CA-CB	6.51	110.42	103.39
1	A	39	PRO	N-CA-CB	6.44	110.01	103.25
1	A	179	VAL	CA-C-N	6.38	126.36	119.78
1	A	179	VAL	C-N-CA	6.38	126.36	119.78
1	A	266	PRO	N-CA-CB	6.36	109.93	103.25
4	F	466	LEU	CA-C-N	6.35	126.27	119.85
4	F	466	LEU	C-N-CA	6.35	126.27	119.85
1	A	1268	PRO	N-CA-CB	6.29	110.19	103.39
1	A	179	VAL	N-CA-C	6.25	114.77	107.77
4	F	312	ALA	N-CA-C	-5.96	105.99	113.20
4	F	500	LYS	N-CA-C	5.96	118.20	108.55
1	A	321	GLY	N-CA-C	-5.91	105.64	112.73
1	A	1033	PRO	N-CA-CB	5.87	109.42	103.25
4	F	511	ASN	N-CA-C	-5.82	104.40	112.03
1	A	244	PRO	N-CA-CB	5.81	109.35	103.25
1	A	1180	ASP	CA-C-N	5.78	125.64	119.28
1	A	1180	ASP	C-N-CA	5.78	125.64	119.28
4	F	414	GLU	N-CA-C	5.74	118.92	110.59
4	F	485	LEU	N-CA-C	-5.71	106.27	113.18
4	F	419	GLY	N-CA-C	-5.70	105.82	115.34
4	F	119	PHE	CB-CA-C	-5.62	110.07	116.54
4	F	626	LEU	CA-C-N	-5.49	112.98	119.84
4	F	626	LEU	C-N-CA	-5.49	112.98	119.84
4	F	135	PRO	N-CA-CB	5.43	110.59	103.42
4	F	594	VAL	N-CA-C	5.38	114.95	108.06
1	A	1303	ASN	N-CA-C	-5.16	106.94	113.18
4	F	480	ASN	N-CA-C	5.08	116.02	108.60

There are no chirality outliers.

There are no planarity outliers.

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	7601	0	5496	211	0
2	B	2210	0	2208	69	0
3	E	688	0	336	4	0
4	F	5735	0	4413	291	0
5	A	1	0	0	0	0
6	F	210	0	195	11	0
7	F	22	0	20	2	0
All	All	16467	0	12668	564	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 19.

All (564) 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)
4:F:607:ARG:HA	4:F:627:PRO:HD3	1.21	1.14
4:F:607:ARG:HA	4:F:627:PRO:CD	1.84	1.07
4:F:626:LEU:O	4:F:628:THR:N	2.02	0.92
4:F:248:GLN:HE21	4:F:447:GLN:HG2	1.37	0.89
4:F:606:ASN:O	4:F:627:PRO:HD2	1.73	0.88
1:A:256:ILE:H	1:A:257:ASN:HA	1.39	0.87
1:A:1274:ILE:HA	1:A:1371:LEU:HD21	1.58	0.86
4:F:75:ASN:CB	4:F:630:SER:O	2.23	0.85
4:F:1008:VAL:HG12	4:F:1009:GLU:H	1.45	0.81
1:A:1373:ILE:HA	1:A:1376:PHE:HD2	1.43	0.81
4:F:601:TYR:HA	4:F:1017:ILE:HG21	1.64	0.79
4:F:238:TYR:HE1	4:F:243:ARG:HD2	1.48	0.77
1:A:367:MET:SD	2:B:352:LEU:HD23	2.24	0.77
4:F:523:VAL:HG12	4:F:524:LEU:HG	1.67	0.77
4:F:626:LEU:O	4:F:628:THR:HG22	1.85	0.75
4:F:169:HIS:HB3	4:F:216:LEU:HB2	1.69	0.75
4:F:570:ASN:HD21	4:F:594:VAL:HG21	1.52	0.75
1:A:983:MET:HG3	4:F:235:ILE:HD12	1.67	0.75
4:F:302:ASP:HB2	4:F:306:PHE:HE1	1.52	0.74
4:F:509:CYS:SG	4:F:561:LEU:N	2.60	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:MET:HE1	2:B:355:SER:CB	2.17	0.74
4:F:346:LEU:O	4:F:353:ARG:NH1	2.22	0.73
2:B:226:MET:H	2:B:310:ALA:HB1	1.53	0.72
1:A:1070:GLU:HA	1:A:1070:GLU:OE2	1.88	0.72
1:A:1067:THR:HA	1:A:1070:GLU:HB2	1.71	0.71
1:A:1233:ALA:HA	1:A:1236:ARG:HE	1.56	0.71
4:F:182:LEU:HD23	4:F:185:LEU:HD12	1.72	0.71
4:F:437:VAL:HA	4:F:469:PHE:HE2	1.55	0.71
4:F:73:GLU:O	4:F:632:TYR:N	2.24	0.71
2:B:99:PHE:HB2	2:B:105:ILE:HG13	1.72	0.70
4:F:607:ARG:CA	4:F:627:PRO:HD3	2.11	0.70
4:F:238:TYR:CE1	4:F:243:ARG:HD2	2.27	0.70
2:B:325:HIS:NE2	2:B:377:CYS:SG	2.65	0.70
4:F:461:VAL:HG22	4:F:484:GLN:HA	1.73	0.69
4:F:502:LEU:O	4:F:622:LEU:HB3	1.92	0.69
4:F:883:UNK:HA	4:F:892:UNK:HA	1.75	0.69
2:B:231:LEU:O	2:B:246:GLN:NE2	2.25	0.69
4:F:345:GLN:O	4:F:348:ASN:ND2	2.26	0.69
4:F:356:CYS:SG	4:F:357:ASN:N	2.61	0.69
1:A:201:LEU:O	1:A:205:PHE:N	2.25	0.69
4:F:184:GLU:HA	4:F:187:TRP:NE1	2.08	0.68
4:F:606:ASN:O	4:F:627:PRO:CD	2.42	0.68
4:F:343:PHE:HE1	4:F:384:VAL:HG11	1.56	0.68
4:F:1009:GLU:O	4:F:1011:LEU:N	2.26	0.68
1:A:367:MET:HE1	2:B:355:SER:HB2	1.75	0.68
4:F:573:LYS:HA	4:F:576:ILE:HD12	1.76	0.68
4:F:212:SER:OG	4:F:213:ALA:N	2.25	0.67
4:F:1004:ARG:NH1	4:F:1035:ILE:O	2.28	0.67
1:A:365:GLY:O	1:A:368:SER:OG	2.11	0.67
4:F:500:LYS:HG2	4:F:501:ARG:O	1.94	0.67
2:B:229:VAL:HG22	2:B:337:ILE:HB	1.76	0.67
2:B:389:GLU:HB2	2:B:395:ALA:HB2	1.77	0.67
1:A:165:ARG:HB3	1:A:579:GLN:HE21	1.60	0.66
4:F:520:ASN:ND2	4:F:560:THR:O	2.29	0.66
4:F:502:LEU:HD12	4:F:512:GLY:HA3	1.78	0.66
4:F:500:LYS:HZ2	4:F:502:LEU:HD13	1.61	0.66
2:B:123:LYS:HG3	2:B:127:MET:HE2	1.76	0.65
4:F:516:ALA:HB3	4:F:1007:HIS:HE1	1.61	0.65
4:F:263:SER:OG	4:F:265:SER:OG	2.14	0.65
4:F:184:GLU:HA	4:F:187:TRP:HE1	1.60	0.65
1:A:1373:ILE:HA	1:A:1376:PHE:CD2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:210:PHE:HB3	4:F:217:ALA:HB3	1.79	0.65
4:F:343:PHE:CE1	4:F:384:VAL:HG11	2.31	0.64
4:F:516:ALA:HB3	4:F:1007:HIS:CE1	2.32	0.64
4:F:1036:GLN:O	4:F:1038:GLU:N	2.30	0.64
4:F:225:TRP:NE1	4:F:236:ASP:OD1	2.31	0.64
4:F:335:TYR:OH	4:F:369:GLU:O	2.05	0.64
1:A:309:TRP:HA	1:A:311:TRP:CD1	2.32	0.64
1:A:644:LEU:O	1:A:648:GLY:N	2.28	0.64
4:F:242:ARG:HH11	4:F:425:THR:HG23	1.61	0.64
4:F:257:LEU:HB3	4:F:360:ILE:HG22	1.79	0.64
4:F:297:ASN:C	4:F:299:ASN:H	2.04	0.64
4:F:680:UNK:O	4:F:682:UNK:N	2.31	0.63
1:A:1034:VAL:O	1:A:1036:ASN:N	2.31	0.63
1:A:165:ARG:HB3	1:A:579:GLN:NE2	2.14	0.63
1:A:90:GLU:HB3	1:A:171:ARG:HH12	1.63	0.62
1:A:1172:PHE:O	1:A:1174:ALA:N	2.33	0.62
4:F:999:CYS:HB2	4:F:1019:ILE:H	1.63	0.62
4:F:585:SER:HB2	4:F:611:TRP:HH2	1.63	0.62
4:F:449:THR:HG22	4:F:463:THR:H	1.64	0.62
4:F:98:ALA:HB1	4:F:199:ARG:HE	1.63	0.62
1:A:211:ALA:O	1:A:215:LEU:N	2.33	0.62
1:A:369:TRP:HZ3	2:B:392:LEU:HA	1.65	0.62
4:F:196:LYS:HD3	4:F:219:TYR:HB2	1.81	0.62
4:F:132:ASP:N	4:F:140:SER:O	2.33	0.61
2:B:234:PRO:HD2	2:B:242:THR:HG23	1.82	0.61
2:B:237:LYS:H	2:B:324:ASN:HD21	1.46	0.61
2:B:341:VAL:HG22	2:B:387:LEU:HD12	1.82	0.61
4:F:95:ARG:NH2	4:F:204:SER:O	2.32	0.61
4:F:311:GLN:HA	4:F:316:ASN:HD22	1.65	0.61
4:F:606:ASN:ND2	6:F:1211:NAG:O7	2.32	0.61
1:A:1370:PHE:HA	1:A:1373:ILE:HD12	1.82	0.61
1:A:1006:SER:O	1:A:1009:THR:OG1	2.16	0.61
3:E:200:LEU:O	3:E:203:SER:OG	2.16	0.61
2:B:56:LYS:HA	2:B:115:ILE:HG13	1.83	0.60
2:B:60:VAL:HA	2:B:96:LYS:HD3	1.83	0.60
4:F:607:ARG:HA	4:F:627:PRO:HD2	1.79	0.60
1:A:309:TRP:O	1:A:312:ILE:HG22	2.01	0.60
4:F:379:ASN:HD21	4:F:382:LYS:HA	1.66	0.60
4:F:1005:ILE:HG22	4:F:1007:HIS:H	1.65	0.60
4:F:500:LYS:HE3	4:F:502:LEU:HB2	1.84	0.60
1:A:645:PHE:O	1:A:649:ASN:N	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:ARG:O	1:A:586:ASP:N	2.31	0.60
4:F:911:UNK:O	4:F:915:UNK:N	2.35	0.60
2:B:290:SER:HG	2:B:292:THR:HG1	1.42	0.60
1:A:288:CYS:HA	1:A:294:TRP:HB3	1.83	0.60
4:F:188:THR:HG23	4:F:189:SER:H	1.67	0.60
1:A:131:PHE:CD1	1:A:164:LEU:HB3	2.37	0.59
4:F:263:SER:O	4:F:265:SER:N	2.36	0.59
1:A:995:PHE:HB3	1:A:1006:SER:HB2	1.85	0.59
4:F:402:GLN:NE2	4:F:1063:PHE:O	2.36	0.59
1:A:602:GLN:O	1:A:605:ILE:HG13	2.02	0.59
1:A:131:PHE:HA	1:A:164:LEU:HD22	1.85	0.59
1:A:973:TYR:HE1	4:F:235:ILE:HG21	1.67	0.59
2:B:252:PHE:HA	2:B:255:HIS:CD2	2.37	0.59
4:F:570:ASN:O	4:F:572:ILE:N	2.33	0.59
2:B:231:LEU:HA	2:B:339:VAL:HB	1.83	0.59
4:F:242:ARG:NH1	4:F:421:ILE:O	2.36	0.58
4:F:298:SER:N	4:F:332:ILE:O	2.37	0.58
1:A:944:CYS:O	1:A:948:GLN:HG2	2.04	0.58
1:A:1070:GLU:O	1:A:1074:THR:N	2.35	0.58
4:F:1008:VAL:HG11	4:F:1013:ASN:HD22	1.67	0.58
1:A:1237:LEU:O	1:A:1241:MET:HG2	2.04	0.58
2:B:390:ASN:OD1	2:B:391:GLN:N	2.35	0.58
4:F:463:THR:HG22	4:F:482:LYS:HA	1.85	0.58
2:B:290:SER:OG	2:B:292:THR:OG1	2.19	0.58
4:F:256:MET:HG3	4:F:285:LEU:HD11	1.84	0.58
1:A:1496:UNK:O	1:A:1500:UNK:N	2.36	0.57
4:F:372:GLN:HA	4:F:375:PHE:CD2	2.39	0.57
4:F:359:ILE:HB	4:F:385:ARG:HB2	1.86	0.57
4:F:210:PHE:CD2	4:F:479:THR:HG22	2.40	0.57
1:A:592:VAL:O	1:A:594:ARG:N	2.36	0.57
4:F:417:SER:OG	4:F:418:ILE:N	2.33	0.57
4:F:470:ASN:HD22	4:F:473:GLY:H	1.53	0.57
4:F:614:VAL:HG12	4:F:616:GLY:H	1.70	0.57
1:A:1336:LYS:C	1:A:1351:THR:HA	2.30	0.57
2:B:88:GLU:N	2:B:91:ASP:OD2	2.37	0.57
4:F:569:GLU:OE2	4:F:571:ASP:N	2.36	0.57
2:B:265:ARG:NH2	2:B:321:ASP:OD2	2.38	0.57
6:F:1209:NAG:HO4	7:F:1217:BMA:HO2	1.51	0.57
1:A:363:LEU:HA	2:B:348:VAL:HG13	1.87	0.56
1:A:592:VAL:C	1:A:594:ARG:H	2.12	0.56
4:F:497:GLU:N	4:F:497:GLU:OE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:SER:O	1:A:326:LEU:HG	2.04	0.56
1:A:1067:THR:O	1:A:1071:GLN:N	2.34	0.56
2:B:241:VAL:O	2:B:245:MET:HG3	2.05	0.56
2:B:341:VAL:HA	2:B:387:LEU:HB2	1.87	0.56
4:F:131:ASP:HA	4:F:141:GLU:HA	1.86	0.56
4:F:662:UNK:O	4:F:666:UNK:N	2.38	0.56
6:F:1203:NAG:O4	6:F:1204:NAG:O7	2.19	0.56
2:B:299:VAL:O	2:B:303:ILE:HG12	2.04	0.56
4:F:254:LYS:HB3	4:F:256:MET:HE2	1.86	0.56
4:F:206:LEU:O	4:F:220:TYR:OH	2.24	0.56
4:F:322:ASP:HA	4:F:325:ASN:ND2	2.20	0.56
4:F:589:THR:HG21	4:F:610:THR:HA	1.88	0.56
4:F:1004:ARG:HG2	4:F:1014:THR:HG22	1.87	0.56
1:A:216:GLU:O	1:A:220:GLY:N	2.35	0.56
1:A:233:ILE:O	1:A:235:ALA:N	2.38	0.56
2:B:261:ILE:HA	2:B:315:LEU:HB2	1.88	0.56
1:A:1043:ILE:HG22	1:A:1047:ILE:HD11	1.89	0.55
4:F:210:PHE:HE1	4:F:212:SER:HB2	1.71	0.55
1:A:1064:VAL:O	1:A:1067:THR:OG1	2.15	0.55
1:A:975:TYR:HE1	1:A:983:MET:HB3	1.71	0.55
4:F:243:ARG:HH12	4:F:455:ALA:H	1.55	0.55
2:B:350:GLN:HA	2:B:364:LEU:HD11	1.89	0.55
4:F:307:GLN:O	4:F:308:HIS:ND1	2.40	0.55
4:F:63:TYR:O	4:F:67:GLN:N	2.40	0.55
4:F:309:LEU:C	4:F:311:GLN:H	2.13	0.55
2:B:353:ILE:HD13	2:B:367:GLN:OE1	2.07	0.55
1:A:34:LEU:O	1:A:36:LEU:N	2.40	0.55
4:F:264:GLY:N	4:F:331:GLY:O	2.36	0.55
4:F:336:LYS:HA	4:F:339:PHE:CD2	2.41	0.55
1:A:218:PHE:O	1:A:222:MET:N	2.40	0.54
1:A:1124:MET:HA	1:A:1127:LEU:HD12	1.88	0.54
4:F:308:HIS:HB2	4:F:309:LEU:HG	1.89	0.54
1:A:1009:THR:O	1:A:1012:THR:OG1	2.22	0.54
2:B:387:LEU:HD21	2:B:399:LEU:HB2	1.89	0.54
4:F:298:SER:HB2	4:F:332:ILE:HG13	1.90	0.54
1:A:268:PRO:C	1:A:271:GLY:H	2.15	0.54
4:F:375:PHE:O	4:F:379:ASN:N	2.32	0.54
1:A:1158:THR:HG21	1:A:1197:VAL:HG21	1.90	0.54
1:A:1239:ARG:HG3	1:A:1242:ARG:CZ	2.38	0.54
4:F:259:LEU:HB3	4:F:296:PHE:HE1	1.72	0.54
4:F:602:ILE:HG22	4:F:603:ASP:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1055:PHE:O	1:A:1059:ILE:HG13	2.08	0.54
2:B:252:PHE:CZ	2:B:396:CYS:HB3	2.43	0.54
1:A:322:SER:O	1:A:325:ILE:HG13	2.08	0.54
4:F:73:GLU:C	4:F:632:TYR:H	2.16	0.54
1:A:656:PHE:CE2	1:A:1057:MET:HG3	2.44	0.53
4:F:182:LEU:HA	4:F:185:LEU:HD12	1.89	0.53
4:F:248:GLN:NE2	4:F:447:GLN:HG2	2.17	0.53
4:F:505:ARG:N	4:F:509:CYS:O	2.29	0.53
4:F:62:ILE:O	4:F:66:TYR:N	2.39	0.53
4:F:1008:VAL:HG12	4:F:1009:GLU:N	2.20	0.53
4:F:282:LEU:C	4:F:317:LYS:HZ2	2.17	0.53
4:F:530:GLN:HB2	4:F:531:PRO:HD3	1.91	0.53
4:F:557:GLU:HB3	4:F:558:PRO:HA	1.90	0.53
2:B:235:SER:OG	2:B:236:LEU:N	2.41	0.53
4:F:414:GLU:O	4:F:423:ILE:HG21	2.08	0.53
1:A:1120:PHE:HA	1:A:1123:LEU:HD12	1.90	0.53
1:A:1146:MET:HA	1:A:1149:ILE:HD12	1.90	0.53
1:A:1186:ASP:HA	1:A:1189:ILE:HD12	1.90	0.53
4:F:76:ASN:O	4:F:78:ARG:N	2.42	0.53
1:A:1056:MET:HA	1:A:1059:ILE:HD12	1.92	0.52
4:F:614:VAL:HB	4:F:618:ASP:O	2.08	0.52
4:F:163:TYR:O	4:F:221:PRO:HD3	2.09	0.52
4:F:256:MET:HB2	4:F:291:VAL:HG22	1.90	0.52
4:F:615:ASN:ND2	6:F:1203:NAG:O5	2.42	0.52
1:A:186:LEU:O	1:A:189:ILE:HG22	2.09	0.52
4:F:411:TYR:CE2	4:F:427:GLU:HG3	2.44	0.52
4:F:500:LYS:HE2	4:F:624:LEU:HD12	1.91	0.52
4:F:503:THR:OG1	4:F:511:ASN:OD1	2.15	0.52
6:F:1203:NAG:O6	6:F:1204:NAG:O7	2.27	0.52
1:A:186:LEU:HA	1:A:189:ILE:HG22	1.90	0.52
1:A:298:LEU:HA	1:A:314:PHE:HE2	1.74	0.52
1:A:581:PHE:HB2	1:A:597:PHE:CD2	2.45	0.52
1:A:997:PHE:HE1	1:A:1006:SER:HB3	1.74	0.52
4:F:595:LYS:HA	4:F:604:LYS:HA	1.90	0.52
1:A:993:ASN:O	1:A:995:PHE:N	2.36	0.52
1:A:1187:PHE:CE2	1:A:1191:ILE:HD11	2.43	0.52
4:F:188:THR:HG23	4:F:189:SER:N	2.24	0.52
4:F:427:GLU:HB3	4:F:431:VAL:HG23	1.91	0.52
1:A:661:VAL:O	1:A:664:LEU:HG	2.09	0.52
4:F:192:ASP:O	4:F:196:LYS:HG2	2.09	0.52
4:F:293:VAL:HG23	4:F:320:LEU:HD21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:391:VAL:HG12	4:F:415:ILE:HB	1.91	0.52
1:A:1014:GLU:OE2	1:A:1324:ALA:HA	2.09	0.52
1:A:1334:TYR:CE1	1:A:1352:CYS:HA	2.44	0.52
1:A:1383:ASN:O	1:A:1387:LEU:N	2.25	0.52
4:F:393:GLN:OE1	4:F:393:GLN:N	2.43	0.52
1:A:1002:SER:O	1:A:1005:MET:HB3	2.10	0.52
4:F:178:SER:HB3	4:F:181:VAL:HG23	1.90	0.52
4:F:191:LEU:HD11	4:F:195:PHE:HE2	1.74	0.52
1:A:287:GLN:O	1:A:290:THR:OG1	2.17	0.52
1:A:962:LYS:O	1:A:964:THR:N	2.43	0.52
4:F:248:GLN:HE22	4:F:448:TRP:C	2.16	0.52
6:F:1209:NAG:O3	7:F:1217:BMA:O5	2.27	0.52
4:F:403:TRP:O	4:F:407:GLU:HB2	2.10	0.51
1:A:954:PHE:O	1:A:956:SER:N	2.43	0.51
1:A:1369:ALA:O	1:A:1373:ILE:HG13	2.09	0.51
2:B:227:ARG:NE	2:B:335:ALA:O	2.24	0.51
1:A:581:PHE:O	1:A:585:TYR:N	2.31	0.51
1:A:651:ILE:HA	1:A:654:ASN:ND2	2.25	0.51
1:A:1131:ASN:O	1:A:1135:LEU:HG	2.10	0.51
2:B:231:LEU:HD23	2:B:249:LEU:HD13	1.93	0.51
4:F:444:LYS:HD3	4:F:469:PHE:CE1	2.45	0.51
1:A:1019:LEU:HG	1:A:1045:PHE:CZ	2.46	0.51
2:B:387:LEU:HD11	2:B:399:LEU:HD22	1.93	0.51
4:F:208:GLN:HA	4:F:481:LEU:HD23	1.92	0.51
1:A:244:PRO:HA	1:A:304:ALA:HB2	1.92	0.51
4:F:167:ALA:HB3	4:F:218:ARG:HB2	1.92	0.51
4:F:192:ASP:HB3	4:F:196:LYS:HE3	1.91	0.51
4:F:242:ARG:HE	4:F:425:THR:CG2	2.24	0.51
4:F:886:UNK:N	4:F:889:UNK:O	2.43	0.51
2:B:263:ILE:HG12	2:B:317:VAL:HB	1.93	0.51
2:B:342:LYS:HE3	2:B:344:SER:HB2	1.93	0.51
4:F:352:SER:O	4:F:354:ALA:N	2.38	0.51
4:F:570:ASN:HD22	4:F:573:LYS:HE3	1.76	0.51
4:F:243:ARG:NH1	4:F:455:ALA:H	2.10	0.50
4:F:266:VAL:HB	4:F:270:THR:HG23	1.92	0.50
1:A:1165:MET:HE2	1:A:1187:PHE:HB2	1.93	0.50
2:B:348:VAL:O	2:B:352:LEU:HG	2.11	0.50
4:F:320:LEU:O	4:F:324:VAL:HG23	2.12	0.50
1:A:124:VAL:HA	1:A:127:PHE:HD2	1.76	0.50
1:A:958:ASN:HD22	1:A:989:GLN:H	1.59	0.50
1:A:128:ILE:O	1:A:131:PHE:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:TRP:HE1	2:B:245:MET:HG2	1.77	0.50
2:B:229:VAL:HB	2:B:317:VAL:HG22	1.94	0.49
2:B:252:PHE:HE2	2:B:400:ALA:HB2	1.78	0.49
4:F:99:LEU:HB3	4:F:466:LEU:CD2	2.42	0.49
4:F:576:ILE:HD13	4:F:609:TYR:OH	2.12	0.49
4:F:580:MET:HG2	4:F:611:TRP:CZ3	2.47	0.49
1:A:1020:LEU:O	1:A:1024:ILE:HG12	2.12	0.49
2:B:66:THR:HG22	2:B:220:TYR:HE1	1.76	0.49
4:F:274:ILE:HD11	4:F:363:PHE:HB2	1.92	0.49
4:F:312:ALA:O	4:F:314:VAL:N	2.43	0.49
1:A:61:ILE:O	1:A:64:ASN:HB2	2.13	0.49
2:B:93:LEU:HB3	2:B:118:ILE:HD13	1.93	0.49
4:F:313:ASN:O	4:F:317:LYS:HB3	2.12	0.49
4:F:505:ARG:HG3	4:F:619:TYR:HE1	1.77	0.49
1:A:663:ASN:HD22	1:A:1061:VAL:HG12	1.78	0.49
1:A:1048:TYR:CZ	1:A:1052:ILE:HD11	2.48	0.49
4:F:297:ASN:C	4:F:299:ASN:N	2.70	0.49
1:A:942:PHE:HA	1:A:945:ILE:HD12	1.95	0.49
1:A:1163:LEU:O	1:A:1167:LEU:HG	2.13	0.49
1:A:1234:PHE:O	1:A:1237:LEU:HB3	2.13	0.49
4:F:281:MET:O	4:F:285:LEU:N	2.45	0.49
4:F:99:LEU:HB3	4:F:466:LEU:HD23	1.95	0.49
4:F:61:ASP:O	4:F:65:LYS:N	2.42	0.49
4:F:1006:PHE:CD1	4:F:1012:MET:HG3	2.48	0.49
1:A:964:THR:HA	1:A:1030:ASP:O	2.13	0.49
1:A:1043:ILE:O	1:A:1047:ILE:HG13	2.12	0.49
4:F:99:LEU:HD21	4:F:481:LEU:HG	1.94	0.49
4:F:594:VAL:HG22	4:F:595:LYS:O	2.12	0.49
1:A:89:LEU:HG	1:A:93:PHE:CE2	2.48	0.48
1:A:647:CYS:O	1:A:650:TYR:HB3	2.13	0.48
1:A:1015:GLY:HA3	1:A:1326:GLN:HE22	1.78	0.48
2:B:93:LEU:HD23	2:B:108:LEU:HA	1.94	0.48
2:B:227:ARG:NH2	2:B:336:PRO:O	2.46	0.48
4:F:109:VAL:HG12	4:F:187:TRP:HB2	1.94	0.48
4:F:214:THR:OG1	4:F:215:GLY:N	2.45	0.48
1:A:1127:LEU:HD13	1:A:1160:ILE:HG21	1.94	0.48
4:F:259:LEU:HD23	4:F:296:PHE:CE1	2.49	0.48
1:A:290:THR:HG21	1:A:616:TRP:HZ2	1.79	0.48
1:A:597:PHE:HE1	1:A:606:SER:HB3	1.78	0.48
1:A:1019:LEU:HG	1:A:1045:PHE:HZ	1.78	0.48
1:A:1144:GLU:O	1:A:1146:MET:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:461:VAL:HG13	4:F:483:ASN:O	2.13	0.48
1:A:581:PHE:HB2	1:A:597:PHE:HD2	1.78	0.48
2:B:326:PRO:HG3	2:B:383:PHE:CZ	2.49	0.48
2:B:340:TYR:HB2	2:B:383:PHE:CD1	2.49	0.48
4:F:186:ASN:HD21	6:F:1207:NAG:H2	1.79	0.48
4:F:238:TYR:OH	4:F:243:ARG:NH2	2.36	0.48
4:F:588:LYS:O	4:F:611:TRP:NE1	2.47	0.48
4:F:609:TYR:CB	4:F:624:LEU:HA	2.43	0.48
1:A:210:TYR:OH	1:A:320:LEU:HD12	2.13	0.48
1:A:367:MET:O	1:A:371:THR:OG1	2.29	0.48
4:F:308:HIS:HA	4:F:309:LEU:HD23	1.95	0.48
4:F:494:VAL:HA	4:F:497:GLU:OE2	2.13	0.48
4:F:518:ASP:HB2	4:F:1007:HIS:CD2	2.47	0.48
4:F:609:TYR:HB2	4:F:624:LEU:HA	1.96	0.48
4:F:88:ILE:O	4:F:92:LEU:HG	2.14	0.48
4:F:299:ASN:OD1	4:F:300:ALA:N	2.46	0.48
4:F:988:ASN:HD22	6:F:1205:NAG:C7	2.27	0.48
4:F:764:UNK:O	4:F:766:UNK:N	2.46	0.48
1:A:455:ASN:O	1:A:459:TRP:N	2.41	0.47
1:A:1147:ASN:O	1:A:1150:SER:OG	2.22	0.47
4:F:218:ARG:NH2	4:F:456:LEU:HD12	2.28	0.47
1:A:131:PHE:HZ	1:A:168:ARG:HH21	1.61	0.47
1:A:179:VAL:HB	1:A:182:LEU:HD12	1.96	0.47
4:F:358:LYS:O	4:F:384:VAL:HA	2.14	0.47
4:F:460:LEU:HD23	4:F:517:ILE:HG23	1.96	0.47
1:A:1476:UNK:O	1:A:1478:UNK:N	2.48	0.47
2:B:55:ALA:HA	2:B:58:LYS:HD2	1.96	0.47
4:F:282:LEU:O	4:F:317:LYS:NZ	2.45	0.47
4:F:606:ASN:O	4:F:627:PRO:CG	2.62	0.47
1:A:216:GLU:HG3	1:A:1240:VAL:HG21	1.97	0.47
1:A:606:SER:O	1:A:609:GLN:HB3	2.14	0.47
4:F:596:SER:C	4:F:602:ILE:HG23	2.40	0.47
4:F:506:PHE:HB2	4:F:618:ASP:HB2	1.96	0.47
1:A:79:ASN:HA	4:F:332:ILE:HA	1.97	0.47
1:A:369:TRP:CD1	2:B:245:MET:HG2	2.50	0.47
1:A:964:THR:O	1:A:966:GLU:N	2.43	0.47
2:B:250:PHE:HE1	2:B:317:VAL:HG12	1.80	0.47
4:F:461:VAL:HG13	4:F:483:ASN:C	2.39	0.47
1:A:1193:SER:O	1:A:1197:VAL:HG23	2.14	0.46
4:F:271:LEU:HA	4:F:274:ILE:HG22	1.97	0.46
4:F:297:ASN:ND2	4:F:330:LYS:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:673:UNK:O	4:F:677:UNK:N	2.47	0.46
1:A:61:ILE:HA	1:A:64:ASN:OD1	2.15	0.46
2:B:349:LEU:HA	2:B:352:LEU:HD12	1.98	0.46
4:F:988:ASN:ND2	6:F:1205:NAG:O7	2.48	0.46
1:A:1066:VAL:O	1:A:1070:GLU:N	2.42	0.46
4:F:1000:GLY:O	4:F:1001:ASN:ND2	2.48	0.46
4:F:1006:PHE:HD1	4:F:1012:MET:HG3	1.79	0.46
2:B:352:LEU:O	2:B:355:SER:OG	2.31	0.46
4:F:485:LEU:O	4:F:489:VAL:HG23	2.15	0.46
4:F:524:LEU:HD21	4:F:1033:LEU:N	2.31	0.46
1:A:369:TRP:NE1	2:B:245:MET:HG2	2.29	0.46
4:F:195:PHE:O	4:F:199:ARG:HG3	2.16	0.46
4:F:263:SER:HA	4:F:297:ASN:HD22	1.81	0.46
4:F:281:MET:SD	4:F:363:PHE:HZ	2.39	0.46
4:F:492:VAL:HG13	4:F:501:ARG:NH1	2.30	0.46
4:F:1063:PHE:HA	4:F:1064:ASP:HA	1.64	0.46
1:A:435:TYR:HA	1:A:436:TRP:HA	1.69	0.46
1:A:649:ASN:O	1:A:653:LEU:HG	2.15	0.46
4:F:626:LEU:C	4:F:628:THR:N	2.73	0.46
2:B:107:ARG:HB3	2:B:115:ILE:HD13	1.97	0.46
4:F:261:ASP:OD2	4:F:263:SER:OG	2.30	0.46
1:A:131:PHE:CE1	1:A:164:LEU:HB3	2.50	0.46
1:A:210:TYR:O	1:A:214:GLY:N	2.37	0.46
1:A:363:LEU:O	1:A:367:MET:HG2	2.16	0.46
1:A:631:SER:OG	1:A:633:PRO:HD2	2.16	0.46
4:F:524:LEU:HD21	4:F:1033:LEU:H	1.81	0.46
1:A:245:CYS:O	1:A:264:GLY:HA2	2.16	0.46
1:A:958:ASN:HA	1:A:959:ASP:HA	1.68	0.46
2:B:65:ARG:N	2:B:221:ASP:O	2.31	0.46
4:F:595:LYS:HB2	6:F:1212:NAG:H83	1.98	0.46
1:A:124:VAL:O	1:A:128:ILE:HG12	2.16	0.46
1:A:326:LEU:O	1:A:330:LEU:HG	2.16	0.46
2:B:237:LYS:H	2:B:324:ASN:ND2	2.10	0.46
2:B:393:GLU:O	2:B:397:GLU:HG2	2.16	0.46
4:F:606:ASN:C	4:F:627:PRO:HG3	2.41	0.46
4:F:254:LYS:HA	4:F:357:ASN:OD1	2.16	0.45
4:F:254:LYS:HG2	4:F:357:ASN:HD21	1.80	0.45
4:F:512:GLY:O	4:F:514:TYR:N	2.43	0.45
4:F:617:THR:HG22	4:F:618:ASP:OD1	2.16	0.45
4:F:858:UNK:O	4:F:862:UNK:HG2	2.17	0.45
1:A:1015:GLY:HA3	1:A:1326:GLN:NE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:THR:HG21	1:A:616:TRP:CZ2	2.51	0.45
1:A:1151:ASP:O	1:A:1155:VAL:HG23	2.17	0.45
4:F:509:CYS:N	4:F:561:LEU:O	2.49	0.45
4:F:587:GLU:O	4:F:589:THR:HG23	2.16	0.45
1:A:614:GLU:OE2	1:A:615:ASP:HB2	2.16	0.45
1:A:1272:LEU:O	1:A:1276:MET:N	2.44	0.45
1:A:1487:UNK:O	1:A:1491:UNK:N	2.50	0.45
4:F:505:ARG:HG3	4:F:619:TYR:CE1	2.52	0.45
4:F:512:GLY:C	4:F:514:TYR:H	2.23	0.45
4:F:576:ILE:HD11	4:F:590:PHE:CZ	2.52	0.45
4:F:591:ARG:HB3	4:F:608:THR:HG22	1.99	0.45
1:A:73:PRO:HA	1:A:74:MET:HA	1.55	0.45
1:A:620:MET:O	1:A:624:ILE:HD12	2.16	0.45
1:A:1142:GLN:HA	1:A:1143:SER:HA	1.63	0.45
4:F:336:LYS:HB3	4:F:374:ILE:HD11	1.98	0.45
1:A:969:ARG:HH21	4:F:177:GLY:HA3	1.81	0.45
1:A:1057:MET:O	1:A:1061:VAL:HG23	2.17	0.45
4:F:75:ASN:CB	4:F:630:SER:C	2.90	0.45
4:F:219:TYR:O	4:F:220:TYR:CG	2.69	0.45
4:F:449:THR:CG2	4:F:463:THR:H	2.26	0.45
4:F:568:LEU:HD12	4:F:596:SER:HA	1.97	0.45
1:A:1372:ILE:HG22	1:A:1376:PHE:CE2	2.52	0.45
4:F:102:LEU:HG	4:F:199:ARG:NH2	2.32	0.45
4:F:130:LYS:N	4:F:141:GLU:O	2.49	0.45
2:B:66:THR:HG22	2:B:220:TYR:CE1	2.52	0.45
4:F:186:ASN:OD1	6:F:1207:NAG:H2	2.16	0.45
4:F:285:LEU:HD23	4:F:286:SER:O	2.17	0.45
4:F:290:PHE:N	4:F:290:PHE:CD1	2.83	0.45
1:A:204:LEU:O	1:A:208:ILE:N	2.50	0.44
1:A:1033:PRO:HA	1:A:1034:VAL:HA	1.74	0.44
4:F:224:PRO:HA	4:F:225:TRP:HA	1.60	0.44
1:A:1329:LEU:HD11	1:A:1358:TYR:CD1	2.52	0.44
4:F:86:ARG:HG2	4:F:90:LYS:HE3	2.00	0.44
4:F:333:THR:HG22	4:F:335:TYR:HB2	1.98	0.44
1:A:930:ASN:O	1:A:934:VAL:HG23	2.17	0.44
1:A:1195:ILE:O	1:A:1199:LEU:HG	2.16	0.44
1:A:1302:ARG:O	1:A:1305:ASN:ND2	2.51	0.44
4:F:184:GLU:O	4:F:188:THR:HG22	2.17	0.44
2:B:65:ARG:HB3	2:B:221:ASP:HB2	2.00	0.44
4:F:509:CYS:SG	4:F:560:THR:HA	2.58	0.44
4:F:1007:HIS:CG	4:F:1008:VAL:H	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:LEU:O	1:A:668:GLU:N	2.45	0.44
1:A:993:ASN:C	1:A:995:PHE:H	2.25	0.44
1:A:1233:ALA:HB2	1:A:1236:ARG:HH21	1.83	0.44
4:F:453:LEU:HB2	4:F:557:GLU:OE2	2.18	0.44
1:A:286:TYR:O	1:A:290:THR:HG23	2.18	0.44
4:F:487:LEU:HD22	4:F:490:MET:SD	2.58	0.44
1:A:205:PHE:O	1:A:209:ILE:N	2.40	0.43
4:F:113:HIS:C	4:F:115:TRP:H	2.25	0.43
4:F:123:GLU:HA	4:F:124:VAL:HA	1.74	0.43
4:F:334:ASP:HB3	4:F:337:LYS:HB2	1.99	0.43
4:F:343:PHE:O	4:F:347:LEU:N	2.51	0.43
1:A:1123:LEU:O	1:A:1127:LEU:HG	2.17	0.43
1:A:366:TYR:HD2	2:B:348:VAL:HG11	1.82	0.43
1:A:647:CYS:O	1:A:651:ILE:HG13	2.18	0.43
1:A:996:HIS:O	1:A:1002:SER:OG	2.25	0.43
4:F:462:ILE:HG13	4:F:485:LEU:HD11	2.00	0.43
1:A:631:SER:OG	1:A:632:TYR:N	2.41	0.43
1:A:942:PHE:HD1	1:A:1044:PHE:CE1	2.36	0.43
1:A:1314:LEU:O	1:A:1317:PHE:N	2.48	0.43
2:B:229:VAL:HB	2:B:317:VAL:HA	2.01	0.43
4:F:98:ALA:HB1	4:F:199:ARG:NE	2.31	0.43
4:F:117:GLU:O	4:F:119:PHE:N	2.51	0.43
4:F:196:LYS:HB3	4:F:196:LYS:HE2	1.81	0.43
4:F:356:CYS:O	4:F:358:LYS:NZ	2.51	0.43
2:B:55:ALA:HB1	2:B:105:ILE:HG21	2.01	0.43
4:F:443:ALA:C	4:F:445:GLN:H	2.27	0.43
4:F:600:ARG:HA	4:F:600:ARG:HD3	1.65	0.43
1:A:194:LEU:O	1:A:196:LEU:N	2.48	0.43
1:A:1185:PHE:HA	1:A:1188:LEU:HD12	2.00	0.43
2:B:353:ILE:HB	2:B:364:LEU:HD13	1.99	0.43
4:F:271:LEU:HD11	4:F:327:ILE:HG23	2.00	0.43
1:A:995:PHE:HE1	1:A:1005:MET:HE3	1.84	0.43
1:A:1046:ILE:O	1:A:1050:ILE:HG13	2.19	0.43
2:B:329:LEU:HB3	2:B:336:PRO:HG3	2.01	0.43
2:B:412:PRO:HA	2:B:413:PRO:HD3	1.92	0.43
1:A:90:GLU:HA	1:A:93:PHE:HD2	1.83	0.43
1:A:458:LEU:O	1:A:462:HIS:N	2.31	0.43
1:A:631:SER:H	1:A:635:VAL:HG23	1.83	0.43
3:E:125:ALA:O	3:E:129:PHE:N	2.52	0.43
4:F:334:ASP:O	4:F:336:LYS:N	2.51	0.43
1:A:1063:PHE:O	1:A:1067:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:158:MET:O	3:E:162:VAL:HG23	2.19	0.43
4:F:465:THR:HG22	4:F:480:ASN:HB3	2.01	0.43
4:F:92:LEU:HD22	4:F:448:TRP:CH2	2.54	0.42
4:F:302:ASP:HB2	4:F:306:PHE:CE1	2.42	0.42
1:A:214:GLY:C	1:A:216:GLU:H	2.26	0.42
1:A:226:CYS:N	1:A:274:HIS:HE2	2.17	0.42
4:F:96:SER:O	4:F:100:VAL:HG23	2.19	0.42
4:F:248:GLN:NE2	4:F:448:TRP:O	2.35	0.42
1:A:958:ASN:ND2	1:A:989:GLN:H	2.16	0.42
1:A:1318:ARG:CZ	1:A:1328:ILE:HD11	2.49	0.42
4:F:390:SER:HB2	4:F:414:GLU:HG2	2.01	0.42
4:F:622:LEU:HD12	4:F:623:ALA:H	1.83	0.42
1:A:1008:PHE:O	1:A:1011:SER:HB3	2.19	0.42
4:F:113:HIS:O	4:F:115:TRP:N	2.39	0.42
4:F:258:ILE:HG13	4:F:361:MET:HE3	2.00	0.42
4:F:309:LEU:C	4:F:311:GLN:N	2.77	0.42
4:F:564:LEU:HD13	4:F:574:VAL:HG22	2.01	0.42
1:A:592:VAL:C	1:A:594:ARG:N	2.77	0.42
1:A:1239:ARG:HG3	1:A:1242:ARG:NH2	2.33	0.42
2:B:326:PRO:HB3	2:B:338:ILE:HG21	2.01	0.42
4:F:335:TYR:CE2	4:F:339:PHE:HE2	2.37	0.42
4:F:609:TYR:HB2	4:F:623:ALA:O	2.19	0.42
4:F:868:UNK:HA	4:F:869:UNK:HA	1.76	0.42
1:A:282:MET:HG2	1:A:286:TYR:CE2	2.55	0.42
4:F:86:ARG:O	4:F:90:LYS:HG3	2.20	0.42
4:F:236:ASP:OD1	4:F:238:TYR:HB3	2.19	0.42
4:F:436:MET:HE1	4:F:443:ALA:HB3	2.02	0.42
1:A:88:LYS:O	1:A:91:TYR:HB3	2.20	0.42
1:A:1178:PHE:O	1:A:1180:ASP:N	2.53	0.42
4:F:107:GLU:OE2	4:F:444:LYS:NZ	2.53	0.42
4:F:470:ASN:HD22	4:F:473:GLY:N	2.14	0.42
4:F:485:LEU:HD23	4:F:485:LEU:HA	1.68	0.42
1:A:87:GLU:HA	1:A:90:GLU:OE1	2.20	0.42
1:A:89:LEU:O	1:A:92:PHE:HB3	2.20	0.42
1:A:210:TYR:HD2	1:A:313:TYR:CE1	2.37	0.42
4:F:359:ILE:CB	4:F:385:ARG:HB2	2.49	0.42
4:F:595:LYS:HB3	4:F:602:ILE:HG21	2.02	0.42
4:F:614:VAL:HG12	4:F:616:GLY:N	2.32	0.41
1:A:943:ALA:HB1	1:A:1000:VAL:HG13	2.02	0.41
1:A:1069:GLN:O	1:A:1073:GLU:N	2.49	0.41
4:F:248:GLN:NE2	4:F:447:GLN:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:528:ASN:O	4:F:531:PRO:HD2	2.20	0.41
4:F:606:ASN:C	4:F:627:PRO:CG	2.93	0.41
1:A:357:GLN:O	1:A:361:GLU:HG2	2.19	0.41
1:A:589:ASP:HA	1:A:590:THR:HA	1.81	0.41
4:F:256:MET:SD	4:F:359:ILE:HD11	2.60	0.41
1:A:309:TRP:HA	1:A:311:TRP:NE1	2.35	0.41
1:A:321:GLY:O	1:A:325:ILE:HG23	2.20	0.41
1:A:937:LEU:HA	1:A:940:PHE:HD2	1.84	0.41
1:A:1375:LEU:O	1:A:1379:VAL:HG23	2.20	0.41
1:A:1184:VAL:O	1:A:1188:LEU:HG	2.20	0.41
4:F:304:SER:O	4:F:305:CYS:SG	2.79	0.41
4:F:488:GLY:O	4:F:492:VAL:HG23	2.20	0.41
4:F:489:VAL:HA	4:F:492:VAL:HB	2.02	0.41
4:F:505:ARG:HG2	4:F:506:PHE:N	2.36	0.41
1:A:1119:TYR:O	1:A:1123:LEU:HG	2.21	0.41
1:A:1293:ALA:N	1:A:1338:CYS:O	2.54	0.41
1:A:1410:UNK:O	1:A:1412:UNK:N	2.53	0.41
4:F:85:ALA:O	4:F:89:GLU:HG3	2.21	0.41
4:F:609:TYR:CG	4:F:624:LEU:HD23	2.55	0.41
1:A:169:VAL:O	1:A:172:PRO:HD2	2.20	0.41
1:A:287:GLN:OE1	1:A:621:TYR:OH	2.32	0.41
1:A:936:THR:O	1:A:939:GLN:HB2	2.21	0.41
4:F:356:CYS:O	4:F:358:LYS:HG3	2.20	0.41
4:F:411:TYR:HB3	4:F:431:VAL:HG21	2.03	0.41
1:A:595:SER:HB3	1:A:605:ILE:HD11	2.03	0.41
1:A:969:ARG:HD2	4:F:177:GLY:HA3	2.03	0.41
4:F:292:ASN:OD1	4:F:308:HIS:HB3	2.20	0.41
4:F:437:VAL:HA	4:F:469:PHE:CE2	2.43	0.41
1:A:1166:ILE:O	1:A:1170:LEU:HG	2.21	0.41
1:A:1372:ILE:HA	1:A:1375:LEU:HD12	2.03	0.41
4:F:335:TYR:CE2	4:F:371:ALA:HB2	2.56	0.41
4:F:444:LYS:HD3	4:F:469:PHE:HE1	1.85	0.41
4:F:505:ARG:HB3	4:F:508:LEU:O	2.20	0.41
1:A:627:TYR:CD2	1:A:637:VAL:HG21	2.56	0.41
2:B:340:TYR:HD2	2:B:386:ILE:HG12	1.86	0.41
3:E:199:LEU:O	3:E:203:SER:N	2.53	0.41
1:A:370:ILE:HD11	2:B:352:LEU:HB3	2.03	0.40
1:A:1016:TRP:N	1:A:1017:PRO:HD2	2.35	0.40
4:F:115:TRP:HA	4:F:183:ASN:OD1	2.21	0.40
4:F:175:TYR:O	4:F:177:GLY:N	2.54	0.40
4:F:460:LEU:H	4:F:460:LEU:HG	1.66	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ARG:O	1:A:168:ARG:HB3	2.21	0.40
4:F:282:LEU:HD23	4:F:282:LEU:HA	1.85	0.40
1:A:632:TYR:H	1:A:633:PRO:HD2	1.86	0.40
1:A:1245:LYS:O	1:A:1248:SER:HB2	2.21	0.40
1:A:1316:LEU:HD11	1:A:1360:TYR:OH	2.20	0.40
4:F:195:PHE:HA	4:F:198:ASN:ND2	2.37	0.40
4:F:418:ILE:C	4:F:420:ALA:H	2.29	0.40
1:A:521:PRO:HA	1:A:522:LEU:HA	1.59	0.40
1:A:642:ILE:O	1:A:646:VAL:HB	2.21	0.40
4:F:554:LYS:O	4:F:555:SER:OG	2.31	0.40
4:F:568:LEU:HD11	4:F:597:GLN:H	1.87	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	1084/1873 (58%)	936 (86%)	75 (7%)	73 (7%)	1	12
2	B	272/356 (76%)	261 (96%)	11 (4%)	0	100	100
3	E	132/222 (60%)	127 (96%)	2 (2%)	3 (2%)	5	29
4	F	617/1106 (56%)	461 (75%)	83 (14%)	73 (12%)	0	4
All	All	2105/3557 (59%)	1785 (85%)	171 (8%)	149 (7%)	2	11

All (149) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	39	PRO
1	A	74	MET
1	A	75	PRO

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Mol	Chain	Res	Type
1	A	242	PRO
1	A	244	PRO
1	A	248	THR
1	A	253	PRO
1	A	266	PRO
1	A	268	PRO
1	A	305	ILE
1	A	518	ALA
1	A	1033	PRO
1	A	1035	TYR
1	A	1106	PRO
1	A	1295	VAL
1	A	1307	GLN
1	A	1340	PRO
1	A	1346	PRO
3	E	130	ARG
4	F	56	VAL
4	F	73	GLU
4	F	74	PRO
4	F	117	GLU
4	F	121	SER
4	F	134	ASP
4	F	142	PRO
4	F	305	CYS
4	F	351	VAL
4	F	510	PRO
4	F	618	ASP
4	F	629	TYR
4	F	630	SER
4	F	638	ILE
4	F	1008	VAL
4	F	1035	ILE
4	F	1036	GLN
4	F	1046	PRO
4	F	1053	PRO
1	A	35	THR
1	A	50	TRP
1	A	51	LYS
1	A	78	ASP
1	A	107	ALA
1	A	262	ARG
1	A	263	GLY

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Mol	Chain	Res	Type
1	A	273	THR
1	A	276	ASP
1	A	589	ASP
1	A	632	TYR
1	A	891	SER
1	A	962	LYS
1	A	963	MET
1	A	966	GLU
1	A	1138	GLN
1	A	1141	HIS
1	A	1173	LYS
3	E	205	PRO
4	F	72	VAL
4	F	77	ALA
4	F	138	ASN
4	F	141	GLU
4	F	264	GLY
4	F	308	HIS
4	F	314	VAL
4	F	347	LEU
4	F	349	TYR
4	F	356	CYS
4	F	409	LYS
4	F	441	ASP
4	F	458	LEU
4	F	470	ASN
4	F	520	ASN
4	F	522	TYR
4	F	639	GLU
4	F	1043	GLY
4	F	1062	CYS
1	A	79	ASN
1	A	131	PHE
1	A	234	VAL
1	A	251	GLY
1	A	466	ILE
1	A	468	ASN
1	A	541	TYR
1	A	631	SER
1	A	892	VAL
1	A	978	GLY
1	A	1145	GLU

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Mol	Chain	Res	Type
1	A	1179	GLY
1	A	1293	ALA
1	A	1341	GLU
1	A	1345	ALA
1	A	1357	ALA
3	E	131	LYS
4	F	118	ASP
4	F	125	VAL
4	F	164	GLN
4	F	265	SER
4	F	335	TYR
4	F	394	HIS
4	F	438	LEU
4	F	475	PHE
4	F	525	LEU
4	F	555	SER
4	F	571	ASP
4	F	1032	ARG
4	F	1037	ALA
4	F	1050	VAL
1	A	36	LEU
1	A	196	LEU
1	A	252	ARG
1	A	261	CYS
1	A	644	LEU
1	A	949	LEU
1	A	1171	ALA
1	A	1302	ARG
1	A	1349	GLU
4	F	163	TYR
4	F	251	ALA
4	F	311	GLN
4	F	330	LYS
4	F	353	ARG
4	F	557	GLU
4	F	627	PRO
4	F	1010	LYS
4	F	1047	CYS
1	A	241	LYS
1	A	254	CYS
1	A	258	GLY
1	A	308	GLU

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Mol	Chain	Res	Type
1	A	977	ASP
1	A	994	ASP
4	F	186	ASN
4	F	348	ASN
4	F	380	LYS
4	F	495	SER
4	F	1007	HIS
1	A	837	ILE
1	A	866	ASN
4	F	137	LYS
4	F	220	TYR
4	F	395	ASN
1	A	1339	ASP
4	F	310	VAL
4	F	499	ILE
1	A	1253	VAL
4	F	634	ILE
4	F	327	ILE
1	A	73	PRO

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	430/1519 (28%)	429 (100%)	1 (0%)	87	85
2	B	240/315 (76%)	240 (100%)	0	100	100
3	E	3/192 (2%)	3 (100%)	0	100	100
4	F	417/706 (59%)	414 (99%)	3 (1%)	76	78
All	All	1090/2732 (40%)	1086 (100%)	4 (0%)	81	82

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1070	GLU
4	F	359	ILE

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Mol	Chain	Res	Type
4	F	626	LEU
4	F	628	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	GLN
1	A	358	GLN
1	A	663	ASN
1	A	958	ASN
1	A	1058	ASN
1	A	1131	ASN
1	A	1154	ASN
1	A	1311	GLN
2	B	49	GLN
2	B	314	GLN
2	B	324	ASN
4	F	316	ASN
4	F	345	GLN
4	F	408	ASN
4	F	570	ASN
4	F	615	ASN
4	F	1007	HIS
4	F	1013	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

Of 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 for Mogul analysis.

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
6	NAG	F	1212	-	14,14,15	0.24	0	17,19,21	0.46	0
6	NAG	F	1211	-	14,14,15	0.26	0	17,19,21	0.39	0
6	NAG	F	1207	-	14,14,15	0.23	0	17,19,21	0.47	0
6	NAG	F	1215	-	14,14,15	0.30	0	17,19,21	0.50	0
6	NAG	F	1214	-	14,14,15	0.29	0	17,19,21	0.44	0
6	NAG	F	1206	-	14,14,15	0.27	0	17,19,21	0.42	0
6	NAG	F	1208	-	14,14,15	0.28	0	17,19,21	0.45	0
6	NAG	F	1213	-	14,14,15	0.29	0	17,19,21	0.39	0
6	NAG	F	1203	-	14,14,15	0.30	0	17,19,21	0.37	0
6	NAG	F	1210	-	14,14,15	0.27	0	17,19,21	0.40	0
6	NAG	F	1201	-	14,14,15	0.24	0	17,19,21	0.58	0
7	BMA	F	1216	-	11,11,12	0.54	0	15,15,17	0.72	0
7	BMA	F	1217	-	11,11,12	0.61	0	15,15,17	0.67	0
6	NAG	F	1209	-	14,14,15	0.27	0	17,19,21	0.40	0
6	NAG	F	1202	-	14,14,15	0.21	0	17,19,21	0.44	0
6	NAG	F	1204	-	14,14,15	0.23	0	17,19,21	0.52	0
6	NAG	F	1205	-	14,14,15	0.23	0	17,19,21	0.42	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
6	NAG	F	1212	-	-	1/6/23/26	0/1/1/1
6	NAG	F	1211	-	-	2/6/23/26	0/1/1/1
6	NAG	F	1207	-	-	2/6/23/26	0/1/1/1
6	NAG	F	1215	-	-	4/6/23/26	0/1/1/1
6	NAG	F	1214	-	-	2/6/23/26	0/1/1/1
6	NAG	F	1206	-	-	0/6/23/26	0/1/1/1
6	NAG	F	1208	-	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	F	1213	-	-	0/6/23/26	0/1/1/1
6	NAG	F	1203	-	-	2/6/23/26	0/1/1/1
6	NAG	F	1210	-	-	0/6/23/26	0/1/1/1
6	NAG	F	1201	-	-	4/6/23/26	0/1/1/1
7	BMA	F	1216	-	-	0/2/19/22	0/1/1/1
7	BMA	F	1217	-	-	0/2/19/22	0/1/1/1
6	NAG	F	1209	-	-	2/6/23/26	0/1/1/1
6	NAG	F	1202	-	-	2/6/23/26	0/1/1/1
6	NAG	F	1204	-	-	0/6/23/26	0/1/1/1
6	NAG	F	1205	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	1201	NAG	O5-C5-C6-O6
6	F	1205	NAG	O5-C5-C6-O6
6	F	1203	NAG	C4-C5-C6-O6
6	F	1202	NAG	O5-C5-C6-O6
6	F	1207	NAG	O5-C5-C6-O6
6	F	1209	NAG	O5-C5-C6-O6
6	F	1211	NAG	O5-C5-C6-O6
6	F	1205	NAG	C4-C5-C6-O6
6	F	1202	NAG	C4-C5-C6-O6
6	F	1209	NAG	C4-C5-C6-O6
6	F	1203	NAG	O5-C5-C6-O6
6	F	1207	NAG	C4-C5-C6-O6
6	F	1201	NAG	C4-C5-C6-O6
6	F	1214	NAG	O5-C5-C6-O6
6	F	1215	NAG	C4-C5-C6-O6
6	F	1211	NAG	C4-C5-C6-O6
6	F	1215	NAG	O5-C5-C6-O6
6	F	1214	NAG	C4-C5-C6-O6
6	F	1201	NAG	C1-C2-N2-C7
6	F	1215	NAG	C1-C2-N2-C7
6	F	1215	NAG	C3-C2-N2-C7
6	F	1212	NAG	O5-C5-C6-O6
6	F	1201	NAG	C3-C2-N2-C7

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	1212	NAG	1	0
6	F	1211	NAG	1	0
6	F	1207	NAG	2	0
6	F	1203	NAG	3	0
7	F	1217	BMA	2	0
6	F	1209	NAG	2	0
6	F	1204	NAG	2	0
6	F	1205	NAG	2	0

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.

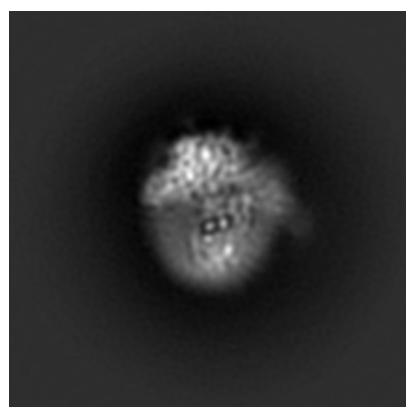
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6475. These allow visual inspection of the internal detail of the map and identification of artifacts.

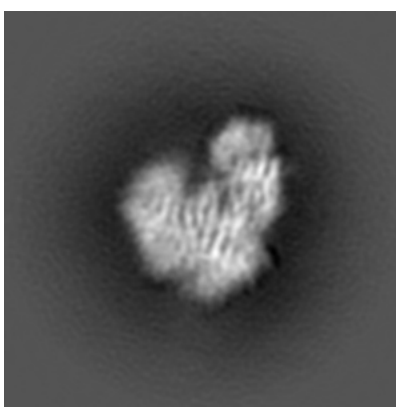
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

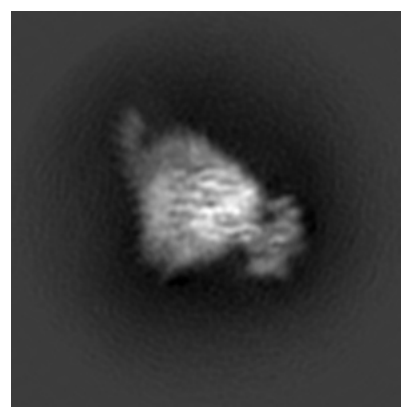
6.1.1 Primary map



X



Y

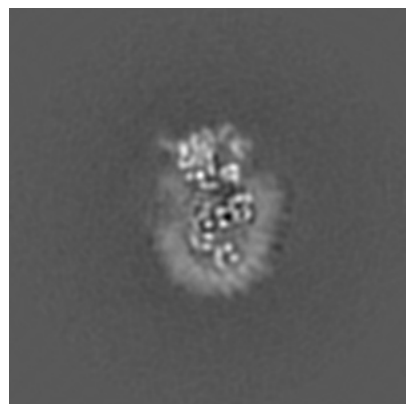


Z

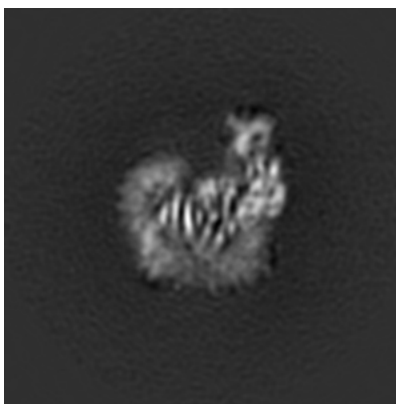
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

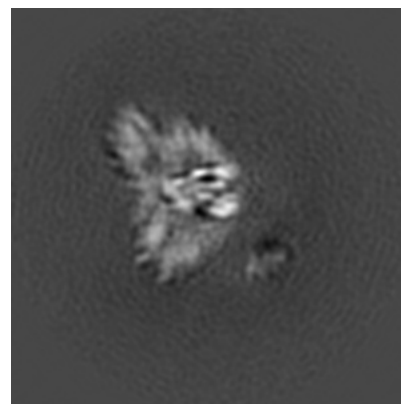
6.2.1 Primary map



X Index: 128



Y Index: 128

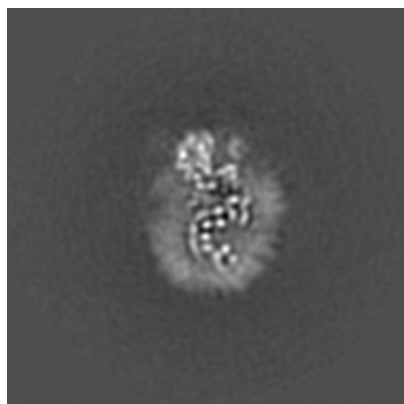


Z Index: 128

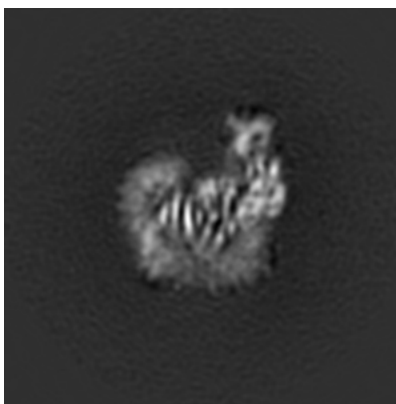
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

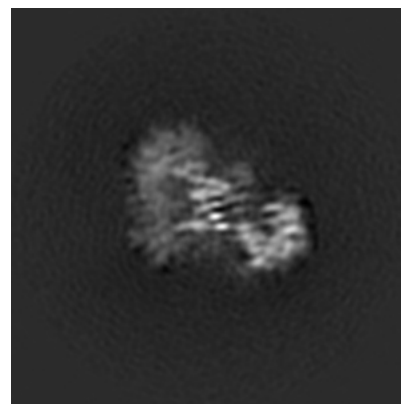
6.3.1 Primary map



X Index: 125



Y Index: 128

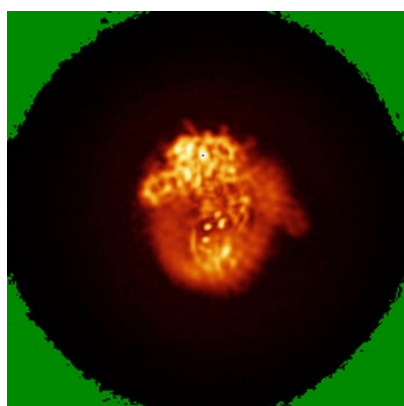


Z Index: 150

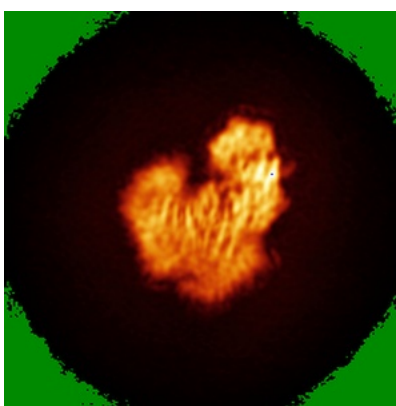
The images above show the largest variance slices of the map in three orthogonal directions.

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

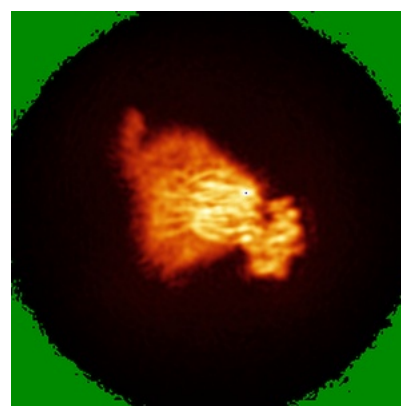
6.4.1 Primary map



X



Y

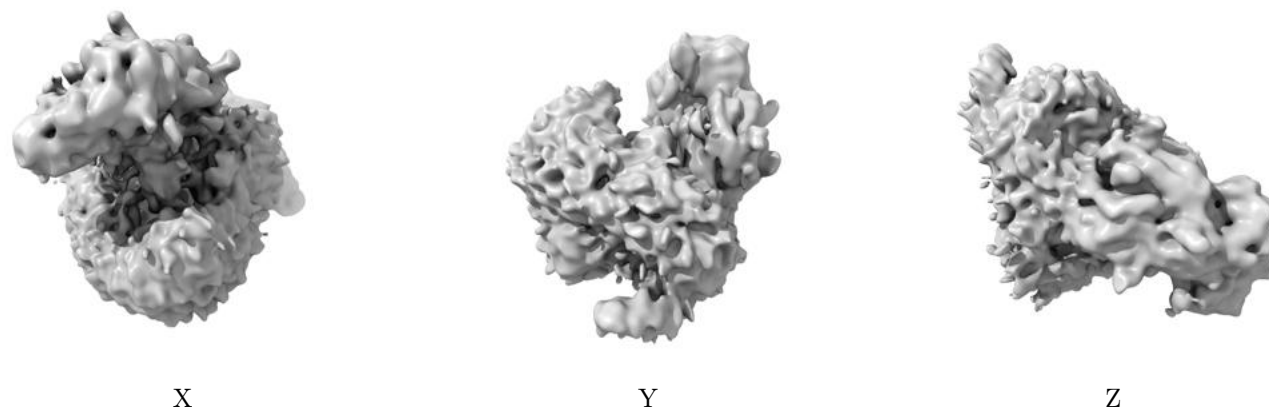


Z

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

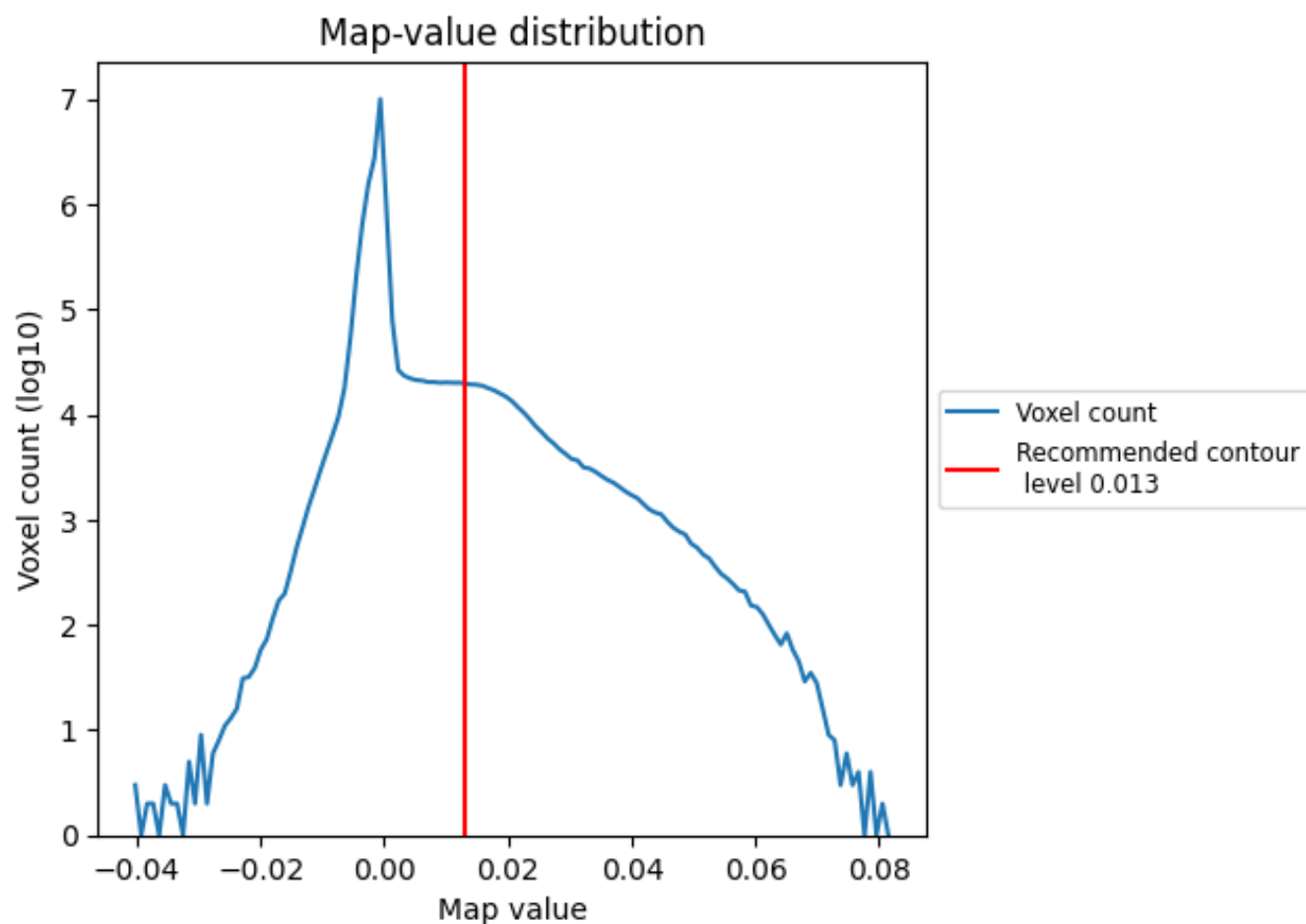
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

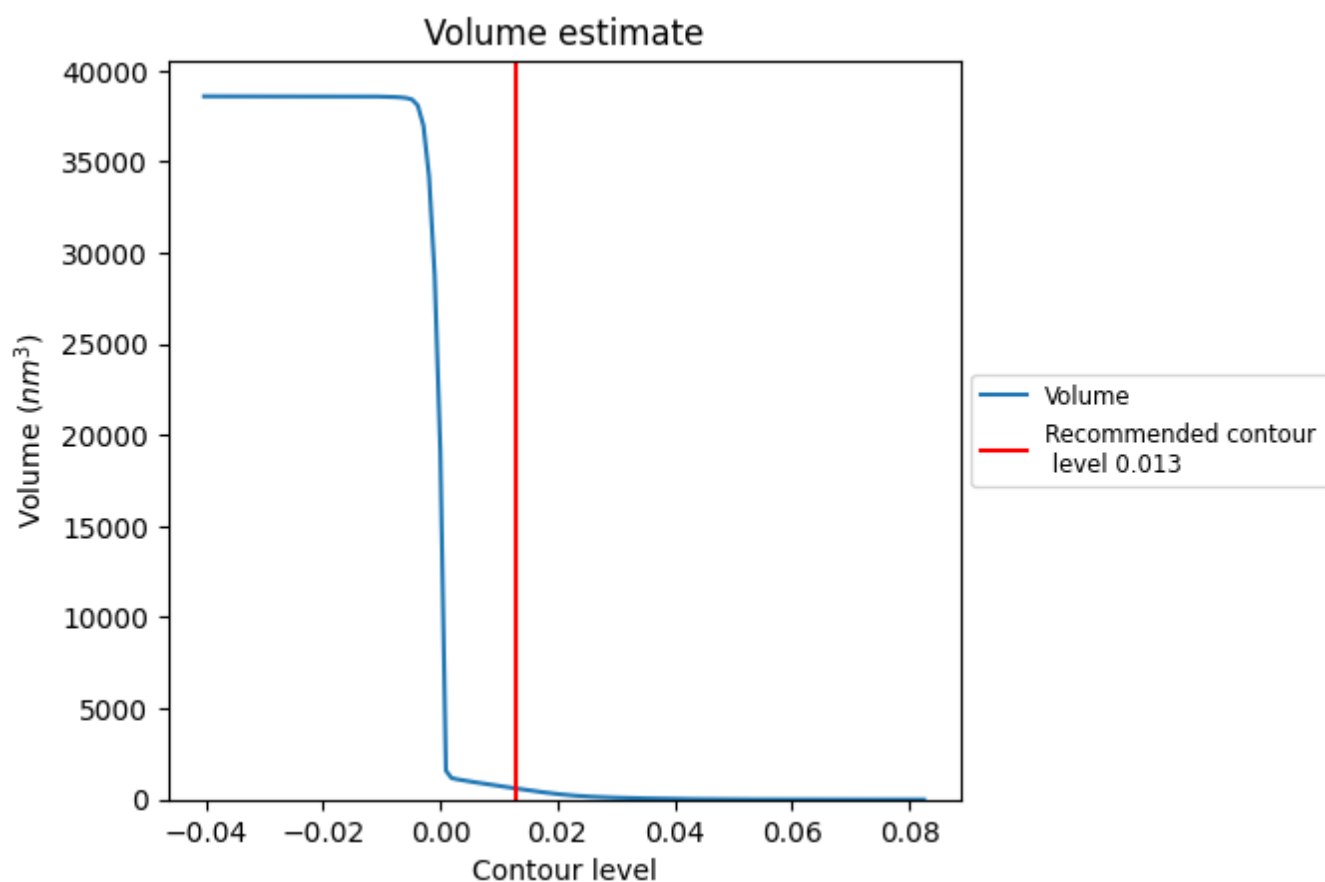
This section contains the results of statistical analysis of the map.

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.

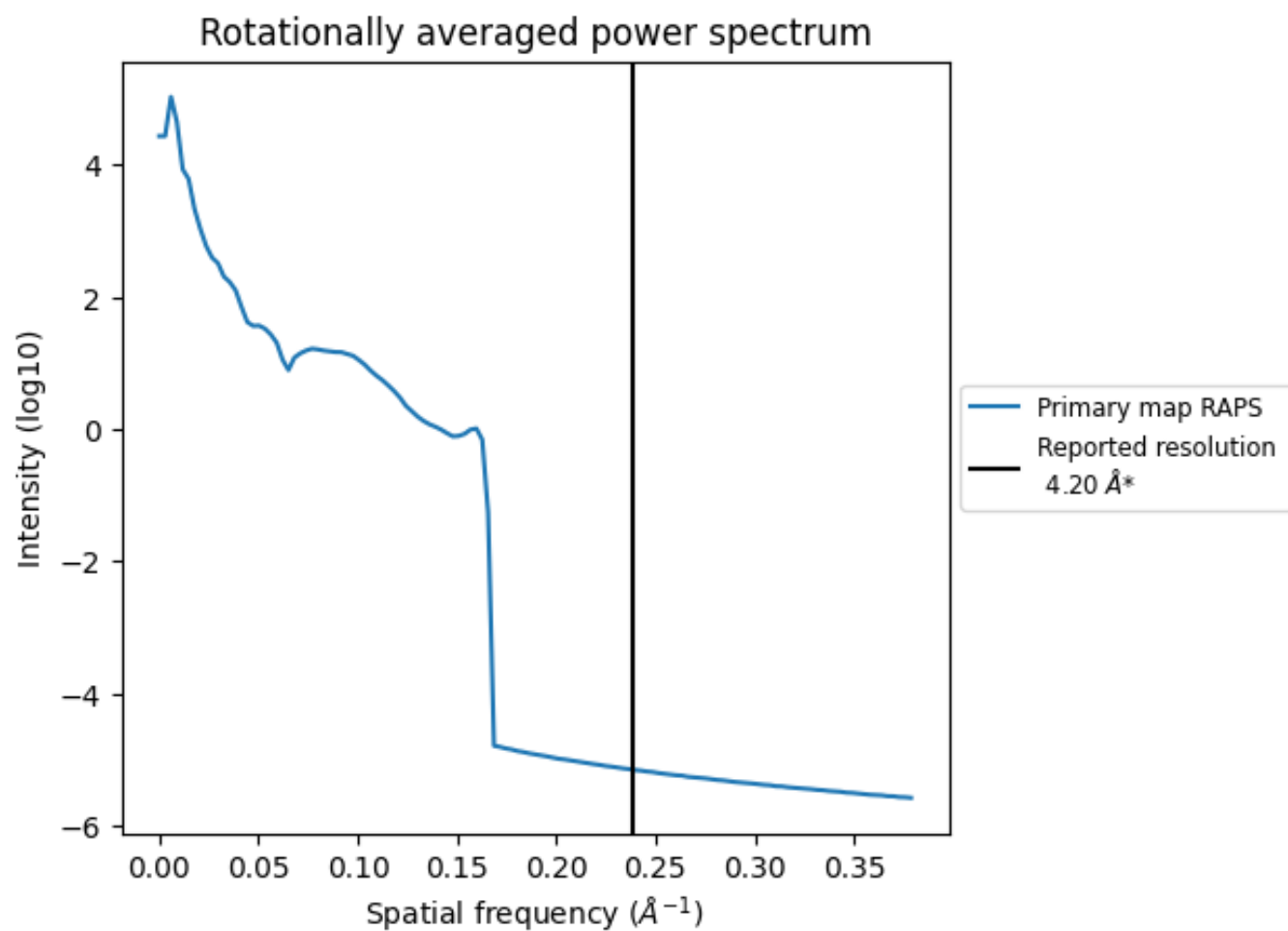
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 607 nm³; this corresponds to an approximate mass of 548 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 0.238 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-6475 and PDB model 3JBR. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

This section was not generated.

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



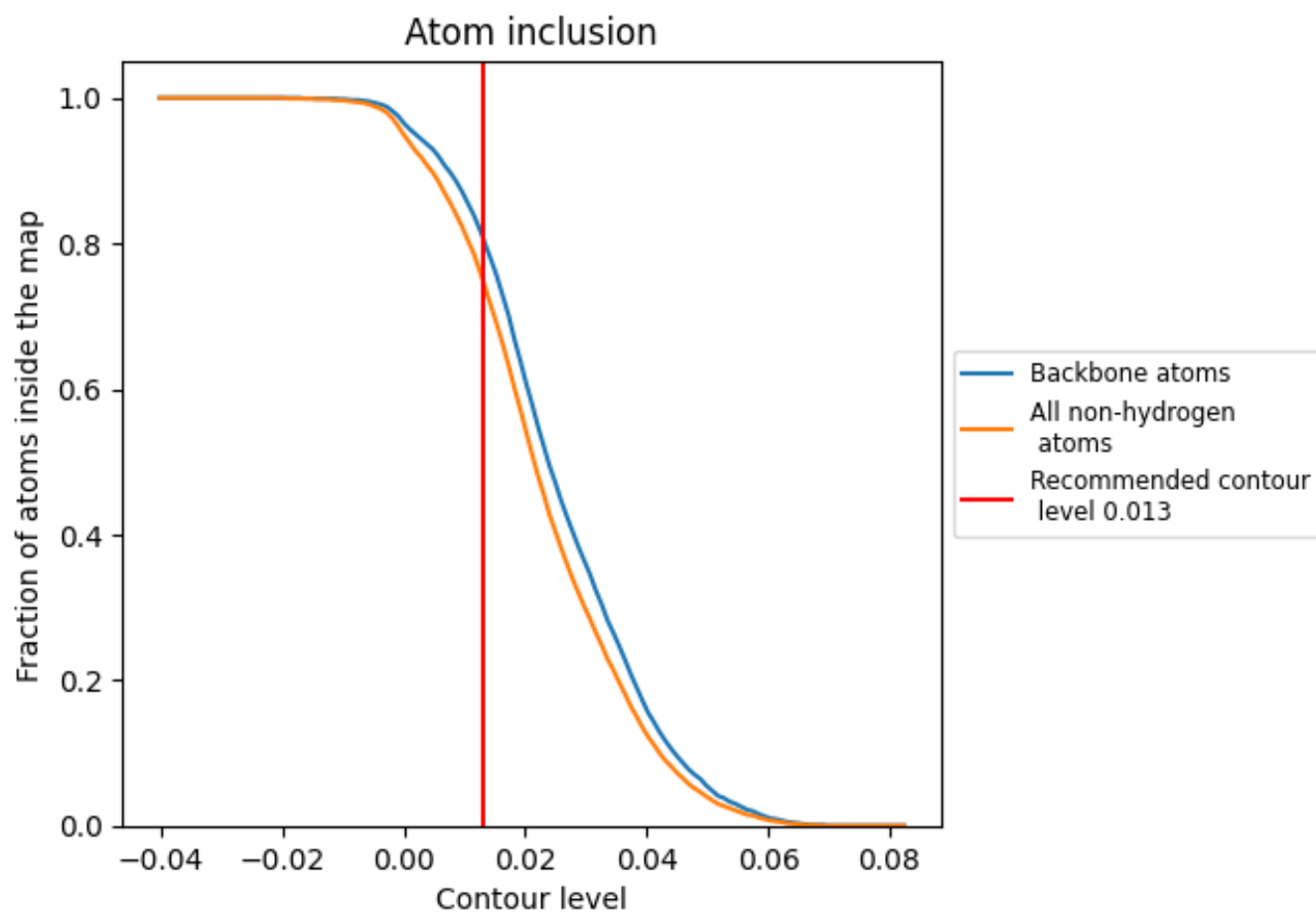
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 75% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7500	0.0880
A	0.7060	0.0570
B	0.4070	0.0330
E	0.8580	0.0570
F	0.9200	0.1520

