



Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 06:40 am GMT

PDB ID : 8B42
EMDB ID : EMD-15837
Title : Structure of heteromeric LRRC8A/C Volume-Regulated Anion Channel.
Authors : Sawicka, M.; Dutzler, R.
Deposited on : 2022-09-19
Resolution : 6.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
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) : 2.39

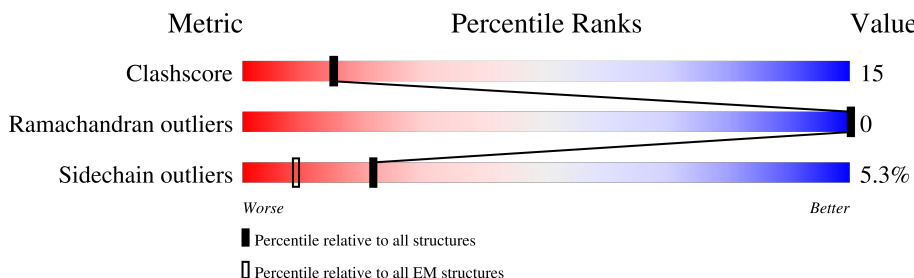
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.60 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	817	
1	B	817	
1	C	817	
1	D	817	
2	E	811	
2	F	811	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 31849 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 Volume-regulated anion channel subunit LRRC8A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	718	Total	C	N	O	S	0	0
			5922	3853	997	1047	25		
1	B	720	Total	C	N	O	S	0	0
			5938	3862	999	1052	25		
1	C	718	Total	C	N	O	S	0	0
			5922	3853	997	1047	25		
1	D	718	Total	C	N	O	S	0	0
			5922	3853	997	1047	25		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q80WG5
A	1	SER	-	expression tag	UNP Q80WG5
A	811	LEU	-	expression tag	UNP Q80WG5
A	812	GLU	-	expression tag	UNP Q80WG5
A	813	VAL	-	expression tag	UNP Q80WG5
A	814	LEU	-	expression tag	UNP Q80WG5
A	815	PHE	-	expression tag	UNP Q80WG5
A	816	GLN	-	expression tag	UNP Q80WG5
B	0	MET	-	initiating methionine	UNP Q80WG5
B	1	SER	-	expression tag	UNP Q80WG5
B	811	LEU	-	expression tag	UNP Q80WG5
B	812	GLU	-	expression tag	UNP Q80WG5
B	813	VAL	-	expression tag	UNP Q80WG5
B	814	LEU	-	expression tag	UNP Q80WG5
B	815	PHE	-	expression tag	UNP Q80WG5
B	816	GLN	-	expression tag	UNP Q80WG5
C	0	MET	-	initiating methionine	UNP Q80WG5
C	1	SER	-	expression tag	UNP Q80WG5
C	811	LEU	-	expression tag	UNP Q80WG5
C	812	GLU	-	expression tag	UNP Q80WG5
C	813	VAL	-	expression tag	UNP Q80WG5
C	814	LEU	-	expression tag	UNP Q80WG5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	815	PHE	-	expression tag	UNP Q80WG5
C	816	GLN	-	expression tag	UNP Q80WG5
D	0	MET	-	initiating methionine	UNP Q80WG5
D	1	SER	-	expression tag	UNP Q80WG5
D	811	LEU	-	expression tag	UNP Q80WG5
D	812	GLU	-	expression tag	UNP Q80WG5
D	813	VAL	-	expression tag	UNP Q80WG5
D	814	LEU	-	expression tag	UNP Q80WG5
D	815	PHE	-	expression tag	UNP Q80WG5
D	816	GLN	-	expression tag	UNP Q80WG5

- Molecule 2 is a protein called Volume-regulated anion channel subunit LRRC8C.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	692	Total	C	N	O	S	0	0
			5638	3678	921	1002	37		
2	F	300	Total	C	N	O	S	0	0
			2507	1657	396	433	21		

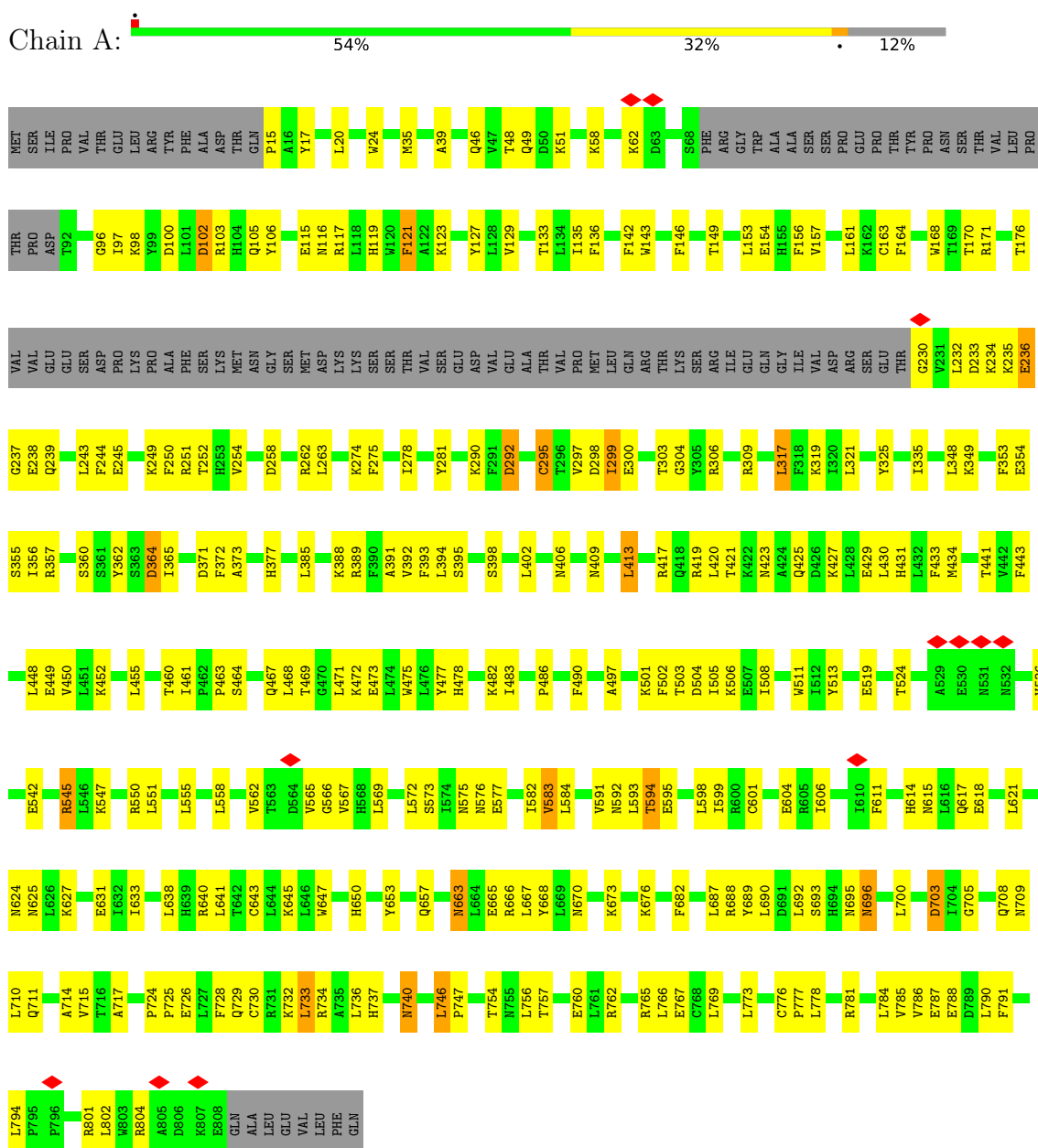
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	MET	-	initiating methionine	UNP Q8R502
E	1	SER	-	expression tag	UNP Q8R502
E	781	ARG	GLY	conflict	UNP Q8R502
E	804	ALA	-	expression tag	UNP Q8R502
E	805	LEU	-	expression tag	UNP Q8R502
E	806	GLU	-	expression tag	UNP Q8R502
E	807	VAL	-	expression tag	UNP Q8R502
E	808	LEU	-	expression tag	UNP Q8R502
E	809	PHE	-	expression tag	UNP Q8R502
E	810	GLN	-	expression tag	UNP Q8R502
F	0	MET	-	initiating methionine	UNP Q8R502
F	1	SER	-	expression tag	UNP Q8R502
F	781	ARG	GLY	conflict	UNP Q8R502
F	804	ALA	-	expression tag	UNP Q8R502
F	805	LEU	-	expression tag	UNP Q8R502
F	806	GLU	-	expression tag	UNP Q8R502
F	807	VAL	-	expression tag	UNP Q8R502
F	808	LEU	-	expression tag	UNP Q8R502
F	809	PHE	-	expression tag	UNP Q8R502
F	810	GLN	-	expression tag	UNP Q8R502

3 Residue-property plots

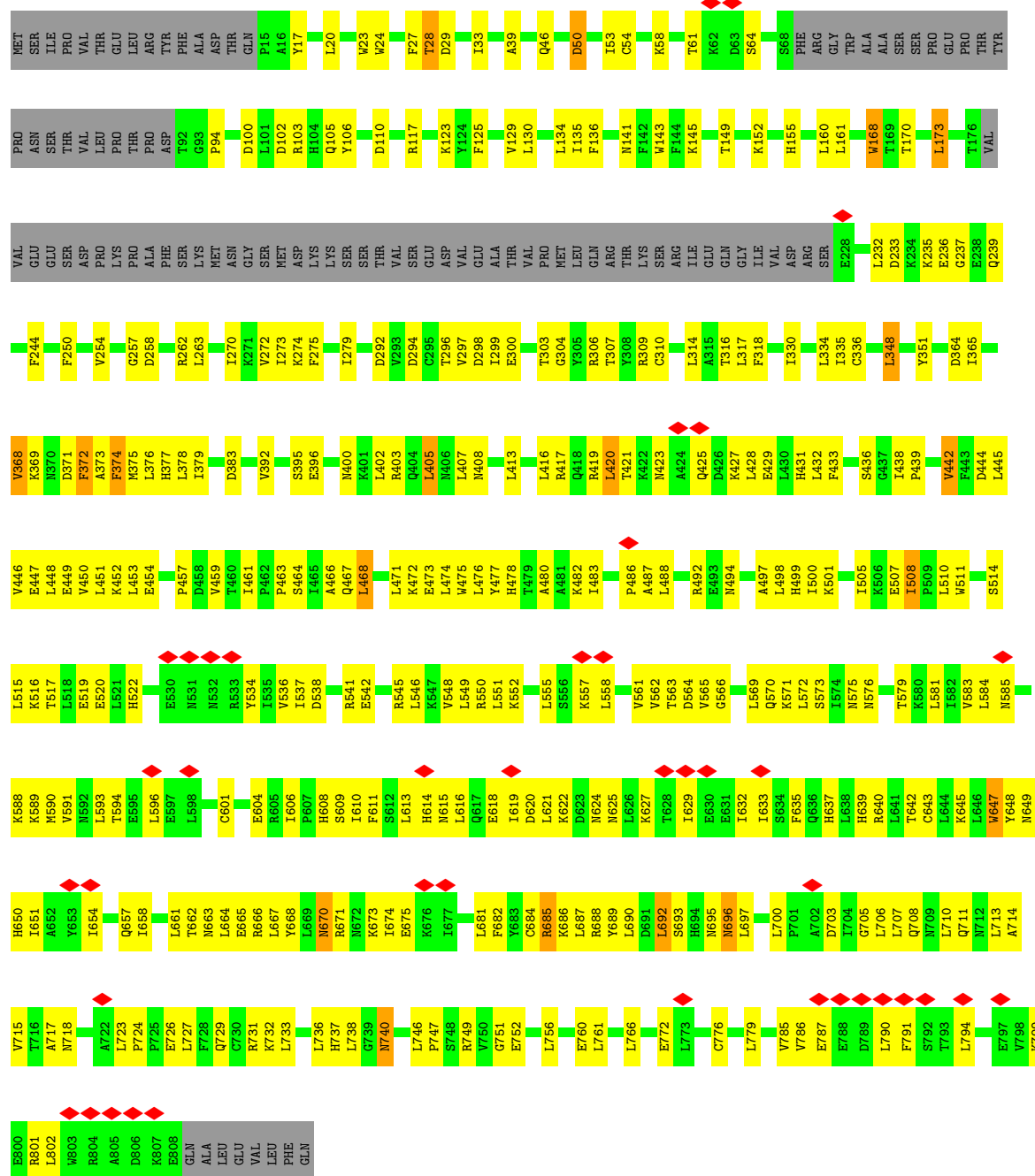
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Volume-regulated anion channel subunit LRRC8A



• Molecule 1: Volume-regulated anion channel subunit LRRC8A

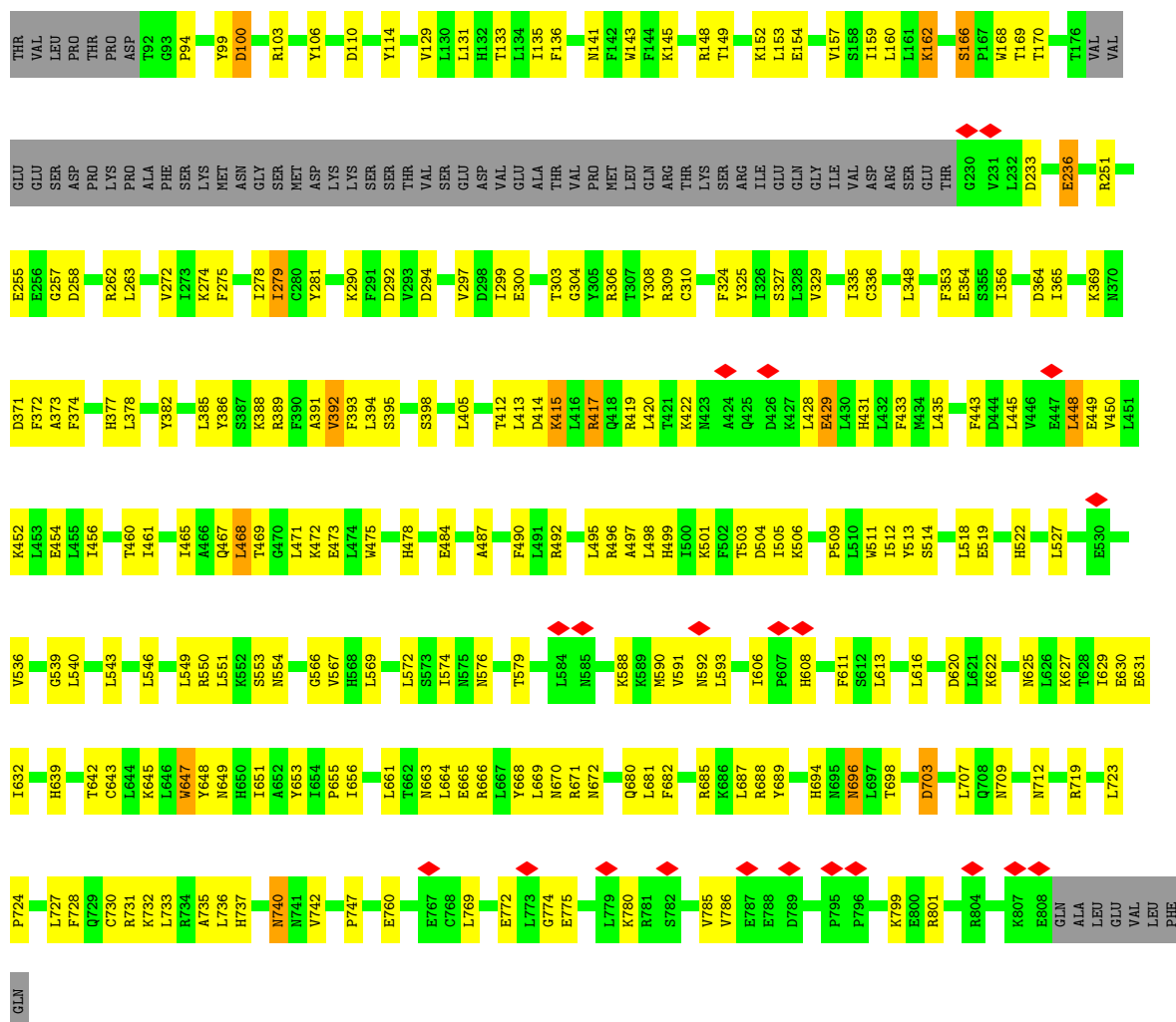
Chain B: 



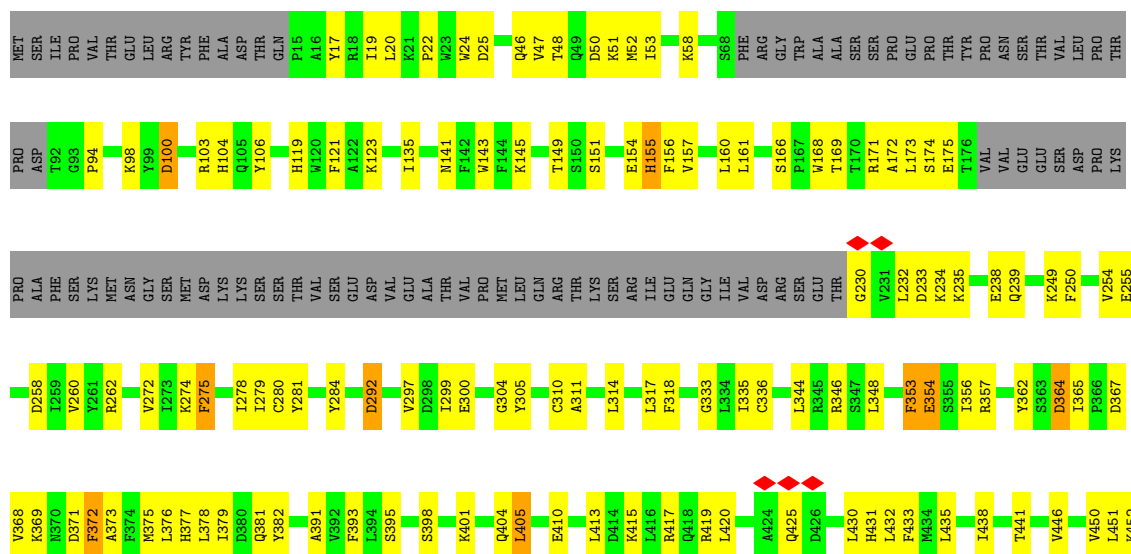
• Molecule 1: Volume-regulated anion channel subunit LRRC8A

Chain C: 

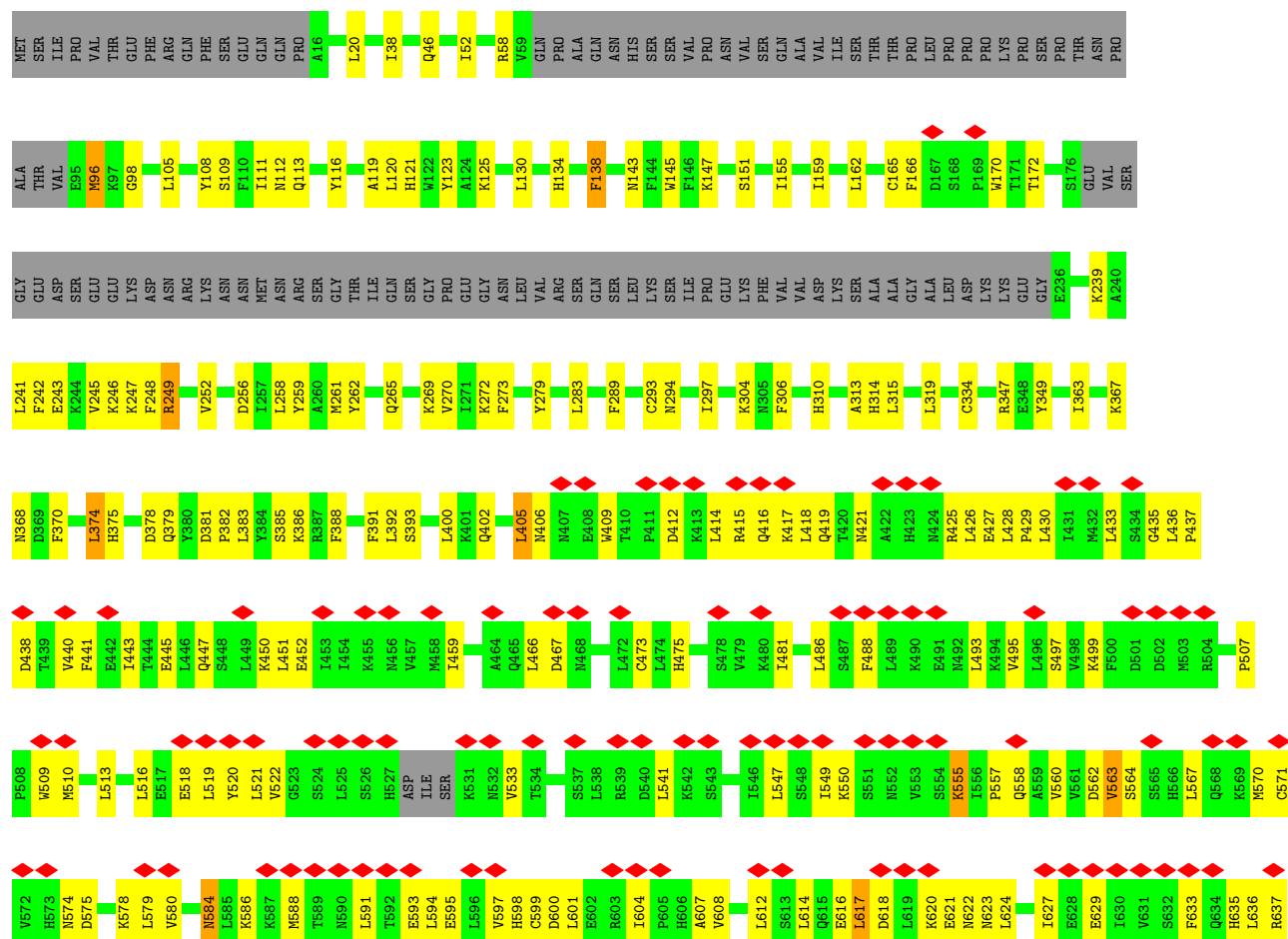


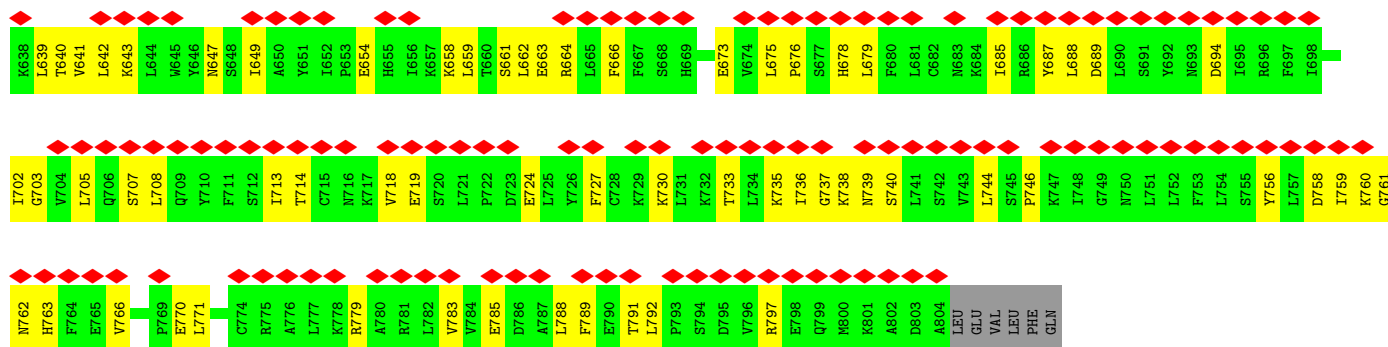


• Molecule 1: Volume-regulated anion channel subunit LRRC8A

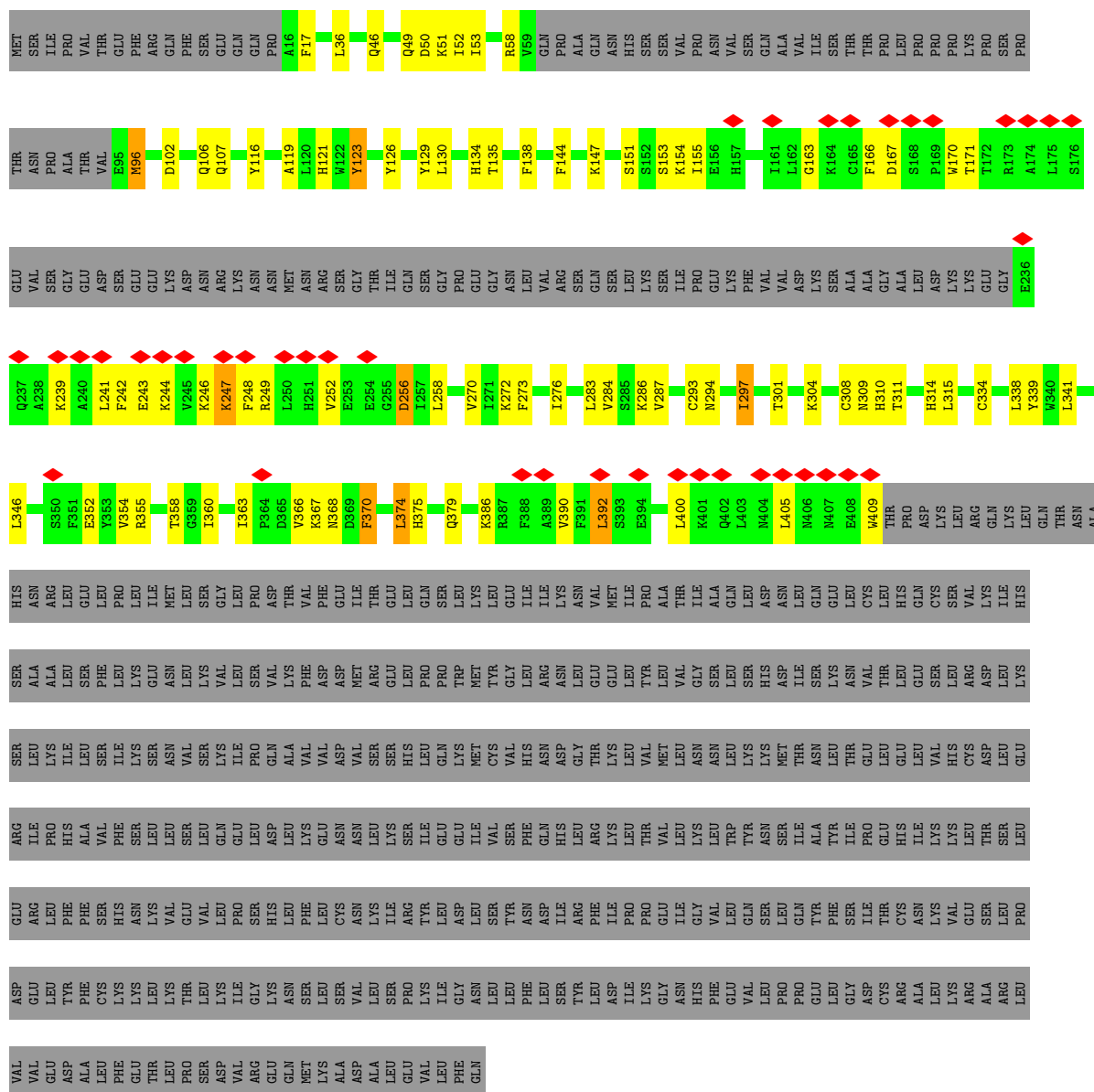


- Molecule 2: Volume-regulated anion channel subunit LRRC8C





• Molecule 2: Volume-regulated anion channel subunit LRRC8C



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	119006	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	67	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.050	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	437.47202, 437.47202, 437.47202	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.302, 1.302, 1.302	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.25	0/6055	0.47	0/8207
1	B	0.25	0/6071	0.48	0/8229
1	C	0.25	0/6055	0.47	0/8207
1	D	0.25	0/6055	0.47	0/8207
2	E	0.25	0/5762	0.45	0/7789
2	F	0.26	0/2576	0.43	0/3481
All	All	0.25	0/32574	0.47	0/44120

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5922	0	6081	182	0
1	B	5938	0	6094	241	0
1	C	5922	0	6081	165	0
1	D	5922	0	6081	168	0
2	E	5638	0	5753	158	0
2	F	2507	0	2490	58	0
All	All	31849	0	32580	955	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 15.

All (955) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:571:LYS:HG3	1:D:595:GLU:HB2	1.60	0.81
1:B:737:HIS:HA	1:B:760:GLU:HB3	1.63	0.80
1:C:449:GLU:HA	1:C:471:LEU:HA	1.65	0.79
1:B:233:ASP:HB3	1:B:236:GLU:HB3	1.65	0.78
2:E:707:SER:HA	2:E:730:LYS:HD2	1.66	0.77
1:A:171:ARG:HH21	1:A:230:GLY:HA3	1.50	0.76
1:B:429:GLU:HB2	1:B:450:VAL:HB	1.68	0.76
2:E:119:ALA:HB2	2:E:293:CYS:HB3	1.69	0.75
1:D:258:ASP:H	1:D:371:ASP:HB2	1.49	0.75
1:A:419:ARG:NH1	1:A:431:HIS:O	2.20	0.74
2:E:620:LYS:HG2	2:E:621:GLU:HG3	1.70	0.73
2:E:702:ILE:HG13	2:E:705:LEU:HD12	1.69	0.73
2:E:497:SER:HA	2:E:520:TYR:HB2	1.71	0.73
1:B:373:ALA:O	1:B:377:HIS:ND1	2.21	0.72
2:F:363:ILE:HG23	2:F:392:LEU:HD12	1.71	0.72
1:A:292:ASP:OD2	1:A:309:ARG:NH2	2.23	0.72
2:E:499:LYS:HG2	2:E:522:VAL:HB	1.72	0.72
1:C:728:PHE:O	1:C:731:ARG:NH1	2.23	0.71
2:E:475:HIS:HA	2:E:499:LYS:HB2	1.72	0.71
2:F:239:LYS:O	2:F:242:PHE:HB2	1.89	0.71
1:D:450:VAL:HG22	1:D:473:GLU:HB2	1.71	0.71
1:A:473:GLU:HG2	1:A:497:ALA:HB3	1.72	0.71
1:A:726:GLU:HA	1:A:729:GLN:HG2	1.72	0.70
2:E:673:GLU:HA	2:E:694:ASP:HB2	1.71	0.70
1:B:633:ILE:HB	1:B:657:GLN:HB3	1.72	0.70
1:B:541:ARG:HG3	1:B:561:VAL:HG23	1.74	0.70
2:E:429:PRO:HA	2:E:450:LYS:HB3	1.73	0.70
1:B:632:ILE:O	1:B:635:PHE:HB2	1.90	0.69
1:B:538:ASP:HA	1:B:561:VAL:HG21	1.73	0.69
2:E:495:VAL:HG13	2:E:518:GLU:HB2	1.75	0.69
2:E:595:GLU:HA	2:E:618:ASP:HB3	1.74	0.69
1:B:522:HIS:HA	1:B:550:ARG:HB3	1.73	0.69
1:B:620:ASP:HA	1:B:645:LYS:HB2	1.73	0.69
2:E:155:ILE:HD11	2:E:258:LEU:HD11	1.75	0.68
1:B:448:LEU:HG	1:B:471:LEU:HD13	1.75	0.68
1:A:103:ARG:HH12	2:F:106:GLN:HE21	1.39	0.68
2:F:239:LYS:HA	2:F:242:PHE:HD1	1.58	0.68
1:A:171:ARG:HD2	1:A:232:LEU:HD11	1.76	0.68
1:B:473:GLU:HG2	1:B:497:ALA:HB3	1.76	0.68
1:B:675:GLU:HG2	1:B:696:ASN:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:469:THR:HA	1:C:490:PHE:HZ	1.57	0.68
1:D:141:ASN:HB3	1:D:145:LYS:HG2	1.76	0.67
1:C:452:LYS:HA	1:C:475:TRP:HB2	1.76	0.67
1:A:364:ASP:N	1:A:364:ASP:OD1	2.25	0.67
2:E:52:ILE:HG12	2:E:310:HIS:HB3	1.77	0.67
2:E:294:ASN:HB3	2:E:304:LYS:HE2	1.75	0.67
2:E:738:LYS:HG2	2:E:761:GLY:HA3	1.76	0.67
1:B:405:LEU:HD13	1:B:408:ASN:HD22	1.60	0.66
1:C:519:GLU:HA	1:C:546:LEU:HA	1.77	0.66
1:B:232:LEU:HD23	1:B:405:LEU:HG	1.78	0.66
2:F:52:ILE:HG12	2:F:310:HIS:HB3	1.77	0.66
1:A:566:GLY:HA2	1:A:569:LEU:HG	1.78	0.66
1:B:794:LEU:O	1:B:799:LYS:NZ	2.28	0.66
1:B:400:ASN:OD1	1:B:403:ARG:NH2	2.28	0.66
1:A:714:ALA:HA	1:A:737:HIS:HB2	1.77	0.66
1:B:736:LEU:HD22	1:B:738:LEU:HD21	1.76	0.66
1:D:373:ALA:O	1:D:377:HIS:ND1	2.26	0.66
2:E:243:GLU:HA	2:E:246:LYS:HE3	1.78	0.66
2:E:618:ASP:HA	2:E:643:LYS:HB2	1.78	0.65
1:A:420:LEU:HD13	1:A:430:LEU:HB2	1.76	0.65
1:D:721:GLU:HA	1:D:743:LEU:HA	1.78	0.65
1:D:675:GLU:HG2	1:D:696:ASN:HB2	1.79	0.65
1:A:389:ARG:HH21	2:F:247:LYS:HE2	1.60	0.65
1:A:709:ASN:HA	1:A:732:LYS:HD2	1.78	0.65
1:A:58:LYS:NZ	1:B:94:PRO:O	2.29	0.65
1:A:693:SER:O	1:A:695:ASN:ND2	2.30	0.65
1:B:576:ASN:HB2	1:B:601:CYS:HA	1.77	0.65
1:D:779:LEU:HG	1:D:802:LEU:HD21	1.79	0.64
1:A:452:LYS:HA	1:A:475:TRP:HB2	1.78	0.64
1:A:692:LEU:HB2	1:A:715:VAL:HG12	1.80	0.64
1:D:567:VAL:O	1:D:592:ASN:ND2	2.29	0.64
1:C:513:TYR:OH	1:C:536:VAL:O	2.13	0.64
1:A:781:ARG:NH1	1:A:784:LEU:O	2.30	0.64
1:C:300:GLU:HA	1:C:304:GLY:H	1.61	0.64
1:B:696:ASN:N	1:B:696:ASN:OD1	2.31	0.64
1:D:354:GLU:HA	1:D:357:ARG:HE	1.63	0.64
1:A:164:PHE:O	1:A:389:ARG:NH1	2.31	0.64
1:B:463:PRO:HB3	1:B:486:PRO:HB2	1.79	0.64
1:B:492:ARG:O	1:B:517:THR:OG1	2.12	0.64
1:B:760:GLU:HA	1:B:785:VAL:HB	1.79	0.64
1:A:760:GLU:HA	1:A:785:VAL:HB	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:ARG:NH1	1:A:573:SER:OG	2.32	0.63
2:E:96:MET:SD	2:E:96:MET:N	2.71	0.63
2:E:239:LYS:O	2:E:242:PHE:HB2	1.99	0.63
2:E:521:LEU:HD23	2:E:549:ILE:HG12	1.79	0.63
2:F:134:HIS:O	2:F:272:LYS:NZ	2.31	0.63
2:E:567:LEU:HD21	2:E:570:MET:HB2	1.79	0.63
1:B:476:LEU:O	1:B:501:LYS:N	2.28	0.63
1:A:292:ASP:OD1	1:A:292:ASP:N	2.32	0.63
1:C:103:ARG:HA	1:C:106:TYR:HD2	1.63	0.63
1:A:450:VAL:HG22	1:A:473:GLU:HB2	1.80	0.62
1:A:232:LEU:O	1:A:409:ASN:ND2	2.31	0.62
1:D:634:SER:O	1:D:637:HIS:ND1	2.31	0.62
1:C:760:GLU:HA	1:C:785:VAL:HB	1.79	0.62
1:A:46:GLN:NE2	1:A:123:LYS:O	2.32	0.62
1:A:582:ILE:HG23	1:A:584:LEU:HG	1.81	0.62
1:A:163:CYS:HA	1:A:243:LEU:HD21	1.81	0.62
1:A:258:ASP:O	1:A:262:ARG:NH1	2.31	0.62
1:A:598:LEU:HB2	1:A:621:LEU:HD23	1.82	0.62
1:D:348:LEU:HD23	1:D:348:LEU:H	1.64	0.62
2:F:171:THR:HA	2:F:390:VAL:HG11	1.82	0.62
1:D:292:ASP:OD1	1:D:292:ASP:N	2.33	0.62
2:F:242:PHE:HE1	2:F:400:LEU:HD23	1.64	0.62
1:A:98:LYS:HE2	2:F:102:ASP:HB2	1.80	0.62
1:B:476:LEU:N	1:B:499:HIS:O	2.31	0.62
1:D:721:GLU:HB3	1:D:742:VAL:HG23	1.81	0.62
1:D:552:LYS:HG3	1:D:575:ASN:HB3	1.82	0.62
1:B:670:ASN:OD1	1:B:670:ASN:N	2.31	0.61
2:F:366:VAL:HB	2:F:370:PHE:HB3	1.83	0.61
1:B:670:ASN:HB3	1:B:693:SER:H	1.64	0.61
1:B:604:GLU:OE1	1:B:627:LYS:NZ	2.32	0.61
1:B:629:ILE:HD13	1:B:651:ILE:HD13	1.81	0.61
1:D:419:ARG:NH1	1:D:431:HIS:O	2.29	0.61
1:B:451:LEU:HB2	1:B:471:LEU:HD11	1.83	0.61
1:D:46:GLN:NE2	1:D:123:LYS:O	2.27	0.61
1:A:696:ASN:OD1	1:A:696:ASN:N	2.34	0.61
2:E:578:LYS:NZ	2:E:600:ASP:O	2.30	0.61
1:B:801:ARG:HH21	1:B:802:LEU:HD23	1.66	0.61
1:C:495:LEU:HD21	1:C:498:LEU:HD13	1.83	0.61
1:D:258:ASP:O	1:D:262:ARG:NH1	2.34	0.60
1:B:453:LEU:HD12	1:B:476:LEU:HD23	1.83	0.60
2:E:421:ASN:OD1	2:E:425:ARG:N	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:513:LEU:HD12	2:E:516:LEU:HD22	1.83	0.60
1:A:591:VAL:O	1:A:615:ASN:ND2	2.34	0.60
1:A:618:GLU:HG2	1:A:643:CYS:HB3	1.84	0.60
1:C:413:LEU:HD22	1:C:417:ARG:HH22	1.66	0.60
1:C:554:ASN:OD1	1:C:579:THR:OG1	2.17	0.60
1:B:24:TRP:O	1:B:28:THR:OG1	2.17	0.60
1:B:613:LEU:HB3	1:B:616:LEU:HD13	1.84	0.60
1:C:472:LYS:HD2	1:C:496:ARG:HG2	1.83	0.60
1:B:463:PRO:HA	1:B:487:ALA:HB2	1.83	0.60
1:C:258:ASP:HA	1:C:371:ASP:HB2	1.83	0.60
1:D:155:HIS:HB3	1:D:250:PHE:CE1	2.37	0.60
1:B:590:MET:HE3	1:B:593:LEU:HD22	1.83	0.59
1:D:300:GLU:HA	1:D:304:GLY:H	1.66	0.59
1:B:423:ASN:HB3	1:B:429:GLU:HB3	1.82	0.59
1:B:368:VAL:HG21	1:B:376:LEU:HD12	1.85	0.59
1:C:499:HIS:HA	1:C:522:HIS:HB2	1.84	0.59
2:E:616:GLU:HA	2:E:641:VAL:HB	1.83	0.59
2:E:771:LEU:HD12	2:E:792:LEU:HD21	1.84	0.59
1:A:392:VAL:O	1:A:395:SER:OG	2.20	0.59
2:E:113:GLN:HG2	2:F:311:THR:HG22	1.85	0.59
2:E:473:CYS:HA	2:E:497:SER:HB2	1.84	0.59
1:B:693:SER:O	1:B:695:ASN:ND2	2.36	0.59
1:D:760:GLU:HA	1:D:785:VAL:HB	1.83	0.59
1:C:255:GLU:HG3	1:C:369:LYS:HB2	1.85	0.59
1:B:756:LEU:HD23	1:B:779:LEU:HD22	1.84	0.59
2:E:586:LYS:HG2	2:E:607:ALA:HA	1.85	0.59
1:A:116:ASN:HB3	1:A:117:ARG:HH11	1.68	0.58
1:A:665:GLU:O	1:A:688:ARG:N	2.29	0.58
1:B:438:ILE:HG13	1:B:459:VAL:HG21	1.86	0.58
1:B:58:LYS:NZ	1:C:94:PRO:O	2.30	0.58
1:D:548:VAL:HG13	1:D:571:LYS:HD3	1.85	0.58
1:D:551:LEU:HD12	1:D:574:ILE:HG12	1.84	0.58
2:E:714:THR:HA	2:E:737:GLY:HA3	1.84	0.58
1:A:135:ILE:HG12	1:A:274:LYS:HZ3	1.66	0.58
2:E:450:LYS:HA	2:E:473:CYS:HB3	1.85	0.58
1:C:620:ASP:HB2	1:C:645:LYS:HD2	1.85	0.58
2:F:96:MET:SD	2:F:96:MET:N	2.72	0.58
1:C:472:LYS:HB3	1:C:496:ARG:HB2	1.84	0.58
1:A:625:ASN:O	1:A:627:LYS:NZ	2.36	0.58
1:B:591:VAL:O	1:B:615:ASN:ND2	2.36	0.58
2:F:153:SER:OG	2:F:154:LYS:NZ	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:481:ILE:HD13	2:E:486:LEU:HB2	1.85	0.58
1:B:272:VAL:HG22	1:B:336:CYS:HB3	1.86	0.57
1:B:292:ASP:OD2	1:B:309:ARG:NH2	2.36	0.57
2:E:438:ASP:HA	2:E:441:PHE:HD2	1.69	0.57
1:B:647:TRP:O	1:B:649:ASN:ND2	2.37	0.57
1:C:251:ARG:O	1:C:255:GLU:HB3	2.04	0.57
2:E:622:ASN:HB3	2:E:624:LEU:HD13	1.86	0.57
1:B:152:LYS:HZ3	1:B:257:GLY:HA3	1.68	0.57
1:C:373:ALA:O	1:C:377:HIS:ND1	2.37	0.57
1:C:429:GLU:HG3	1:C:452:LYS:HE3	1.86	0.57
2:F:352:GLU:OE1	2:F:355:ARG:NH2	2.37	0.57
1:D:364:ASP:OD1	1:D:364:ASP:N	2.38	0.57
1:C:135:ILE:HG23	1:C:274:LYS:HZ2	1.69	0.57
2:E:608:VAL:HG11	2:E:617:LEU:HD11	1.86	0.57
1:A:300:GLU:HA	1:A:304:GLY:H	1.69	0.57
1:C:696:ASN:OD1	1:C:696:ASN:N	2.37	0.57
1:B:620:ASP:HB2	1:B:645:LYS:HD2	1.85	0.57
1:B:670:ASN:HB3	1:B:693:SER:N	2.20	0.57
1:A:711:GLN:O	1:A:734:ARG:N	2.28	0.57
1:D:454:GLU:HG2	1:D:455:LEU:HG	1.86	0.57
1:D:473:GLU:HG2	1:D:497:ALA:HB3	1.87	0.57
2:E:52:ILE:HD11	2:E:120:LEU:HD22	1.85	0.57
1:B:24:TRP:HB2	1:B:335:ILE:HG23	1.86	0.56
1:B:431:HIS:HA	1:B:452:LYS:HB2	1.85	0.56
2:E:419:GLN:O	2:E:427:GLU:N	2.34	0.56
2:E:170:TRP:CZ2	2:E:400:LEU:HB2	2.39	0.56
2:F:126:TYR:HA	2:F:129:TYR:HD2	1.70	0.56
1:A:776:CYS:O	1:A:801:ARG:NH2	2.39	0.56
1:B:364:ASP:HB3	1:B:396:GLU:HB3	1.88	0.56
1:B:649:ASN:O	1:B:673:LYS:NZ	2.38	0.56
1:B:733:LEU:HD21	1:B:736:LEU:HD21	1.87	0.56
1:C:518:LEU:HB3	1:C:543:LEU:HD22	1.86	0.56
2:E:113:GLN:HE22	2:F:53:ILE:HB	1.70	0.56
2:E:588:MET:HB3	2:E:591:LEU:HB2	1.87	0.56
1:A:567:VAL:O	1:A:592:ASN:ND2	2.38	0.56
1:C:58:LYS:NZ	1:D:94:PRO:O	2.38	0.56
1:C:258:ASP:O	1:C:262:ARG:NH1	2.39	0.56
1:C:513:TYR:CG	1:C:539:GLY:HA3	2.41	0.56
1:C:629:ILE:HD13	1:C:651:ILE:HD13	1.88	0.56
1:D:665:GLU:O	1:D:688:ARG:N	2.29	0.56
1:B:348:LEU:HD12	1:B:374:PHE:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:717:ALA:HA	1:B:740:ASN:HB2	1.88	0.56
1:C:169:THR:HG23	1:C:393:PHE:HE1	1.71	0.56
1:B:658:ILE:HG13	1:B:661:LEU:HD22	1.87	0.56
1:D:742:VAL:HA	1:D:765:ARG:HD3	1.86	0.56
2:E:245:VAL:HG21	2:E:391:PHE:HB3	1.87	0.56
2:E:459:ILE:HB	2:E:481:ILE:HG22	1.88	0.56
2:F:121:HIS:HE1	2:F:283:LEU:HD22	1.71	0.56
2:E:766:VAL:HA	2:E:791:THR:HG21	1.87	0.56
1:B:715:VAL:O	1:B:718:ASN:ND2	2.39	0.56
1:D:632:ILE:O	1:D:635:PHE:HB2	2.06	0.56
1:B:576:ASN:HD22	1:B:579:THR:HB	1.71	0.56
1:C:551:LEU:HD12	1:C:574:ILE:HG12	1.88	0.56
1:C:567:VAL:O	1:C:592:ASN:ND2	2.25	0.56
2:E:436:LEU:HD11	2:E:459:ILE:HG12	1.88	0.56
2:E:705:LEU:HB3	2:E:708:LEU:HB2	1.88	0.56
1:A:234:LYS:O	1:A:238:GLU:HG2	2.05	0.56
1:B:446:VAL:HA	1:B:468:LEU:HA	1.88	0.56
1:B:448:LEU:HD21	1:B:451:LEU:HD13	1.88	0.55
1:B:453:LEU:O	1:B:477:TYR:HB2	2.06	0.55
1:C:647:TRP:H	1:C:647:TRP:HD1	1.51	0.55
2:E:785:GLU:HG2	2:E:788:LEU:HD22	1.88	0.55
1:A:558:LEU:HD22	1:A:583:VAL:HG12	1.89	0.55
2:F:270:VAL:HG22	2:F:334:CYS:HB3	1.89	0.55
2:E:687:TYR:HE1	2:E:689:ASP:HB2	1.72	0.55
2:E:737:GLY:O	2:E:762:ASN:ND2	2.37	0.55
1:B:476:LEU:HD12	1:B:500:ILE:HG23	1.88	0.55
2:F:294:ASN:HB3	2:F:304:LYS:HE2	1.88	0.55
1:B:292:ASP:OD1	1:B:292:ASP:N	2.40	0.55
1:B:461:ILE:HB	1:B:483:ILE:HG13	1.88	0.55
1:B:662:THR:HA	1:B:684:CYS:HA	1.89	0.55
1:D:438:ILE:HG13	1:D:459:VAL:HG21	1.89	0.55
2:E:736:ILE:O	2:E:739:ASN:ND2	2.40	0.55
1:D:550:ARG:NH1	1:D:573:SER:OG	2.39	0.55
1:B:416:LEU:HD13	1:B:442:VAL:HA	1.88	0.55
1:C:774:GLY:O	1:C:801:ARG:NH2	2.40	0.55
1:D:24:TRP:HB2	1:D:335:ILE:HG23	1.89	0.55
1:C:712:ASN:HA	1:C:735:ALA:HB3	1.88	0.55
2:E:430:LEU:HD12	2:E:451:LEU:HG	1.89	0.55
1:C:665:GLU:OE1	1:C:688:ARG:NE	2.36	0.54
1:D:53:ILE:O	1:D:310:CYS:HA	2.07	0.54
1:B:348:LEU:H	1:B:348:LEU:HD23	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:711:GLN:HA	1:B:733:LEU:HA	1.89	0.54
1:C:632:ILE:HD11	1:C:655:PRO:HB2	1.88	0.54
1:A:373:ALA:O	1:A:377:HIS:ND1	2.39	0.54
1:C:509:PRO:HB2	1:C:512:ILE:HG23	1.89	0.54
1:B:550:ARG:HH12	1:B:575:ASN:HB2	1.73	0.54
1:B:700:LEU:HB2	1:B:724:PRO:HG3	1.89	0.54
1:B:766:LEU:HB2	1:B:790:LEU:HD13	1.90	0.54
1:C:689:TYR:HA	1:C:712:ASN:HB2	1.89	0.54
1:D:272:VAL:HG22	1:D:336:CYS:HB3	1.88	0.54
1:D:688:ARG:HA	1:D:710:LEU:HA	1.89	0.54
2:E:597:VAL:HG22	2:E:620:LYS:HB3	1.89	0.54
2:E:659:LEU:HB3	2:E:662:LEU:HG	1.87	0.54
2:E:405:LEU:HG	2:E:409:TRP:HD1	1.72	0.54
2:E:570:MET:H	2:E:591:LEU:HD11	1.72	0.54
1:A:504:ASP:OD1	1:A:505:ILE:N	2.38	0.54
1:C:492:ARG:HH21	1:C:514:SER:HB2	1.73	0.54
1:A:688:ARG:HA	1:A:710:LEU:HA	1.90	0.54
1:B:664:LEU:HB2	1:B:684:CYS:HB3	1.88	0.54
1:C:669:LEU:O	1:C:672:ASN:ND2	2.40	0.54
2:E:627:ILE:HD13	2:E:649:ILE:HD13	1.89	0.54
2:F:243:GLU:O	2:F:246:LYS:HG2	2.06	0.54
1:A:356:ILE:HD13	1:A:391:ALA:HB3	1.90	0.54
1:B:46:GLN:HB2	1:B:318:PHE:HZ	1.72	0.54
1:C:52:MET:HG3	1:C:114:TYR:HD1	1.72	0.54
1:B:258:ASP:O	1:B:262:ARG:NH1	2.41	0.54
1:B:551:LEU:O	1:B:575:ASN:N	2.30	0.54
2:F:354:VAL:O	2:F:358:THR:OG1	2.24	0.54
1:A:460:THR:HA	1:A:482:LYS:O	2.07	0.53
1:B:416:LEU:HB3	1:B:445:LEU:HD11	1.90	0.53
1:B:520:GLU:HA	1:B:548:VAL:HB	1.90	0.53
1:C:608:HIS:HA	1:C:611:PHE:HD2	1.73	0.53
1:D:149:THR:HG22	1:D:260:VAL:HG22	1.90	0.53
1:D:156:PHE:HD1	1:D:250:PHE:HE2	1.56	0.53
2:E:406:ASN:ND2	2:E:437:PRO:HA	2.23	0.53
2:E:467:ASP:HA	2:E:488:PHE:HZ	1.73	0.53
1:A:788:GLU:HA	1:A:791:PHE:HB3	1.90	0.53
2:E:414:LEU:HD22	2:E:428:LEU:HD21	1.91	0.53
1:A:49:GLN:O	1:A:51:LYS:NZ	2.41	0.53
1:A:663:ASN:OD1	1:A:663:ASN:N	2.39	0.53
1:C:698:THR:HG22	1:C:719:ARG:HB2	1.90	0.53
1:B:17:TYR:HA	1:B:20:LEU:HD23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:ILE:N	1:B:522:HIS:O	2.38	0.53
1:C:166:SER:O	1:C:169:THR:OG1	2.26	0.53
1:D:580:LYS:NZ	1:D:603:LEU:O	2.41	0.53
1:D:47:VAL:HG12	1:D:48:THR:HG23	1.90	0.53
2:E:426:LEU:HB3	2:E:447:GLN:H	1.73	0.53
1:B:498:LEU:N	1:B:520:GLU:O	2.36	0.53
1:C:670:ASN:HD22	1:C:671:ARG:HG2	1.73	0.53
1:D:103:ARG:HA	1:D:106:TYR:HD2	1.74	0.53
1:D:629:ILE:HD13	1:D:651:ILE:HD13	1.90	0.53
1:D:740:ASN:N	1:D:762:ARG:O	2.41	0.53
1:C:671:ARG:HD3	1:C:694:HIS:HB2	1.91	0.53
1:D:670:ASN:OD1	1:D:670:ASN:N	2.33	0.53
1:B:505:ILE:HD12	1:B:536:VAL:HG11	1.91	0.52
1:C:39:ALA:HB2	1:C:129:VAL:HG12	1.91	0.52
1:D:693:SER:O	1:D:695:ASN:ND2	2.43	0.52
1:B:379:ILE:O	1:B:383:ASP:N	2.32	0.52
1:D:726:GLU:HA	1:D:729:GLN:HG2	1.90	0.52
2:E:746:PRO:HB3	2:E:770:GLU:HG3	1.91	0.52
1:C:473:GLU:HG2	1:C:497:ALA:HB3	1.91	0.52
1:B:452:LYS:HA	1:B:475:TRP:HB2	1.91	0.52
1:C:723:LEU:HB2	1:C:747:PRO:HG2	1.90	0.52
2:E:38:ILE:HG23	2:E:319:LEU:HD11	1.92	0.52
1:A:237:GLY:HA3	1:A:406:ASN:HD21	1.73	0.52
1:A:505:ILE:HD12	1:A:536:VAL:HG11	1.91	0.52
1:C:364:ASP:O	1:C:395:SER:HA	2.08	0.52
1:A:705:GLY:O	1:A:708:GLN:NE2	2.43	0.52
1:B:692:LEU:HD22	1:B:697:LEU:HD11	1.92	0.52
1:A:429:GLU:HG3	1:A:452:LYS:HE3	1.91	0.52
1:B:642:THR:HG22	1:B:665:GLU:HG3	1.92	0.52
1:C:54:CYS:N	1:C:110:ASP:OD1	2.43	0.52
2:F:144:PHE:HA	2:F:147:LYS:HB2	1.91	0.52
1:A:725:PRO:HA	1:A:728:PHE:HD2	1.74	0.52
1:B:298:ASP:OD1	1:B:306:ARG:NH1	2.43	0.52
1:B:299:ILE:O	1:B:303:THR:OG1	2.26	0.52
1:D:794:LEU:O	1:D:799:LYS:NZ	2.30	0.52
2:E:405:LEU:HG	2:E:409:TRP:CD1	2.45	0.52
2:E:52:ILE:HD12	2:E:116:TYR:HA	1.92	0.52
1:D:235:LYS:O	1:D:239:GLN:HG2	2.09	0.51
1:A:633:ILE:HD13	1:A:657:GLN:HG2	1.92	0.51
1:B:294:ASP:OD1	1:B:309:ARG:NH1	2.43	0.51
1:D:232:LEU:HD23	1:D:405:LEU:HG	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:516:LEU:HD21	2:E:519:LEU:HD13	1.90	0.51
1:C:630:GLU:OE2	1:C:653:TYR:OH	2.21	0.51
1:D:602:ASP:OD1	1:D:625:ASN:ND2	2.44	0.51
2:E:564:SER:HA	2:E:567:LEU:HB3	1.91	0.51
2:E:675:LEU:HD23	2:E:675:LEU:H	1.75	0.51
1:B:431:HIS:CE1	1:B:454:GLU:HB2	2.46	0.51
1:C:46:GLN:HA	1:C:50:ASP:HB2	1.92	0.51
2:E:46:GLN:NE2	2:E:125:LYS:O	2.43	0.51
2:E:417:LYS:NZ	2:E:429:PRO:O	2.26	0.51
2:E:654:GLU:HA	2:E:678:HIS:CD2	2.46	0.51
1:C:546:LEU:HD21	1:C:549:LEU:HD13	1.92	0.51
1:D:478:HIS:N	1:D:501:LYS:O	2.43	0.51
2:E:493:LEU:HD23	2:E:513:LEU:HD13	1.93	0.51
1:A:115:GLU:OE2	1:B:316:THR:OG1	2.28	0.51
1:B:658:ILE:HA	1:B:661:LEU:HD13	1.92	0.51
1:C:53:ILE:O	1:C:310:CYS:HA	2.10	0.51
2:E:108:TYR:O	2:E:112:ASN:ND2	2.43	0.51
2:E:637:ARG:NH1	2:E:658:LYS:O	2.43	0.51
2:E:713:ILE:HD12	2:E:718:VAL:HG21	1.92	0.51
1:A:611:PHE:HZ	1:A:631:GLU:HB3	1.76	0.51
1:A:773:LEU:HD23	1:A:794:LEU:HD21	1.92	0.51
1:B:499:HIS:HA	1:B:522:HIS:HB2	1.92	0.51
1:B:714:ALA:HA	1:B:737:HIS:HB2	1.93	0.51
1:C:160:LEU:HD11	1:C:386:TYR:HB3	1.92	0.51
1:D:658:ILE:HA	1:D:661:LEU:HD13	1.93	0.51
1:C:419:ARG:NH2	1:C:431:HIS:O	2.39	0.51
2:E:788:LEU:O	2:E:791:THR:OG1	2.26	0.51
2:F:119:ALA:HB2	2:F:293:CYS:HB3	1.91	0.51
2:F:354:VAL:HG12	2:F:360:ILE:HD11	1.92	0.51
1:B:658:ILE:HD13	1:B:681:LEU:HD13	1.93	0.51
1:A:103:ARG:HH12	2:F:106:GLN:HB2	1.76	0.51
1:A:119:HIS:CD2	1:A:121:PHE:HB3	2.46	0.51
1:C:299:ILE:O	1:C:303:THR:OG1	2.19	0.51
1:C:665:GLU:HA	1:C:687:LEU:HA	1.92	0.51
1:D:415:LYS:O	1:D:419:ARG:HB2	2.11	0.51
2:E:688:LEU:HB2	2:E:708:LEU:HD11	1.93	0.51
1:A:477:TYR:HA	1:A:501:LYS:HB3	1.92	0.50
1:D:453:LEU:O	1:D:477:TYR:N	2.40	0.50
1:A:463:PRO:HB3	1:A:486:PRO:HB2	1.94	0.50
1:A:615:ASN:HA	1:A:640:ARG:HH21	1.76	0.50
1:C:422:LYS:HG2	1:C:428:LEU:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ASP:H	1:A:105:GLN:HE21	1.59	0.50
1:B:46:GLN:O	1:B:50:ASP:HB3	2.11	0.50
1:B:618:GLU:HG3	1:B:643:CYS:HB3	1.93	0.50
1:A:354:GLU:HA	1:A:357:ARG:HG2	1.93	0.50
2:E:412:ASP:OD1	2:E:416:GLN:NE2	2.45	0.50
1:B:427:LYS:HB3	1:B:449:GLU:HB3	1.94	0.50
1:B:475:TRP:HA	1:B:499:HIS:HB2	1.92	0.50
1:D:413:LEU:HB3	1:D:417:ARG:HH22	1.75	0.50
1:A:469:THR:HA	1:A:490:PHE:HZ	1.76	0.50
1:B:61:THR:N	1:B:64:SER:O	2.43	0.50
1:D:632:ILE:O	1:D:661:LEU:HD11	2.12	0.50
2:E:574:ASN:HD21	2:E:599:CYS:HA	1.77	0.50
2:E:759:ILE:O	2:E:762:ASN:ND2	2.44	0.50
2:F:155:ILE:HD11	2:F:258:LEU:HD11	1.94	0.50
1:B:451:LEU:O	1:B:475:TRP:N	2.44	0.50
1:B:776:CYS:HB2	1:B:779:LEU:HB3	1.94	0.50
1:C:135:ILE:HG23	1:C:274:LYS:NZ	2.27	0.50
1:A:614:HIS:O	1:A:640:ARG:NH2	2.45	0.50
1:B:258:ASP:HA	1:B:371:ASP:HB2	1.93	0.50
1:B:665:GLU:O	1:B:688:ARG:N	2.44	0.50
1:D:452:LYS:HA	1:D:475:TRP:HB2	1.93	0.50
1:D:534:TYR:HB3	1:D:559:PRO:HB3	1.92	0.50
1:D:690:LEU:HD23	1:D:713:LEU:HD13	1.94	0.50
2:E:421:ASN:ND2	2:E:425:ARG:HB2	2.27	0.50
1:C:433:PHE:HD1	1:C:454:GLU:HB3	1.77	0.49
1:D:254:VAL:HB	1:D:372:PHE:HE1	1.76	0.49
2:E:143:ASN:O	2:E:147:LYS:HG2	2.12	0.49
2:E:270:VAL:HG22	2:E:334:CYS:HB3	1.94	0.49
1:B:555:LEU:O	1:B:576:ASN:ND2	2.32	0.49
1:D:474:LEU:O	1:D:499:HIS:N	2.45	0.49
2:E:719:GLU:HG2	2:E:740:SER:HB3	1.94	0.49
2:F:121:HIS:CE1	2:F:123:TYR:HB3	2.47	0.49
2:E:441:PHE:HA	2:E:466:LEU:HD21	1.94	0.49
1:A:299:ILE:O	1:A:303:THR:OG1	2.20	0.49
1:A:601:CYS:N	1:A:624:ASN:OD1	2.45	0.49
1:A:645:LYS:HG2	1:A:668:TYR:HB2	1.94	0.49
1:B:648:TYR:HA	1:B:671:ARG:HB2	1.94	0.49
1:C:365:ILE:HD13	1:C:391:ALA:HB1	1.94	0.49
1:C:504:ASP:OD1	1:C:505:ILE:N	2.46	0.49
1:B:492:ARG:NH1	1:B:514:SER:O	2.42	0.49
1:D:357:ARG:NH1	1:D:365:ILE:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:THR:O	1:A:153:LEU:HG	2.13	0.49
1:A:519:GLU:HG2	1:A:545:ARG:HG3	1.95	0.49
1:D:571:LYS:NZ	1:D:573:SER:HB2	2.28	0.49
2:F:151:SER:HB2	2:F:258:LEU:HD13	1.95	0.49
1:A:103:ARG:HA	1:A:106:TYR:HD2	1.76	0.49
1:A:551:LEU:HD11	1:A:562:VAL:HG11	1.95	0.49
1:A:777:PRO:HB2	1:A:778:LEU:HD12	1.95	0.49
1:C:272:VAL:HG22	1:C:336:CYS:HB3	1.94	0.49
1:C:429:GLU:HB2	1:C:450:VAL:HB	1.95	0.49
1:D:583:VAL:HG23	1:D:585:ASN:H	1.78	0.49
2:E:111:ILE:HD13	2:E:306:PHE:CE1	2.48	0.49
1:B:135:ILE:HG12	1:B:274:LYS:HZ3	1.78	0.49
1:B:588:LYS:HB3	1:B:609:SER:HA	1.95	0.49
1:B:751:GLY:HA3	1:B:772:GLU:HB3	1.94	0.49
1:C:50:ASP:OD2	1:C:114:TYR:OH	2.20	0.49
1:D:46:GLN:HA	1:D:50:ASP:HB2	1.95	0.49
1:D:297:VAL:HG23	1:D:299:ILE:HG12	1.95	0.49
1:B:546:LEU:HD21	1:B:549:LEU:HD13	1.95	0.49
1:D:119:HIS:ND1	1:D:121:PHE:HB3	2.27	0.49
2:F:346:LEU:HD22	2:F:375:HIS:CG	2.47	0.49
1:A:513:TYR:HB3	1:A:542:GLU:HB2	1.95	0.48
1:A:714:ALA:HB2	1:A:737:HIS:HD2	1.78	0.48
1:A:348:LEU:HD22	1:A:377:HIS:CG	2.49	0.48
1:B:413:LEU:HD13	1:B:444:ASP:HB2	1.95	0.48
1:B:608:HIS:HA	1:B:611:PHE:HD2	1.77	0.48
1:B:654:ILE:HD13	1:B:681:LEU:HD22	1.95	0.48
1:B:413:LEU:HA	1:B:416:LEU:HD12	1.95	0.48
1:B:423:ASN:ND2	1:B:425:GLN:OE1	2.46	0.48
1:B:472:LYS:HD3	1:B:494:ASN:O	2.13	0.48
1:B:682:PHE:CD2	1:B:703:ASP:HB2	2.48	0.48
1:A:365:ILE:HD13	1:A:391:ALA:HB1	1.96	0.48
1:C:100:ASP:HB3	1:D:98:LYS:HE2	1.95	0.48
1:D:255:GLU:HG2	1:D:369:LYS:HB2	1.95	0.48
1:D:432:LEU:HB3	1:D:435:LEU:HD12	1.94	0.48
1:D:712:ASN:HD21	1:D:735:ALA:HB3	1.79	0.48
1:B:546:LEU:HG	1:B:569:LEU:HD21	1.95	0.48
1:C:461:ILE:O	1:C:484:GLU:HG2	2.13	0.48
1:C:769:LEU:HD21	1:C:786:VAL:HG21	1.95	0.48
1:D:175:GLU:HG3	1:D:401:LYS:HE2	1.96	0.48
2:E:740:SER:HA	2:E:763:HIS:CE1	2.48	0.48
1:A:717:ALA:HA	1:A:740:ASN:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:338:LEU:HD12	2:F:341:LEU:HD12	1.96	0.48
1:A:164:PHE:HD1	1:A:389:ARG:HG3	1.79	0.48
1:A:461:ILE:HB	1:A:483:ILE:HG13	1.95	0.48
1:B:46:GLN:NE2	1:B:123:LYS:O	2.47	0.48
1:B:250:PHE:CZ	1:B:254:VAL:HG21	2.49	0.48
1:B:687:LEU:HD23	1:B:707:LEU:HD13	1.96	0.48
1:D:582:ILE:HG22	1:D:584:LEU:HG	1.96	0.48
1:C:294:ASP:OD2	1:C:309:ARG:NH1	2.45	0.48
1:D:234:LYS:O	1:D:238:GLU:HG2	2.14	0.48
2:E:105:LEU:HA	2:E:108:TYR:CD2	2.49	0.48
1:A:348:LEU:HD22	1:A:377:HIS:CD2	2.49	0.48
1:A:472:LYS:HA	1:A:472:LYS:HD3	1.68	0.48
1:A:478:HIS:CE1	1:A:503:THR:HG23	2.49	0.48
1:C:665:GLU:HB3	1:C:688:ARG:HE	1.78	0.48
2:E:452:GLU:HA	2:E:475:HIS:HB2	1.95	0.48
1:A:627:LYS:HG2	1:A:650:HIS:HB2	1.94	0.48
1:B:446:VAL:HG12	1:B:467:GLN:HB3	1.95	0.48
1:B:710:LEU:HD21	1:B:713:LEU:HB2	1.95	0.48
2:E:437:PRO:HB2	2:E:440:VAL:HG23	1.95	0.48
1:B:431:HIS:HE1	1:B:454:GLU:HB2	1.79	0.47
1:C:392:VAL:O	1:C:395:SER:OG	2.25	0.47
1:C:103:ARG:HA	1:C:106:TYR:CD2	2.47	0.47
1:D:803:TRP:O	1:D:807:LYS:HG2	2.14	0.47
2:E:378:ASP:OD2	2:E:379:GLN:NE2	2.47	0.47
2:E:418:LEU:HD22	2:E:426:LEU:HG	1.96	0.47
1:A:136:PHE:CE1	1:A:274:LYS:HE3	2.49	0.47
1:A:791:PHE:HE1	1:A:802:LEU:HD23	1.78	0.47
1:B:29:ASP:O	1:B:33:ILE:HG12	2.14	0.47
1:B:648:TYR:CZ	1:B:671:ARG:HG3	2.49	0.47
1:C:606:ILE:HD12	1:C:631:GLU:HB2	1.96	0.47
1:D:365:ILE:HD13	1:D:391:ALA:HB1	1.96	0.47
2:E:451:LEU:O	2:E:475:HIS:N	2.42	0.47
1:B:368:VAL:HG12	1:B:372:PHE:HB3	1.96	0.47
1:C:737:HIS:HA	1:C:760:GLU:HB2	1.96	0.47
1:D:651:ILE:O	1:D:672:ASN:HB3	2.15	0.47
2:E:604:ILE:HD12	2:E:629:GLU:HB2	1.96	0.47
2:E:733:THR:HG23	2:E:756:TYR:HB3	1.95	0.47
1:C:443:PHE:O	1:C:467:GLN:NE2	2.48	0.47
1:C:505:ILE:HD11	1:C:527:LEU:HA	1.96	0.47
2:E:349:TYR:HD1	2:E:375:HIS:CE1	2.33	0.47
1:A:682:PHE:CD2	1:A:703:ASP:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:PHE:CZ	1:C:378:LEU:HD11	2.49	0.47
1:D:119:HIS:CE1	1:D:121:PHE:HB3	2.50	0.47
2:E:421:ASN:HB3	2:E:427:GLU:HB2	1.96	0.47
1:A:48:THR:HG23	1:A:49:GLN:HG3	1.96	0.47
1:A:449:GLU:HA	1:A:471:LEU:HA	1.96	0.47
1:B:570:GLN:OE1	1:B:594:THR:OG1	2.33	0.47
1:B:665:GLU:CD	1:B:686:LYS:HB3	2.35	0.47
1:B:674:ILE:HD12	1:B:692:LEU:HD21	1.97	0.47
1:B:685:ARG:HH21	1:B:706:LEU:HB3	1.80	0.47
1:C:465:ILE:HD11	1:C:487:ALA:HA	1.96	0.47
1:C:498:LEU:HB2	1:C:518:LEU:HD11	1.97	0.47
1:D:151:SER:O	1:D:154:GLU:HG2	2.14	0.47
1:D:249:LYS:HE3	2:E:172:THR:HG23	1.96	0.47
1:D:454:GLU:HA	1:D:477:TYR:HB2	1.95	0.47
2:E:246:LYS:O	2:E:249:ARG:HG3	2.15	0.47
2:E:415:ARG:HA	2:E:418:LEU:HD12	1.96	0.47
2:E:560:VAL:HG11	2:E:570:MET:SD	2.55	0.47
1:A:734:ARG:HA	1:A:756:LEU:HA	1.97	0.47
1:B:420:LEU:HB3	1:B:428:LEU:HD22	1.97	0.47
1:B:450:VAL:HG13	1:B:473:GLU:HB2	1.96	0.47
1:B:464:SER:OG	1:B:467:GLN:NE2	2.48	0.47
1:C:431:HIS:HA	1:C:452:LYS:HB2	1.96	0.47
1:C:540:LEU:HD12	1:C:543:LEU:HD12	1.96	0.47
1:D:58:LYS:NZ	1:D:305:TYR:OH	2.48	0.47
2:E:623:ASN:HA	2:E:647:ASN:HA	1.97	0.47
1:A:250:PHE:CE1	1:A:254:VAL:HG21	2.50	0.47
1:B:433:PHE:HD1	1:B:454:GLU:HB3	1.79	0.47
1:B:705:GLY:O	1:B:708:GLN:NE2	2.48	0.47
1:C:639:HIS:O	1:C:663:ASN:ND2	2.48	0.47
2:E:584:ASN:OD1	2:E:584:ASN:N	2.47	0.47
2:E:666:PHE:HA	2:E:689:ASP:HB3	1.97	0.47
1:B:498:LEU:HD12	1:B:499:HIS:H	1.80	0.47
1:C:522:HIS:HA	1:C:550:ARG:HB3	1.97	0.47
1:D:172:ALA:O	1:D:362:TYR:OH	2.33	0.47
1:C:625:ASN:O	1:C:627:LYS:NZ	2.47	0.46
1:C:661:LEU:HB3	1:C:664:LEU:HG	1.95	0.46
1:D:734:ARG:O	1:D:757:THR:N	2.27	0.46
2:E:617:LEU:HB3	2:E:642:LEU:HD23	1.96	0.46
1:B:23:TRP:O	1:B:27:PHE:HD1	1.97	0.46
2:E:703:GLY:HA3	2:E:724:GLU:HB3	1.97	0.46
2:F:284:VAL:O	2:F:287:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:TYR:HA	1:A:20:LEU:HD23	1.97	0.46
1:B:713:LEU:O	1:B:737:HIS:ND1	2.39	0.46
1:D:478:HIS:CD2	1:D:503:THR:HG23	2.51	0.46
1:A:730:CYS:HB2	1:A:733:LEU:HD13	1.97	0.46
2:E:138:PHE:HE1	2:E:269:LYS:HA	1.79	0.46
2:F:53:ILE:O	2:F:308:CYS:HA	2.16	0.46
1:B:50:ASP:HB2	1:B:314:LEU:HD12	1.98	0.46
1:D:22:PRO:HD2	1:D:25:ASP:HB2	1.98	0.46
2:E:130:LEU:HD11	2:E:279:TYR:OH	2.16	0.46
2:E:165:CYS:SG	2:E:388:PHE:HA	2.55	0.46
2:E:248:PHE:CZ	2:E:252:VAL:HG21	2.51	0.46
2:E:736:ILE:N	2:E:758:ASP:O	2.45	0.46
1:A:746:LEU:HD23	1:A:747:PRO:HD2	1.97	0.46
1:C:478:HIS:CE1	1:C:503:THR:HG23	2.51	0.46
1:D:377:HIS:O	1:D:381:GLN:HG2	2.15	0.46
1:D:555:LEU:H	1:D:576:ASN:HD22	1.64	0.46
1:D:687:LEU:HD23	1:D:707:LEU:HD13	1.97	0.46
1:D:736:LEU:HD13	1:D:738:LEU:HD11	1.97	0.46
2:E:591:LEU:HD21	2:E:594:LEU:HD13	1.98	0.46
2:E:766:VAL:HG23	2:E:791:THR:HB	1.97	0.46
2:F:49:GLN:O	2:F:51:LYS:NZ	2.47	0.46
1:B:541:ARG:HE	1:B:564:ASP:HB2	1.81	0.46
1:D:420:LEU:HD23	1:D:430:LEU:HB2	1.97	0.46
1:D:643:CYS:SG	1:D:644:LEU:N	2.89	0.46
1:A:96:GLY:N	2:F:102:ASP:OD2	2.49	0.46
1:B:436:SER:HA	1:B:457:PRO:HD2	1.97	0.46
1:B:791:PHE:HE1	1:B:802:LEU:HD12	1.81	0.46
1:D:622:LYS:HG3	1:D:648:TYR:HB2	1.97	0.46
1:B:233:ASP:O	1:B:237:GLY:N	2.38	0.46
1:B:365:ILE:HG12	1:B:395:SER:HB2	1.98	0.46
1:B:480:ALA:HB2	1:B:507:GLU:HA	1.98	0.46
1:B:550:ARG:HH22	1:B:575:ASN:HD22	1.64	0.46
1:B:596:LEU:O	1:B:619:ILE:HA	2.15	0.46
2:E:557:PRO:HG2	2:E:560:VAL:HG23	1.97	0.46
1:A:733:LEU:HG	1:A:736:LEU:HD21	1.97	0.46
1:A:754:THR:HB	1:A:777:PRO:HG2	1.98	0.46
1:B:550:ARG:HD2	1:B:573:SER:HB3	1.97	0.46
1:B:562:VAL:HA	1:B:565:VAL:HG12	1.98	0.46
2:E:533:VAL:H	2:E:555:LYS:HE3	1.81	0.46
1:A:39:ALA:HB2	1:A:129:VAL:HG12	1.98	0.45
1:A:762:ARG:HE	1:A:787:GLU:HG3	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:486:LEU:HD13	2:E:509:TRP:HB2	1.97	0.45
2:F:170:TRP:CZ2	2:F:400:LEU:HB2	2.51	0.45
1:A:483:ILE:HB	1:A:511:TRP:CZ2	2.51	0.45
1:A:665:GLU:HA	1:A:687:LEU:HA	1.98	0.45
1:C:647:TRP:CE3	1:C:668:TYR:HB3	2.51	0.45
1:D:620:ASP:HA	1:D:645:LYS:HB2	1.98	0.45
1:A:46:GLN:OE1	1:A:127:TYR:OH	2.28	0.45
1:A:317:LEU:O	1:A:321:LEU:HG	2.15	0.45
1:B:492:ARG:HA	1:B:515:LEU:HA	1.99	0.45
1:D:473:GLU:HB3	1:D:499:HIS:HE1	1.80	0.45
1:D:518:LEU:HD23	1:D:543:LEU:HD13	1.98	0.45
2:E:252:VAL:HB	2:E:370:PHE:HE1	1.82	0.45
1:A:129:VAL:HG13	1:A:325:TYR:CE1	2.52	0.45
1:B:407:LEU:HG	1:B:439:PRO:HG3	1.97	0.45
1:C:733:LEU:HD21	1:C:736:LEU:HD21	1.98	0.45
1:B:423:ASN:HB3	1:B:429:GLU:CB	2.46	0.45
1:C:154:GLU:HA	1:C:157:VAL:HG12	1.98	0.45
2:E:418:LEU:HD11	2:E:443:ILE:HG21	1.98	0.45
1:A:638:LEU:HD22	1:A:641:LEU:HD22	1.98	0.45
1:A:666:ARG:HG2	1:A:689:TYR:HB2	1.98	0.45
1:C:149:THR:O	1:C:153:LEU:HG	2.16	0.45
1:C:325:TYR:O	1:C:329:VAL:HG23	2.15	0.45
1:A:156:PHE:HB2	1:A:250:PHE:CZ	2.52	0.45
1:B:583:VAL:HG23	1:B:585:ASN:H	1.81	0.45
1:B:296:THR:HG23	1:B:307:THR:HG22	1.99	0.45
1:C:129:VAL:O	1:C:133:THR:HG23	2.17	0.45
1:D:168:TRP:CZ3	1:D:398:SER:HB2	2.52	0.45
2:F:121:HIS:ND1	2:F:286:LYS:HG2	2.32	0.45
1:A:251:ARG:HD2	1:A:394:LEU:HD11	1.99	0.45
1:A:769:LEU:HG	1:A:790:LEU:HG	1.99	0.45
1:C:365:ILE:HG23	1:C:394:LEU:HD23	1.98	0.45
1:C:420:LEU:HD11	1:C:448:LEU:HD11	1.99	0.45
1:D:704:ILE:HD13	1:D:727:LEU:HA	1.99	0.45
1:B:39:ALA:HB2	1:B:129:VAL:HG12	1.98	0.44
1:B:102:ASP:OD1	1:B:105:GLN:NE2	2.42	0.44
1:B:300:GLU:O	1:B:304:GLY:N	2.49	0.44
1:B:731:ARG:CZ	1:B:752:GLU:HB3	2.47	0.44
1:D:534:TYR:HE2	1:D:557:LYS:HE3	1.82	0.44
1:B:405:LEU:HD13	1:B:405:LEU:HA	1.69	0.44
1:B:542:GLU:OE1	1:B:542:GLU:N	2.49	0.44
1:C:131:LEU:O	1:C:135:ILE:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:LEU:O	1:D:318:PHE:N	2.38	0.44
1:D:729:GLN:OE1	1:D:749:ARG:NH2	2.39	0.44
2:E:374:LEU:HD11	2:E:385:SER:HB2	1.99	0.44
1:B:500:ILE:HG21	1:B:508:ILE:HG23	1.99	0.44
1:B:663:ASN:HA	1:B:686:LYS:HD2	1.99	0.44
1:C:152:LYS:NZ	1:C:257:GLY:HA3	2.33	0.44
1:C:415:LYS:HE2	1:C:415:LYS:HB3	1.72	0.44
1:C:435:LEU:H	1:C:456:ILE:HG12	1.82	0.44
2:E:522:VAL:HA	2:E:550:LYS:HB2	1.99	0.44
2:F:297:ILE:O	2:F:301:THR:N	2.38	0.44
1:A:258:ASP:OD1	1:A:349:LYS:NZ	2.46	0.44
1:A:737:HIS:HA	1:A:760:GLU:HB2	1.99	0.44
1:B:173:LEU:HD21	1:B:392:VAL:HG21	2.00	0.44
1:B:642:THR:O	1:B:665:GLU:N	2.43	0.44
1:C:588:LYS:HA	1:C:613:LEU:HD21	2.00	0.44
1:C:656:ILE:HB	1:C:680:GLN:HB2	2.00	0.44
1:D:801:ARG:HA	1:D:804:ARG:HE	1.81	0.44
2:E:415:ARG:NE	2:E:445:GLU:OE2	2.50	0.44
2:E:430:LEU:HD13	2:E:433:LEU:HD12	1.99	0.44
1:A:364:ASP:O	1:A:395:SER:HA	2.17	0.44
1:A:767:GLU:HG2	1:B:711:GLN:HE21	1.83	0.44
1:C:152:LYS:HZ1	1:C:257:GLY:HA3	1.82	0.44
1:C:159:ILE:HA	1:C:162:LYS:HD2	1.99	0.44
1:C:527:LEU:HG	1:C:553:SER:HB3	1.99	0.44
2:E:170:TRP:NE1	2:E:400:LEU:HD13	2.33	0.44
2:E:507:PRO:O	2:E:510:MET:HG2	2.17	0.44
1:A:24:TRP:HB2	1:A:335:ILE:HG23	1.99	0.44
1:A:434:MET:HA	1:A:455:LEU:O	2.18	0.44
1:A:667:LEU:O	1:A:690:LEU:HA	2.18	0.44
1:B:368:VAL:HB	1:B:373:ALA:HB2	1.99	0.44
1:B:432:LEU:O	1:B:454:GLU:N	2.50	0.44
1:D:168:TRP:CZ3	1:D:172:ALA:HB2	2.53	0.44
1:D:517:THR:HA	1:D:545:ARG:HD3	2.00	0.44
1:D:571:LYS:HZ1	1:D:573:SER:HB2	1.82	0.44
2:E:641:VAL:HG22	2:E:664:ARG:HD3	2.00	0.44
1:A:319:LYS:HE3	1:A:319:LYS:HB2	1.77	0.44
1:A:555:LEU:HB2	1:A:576:ASN:ND2	2.32	0.44
1:B:374:PHE:CZ	1:B:378:LEU:HD11	2.52	0.44
1:C:56:PRO:HG2	1:C:99:TYR:CD1	2.53	0.44
2:E:20:LEU:HD11	2:E:159:ILE:HD11	1.98	0.44
2:E:347:ARG:O	2:E:368:ASN:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:LYS:HG2	1:B:475:TRP:CD1	2.52	0.44
1:C:24:TRP:HB2	1:C:335:ILE:HG23	2.00	0.44
1:C:324:PHE:O	1:C:327:SER:OG	2.26	0.44
1:C:354:GLU:OE1	1:C:354:GLU:N	2.41	0.44
1:D:17:TYR:HA	1:D:20:LEU:HD23	2.00	0.44
1:D:100:ASP:O	2:E:98:GLY:HA3	2.18	0.44
2:E:134:HIS:O	2:E:272:LYS:NZ	2.47	0.44
2:E:579:LEU:HB3	2:E:601:LEU:HD21	2.00	0.44
2:F:36:LEU:N	2:F:135:THR:HG21	2.33	0.44
1:A:232:LEU:HB2	1:A:409:ASN:HD21	1.81	0.44
1:A:433:PHE:HE1	1:A:455:LEU:HD12	1.83	0.43
1:A:502:PHE:CE1	1:A:508:ILE:HD11	2.53	0.43
1:D:502:PHE:HB2	1:D:507:GLU:HB2	1.98	0.43
2:E:383:LEU:HD22	2:E:386:LYS:HB3	2.00	0.43
2:E:760:LYS:HB2	2:E:783:VAL:HG12	1.99	0.43
2:F:46:GLN:HA	2:F:50:ASP:HB2	1.99	0.43
1:A:168:TRP:CD1	1:A:402:LEU:HD23	2.53	0.43
1:A:575:ASN:HA	1:A:599:ILE:O	2.18	0.43
1:B:461:ILE:HB	1:B:483:ILE:HA	2.01	0.43
1:B:618:GLU:HA	1:B:643:CYS:HB3	2.00	0.43
1:D:502:PHE:HZ	1:D:527:LEU:HB3	1.83	0.43
2:E:612:LEU:HD11	2:E:635:HIS:CE1	2.53	0.43
2:E:614:LEU:HD12	2:E:614:LEU:HA	1.74	0.43
2:F:294:ASN:HA	2:F:304:LYS:O	2.18	0.43
1:B:488:LEU:HD12	1:B:515:LEU:HD21	2.00	0.43
1:B:557:LYS:NZ	1:B:558:LEU:O	2.46	0.43
1:B:726:GLU:HA	1:B:729:GLN:HG2	2.00	0.43
1:C:129:VAL:HG13	1:C:325:TYR:CE1	2.53	0.43
1:C:740:ASN:OD1	1:C:740:ASN:N	2.51	0.43
1:B:593:LEU:HD23	1:B:616:LEU:HD11	2.00	0.43
1:C:566:GLY:HA3	1:C:590:MET:HG2	1.99	0.43
2:E:363:ILE:HD11	2:E:393:SER:HB2	1.98	0.43
2:F:354:VAL:HG22	2:F:386:LYS:HD3	2.01	0.43
1:A:154:GLU:HA	1:A:157:VAL:HG12	2.00	0.43
1:A:233:ASP:O	1:A:236:GLU:HG3	2.19	0.43
1:A:673:LYS:O	1:A:696:ASN:ND2	2.47	0.43
1:A:700:LEU:HD12	1:A:724:PRO:HD2	1.99	0.43
1:B:54:CYS:HB2	1:B:110:ASP:OD1	2.18	0.43
1:C:141:ASN:O	1:C:145:LYS:HG2	2.18	0.43
1:C:450:VAL:HG22	1:C:473:GLU:HB2	2.00	0.43
1:C:511:TRP:O	1:C:514:SER:OG	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:620:ASP:HA	1:C:645:LYS:HB2	1.99	0.43
1:D:171:ARG:HH22	1:D:230:GLY:HA3	1.83	0.43
1:D:233:ASP:OD1	1:D:234:LYS:N	2.51	0.43
2:E:550:LYS:HB3	2:E:550:LYS:HE3	1.83	0.43
1:A:117:ARG:HB2	1:A:295:CYS:HB3	1.99	0.43
1:A:129:VAL:HG22	1:A:325:TYR:CE2	2.54	0.43
1:A:298:ASP:OD1	1:A:306:ARG:NH1	2.45	0.43
1:B:155:HIS:HB3	1:B:250:PHE:CE1	2.54	0.43
1:B:235:LYS:O	1:B:239:GLN:HG2	2.18	0.43
1:B:474:LEU:O	1:B:499:HIS:N	2.52	0.43
2:E:289:PHE:HA	2:E:313:ALA:HB3	1.99	0.43
2:F:374:LEU:HD22	2:F:374:LEU:HA	1.87	0.43
1:B:53:ILE:O	1:B:310:CYS:HA	2.19	0.43
1:B:168:TRP:NE1	1:B:402:LEU:HD23	2.33	0.43
1:C:572:LEU:N	1:C:593:LEU:HD11	2.33	0.43
1:D:160:LEU:HD21	1:D:379:ILE:HG21	2.00	0.43
1:D:254:VAL:HB	1:D:372:PHE:CE1	2.53	0.43
2:E:402:GLN:HE22	2:E:435:GLY:HA3	1.84	0.43
2:F:163:GLY:O	2:F:167:ASP:HB2	2.18	0.43
1:B:447:GLU:CD	1:B:447:GLU:H	2.22	0.43
1:B:625:ASN:N	1:B:649:ASN:OD1	2.52	0.43
1:B:666:ARG:HG2	1:B:689:TYR:HB2	2.01	0.43
1:C:58:LYS:HE3	1:C:58:LYS:HB3	1.84	0.43
1:C:297:VAL:HG23	1:C:299:ILE:HG12	2.00	0.43
1:C:513:TYR:CD2	1:C:539:GLY:HA3	2.53	0.43
2:F:338:LEU:HD12	2:F:338:LEU:HA	1.89	0.43
1:B:155:HIS:HB3	1:B:250:PHE:HE1	1.83	0.43
1:C:543:LEU:HB3	1:C:546:LEU:HB2	2.01	0.43
1:C:642:THR:HA	1:C:664:LEU:HA	2.00	0.43
2:E:633:PHE:HB3	2:E:659:LEU:HD11	2.00	0.43
2:E:676:PRO:HG2	2:E:679:LEU:HB2	2.01	0.43
2:F:246:LYS:HB3	2:F:246:LYS:HE2	1.87	0.43
1:A:62:LYS:HB2	1:A:62:LYS:HE3	1.70	0.43
1:A:448:LEU:HD11	1:A:450:VAL:O	2.19	0.43
1:B:330:ILE:O	1:B:334:LEU:HG	2.19	0.43
1:B:428:LEU:HD23	1:B:428:LEU:HA	1.80	0.43
1:D:566:GLY:HA3	1:D:590:MET:HG2	2.01	0.43
1:D:645:LYS:HG2	1:D:668:TYR:HD1	1.84	0.43
2:E:289:PHE:HA	2:E:313:ALA:CB	2.49	0.43
1:B:463:PRO:O	1:B:466:ALA:HB3	2.19	0.42
1:B:534:TYR:HA	1:B:537:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:625:ASN:N	1:C:649:ASN:OD1	2.52	0.42
1:C:709:ASN:HA	1:C:732:LYS:HD2	2.00	0.42
1:D:135:ILE:HG12	1:D:274:LYS:HZ3	1.84	0.42
1:D:173:LEU:HD13	1:D:173:LEU:HA	1.93	0.42
1:D:513:TYR:OH	1:D:536:VAL:O	2.37	0.42
1:D:551:LEU:O	1:D:575:ASN:N	2.48	0.42
1:D:587:LEU:HD21	1:D:596:LEU:HD21	2.00	0.42
1:A:431:HIS:HB2	1:A:452:LYS:HD2	2.01	0.42
1:A:594:THR:O	1:A:617:GLN:N	2.38	0.42
1:B:149:THR:HG21	1:B:263:LEU:HD12	2.00	0.42
1:B:473:GLU:HB3	1:B:499:HIS:HE1	1.82	0.42
1:C:148:ARG:HE	1:C:148:ARG:HB2	1.60	0.42
1:C:233:ASP:O	1:C:236:GLU:HG3	2.18	0.42
1:D:546:LEU:O	1:D:568:HIS:ND1	2.51	0.42
2:E:452:GLU:HG2	2:E:475:HIS:HB2	2.00	0.42
2:F:147:LYS:HA	2:F:147:LYS:HD3	1.83	0.42
1:A:176:THR:HG22	1:A:360:SER:HA	2.00	0.42
1:A:357:ARG:HB2	1:A:362:TYR:O	2.20	0.42
1:A:595:GLU:HG2	1:A:618:GLU:HB2	2.02	0.42
1:B:723:LEU:HD12	1:B:747:PRO:HD2	2.00	0.42
1:D:348:LEU:HB2	1:D:377:HIS:ND1	2.34	0.42
1:D:364:ASP:O	1:D:395:SER:HA	2.19	0.42
1:D:534:TYR:CE2	1:D:557:LYS:HE3	2.54	0.42
1:D:712:ASN:ND2	1:D:735:ALA:HB3	2.34	0.42
1:A:645:LYS:HZ1	1:A:666:ARG:HH12	1.66	0.42
1:A:766:LEU:HD23	1:A:790:LEU:HD21	1.99	0.42
1:B:270:ILE:O	1:B:273:ILE:HG13	2.19	0.42
1:B:375:MET:O	1:B:379:ILE:HG12	2.18	0.42
1:B:519:GLU:OE2	1:B:545:ARG:NH2	2.53	0.42
1:B:572:LEU:O	1:B:596:LEU:HD12	2.19	0.42
1:B:761:LEU:HB2	1:B:786:VAL:HG23	2.01	0.42
1:C:569:LEU:HD12	1:C:590:MET:HE3	2.01	0.42
1:D:19:ILE:HG22	1:D:382:TYR:CZ	2.54	0.42
1:D:453:LEU:N	1:D:475:TRP:O	2.41	0.42
2:F:126:TYR:O	2:F:130:LEU:N	2.40	0.42
1:A:392:VAL:O	1:A:398:SER:OG	2.30	0.42
1:A:478:HIS:ND1	1:A:503:THR:HG23	2.33	0.42
1:A:740:ASN:OD1	1:A:740:ASN:N	2.52	0.42
1:B:58:LYS:HE3	1:B:58:LYS:HB3	1.80	0.42
1:B:583:VAL:O	1:B:584:LEU:HG	2.20	0.42
1:B:787:GLU:HB2	1:B:790:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:616:LEU:HD12	1:C:616:LEU:HA	1.87	0.42
1:D:461:ILE:HG12	1:D:482:LYS:O	2.20	0.42
2:E:375:HIS:O	2:E:379:GLN:HG2	2.20	0.42
1:A:245:GLU:O	1:A:249:LYS:HG2	2.20	0.42
1:B:160:LEU:HD21	1:B:379:ILE:HG21	2.01	0.42
1:B:622:LYS:HB2	1:B:647:TRP:HE1	1.84	0.42
1:B:622:LYS:HB2	1:B:647:TRP:NE1	2.35	0.42
1:D:425:GLN:N	1:D:425:GLN:OE1	2.53	0.42
1:D:742:VAL:HG12	1:D:765:ARG:NH1	2.35	0.42
2:E:558:GLN:NE2	2:E:562:ASP:OD1	2.52	0.42
1:A:129:VAL:O	1:A:133:THR:HG23	2.19	0.42
1:A:278:ILE:HA	1:A:281:TYR:CE2	2.55	0.42
1:A:413:LEU:HD22	1:A:417:ARG:HH12	1.84	0.42
1:B:566:GLY:HA2	1:B:569:LEU:HD12	2.02	0.42
1:B:620:ASP:O	1:B:621:LEU:HD23	2.19	0.42
1:C:576:ASN:HB3	1:C:579:THR:HB	2.00	0.42
1:D:550:ARG:HA	1:D:573:SER:HB3	2.01	0.42
2:E:121:HIS:HE1	2:E:283:LEU:HD22	1.85	0.42
1:A:164:PHE:CD1	1:A:389:ARG:HG3	2.54	0.42
1:B:417:ARG:HE	1:B:447:GLU:CD	2.23	0.42
1:B:508:ILE:H	1:B:508:ILE:HG13	1.61	0.42
1:D:171:ARG:O	1:D:175:GLU:HG2	2.20	0.42
2:E:663:GLU:HA	2:E:685:ILE:HA	2.01	0.42
1:A:295:CYS:HB2	1:A:297:VAL:HG13	2.02	0.42
1:A:423:ASN:ND2	1:A:450:VAL:HG21	2.34	0.42
1:C:278:ILE:HA	1:C:281:TYR:CD1	2.55	0.42
1:C:608:HIS:HA	1:C:611:PHE:CD2	2.52	0.42
1:C:682:PHE:CD2	1:C:703:ASP:HB2	2.55	0.42
1:A:421:THR:OG1	1:A:429:GLU:OE1	2.32	0.42
1:B:141:ASN:O	1:B:145:LYS:HG2	2.20	0.42
1:B:419:ARG:O	1:B:421:THR:HG23	2.20	0.42
1:B:516:LYS:NZ	1:B:542:GLU:HB3	2.35	0.42
1:B:550:ARG:HH22	1:B:575:ASN:HB2	1.84	0.42
1:C:44:THR:O	1:C:48:THR:OG1	2.27	0.42
1:C:622:LYS:HE3	1:C:648:TYR:CD1	2.55	0.42
1:D:737:HIS:HA	1:D:760:GLU:HB3	2.02	0.42
2:E:636:LEU:HB2	2:E:639:LEU:HB2	2.02	0.42
2:F:241:LEU:HD22	2:F:244:LYS:HB3	2.02	0.42
2:F:248:PHE:CZ	2:F:252:VAL:HG21	2.55	0.42
1:B:615:ASN:HA	1:B:640:ARG:NH2	2.34	0.41
1:D:646:LEU:O	1:D:649:ASN:ND2	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:261:MET:HG3	2:E:265:GLN:HE21	1.85	0.41
1:C:356:ILE:HD12	1:C:388:LYS:HG2	2.02	0.41
1:C:473:GLU:HA	1:C:497:ALA:HB3	2.01	0.41
1:C:478:HIS:CE1	1:C:501:LYS:HG2	2.55	0.41
1:D:154:GLU:HA	1:D:157:VAL:HG12	2.02	0.41
1:D:305:TYR:HA	2:E:96:MET:HG3	2.01	0.41
1:D:646:LEU:HB2	1:D:669:LEU:HD22	2.01	0.41
1:A:15:PRO:HB2	1:A:17:TYR:HD1	1.86	0.41
1:A:290:LYS:HE3	1:A:290:LYS:HB2	1.73	0.41
1:A:504:ASP:OD2	1:A:506:LYS:NZ	2.42	0.41
1:A:604:GLU:HG2	1:A:625:ASN:HB2	2.01	0.41
1:B:135:ILE:HG23	1:B:274:LYS:HZ2	1.85	0.41
1:B:601:CYS:H	1:B:624:ASN:ND2	2.18	0.41
1:C:703:ASP:OD1	1:C:703:ASP:N	2.52	0.41
2:E:381:ASP:HA	2:E:382:PRO:HD3	1.90	0.41
2:F:52:ILE:HD12	2:F:116:TYR:HA	2.01	0.41
2:F:256:ASP:HB2	2:F:368:ASN:HB2	2.02	0.41
1:B:581:LEU:HB3	1:B:601:CYS:HB3	2.01	0.41
1:C:445:LEU:O	1:C:468:LEU:HB3	2.20	0.41
1:D:667:LEU:O	1:D:690:LEU:HA	2.20	0.41
2:E:563:VAL:HG13	2:E:567:LEU:HB2	2.01	0.41
1:A:765:ARG:H	1:A:765:ARG:HG2	1.68	0.41
1:B:615:ASN:HA	1:B:640:ARG:HH21	1.86	0.41
1:C:566:GLY:HA2	1:C:569:LEU:HB2	2.01	0.41
1:C:647:TRP:O	1:C:649:ASN:ND2	2.53	0.41
2:E:151:SER:HB2	2:E:258:LEU:HD13	2.03	0.41
2:F:375:HIS:O	2:F:379:GLN:HG2	2.20	0.41
2:F:405:LEU:HG	2:F:409:TRP:CD1	2.55	0.41
1:A:97:ILE:O	2:F:107:GLN:NE2	2.48	0.41
1:A:168:TRP:CZ3	1:A:398:SER:HB2	2.55	0.41
1:B:296:THR:HG22	1:B:306:ARG:HH21	1.86	0.41
1:B:618:GLU:OE2	1:B:642:THR:OG1	2.30	0.41
1:D:504:ASP:OD1	1:D:505:ILE:N	2.53	0.41
1:D:583:VAL:O	1:D:586:SER:OG	2.36	0.41
2:E:145:TRP:CZ2	2:E:262:TYR:HB2	2.56	0.41
1:A:235:LYS:O	1:A:239:GLN:HG2	2.20	0.41
1:A:258:ASP:H	1:A:371:ASP:HB2	1.86	0.41
1:A:572:LEU:N	1:A:593:LEU:HD11	2.35	0.41
1:C:149:THR:HG21	1:C:263:LEU:HD12	2.02	0.41
1:C:417:ARG:NH2	1:C:445:LEU:HD11	2.36	0.41
1:C:496:ARG:HD3	1:C:496:ARG:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:PHE:CE1	1:D:333:GLY:HA3	2.56	0.41
1:D:433:PHE:HD1	1:D:454:GLU:HB3	1.86	0.41
1:D:787:GLU:OE1	1:D:787:GLU:N	2.49	0.41
2:E:789:PHE:CE2	2:E:797:ARG:HB2	2.55	0.41
1:A:482:LYS:HE2	1:A:482:LYS:HB2	1.92	0.41
1:B:461:ILE:N	1:B:482:LYS:O	2.50	0.41
1:B:645:LYS:HG2	1:B:668:TYR:HB2	2.03	0.41
1:D:52:MET:HA	1:D:311:ALA:O	2.20	0.41
1:D:278:ILE:HA	1:D:281:TYR:CD1	2.56	0.41
1:D:580:LYS:HA	1:D:601:CYS:O	2.21	0.41
1:D:585:ASN:OD1	1:D:609:SER:OG	2.38	0.41
2:E:640:THR:HA	2:E:661:SER:O	2.19	0.41
2:E:735:LYS:HA	2:E:758:ASP:HB3	2.01	0.41
2:F:405:LEU:HG	2:F:409:TRP:HD1	1.85	0.41
1:A:385:LEU:HA	1:A:388:LYS:HE3	2.02	0.41
1:B:548:VAL:HA	1:B:571:LYS:O	2.21	0.41
1:C:279:ILE:HD13	1:C:279:ILE:HA	1.91	0.41
1:C:385:LEU:O	1:C:389:ARG:HG2	2.21	0.41
1:C:590:MET:HE1	1:C:593:LEU:HD22	2.03	0.41
1:C:772:GLU:O	1:C:775:GLU:HG2	2.20	0.41
1:D:24:TRP:HB2	1:D:335:ILE:CG2	2.51	0.41
1:D:718:ASN:HB2	1:D:741:ASN:HD21	1.86	0.41
1:D:718:ASN:HB2	1:D:741:ASN:ND2	2.36	0.41
2:E:513:LEU:O	2:E:541:LEU:HA	2.21	0.41
2:E:547:LEU:O	2:E:571:CYS:N	2.44	0.41
2:E:593:GLU:HB3	2:E:616:GLU:HB2	2.03	0.41
2:E:724:GLU:O	2:E:727:PHE:HB2	2.21	0.41
1:A:427:LYS:HB3	1:A:449:GLU:HB3	2.02	0.41
1:B:477:TYR:CE2	1:B:501:LYS:HD3	2.56	0.41
1:B:614:HIS:CE1	1:B:637:HIS:HB3	2.55	0.41
1:B:627:LYS:HE3	1:B:650:HIS:HD2	1.85	0.41
1:B:749:ARG:HE	1:B:749:ARG:HB3	1.61	0.41
1:C:19:ILE:HG22	1:C:382:TYR:CZ	2.55	0.41
1:C:799:LYS:HE2	1:C:799:LYS:HB3	1.91	0.41
1:D:669:LEU:O	1:D:672:ASN:ND2	2.53	0.41
1:A:103:ARG:HA	1:A:103:ARG:HD2	1.80	0.40
1:A:443:PHE:HA	1:A:468:LEU:HD11	2.02	0.40
1:A:804:ARG:HD2	1:A:804:ARG:HA	1.84	0.40
1:B:103:ARG:HA	1:B:106:TYR:HD2	1.85	0.40
1:C:49:GLN:HE21	1:C:49:GLN:HB2	1.76	0.40
1:C:60:VAL:HG21	1:C:306:ARG:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:ILE:HA	1:C:281:TYR:CE1	2.56	0.40
1:D:346:ARG:HG3	1:D:348:LEU:HB3	2.01	0.40
1:D:698:THR:HB	1:D:719:ARG:HB2	2.03	0.40
1:A:100:ASP:N	1:A:100:ASP:OD1	2.54	0.40
1:A:354:GLU:OE1	1:A:354:GLU:N	2.51	0.40
1:A:423:ASN:HD21	1:A:425:GLN:HB2	1.86	0.40
1:A:545:ARG:O	1:A:547:LYS:HG2	2.21	0.40
1:B:369:LYS:HE3	1:B:369:LYS:HB3	1.86	0.40
1:B:572:LEU:N	1:B:593:LEU:HD11	2.36	0.40
1:B:593:LEU:HD21	1:B:596:LEU:HD13	2.02	0.40
1:C:169:THR:HG22	1:C:392:VAL:HG11	2.03	0.40
1:C:649:ASN:O	1:C:672:ASN:HA	2.21	0.40
1:C:724:PRO:HG2	1:C:727:LEU:HB2	2.03	0.40
1:D:166:SER:HB3	1:D:169:THR:HG23	2.03	0.40
1:D:375:MET:O	1:D:379:ILE:HG12	2.21	0.40
1:D:378:LEU:HD23	1:D:378:LEU:HA	1.97	0.40
1:D:499:HIS:HD2	1:D:522:HIS:CG	2.39	0.40
1:D:534:TYR:HE1	1:D:555:LEU:HD22	1.86	0.40
1:A:142:PHE:O	1:A:146:PHE:N	2.54	0.40
1:A:464:SER:O	1:A:467:GLN:HB2	2.22	0.40
1:B:161:LEU:HD23	1:B:161:LEU:HA	1.87	0.40
1:B:454:GLU:HA	1:B:477:TYR:O	2.20	0.40
1:B:552:LYS:HA	1:B:575:ASN:O	2.21	0.40
1:B:596:LEU:HD23	1:B:616:LEU:HD21	2.04	0.40
1:B:606:ILE:HG23	1:B:610:ILE:HD12	2.02	0.40
1:C:274:LYS:HB3	1:C:274:LYS:HE2	1.74	0.40
1:C:290:LYS:HE3	1:C:290:LYS:HB2	1.93	0.40
1:D:51:LYS:NZ	1:D:51:LYS:HB2	2.36	0.40
1:D:565:VAL:HG22	1:D:568:HIS:CE1	2.55	0.40
1:D:677:ILE:HG23	1:D:681:LEU:HD23	2.03	0.40
1:D:700:LEU:HB2	1:D:724:PRO:HD3	2.03	0.40
1:A:35:MET:HE2	1:A:325:TYR:HE1	1.86	0.40
1:A:232:LEU:HB2	1:A:409:ASN:ND2	2.36	0.40
1:C:168:TRP:CH2	1:C:398:SER:HB2	2.57	0.40
1:C:263:LEU:HD23	1:C:263:LEU:HA	1.85	0.40
1:C:292:ASP:OD1	1:C:292:ASP:N	2.54	0.40
1:C:643:CYS:HA	1:C:666:ARG:O	2.21	0.40
1:C:685:ARG:HA	1:C:707:LEU:HD22	2.03	0.40
1:D:250:PHE:CZ	1:D:254:VAL:HG21	2.57	0.40
1:D:357:ARG:NH2	1:D:367:ASP:OD1	2.55	0.40
1:D:451:LEU:HB3	1:D:474:LEU:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:134:HIS:CG	2:F:276:ILE:HD11	2.56	0.40
1:A:244:PHE:CE2	1:A:393:PHE:HA	2.57	0.40
1:A:583:VAL:HG23	1:A:584:LEU:H	1.86	0.40
1:A:606:ILE:HD12	1:A:631:GLU:HB2	2.03	0.40
1:B:130:LEU:O	1:B:134:LEU:HG	2.21	0.40
1:B:563:THR:HG21	1:B:589:LYS:HD2	2.03	0.40
1:B:648:TYR:CE2	1:B:671:ARG:HG3	2.56	0.40
1:B:667:LEU:O	1:B:690:LEU:HA	2.21	0.40
1:C:780:LYS:HE3	1:C:780:LYS:HB2	1.88	0.40
1:D:353:PHE:HD1	1:D:353:PHE:HA	1.77	0.40
1:D:404:GLN:NE2	1:D:438:ILE:O	2.51	0.40
1:D:759:ILE:N	1:D:783:GLY:O	2.36	0.40
2:F:170:TRP:NE1	2:F:400:LEU:HD13	2.36	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	712/817 (87%)	687 (96%)	25 (4%)	0	100	100
1	B	714/817 (87%)	687 (96%)	27 (4%)	0	100	100
1	C	712/817 (87%)	685 (96%)	27 (4%)	0	100	100
1	D	712/817 (87%)	692 (97%)	20 (3%)	0	100	100
2	E	684/811 (84%)	650 (95%)	34 (5%)	0	100	100
2	F	294/811 (36%)	279 (95%)	15 (5%)	0	100	100
All	All	3828/4890 (78%)	3680 (96%)	148 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	666/756 (88%)	629 (94%)	37 (6%)	17	38
1	B	668/756 (88%)	630 (94%)	38 (6%)	17	38
1	C	666/756 (88%)	634 (95%)	32 (5%)	21	43
1	D	666/756 (88%)	631 (95%)	35 (5%)	19	40
2	E	640/755 (85%)	611 (96%)	29 (4%)	23	45
2	F	278/755 (37%)	259 (93%)	19 (7%)	13	34
All	All	3584/4534 (79%)	3394 (95%)	190 (5%)	21	40

All (190) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	ASP
1	A	121	PHE
1	A	143	TRP
1	A	161	LEU
1	A	170	THR
1	A	236	GLU
1	A	252	THR
1	A	263	LEU
1	A	275	PHE
1	A	292	ASP
1	A	295	CYS
1	A	299	ILE
1	A	317	LEU
1	A	353	PHE
1	A	355	SER
1	A	364	ASP
1	A	372	PHE
1	A	413	LEU
1	A	441	THR
1	A	524	THR
1	A	545	ARG
1	A	565	VAL

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Mol	Chain	Res	Type
1	A	577	GLU
1	A	583	VAL
1	A	594	THR
1	A	647	TRP
1	A	653	TYR
1	A	663	ASN
1	A	670	ASN
1	A	676	LYS
1	A	696	ASN
1	A	703	ASP
1	A	733	LEU
1	A	740	ASN
1	A	746	LEU
1	A	757	THR
1	A	786	VAL
1	B	28	THR
1	B	50	ASP
1	B	100	ASP
1	B	117	ARG
1	B	125	PHE
1	B	136	PHE
1	B	143	TRP
1	B	168	TRP
1	B	170	THR
1	B	173	LEU
1	B	244	PHE
1	B	275	PHE
1	B	279	ILE
1	B	297	VAL
1	B	317	LEU
1	B	348	LEU
1	B	351	TYR
1	B	368	VAL
1	B	372	PHE
1	B	374	PHE
1	B	405	LEU
1	B	420	LEU
1	B	442	VAL
1	B	468	LEU
1	B	478	HIS
1	B	508	ILE
1	B	510	LEU

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Mol	Chain	Res	Type
1	B	511	TRP
1	B	639	HIS
1	B	647	TRP
1	B	670	ASN
1	B	685	ARG
1	B	692	LEU
1	B	696	ASN
1	B	727	LEU
1	B	732	LYS
1	B	740	ASN
1	B	746	LEU
1	C	100	ASP
1	C	136	PHE
1	C	143	TRP
1	C	162	LYS
1	C	166	SER
1	C	170	THR
1	C	236	GLU
1	C	275	PHE
1	C	279	ILE
1	C	308	TYR
1	C	348	LEU
1	C	353	PHE
1	C	372	PHE
1	C	392	VAL
1	C	405	LEU
1	C	412	THR
1	C	414	ASP
1	C	415	LYS
1	C	417	ARG
1	C	429	GLU
1	C	448	LEU
1	C	460	THR
1	C	468	LEU
1	C	506	LYS
1	C	591	VAL
1	C	647	TRP
1	C	681	LEU
1	C	696	ASN
1	C	703	ASP
1	C	730	CYS
1	C	740	ASN

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Mol	Chain	Res	Type
1	C	742	VAL
1	D	100	ASP
1	D	104	HIS
1	D	143	TRP
1	D	155	HIS
1	D	161	LEU
1	D	174	SER
1	D	275	PHE
1	D	279	ILE
1	D	280	CYS
1	D	284	TYR
1	D	292	ASP
1	D	317	LEU
1	D	344	LEU
1	D	353	PHE
1	D	354	GLU
1	D	356	ILE
1	D	364	ASP
1	D	368	VAL
1	D	372	PHE
1	D	376	LEU
1	D	393	PHE
1	D	405	LEU
1	D	410	GLU
1	D	441	THR
1	D	446	VAL
1	D	584	LEU
1	D	635	PHE
1	D	647	TRP
1	D	670	ASN
1	D	679	THR
1	D	684	CYS
1	D	727	LEU
1	D	737	HIS
1	D	743	LEU
1	D	793	THR
2	E	58	ARG
2	E	96	MET
2	E	109	SER
2	E	123	TYR
2	E	138	PHE
2	E	162	LEU

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Mol	Chain	Res	Type
2	E	166	PHE
2	E	241	LEU
2	E	247	LYS
2	E	249	ARG
2	E	256	ASP
2	E	259	TYR
2	E	273	PHE
2	E	297	ILE
2	E	314	HIS
2	E	315	LEU
2	E	367	LYS
2	E	374	LEU
2	E	392	LEU
2	E	405	LEU
2	E	555	LYS
2	E	563	VAL
2	E	575	ASP
2	E	580	VAL
2	E	584	ASN
2	E	598	HIS
2	E	617	LEU
2	E	744	LEU
2	E	779	ARG
2	F	17	PHE
2	F	58	ARG
2	F	96	MET
2	F	123	TYR
2	F	138	PHE
2	F	166	PHE
2	F	247	LYS
2	F	249	ARG
2	F	256	ASP
2	F	273	PHE
2	F	297	ILE
2	F	309	ASN
2	F	314	HIS
2	F	315	LEU
2	F	339	TYR
2	F	367	LYS
2	F	370	PHE
2	F	374	LEU
2	F	392	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	105	GLN
1	A	119	HIS
1	A	381	GLN
1	A	431	HIS
1	A	467	GLN
1	A	522	HIS
1	A	615	ASN
1	A	708	GLN
1	A	712	ASN
1	B	104	HIS
1	B	116	ASN
1	B	467	GLN
1	B	554	ASN
1	B	614	HIS
1	B	624	ASN
1	B	663	ASN
1	C	404	GLN
1	C	408	ASN
1	C	494	ASN
1	C	660	ASN
1	C	712	ASN
1	D	400	ASN
1	D	418	GLN
1	D	615	ASN
1	D	696	ASN
1	D	709	ASN
1	D	741	ASN
2	E	113	GLN
2	E	121	HIS
2	E	309	ASN
2	E	375	HIS
2	E	379	GLN
2	E	406	ASN
2	E	606	HIS
2	F	106	GLN
2	F	121	HIS
2	F	309	ASN
2	F	402	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

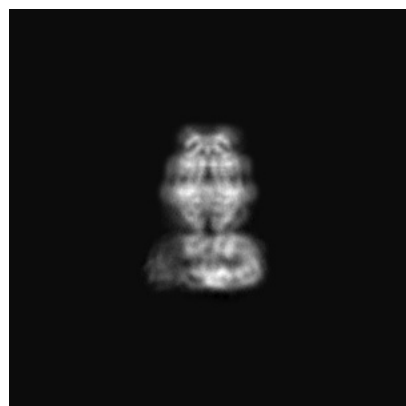
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15837. These allow visual inspection of the internal detail of the map and identification of artifacts.

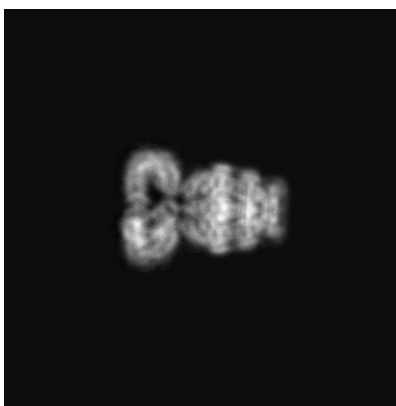
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

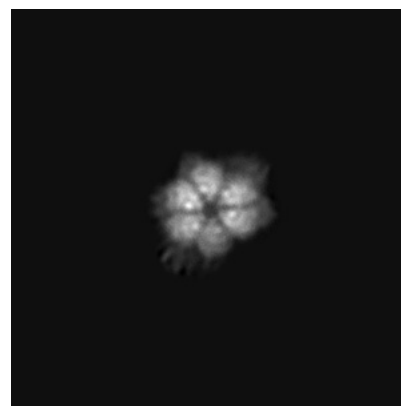
6.1.1 Primary map



X

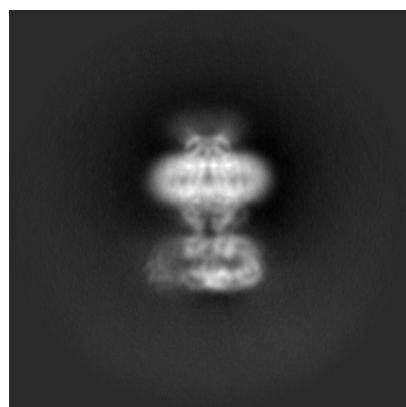


Y

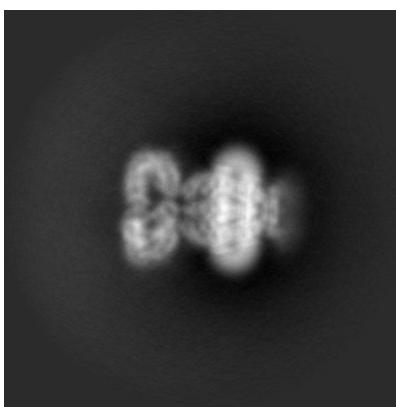


Z

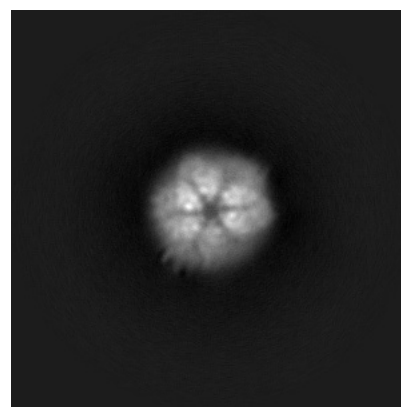
6.1.2 Raw map



X



Y



Z

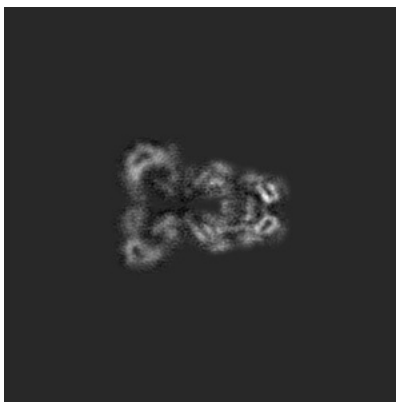
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

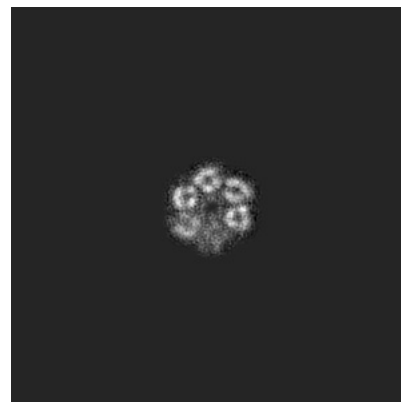
6.2.1 Primary map



X Index: 168

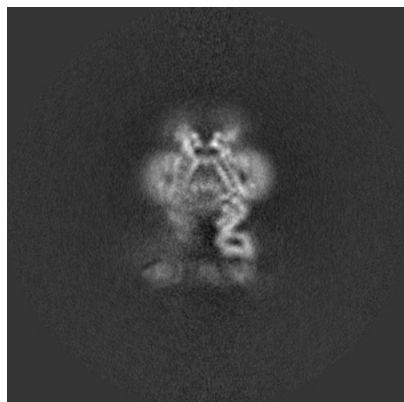


Y Index: 168

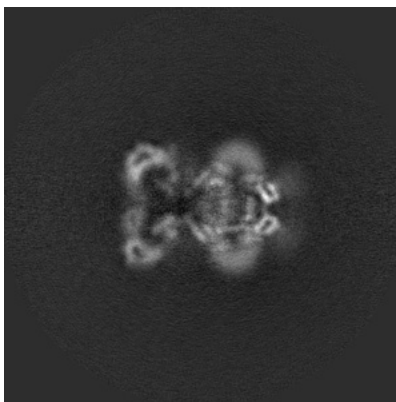


Z Index: 168

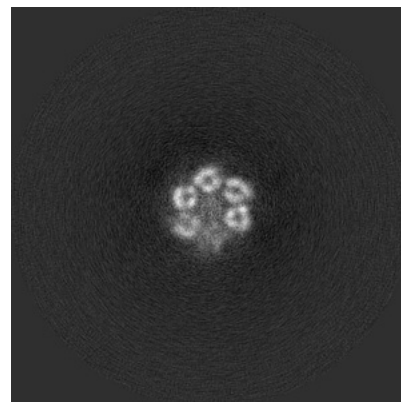
6.2.2 Raw map



X Index: 168



Y Index: 168



Z Index: 168

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

6.3 Largest variance slices [i](#)

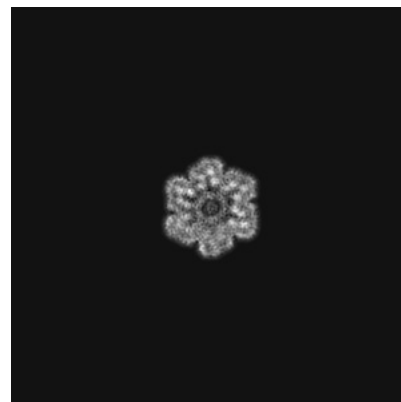
6.3.1 Primary map



X Index: 149

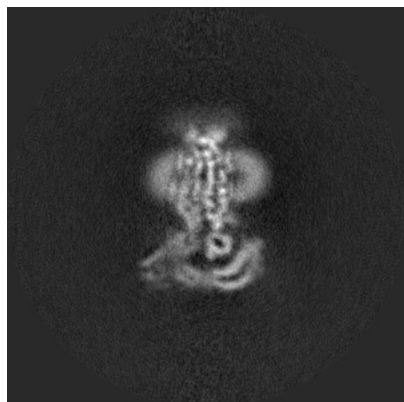


Y Index: 181

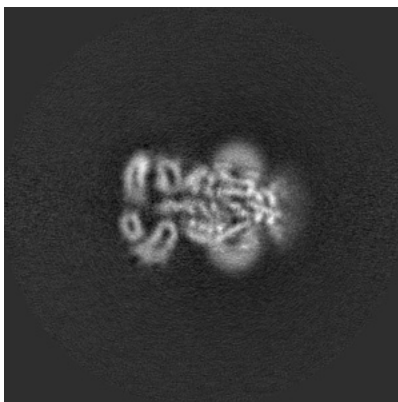


Z Index: 182

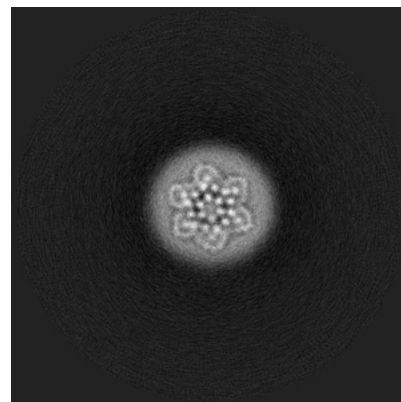
6.3.2 Raw map



X Index: 149



Y Index: 181

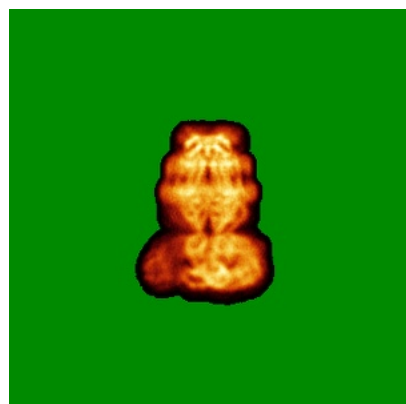


Z Index: 205

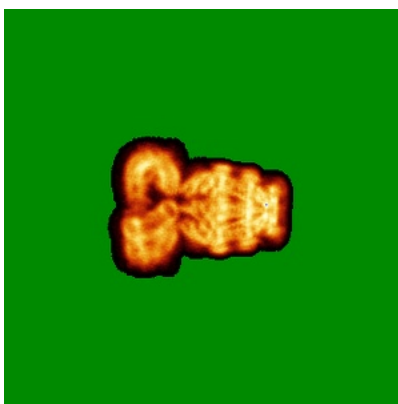
The images above show the largest variance slices of the map in three orthogonal directions.

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

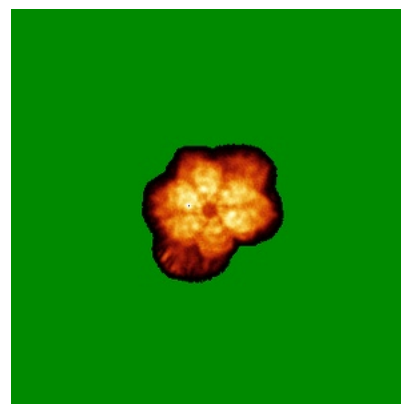
6.4.1 Primary map



X



Y

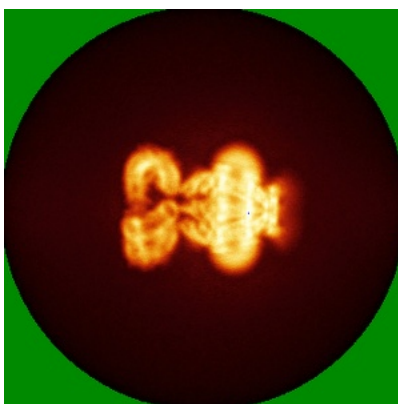


Z

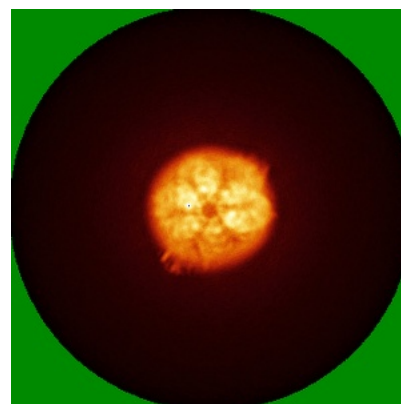
6.4.2 Raw map



X



Y

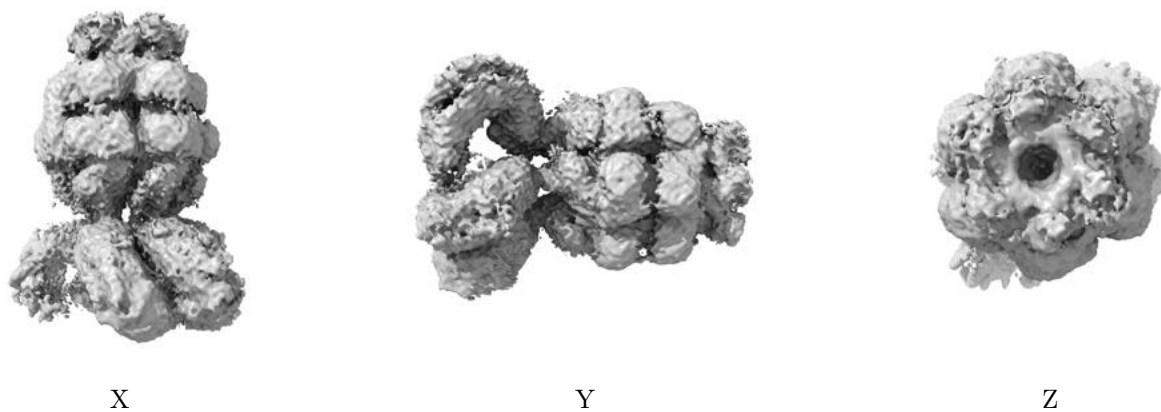


Z

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

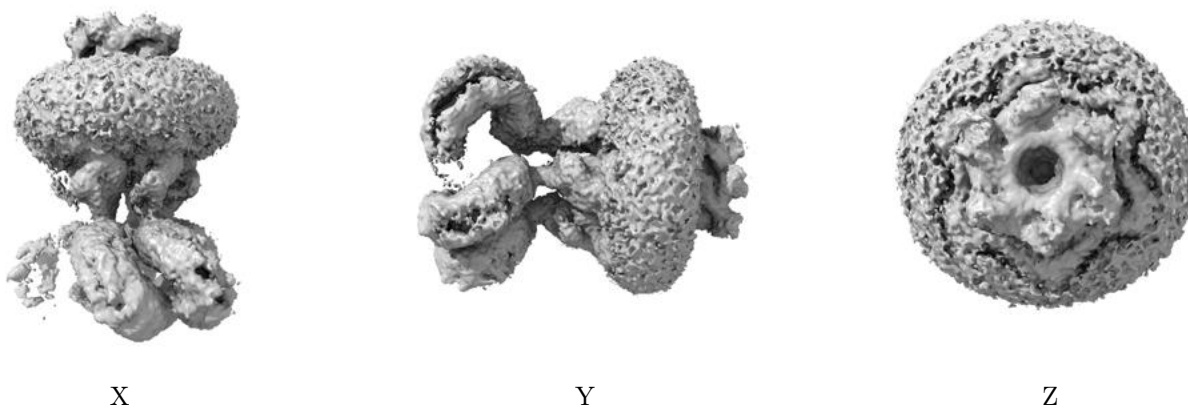
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

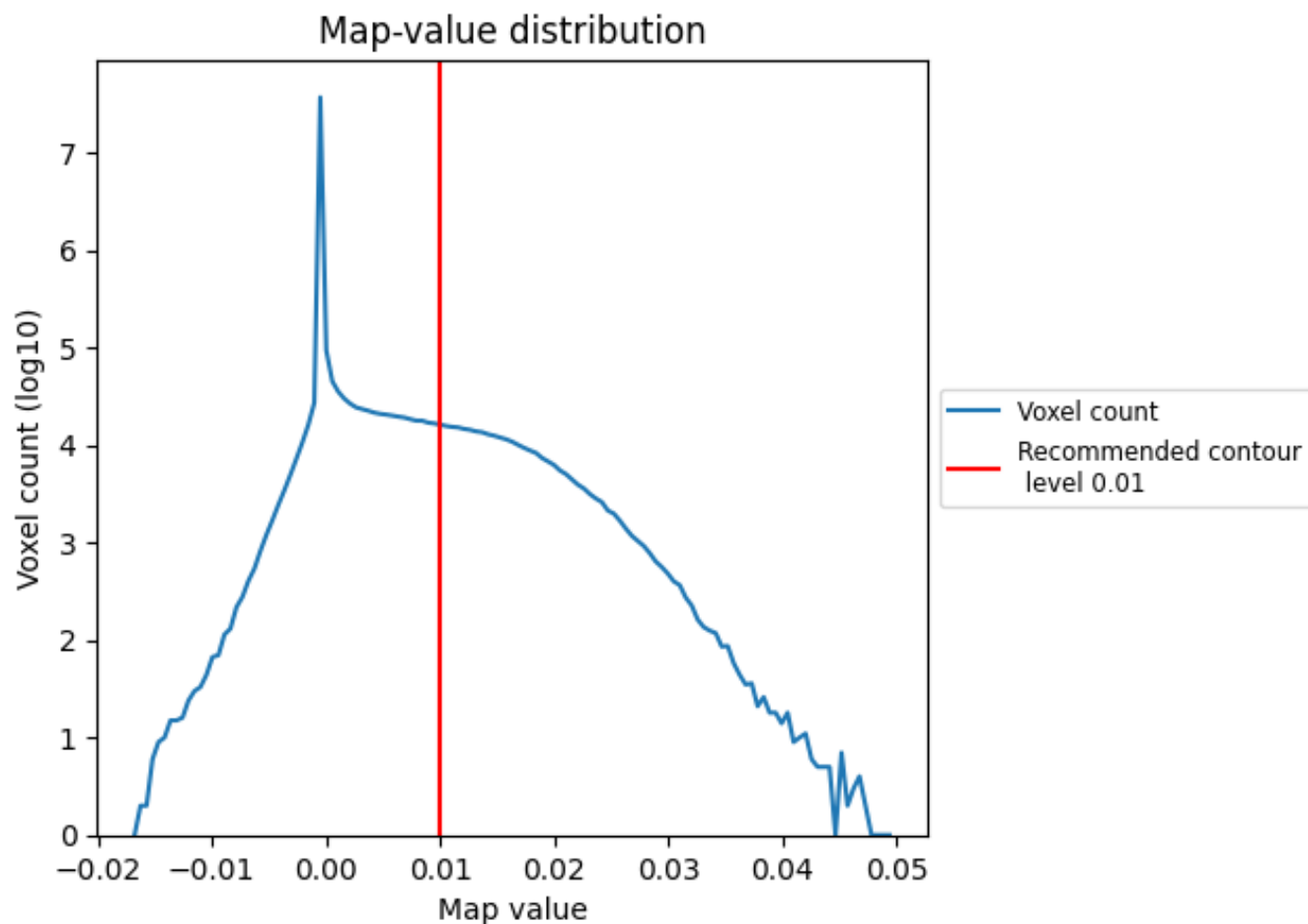
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

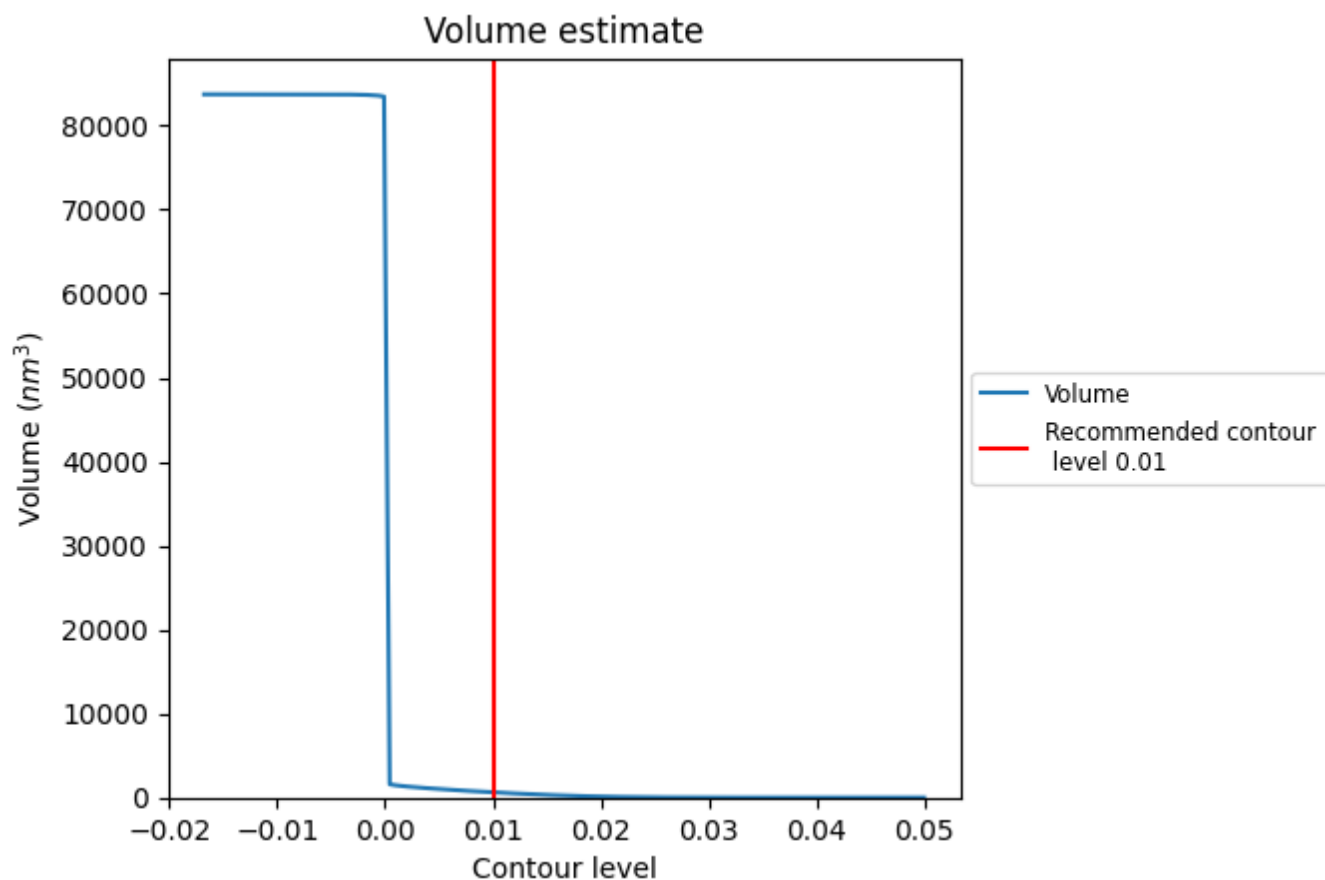
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

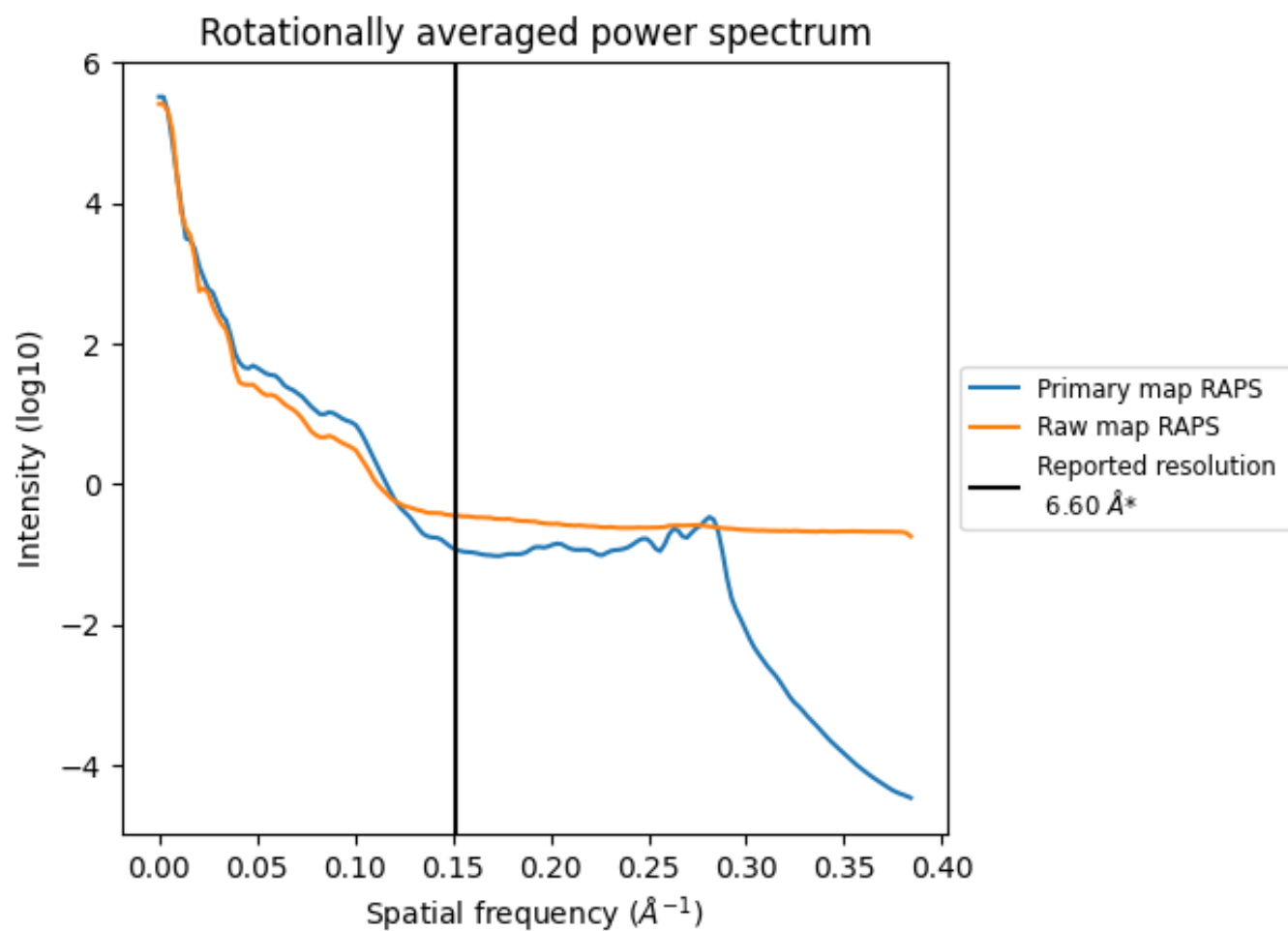
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 624 nm^3 ; this corresponds to an approximate mass of 564 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 ⓘ

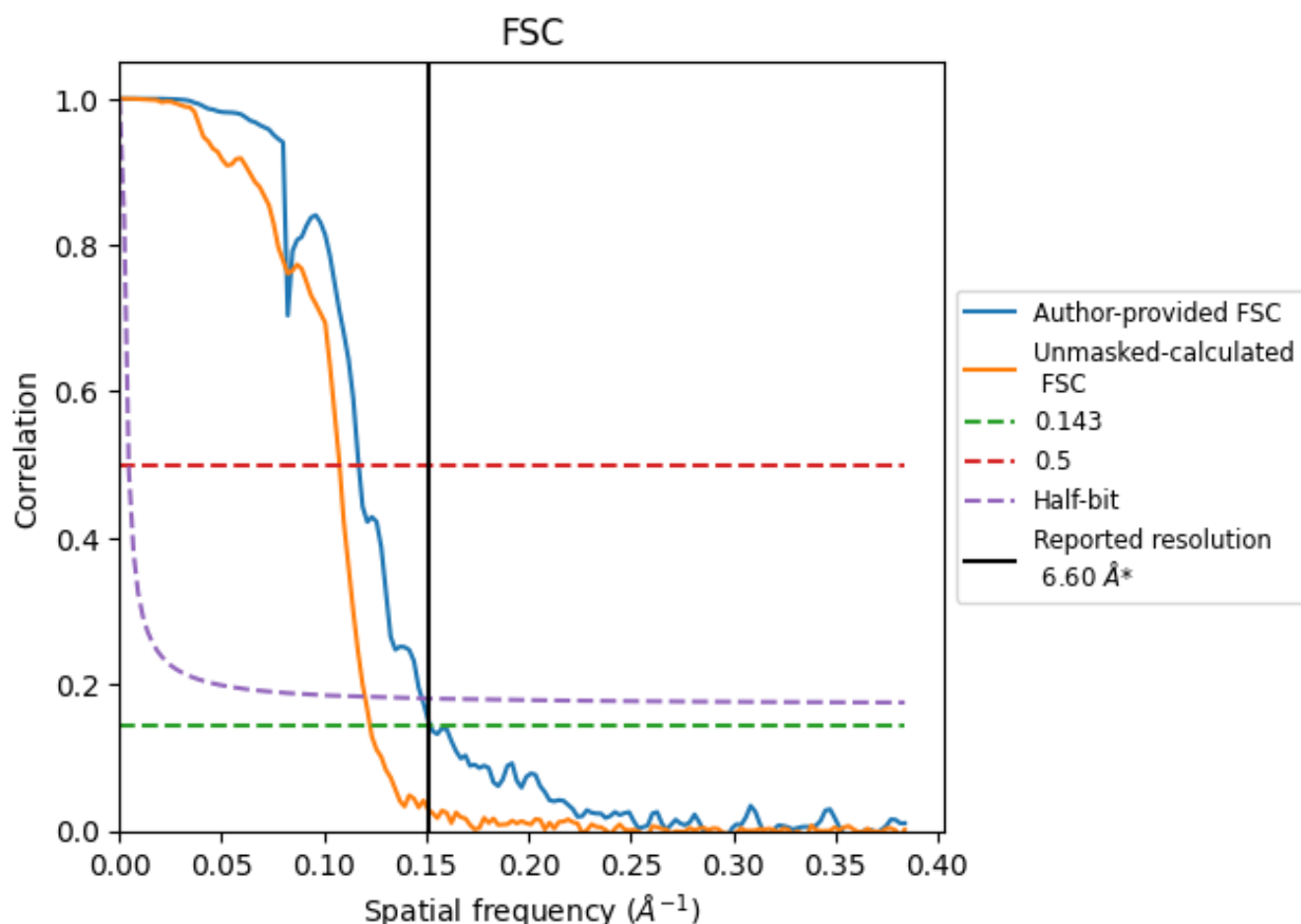


*Reported resolution corresponds to spatial frequency of 0.152 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.152 Å⁻¹

8.2 Resolution estimates [i](#)

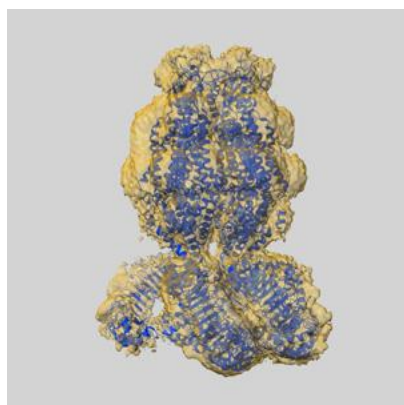
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.60	-	-
Author-provided FSC curve	6.57	8.55	6.76
Unmasked-calculated*	8.16	9.29	8.33

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.16 differs from the reported value 6.6 by more than 10 %

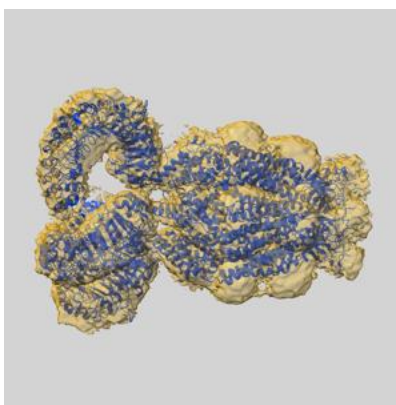
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15837 and PDB model 8B42. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

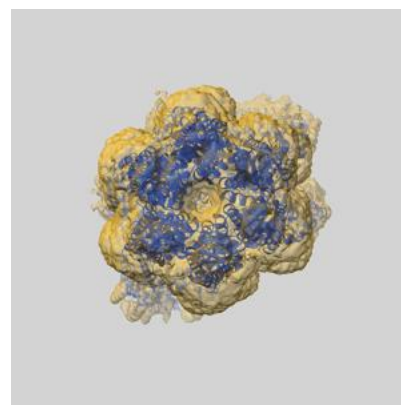
9.1 Map-model overlay [i](#)



X



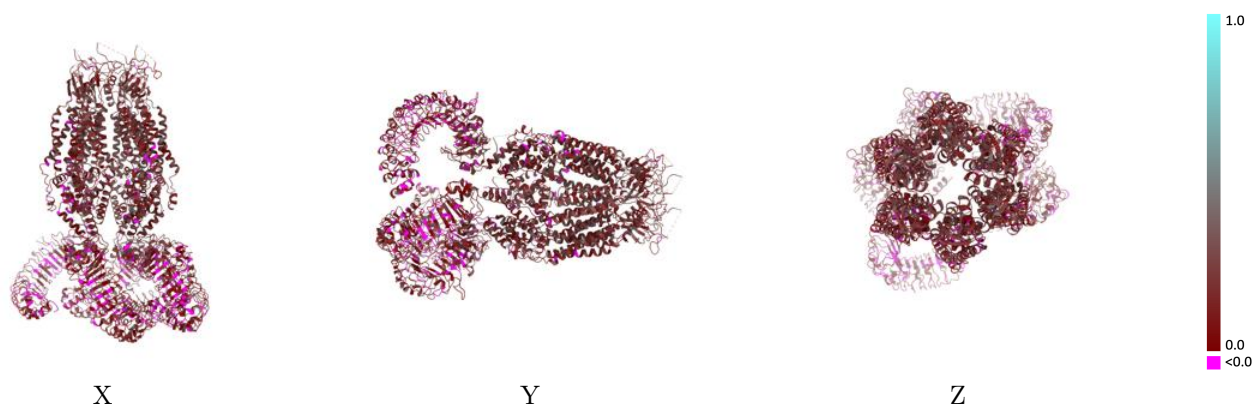
Y



Z

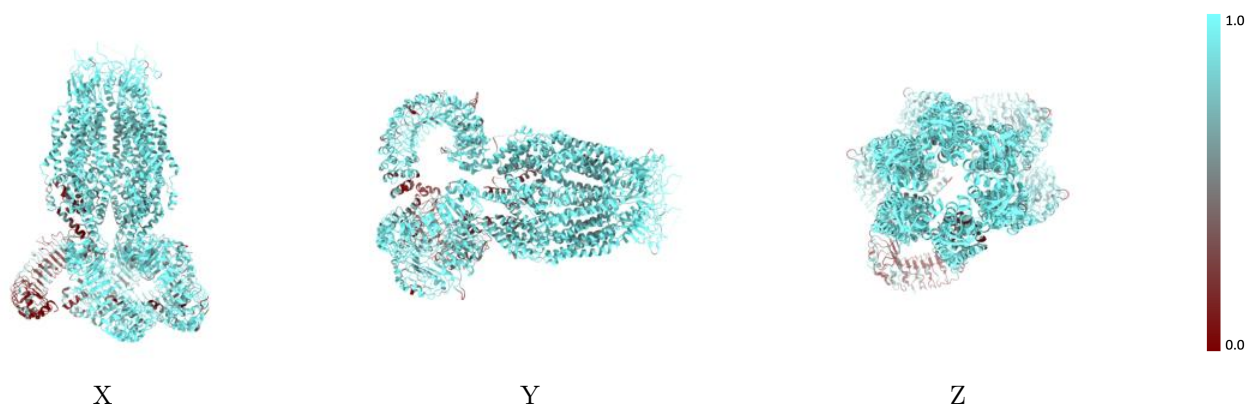
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



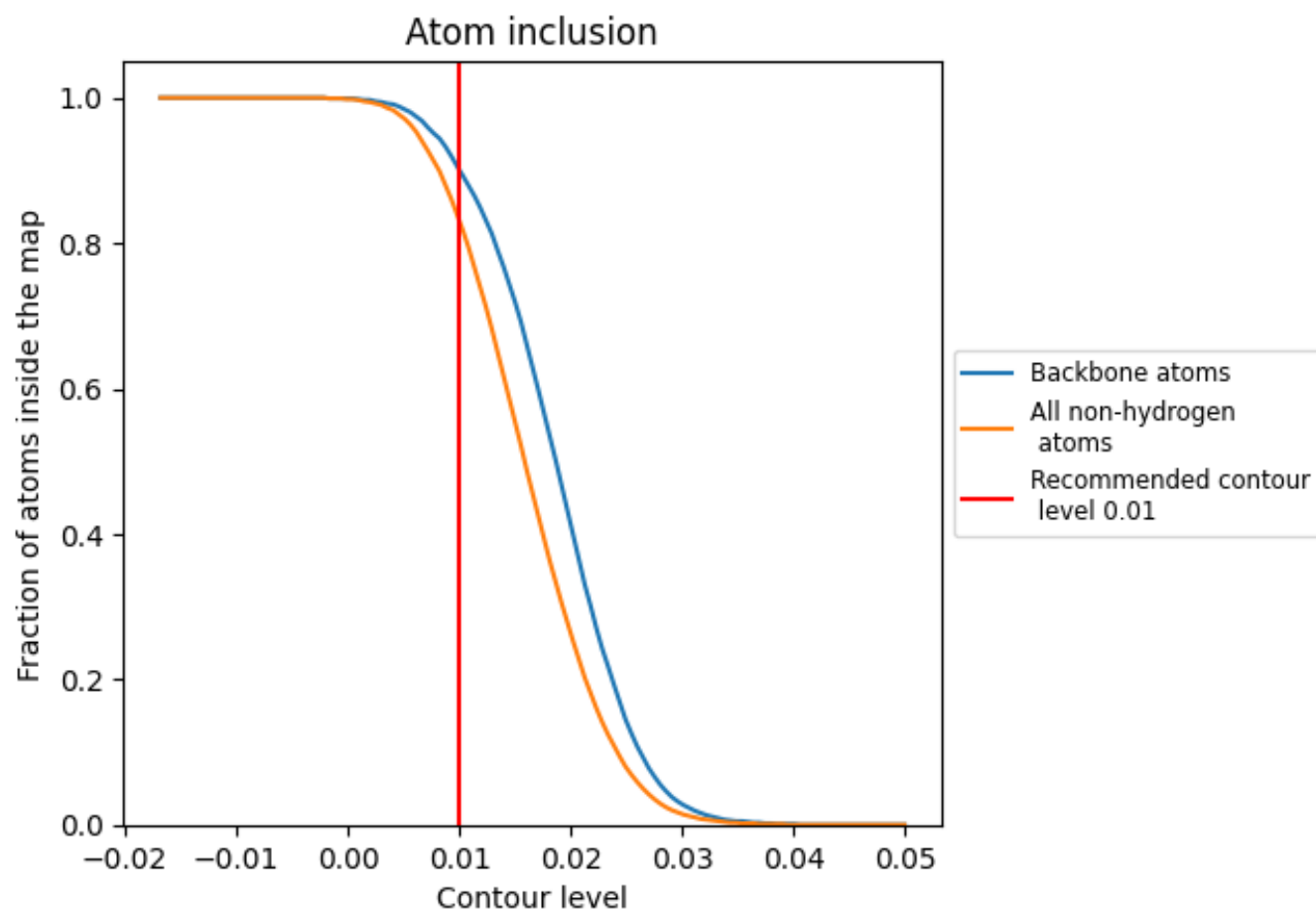
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 83% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8320</div>	<div><div></div>0.1670</div>
A	<div><div></div>0.9230</div>	<div><div></div>0.1710</div>
B	<div><div></div>0.8650</div>	<div><div></div>0.1650</div>
C	<div><div></div>0.8920</div>	<div><div></div>0.1780</div>
D	<div><div></div>0.8790</div>	<div><div></div>0.1700</div>
E	<div><div></div>0.6060</div>	<div><div></div>0.1430</div>
F	<div><div></div>0.7960</div>	<div><div></div>0.1820</div>

1.0

0.0

<0.0