Full wwPDB EM Validation Report (i)

Sep 21, 2026 – 07:26 pm BST

PDB ID	:	9T5N / pdb_00009t5n
EMDB ID	:	EMD-55590
Title	:	Structure of heteromeric mouse LRRC8A/D Volume-Regulated Anion Channel in complex with synthetic nanobody Sb1, Conformation 1
Authors	:	Lehmann, E.F.; Deneka, D.; Stierli, F.; Rutz, S.; Dutzler, R.
Deposited on	:	2025-11-05
Resolution	:	3.02 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 (i) 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 (i)) were used in the production of this report:

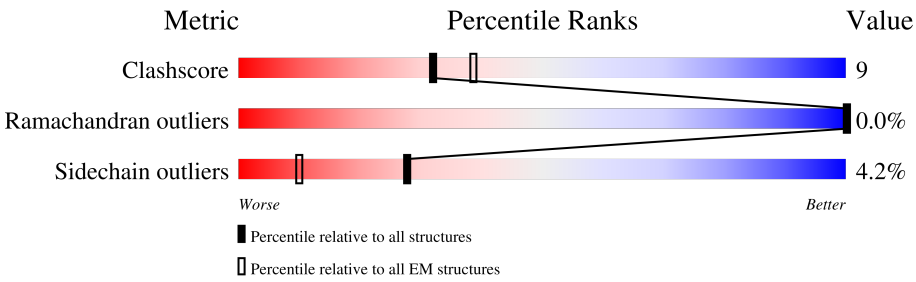
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

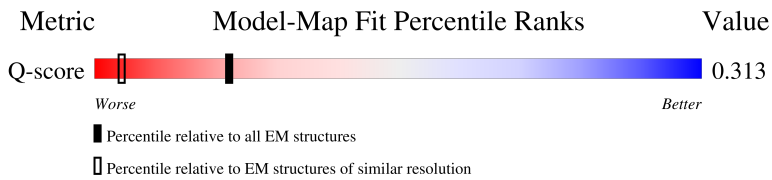
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.02 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	13913 (2.52 - 3.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	818	68% 19% • 12%
1	B	818	69% 18% • 11%
1	C	818	• 64% 23% 12%
1	D	818	5% 67% 22% • 11%

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Mol	Chain	Length	Quality of chain
2	G	118	64% 31%
2	H	118	69% 24%
2	I	118	14% 67% 30%
2	J	118	93% 79% 17%
3	E	924	14% 55% 19% 24%
3	F	924	30% 54% 20% 24%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 38972 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
			Total	C	N	O	S		
1	A	718	5922	3853	997	1047	25	0	0
1	B	732	6030	3916	1018	1071	25	0	0
1	C	718	5922	3853	997	1047	25	0	0
1	D	732	6030	3916	1018	1071	25	0	0

There are 36 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	ALA	-	expression tag	UNP Q80WG5
A	812	LEU	-	expression tag	UNP Q80WG5
A	813	GLU	-	expression tag	UNP Q80WG5
A	814	VAL	-	expression tag	UNP Q80WG5
A	815	LEU	-	expression tag	UNP Q80WG5
A	816	PHE	-	expression tag	UNP Q80WG5
A	817	GLN	-	expression tag	UNP Q80WG5
B	0	MET	-	initiating methionine	UNP Q80WG5
B	1	SER	-	expression tag	UNP Q80WG5
B	811	ALA	-	expression tag	UNP Q80WG5
B	812	LEU	-	expression tag	UNP Q80WG5
B	813	GLU	-	expression tag	UNP Q80WG5
B	814	VAL	-	expression tag	UNP Q80WG5
B	815	LEU	-	expression tag	UNP Q80WG5
B	816	PHE	-	expression tag	UNP Q80WG5
B	817	GLN	-	expression tag	UNP Q80WG5
C	0	MET	-	initiating methionine	UNP Q80WG5
C	1	SER	-	expression tag	UNP Q80WG5
C	811	ALA	-	expression tag	UNP Q80WG5
C	812	LEU	-	expression tag	UNP Q80WG5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	813	GLU	-	expression tag	UNP Q80WG5
C	814	VAL	-	expression tag	UNP Q80WG5
C	815	LEU	-	expression tag	UNP Q80WG5
C	816	PHE	-	expression tag	UNP Q80WG5
C	817	GLN	-	expression tag	UNP Q80WG5
D	0	MET	-	initiating methionine	UNP Q80WG5
D	1	SER	-	expression tag	UNP Q80WG5
D	811	ALA	-	expression tag	UNP Q80WG5
D	812	LEU	-	expression tag	UNP Q80WG5
D	813	GLU	-	expression tag	UNP Q80WG5
D	814	VAL	-	expression tag	UNP Q80WG5
D	815	LEU	-	expression tag	UNP Q80WG5
D	816	PHE	-	expression tag	UNP Q80WG5
D	817	GLN	-	expression tag	UNP Q80WG5

- Molecule 2 is a protein called Sb1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	G	114	903	575	152	172	4	0	0
2	H	114	903	575	152	172	4	0	0
2	I	114	903	575	152	172	4	0	0
2	J	114	903	575	152	172	4	0	0

- Molecule 3 is a protein called Volume-regulated anion channel subunit LRRC8D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	702	5728	3729	951	1013	35	1	0
3	F	702	5728	3729	951	1013	35	1	0

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	MET	-	initiating methionine	UNP Q8BGR2
E	1	SER	-	expression tag	UNP Q8BGR2
E	61N	VAL	ILE	conflict	UNP Q8BGR2
E	63O	VAL	ALA	conflict	UNP Q8BGR2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	313	VAL	LEU	conflict	UNP Q8BGR2
E	347	ILE	THR	conflict	UNP Q8BGR2
E	859	ALA	-	expression tag	UNP Q8BGR2
E	860	LEU	-	expression tag	UNP Q8BGR2
E	861	GLU	-	expression tag	UNP Q8BGR2
E	862	VAL	-	expression tag	UNP Q8BGR2
E	863	LEU	-	expression tag	UNP Q8BGR2
E	864	PHE	-	expression tag	UNP Q8BGR2
E	865	GLN	-	expression tag	UNP Q8BGR2
E	866	GLY	-	expression tag	UNP Q8BGR2
E	867	PRO	-	expression tag	UNP Q8BGR2
E	868	GLN	-	expression tag	UNP Q8BGR2
E	869	GLY	-	expression tag	UNP Q8BGR2
E	870	THR	-	expression tag	UNP Q8BGR2
E	871	GLU	-	expression tag	UNP Q8BGR2
E	872	GLN	-	expression tag	UNP Q8BGR2
E	873	LYS	-	expression tag	UNP Q8BGR2
E	874	LEU	-	expression tag	UNP Q8BGR2
E	875	ILE	-	expression tag	UNP Q8BGR2
E	876	SER	-	expression tag	UNP Q8BGR2
E	877	GLU	-	expression tag	UNP Q8BGR2
E	878	GLU	-	expression tag	UNP Q8BGR2
E	879	ASP	-	expression tag	UNP Q8BGR2
E	880	LEU	-	expression tag	UNP Q8BGR2
E	881	ARG	-	expression tag	UNP Q8BGR2
E	882	GLY	-	expression tag	UNP Q8BGR2
E	883	ALA	-	expression tag	UNP Q8BGR2
E	884	SER	-	expression tag	UNP Q8BGR2
E	885	MET	-	expression tag	UNP Q8BGR2
E	886	ASP	-	expression tag	UNP Q8BGR2
E	887	GLU	-	expression tag	UNP Q8BGR2
E	888	LYS	-	expression tag	UNP Q8BGR2
E	889	THR	-	expression tag	UNP Q8BGR2
E	890	THR	-	expression tag	UNP Q8BGR2
E	891	GLY	-	expression tag	UNP Q8BGR2
E	892	TRP	-	expression tag	UNP Q8BGR2
E	893	ARG	-	expression tag	UNP Q8BGR2
E	894	GLY	-	expression tag	UNP Q8BGR2
E	895	GLY	-	expression tag	UNP Q8BGR2
E	896	HIS	-	expression tag	UNP Q8BGR2
E	897	VAL	-	expression tag	UNP Q8BGR2
E	898	VAL	-	expression tag	UNP Q8BGR2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	899	GLU	-	expression tag	UNP Q8BGR2
E	900	GLY	-	expression tag	UNP Q8BGR2
E	901	LEU	-	expression tag	UNP Q8BGR2
E	902	ALA	-	expression tag	UNP Q8BGR2
E	903	GLY	-	expression tag	UNP Q8BGR2
E	904	GLU	-	expression tag	UNP Q8BGR2
E	905	LEU	-	expression tag	UNP Q8BGR2
E	906	GLU	-	expression tag	UNP Q8BGR2
E	907	GLN	-	expression tag	UNP Q8BGR2
E	908	LEU	-	expression tag	UNP Q8BGR2
E	909	ARG	-	expression tag	UNP Q8BGR2
E	910	ALA	-	expression tag	UNP Q8BGR2
E	911	ARG	-	expression tag	UNP Q8BGR2
E	912	LEU	-	expression tag	UNP Q8BGR2
E	913	GLU	-	expression tag	UNP Q8BGR2
E	914	HIS	-	expression tag	UNP Q8BGR2
E	915	HIS	-	expression tag	UNP Q8BGR2
E	916	PRO	-	expression tag	UNP Q8BGR2
E	917	GLN	-	expression tag	UNP Q8BGR2
E	918	GLY	-	expression tag	UNP Q8BGR2
E	919	GLN	-	expression tag	UNP Q8BGR2
E	920	ARG	-	expression tag	UNP Q8BGR2
E	921	GLU	-	expression tag	UNP Q8BGR2
E	922	PRO	-	expression tag	UNP Q8BGR2
F	0	MET	-	initiating methionine	UNP Q8BGR2
F	1	SER	-	expression tag	UNP Q8BGR2
F	61N	VAL	ILE	conflict	UNP Q8BGR2
F	63O	VAL	ALA	conflict	UNP Q8BGR2
F	313	VAL	LEU	conflict	UNP Q8BGR2
F	347	ILE	THR	conflict	UNP Q8BGR2
F	859	ALA	-	expression tag	UNP Q8BGR2
F	860	LEU	-	expression tag	UNP Q8BGR2
F	861	GLU	-	expression tag	UNP Q8BGR2
F	862	VAL	-	expression tag	UNP Q8BGR2
F	863	LEU	-	expression tag	UNP Q8BGR2
F	864	PHE	-	expression tag	UNP Q8BGR2
F	865	GLN	-	expression tag	UNP Q8BGR2
F	866	GLY	-	expression tag	UNP Q8BGR2
F	867	PRO	-	expression tag	UNP Q8BGR2
F	868	GLN	-	expression tag	UNP Q8BGR2
F	869	GLY	-	expression tag	UNP Q8BGR2
F	870	THR	-	expression tag	UNP Q8BGR2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	871	GLU	-	expression tag	UNP Q8BGR2
F	872	GLN	-	expression tag	UNP Q8BGR2
F	873	LYS	-	expression tag	UNP Q8BGR2
F	874	LEU	-	expression tag	UNP Q8BGR2
F	875	ILE	-	expression tag	UNP Q8BGR2
F	876	SER	-	expression tag	UNP Q8BGR2
F	877	GLU	-	expression tag	UNP Q8BGR2
F	878	GLU	-	expression tag	UNP Q8BGR2
F	879	ASP	-	expression tag	UNP Q8BGR2
F	880	LEU	-	expression tag	UNP Q8BGR2
F	881	ARG	-	expression tag	UNP Q8BGR2
F	882	GLY	-	expression tag	UNP Q8BGR2
F	883	ALA	-	expression tag	UNP Q8BGR2
F	884	SER	-	expression tag	UNP Q8BGR2
F	885	MET	-	expression tag	UNP Q8BGR2
F	886	ASP	-	expression tag	UNP Q8BGR2
F	887	GLU	-	expression tag	UNP Q8BGR2
F	888	LYS	-	expression tag	UNP Q8BGR2
F	889	THR	-	expression tag	UNP Q8BGR2
F	890	THR	-	expression tag	UNP Q8BGR2
F	891	GLY	-	expression tag	UNP Q8BGR2
F	892	TRP	-	expression tag	UNP Q8BGR2
F	893	ARG	-	expression tag	UNP Q8BGR2
F	894	GLY	-	expression tag	UNP Q8BGR2
F	895	GLY	-	expression tag	UNP Q8BGR2
F	896	HIS	-	expression tag	UNP Q8BGR2
F	897	VAL	-	expression tag	UNP Q8BGR2
F	898	VAL	-	expression tag	UNP Q8BGR2
F	899	GLU	-	expression tag	UNP Q8BGR2
F	900	GLY	-	expression tag	UNP Q8BGR2
F	901	LEU	-	expression tag	UNP Q8BGR2
F	902	ALA	-	expression tag	UNP Q8BGR2
F	903	GLY	-	expression tag	UNP Q8BGR2
F	904	GLU	-	expression tag	UNP Q8BGR2
F	905	LEU	-	expression tag	UNP Q8BGR2
F	906	GLU	-	expression tag	UNP Q8BGR2
F	907	GLN	-	expression tag	UNP Q8BGR2
F	908	LEU	-	expression tag	UNP Q8BGR2
F	909	ARG	-	expression tag	UNP Q8BGR2
F	910	ALA	-	expression tag	UNP Q8BGR2
F	911	ARG	-	expression tag	UNP Q8BGR2
F	912	LEU	-	expression tag	UNP Q8BGR2

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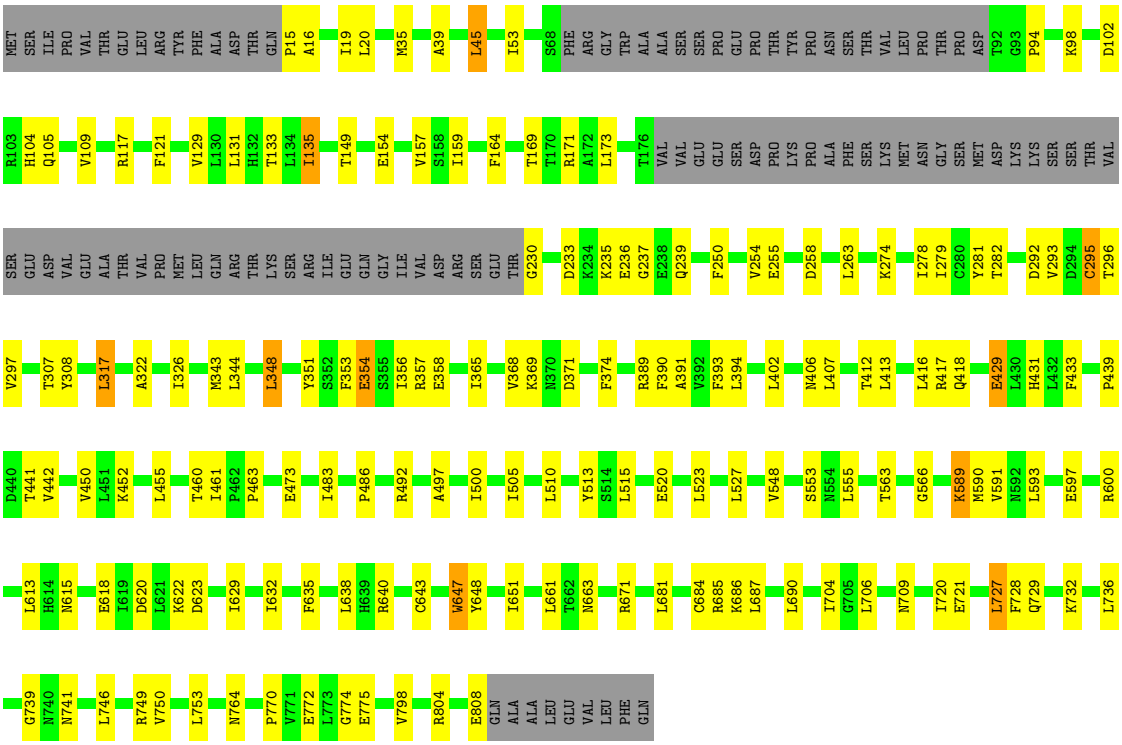
Chain	Residue	Modelled	Actual	Comment	Reference
F	913	GLU	-	expression tag	UNP Q8BGR2
F	914	HIS	-	expression tag	UNP Q8BGR2
F	915	HIS	-	expression tag	UNP Q8BGR2
F	916	PRO	-	expression tag	UNP Q8BGR2
F	917	GLN	-	expression tag	UNP Q8BGR2
F	918	GLY	-	expression tag	UNP Q8BGR2
F	919	GLN	-	expression tag	UNP Q8BGR2
F	920	ARG	-	expression tag	UNP Q8BGR2
F	921	GLU	-	expression tag	UNP Q8BGR2
F	922	PRO	-	expression tag	UNP Q8BGR2

3 Residue-property plots (i)

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

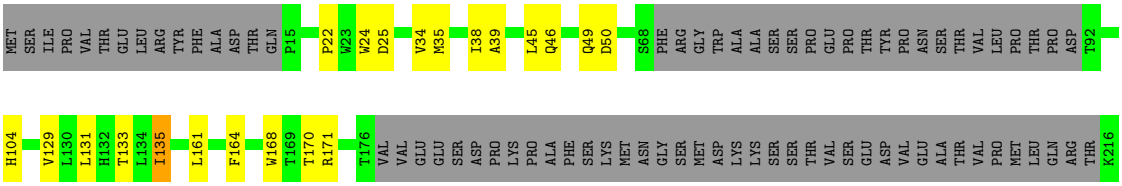
• Molecule 1: Volume-regulated anion channel subunit LRRC8A

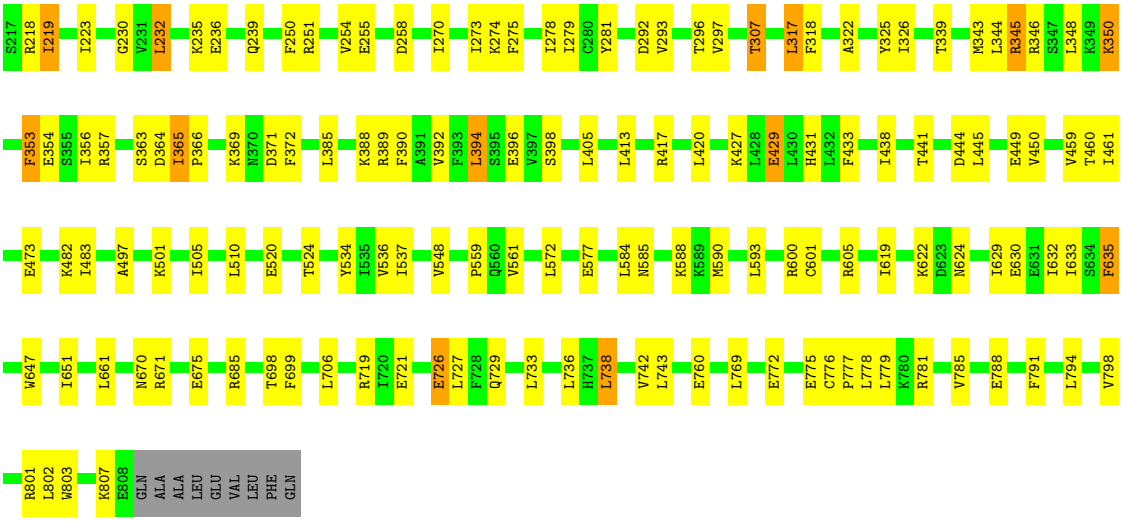
Chain A:



• Molecule 1: Volume-regulated anion channel subunit LRRC8A

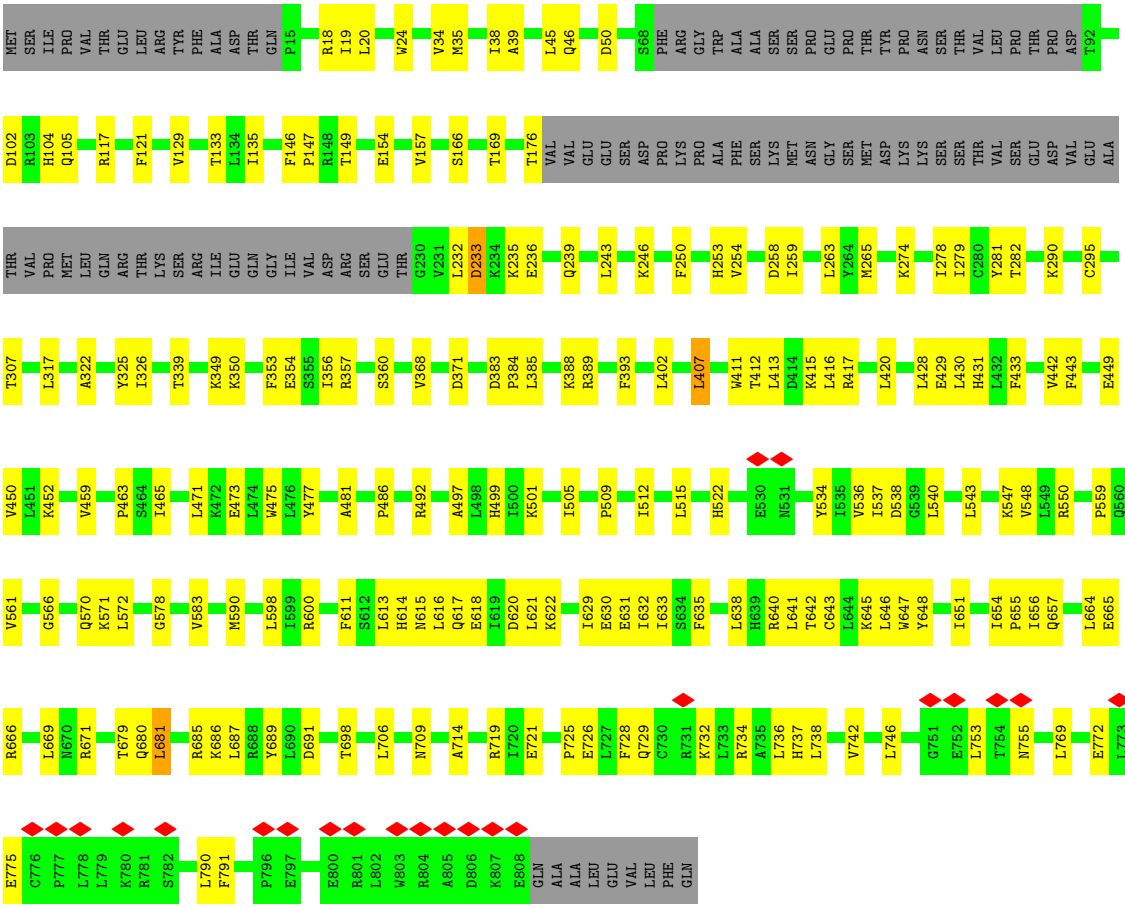
Chain B:





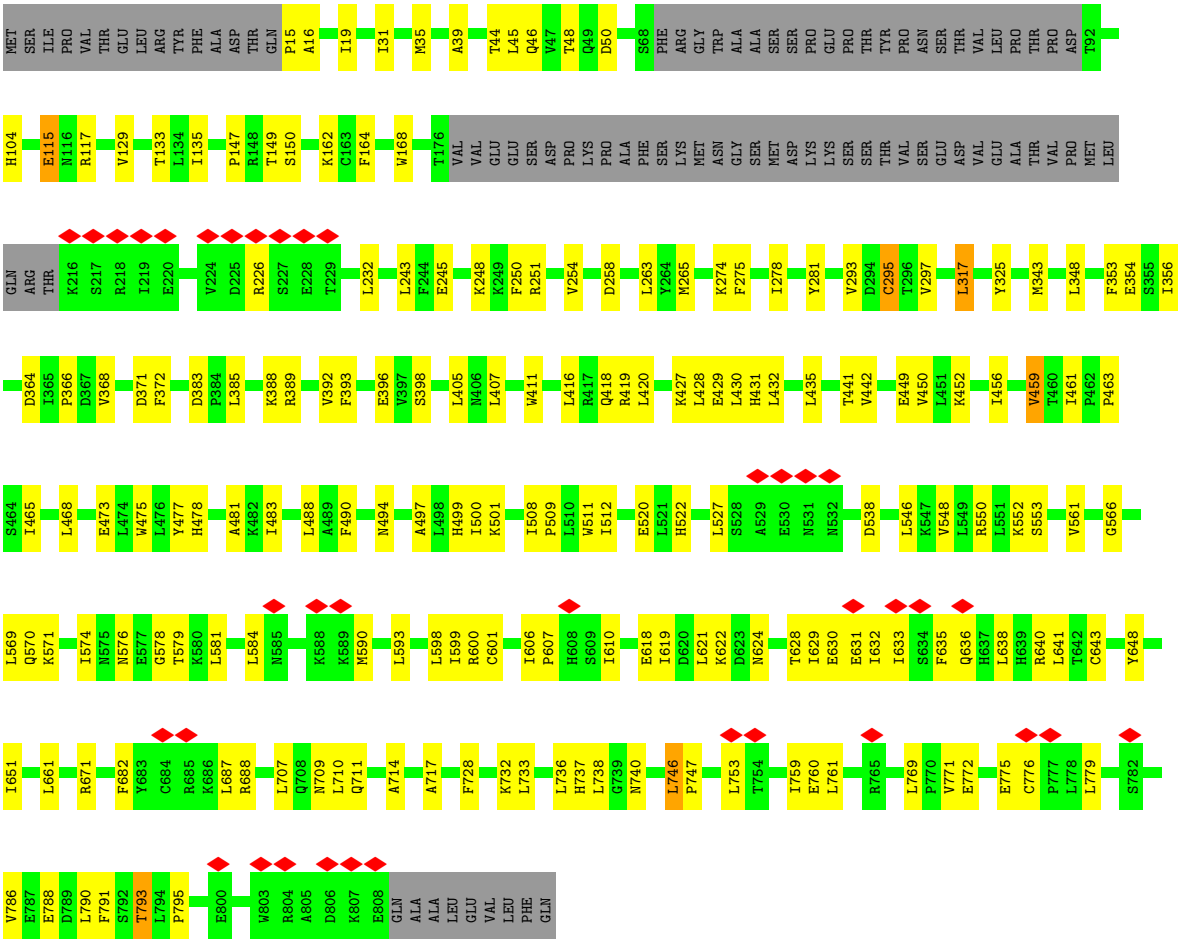
• Molecule 1: Volume-regulated anion channel subunit LRRC8A

Chain C:



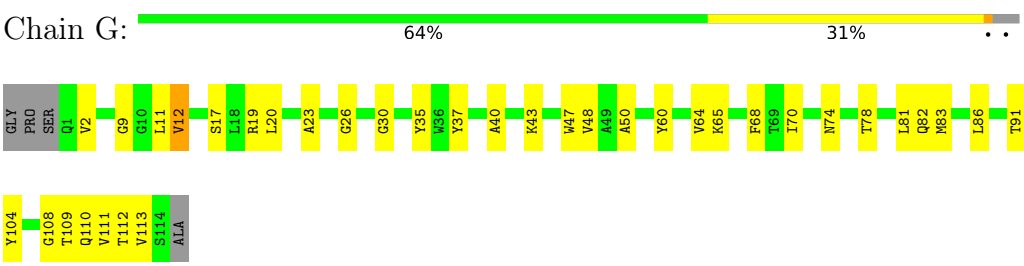
• Molecule 1: Volume-regulated anion channel subunit LRRC8A

Chain D:



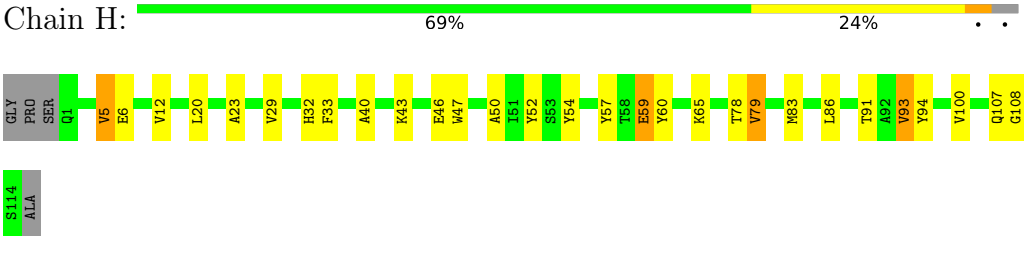
- Molecule 2: Sb1

Chain G:



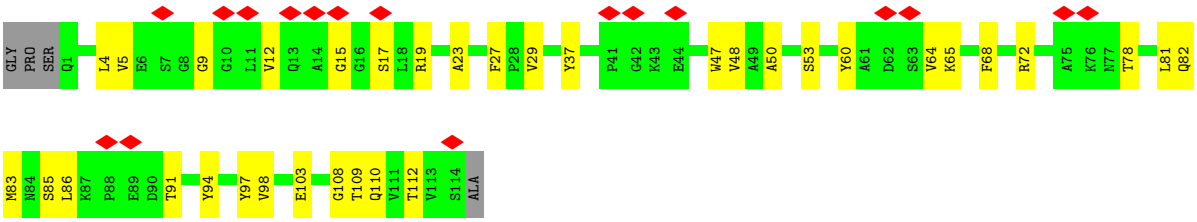
- Molecule 2: Sb1

Chain H:



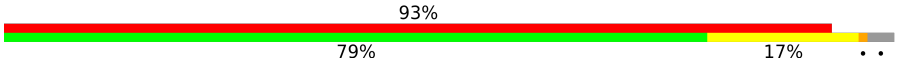
- Molecule 2: Sb1

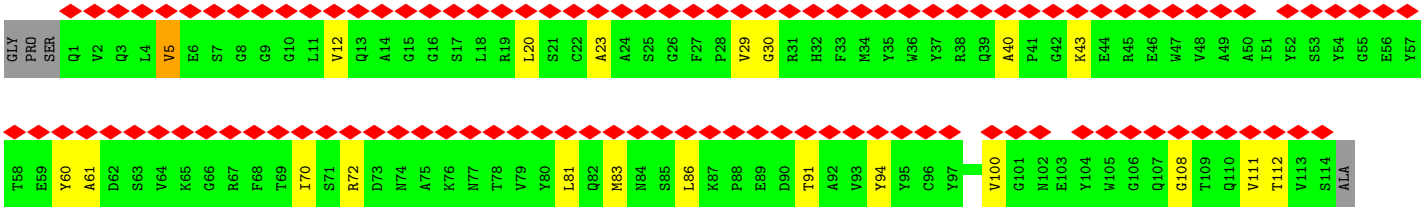
Chain I:



• Molecule 2: Sb1

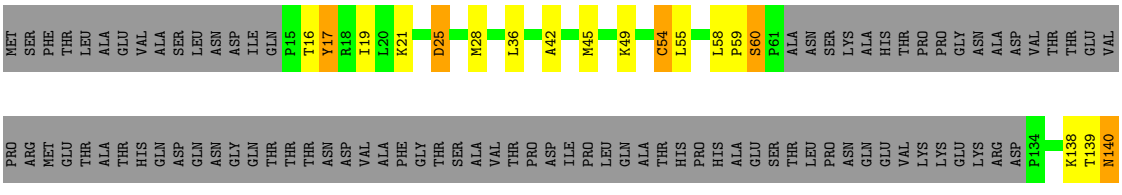
Chain J:

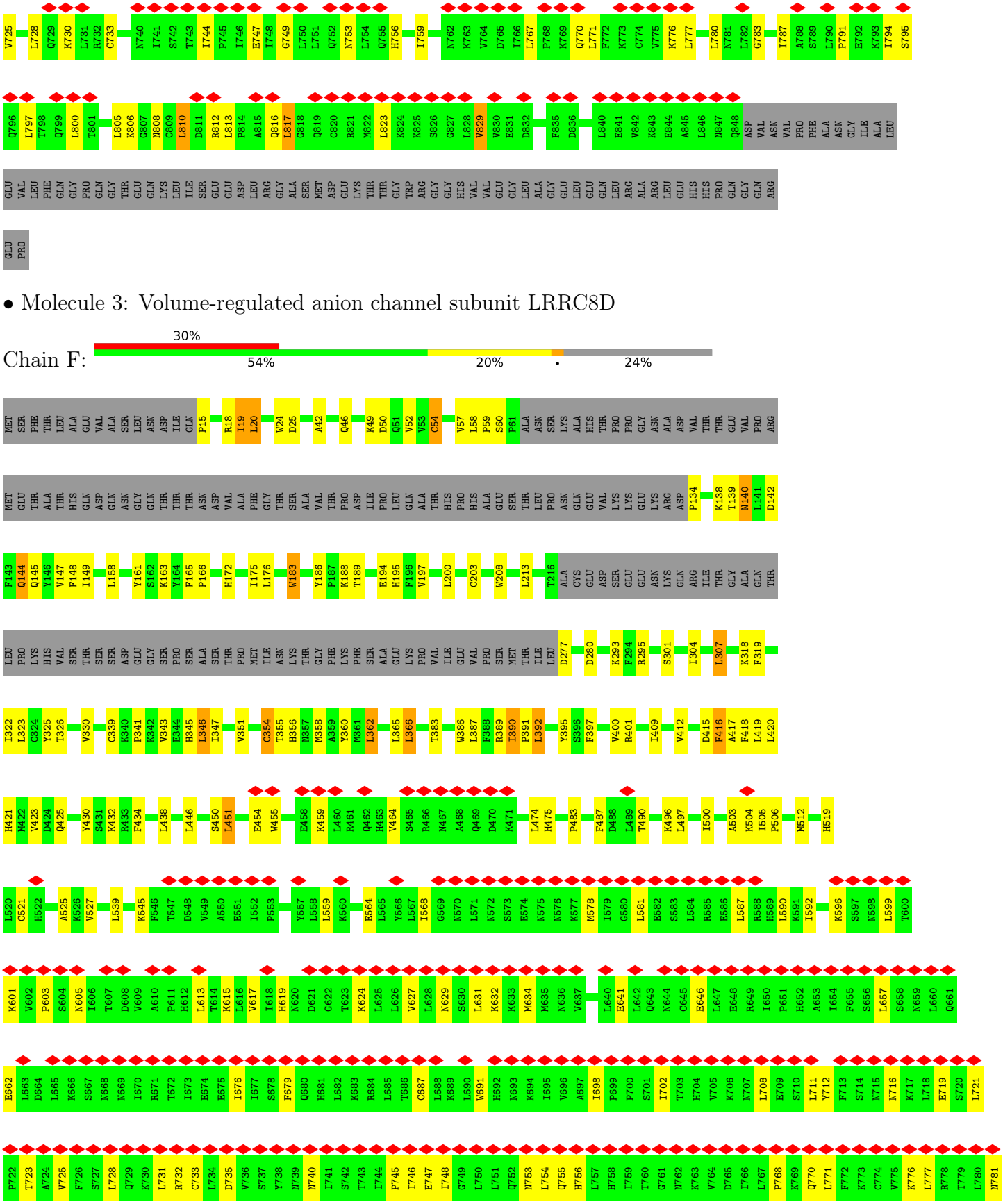




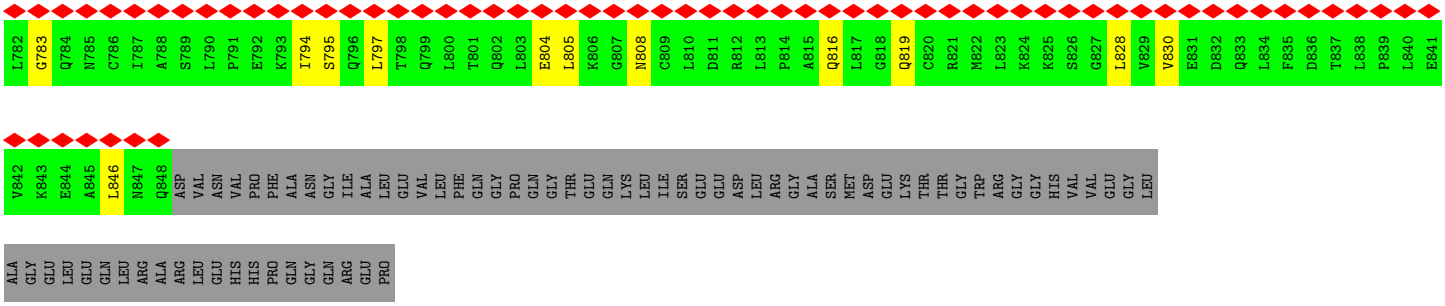
• Molecule 3: Volume-regulated anion channel subunit LRRC8D

Chain E:





• Molecule 3: Volume-regulated anion channel subunit LRRC8D


L782
G783
Q784
N785
C786
I787
A788
S789
L790
P791
E792
K793
I794
S795
Q796
L797
T798
Q799
L800
T801
Q802
L803
E804
L805
K806
G807
N808
C809
L810
D811
R812
L813
P814
A815
Q816
L817
G818
Q819
C820
R821
M822
L823
K824
K825
S826
G827
L828
V829
V830
E831
D832
Q833
L834
F835
D836
T837
L838
P839
L840
E841
V842
K843
E844
A845
L846
N847
Q848
ASP
VAL
ASN
VAL
PRO
PHE
ALA
ASN
GLY
ILE
ALA
LEU
GLU
VAL
LEU
PHE
GLN
GLY
PRO
GLN
GLY
THR
GLU
GLN
LYS
LEU
ILE
SER
GLU
GLU
ASP
LEU
ARG
GLY
ALA
SER
MET
ASP
GLU
LYS
THR
THR
GLY
TRP
ARG
GLY
GLY
HIS
VAL
VAL
GLU
GLY
LEU
ALA
GLY
GLU
LEU
GLU
GLN
LEU
ARG
ALA
ARG
LEU
GLU
HIS
HIS
PRO
GLN
GLY
GLN
ARG
GLU
PRO

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	387972	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	63.03	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.447	Depositor
Minimum map value	-0.500	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.0945	Depositor
Map size (Å)	476.532, 476.532, 476.532	wwPDB
Map dimensions	366, 366, 366	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	0.21	0/6055	0.30	0/8207
1	B	0.20	0/6163	0.29	0/8352
1	C	0.17	0/6055	0.28	0/8207
1	D	0.15	0/6163	0.27	0/8352
2	G	0.10	0/927	0.28	0/1258
2	H	0.09	0/927	0.26	0/1258
2	I	0.08	0/927	0.24	0/1258
2	J	0.07	0/927	0.24	0/1258
3	E	0.13	0/5860	0.25	0/7934
3	F	0.14	0/5860	0.26	0/7934
All	All	0.16	0/39864	0.27	0/54018

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	86	0
1	B	6030	0	6184	91	0
1	C	5922	0	6081	110	0
1	D	6030	0	6184	112	0
2	G	903	0	852	22	0
2	H	903	0	852	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	903	0	852	20	0
2	J	903	0	852	14	0
3	E	5728	0	5887	107	0
3	F	5728	0	5887	112	0
All	All	38972	0	39712	679	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 9.

All (679) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:94:TYR:O	2:I:108:GLY:HA2	1.66	0.95
2:G:94:TYR:O	2:G:108:GLY:HA2	1.67	0.95
2:I:17:SER:HA	2:I:83:MET:O	1.72	0.89
3:F:149:ILE:HD11	3:F:347:ILE:HG13	1.61	0.82
3:E:149:ILE:HD11	3:E:347:ILE:HG13	1.64	0.80
2:G:17:SER:HA	2:G:83:MET:O	1.83	0.79
3:F:142:ASP:HB2	3:F:145:GLN:HE21	1.48	0.78
1:C:714:ALA:HA	1:C:737:HIS:HB2	1.69	0.74
2:J:94:TYR:O	2:J:108:GLY:HA2	1.90	0.72
2:G:83:MET:HB3	2:G:86:LEU:HD21	1.71	0.72
1:C:691:ASP:HA	1:C:714:ALA:HB3	1.72	0.71
3:F:723:THR:HG23	3:F:747:GLU:HG2	1.70	0.71
1:C:522:HIS:HA	1:C:550:ARG:HB3	1.73	0.70
1:B:520:GLU:HG2	1:B:548:VAL:HB	1.74	0.70
2:G:19:ARG:HH11	2:G:82:GLN:HB2	1.57	0.69
3:F:521:CYS:HA	3:F:545:LYS:HB2	1.75	0.69
2:J:20:LEU:HD11	2:J:83:MET:HE2	1.75	0.69
1:D:477:TYR:HA	1:D:501:LYS:HB3	1.75	0.68
1:B:135:ILE:HG13	1:B:274:LYS:HZ2	1.59	0.68
3:F:58:LEU:HD11	3:F:139:THR:HG22	1.76	0.68
1:B:632:ILE:O	1:B:635:PHE:HB2	1.94	0.67
3:E:58:LEU:HD11	3:E:139:THR:HG22	1.77	0.67
3:E:521:CYS:HA	3:E:545:LYS:HB3	1.75	0.67
2:G:2:VAL:HA	2:G:26:GLY:HA3	1.77	0.67
3:E:805:LEU:HD21	3:E:810:LEU:HD22	1.77	0.67
1:C:632:ILE:O	1:C:635:PHE:HB2	1.95	0.66
2:H:94:TYR:O	2:H:108:GLY:HA2	1.95	0.66
1:D:629:ILE:HD13	1:D:651:ILE:HD13	1.77	0.66
3:F:676:ILE:HD13	3:F:702:ILE:HG22	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:47:TRP:HE1	2:H:50:ALA:HB2	1.62	0.65
3:F:728:LEU:HD12	3:F:731:LEU:HD22	1.78	0.65
1:C:35:MET:HE2	1:C:133:THR:HG22	1.78	0.65
2:I:19:ARG:HH11	2:I:82:GLN:HB2	1.60	0.65
1:A:687:LEU:HD21	1:A:690:LEU:HB2	1.79	0.65
3:E:733:CYS:HA	3:E:756:HIS:HB2	1.79	0.65
2:G:23:ALA:HA	2:G:78:THR:HG22	1.79	0.64
1:B:345:ARG:HH21	1:B:346:ARG:HB2	1.62	0.64
1:D:461:ILE:HB	1:D:483:ILE:HG13	1.78	0.64
1:D:714:ALA:HA	1:D:737:HIS:HB2	1.79	0.64
3:E:45:MET:HB3	3:E:358:MET:HE1	1.78	0.64
1:A:35:MET:HE2	1:A:133:THR:HG22	1.80	0.64
3:E:601:LYS:HG3	3:E:627:VAL:HB	1.80	0.64
1:C:656:ILE:HB	1:C:680:GLN:HB2	1.80	0.64
1:A:237:GLY:HA3	1:A:406:ASN:HD21	1.63	0.64
1:D:104:HIS:CE1	3:E:150:ASN:HD21	2.16	0.63
1:D:258:ASP:H	1:D:371:ASP:HB2	1.62	0.63
1:C:615:ASN:HA	1:C:640:ARG:HE	1.62	0.63
1:D:356:ILE:HD12	1:D:388:LYS:HD2	1.80	0.63
3:E:581:LEU:HD13	3:E:603:PRO:HB3	1.80	0.63
1:A:171:ARG:HH21	1:A:230:GLY:HA3	1.64	0.63
1:A:94:PRO:HD2	3:F:59:PRO:HD3	1.80	0.62
1:D:45:LEU:HD21	1:D:317:LEU:HD13	1.81	0.62
3:F:753:ASN:HA	3:F:776:LYS:HD2	1.81	0.62
1:B:255:GLU:HB2	1:B:369:LYS:HB2	1.82	0.62
1:B:760:GLU:HA	1:B:785:VAL:HB	1.82	0.62
1:C:618:GLU:HA	1:C:643:CYS:HB3	1.82	0.62
1:D:632:ILE:O	1:D:635:PHE:HB2	2.00	0.62
3:E:607:THR:HA	3:E:610:ALA:HB2	1.80	0.62
1:C:709:ASN:HA	1:C:732:LYS:HD2	1.82	0.62
1:B:698:THR:HG23	1:B:699:PHE:HD1	1.64	0.62
1:B:473:GLU:HG2	1:B:497:ALA:HB3	1.82	0.61
3:E:753:ASN:HA	3:E:776:LYS:HD2	1.80	0.61
3:F:475:HIS:HA	3:F:496:LYS:HB2	1.82	0.61
2:J:83:MET:HE1	2:J:111:VAL:HG11	1.82	0.61
3:E:708:LEU:HD11	3:E:728:LEU:HD13	1.81	0.61
2:I:23:ALA:HA	2:I:78:THR:HG22	1.81	0.61
3:E:812:ARG:HH21	3:F:732:ARG:HD2	1.66	0.61
3:F:400:VAL:HA	3:F:432:LYS:HE3	1.81	0.61
1:D:135:ILE:HG12	1:D:274:LYS:HZ2	1.65	0.60
1:B:35:MET:HE2	1:B:133:THR:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:LEU:HD23	1:B:405:LEU:HG	1.84	0.60
1:D:265:MET:HE2	1:D:343:MET:HE2	1.82	0.60
1:B:781:ARG:HB2	1:B:802:LEU:HB3	1.83	0.60
3:E:496:LYS:HA	3:E:519:HIS:HB2	1.83	0.60
1:C:473:GLU:HG2	1:C:497:ALA:HB3	1.84	0.60
2:G:68:PHE:HB3	2:G:81:LEU:HD11	1.84	0.60
3:F:805:LEU:HB2	3:F:830:VAL:HG12	1.82	0.60
1:A:429:GLU:HB2	1:A:450:VAL:HB	1.84	0.60
1:B:258:ASP:HA	1:B:371:ASP:HB2	1.84	0.60
2:I:91:THR:HG23	2:I:112:THR:HA	1.84	0.59
1:A:169:THR:HG22	1:A:393:PHE:HE1	1.68	0.59
1:A:566:GLY:HA3	1:A:590:MET:HE3	1.84	0.59
3:F:712:TYR:HA	3:F:735:ASP:HB3	1.84	0.59
1:C:499:HIS:HA	1:C:522:HIS:HB2	1.82	0.59
2:J:12:VAL:HG11	2:J:86:LEU:HD22	1.83	0.59
1:D:117:ARG:HB2	1:D:295:CYS:HB3	1.83	0.59
3:E:543:HIS:HA	3:E:566:TYR:HB2	1.85	0.59
1:B:364:ASP:HB3	1:B:396:GLU:H	1.66	0.59
1:C:420:LEU:HD21	1:C:428:LEU:HD21	1.83	0.59
1:A:597:GLU:HG3	1:A:620:ASP:HB3	1.85	0.59
1:B:736:LEU:HD22	1:B:738:LEU:HD21	1.84	0.59
1:C:492:ARG:HG2	1:C:515:LEU:HA	1.84	0.59
1:D:35:MET:HE3	1:D:133:THR:HG22	1.84	0.59
3:F:676:ILE:HG13	3:F:679:PHE:HD2	1.68	0.59
2:G:60:TYR:HB2	2:G:65:LYS:HG3	1.85	0.58
3:F:42:ALA:HB1	3:F:166:PRO:HG3	1.85	0.58
3:F:503:ALA:HB3	3:F:525:ALA:HA	1.83	0.58
1:A:527:LEU:HG	1:A:553:SER:HB3	1.85	0.58
1:D:578:GLY:H	1:D:600:ARG:HB3	1.68	0.58
2:G:91:THR:HA	2:G:111:VAL:O	2.03	0.58
1:C:654:ILE:HD13	1:C:681:LEU:HD13	1.86	0.58
3:F:54:CYS:HA	3:F:354:CYS:HA	1.86	0.58
1:A:685:ARG:HE	1:A:706:LEU:HB3	1.68	0.58
1:B:798:VAL:HG13	1:B:801:ARG:HH21	1.67	0.58
2:G:47:TRP:HE1	2:G:50:ALA:HB2	1.69	0.58
3:F:464:VAL:HG22	3:F:474:LEU:HB2	1.86	0.58
1:C:548:VAL:HG22	1:C:571:LYS:HB3	1.85	0.57
3:F:172:HIS:CE1	3:F:176:LEU:HD22	2.39	0.57
3:F:496:LYS:HA	3:F:519:HIS:HB2	1.84	0.57
1:A:804:ARG:HH12	1:A:808:GLU:HB3	1.69	0.57
1:D:500:ILE:HG21	1:D:508:ILE:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:587:LEU:HB3	3:F:590:LEU:HB2	1.85	0.57
1:A:473:GLU:HG2	1:A:497:ALA:HB3	1.86	0.57
1:C:452:LYS:HA	1:C:475:TRP:HB2	1.86	0.57
1:C:463:PRO:HB3	1:C:486:PRO:HB2	1.85	0.57
1:B:450:VAL:HG22	1:B:473:GLU:HB2	1.85	0.57
3:E:567:LEU:HD12	3:E:595:VAL:HG22	1.87	0.57
2:I:53:SER:HA	2:I:72:ARG:HH12	1.69	0.57
1:A:19:ILE:HD11	1:A:157:VAL:HG23	1.87	0.56
3:F:52:VAL:HG12	3:F:356:HIS:HA	1.87	0.56
1:C:629:ILE:HD13	1:C:651:ILE:HD13	1.85	0.56
1:A:416:LEU:HD13	1:A:442:VAL:HG12	1.88	0.56
1:B:438:ILE:HG13	1:B:459:VAL:HG21	1.86	0.56
1:C:646:LEU:HB2	1:C:669:LEU:HD22	1.86	0.56
3:F:175:ILE:HG21	3:F:318:LYS:HE3	1.88	0.56
1:D:566:GLY:HA2	1:D:569:LEU:HB2	1.87	0.56
2:G:9:GLY:HA3	2:G:109:THR:HB	1.87	0.56
1:C:618:GLU:HG2	1:C:666:ARG:HH22	1.71	0.56
1:D:618:GLU:HG3	1:D:643:CYS:HB3	1.87	0.56
2:I:9:GLY:HA3	2:I:109:THR:HB	1.87	0.56
3:E:795:SER:HB3	3:E:816:GLN:HB3	1.87	0.56
3:F:617:VAL:HG13	3:F:641:GLU:HB2	1.88	0.56
1:D:793:THR:HA	3:E:684:ARG:HH12	1.69	0.56
3:E:28:MET:HB3	3:E:379:ILE:HD11	1.88	0.56
1:B:777:PRO:HB2	1:B:778:LEU:HD12	1.87	0.56
3:F:601:LYS:HG3	3:F:627:VAL:HB	1.88	0.56
1:D:499:HIS:HA	1:D:522:HIS:HB2	1.88	0.55
1:D:44:THR:O	1:D:48:THR:HG22	2.05	0.55
2:H:23:ALA:HA	2:H:78:THR:HG22	1.87	0.55
1:B:413:LEU:HD21	1:B:417:ARG:HH22	1.71	0.55
2:H:20:LEU:HD11	2:H:83:MET:HE2	1.88	0.55
1:A:600:ARG:HG2	1:A:623:ASP:HB3	1.87	0.55
1:C:613:LEU:HB3	1:C:616:LEU:HD13	1.87	0.55
2:J:83:MET:HE3	2:J:86:LEU:HD21	1.89	0.55
1:A:450:VAL:HG22	1:A:473:GLU:HB2	1.87	0.55
1:B:218:ARG:HG3	1:B:223:ILE:HB	1.89	0.55
1:D:590:MET:HE3	1:D:593:LEU:HD22	1.89	0.55
3:E:350:GLU:HG2	3:E:351:VAL:HG23	1.88	0.55
3:E:464:VAL:HG21	3:E:492:LEU:HD21	1.87	0.55
3:F:581:LEU:HD13	3:F:603:PRO:HB3	1.87	0.55
3:F:795:SER:HB3	3:F:816:GLN:HB3	1.87	0.55
1:A:629:ILE:HD13	1:A:651:ILE:HD13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ALA:HB2	1:C:129:VAL:HG12	1.88	0.55
2:G:20:LEU:HD12	2:G:81:LEU:HD23	1.87	0.55
1:D:39:ALA:HB2	1:D:129:VAL:HG12	1.89	0.55
3:F:497:LEU:HB3	3:F:500:ILE:HD12	1.89	0.55
1:D:465:ILE:HG13	1:D:468:LEU:HD12	1.89	0.55
1:B:356:ILE:HD12	1:B:388:LYS:HG2	1.89	0.54
1:D:636:GLN:HE22	2:J:61:ALA:HA	1.71	0.54
1:D:736:LEU:HD22	1:D:738:LEU:HD21	1.88	0.54
2:H:83:MET:HE3	2:H:86:LEU:HD21	1.88	0.54
1:B:505:ILE:HD12	1:B:536:VAL:HG11	1.90	0.54
3:F:46:GLN:HA	3:F:50:ASP:HB2	1.87	0.54
1:A:117:ARG:HG2	1:A:295:CYS:HA	1.90	0.54
3:E:460:LEU:HD22	3:E:474:LEU:HD21	1.88	0.54
1:B:537:ILE:HG13	1:B:561:VAL:HG11	1.88	0.54
1:D:46:GLN:O	1:D:50:ASP:HB3	2.07	0.54
1:D:638:LEU:HB3	1:D:641:LEU:HB2	1.90	0.54
2:I:47:TRP:HE1	2:I:50:ALA:HB2	1.73	0.54
1:B:726:GLU:HA	1:B:729:GLN:HG2	1.90	0.54
1:C:459:VAL:HG23	1:C:481:ALA:HA	1.88	0.54
1:C:509:PRO:HB2	1:C:512:ILE:HG23	1.90	0.54
1:D:599:ILE:HG13	1:D:622:LYS:HB3	1.88	0.54
3:E:460:LEU:HB3	3:E:489:LEU:HD11	1.90	0.54
1:D:769:LEU:HG	1:D:790:LEU:HB3	1.90	0.54
1:B:601:CYS:HB2	1:B:624:ASN:HD21	1.73	0.54
1:D:606:ILE:HD12	1:D:631:GLU:HB2	1.88	0.54
3:F:345:HIS:HD2	3:F:346:LEU:HD13	1.73	0.54
3:E:777:LEU:HD21	3:E:780:LEU:HD13	1.90	0.53
3:F:277:ASP:HB3	3:F:280:ASP:HB3	1.89	0.53
1:A:135:ILE:HD11	1:A:274:LYS:HG2	1.89	0.53
1:D:688:ARG:HA	1:D:710:LEU:HA	1.90	0.53
2:G:48:VAL:HG13	2:G:64:VAL:HG21	1.90	0.53
3:E:666:LYS:HB2	3:E:691:TRP:HE1	1.72	0.53
3:E:806:LYS:HE3	3:E:829:VAL:HB	1.91	0.53
1:A:618:GLU:HG2	1:A:643:CYS:HB3	1.89	0.53
2:G:40:ALA:HB3	2:G:43:LYS:HB3	1.90	0.53
3:F:539:LEU:HD23	3:F:559:LEU:HD13	1.90	0.53
1:D:711:GLN:HA	1:D:733:LEU:HA	1.90	0.53
1:B:251:ARG:HH22	1:B:366:PRO:HG2	1.74	0.53
1:D:364:ASP:HB3	1:D:396:GLU:HB3	1.90	0.53
2:G:91:THR:HG23	2:G:112:THR:HA	1.91	0.53
3:E:657:LEU:HD12	3:E:660:LEU:HD22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:395:TYR:HB3	3:F:412:VAL:HG22	1.91	0.53
1:D:576:ASN:HB3	1:D:579:THR:HB	1.91	0.53
1:D:737:HIS:HA	1:D:760:GLU:HB3	1.89	0.53
1:C:537:ILE:HG13	1:C:561:VAL:HG11	1.91	0.52
2:J:5:VAL:HG13	2:J:23:ALA:HB3	1.92	0.52
3:F:691:TRP:HA	3:F:716:ASN:HD21	1.74	0.52
1:D:420:LEU:HD23	1:D:430:LEU:HD13	1.92	0.52
3:F:748:ILE:HG22	3:F:770:GLN:HE21	1.74	0.52
1:C:572:LEU:HD22	1:C:590:MET:HE1	1.90	0.52
2:H:91:THR:HG23	2:H:112:THR:HA	1.92	0.52
1:B:348:LEU:H	1:B:348:LEU:HD23	1.74	0.52
1:C:102:ASP:HB2	1:C:105:GLN:HG3	1.90	0.52
3:F:42:ALA:HB2	3:F:365:LEU:HD23	1.92	0.52
3:E:794:ILE:HD12	3:E:797:LEU:HD23	1.91	0.52
1:A:407:LEU:HG	1:A:439:PRO:HG3	1.92	0.52
1:D:619:ILE:HG22	1:D:641:LEU:HD11	1.91	0.52
1:A:429:GLU:HG3	1:A:452:LYS:HE3	1.93	0.51
3:E:204:PHE:HA	3:E:433:ARG:HG2	1.91	0.51
1:A:774:GLY:HA3	1:A:798:VAL:HG22	1.92	0.51
3:F:200:LEU:HD11	3:F:430:TYR:HB3	1.92	0.51
1:A:102:ASP:HB2	1:A:105:GLN:HG3	1.93	0.51
1:B:429:GLU:HB2	1:B:450:VAL:HB	1.93	0.51
1:C:769:LEU:HG	1:C:790:LEU:HG	1.92	0.51
2:H:60:TYR:HB2	2:H:65:LYS:HD3	1.92	0.51
3:E:489:LEU:HB3	3:E:492:LEU:HD23	1.91	0.51
1:C:620:ASP:HA	1:C:645:LYS:HB2	1.93	0.51
3:E:783:GLY:HA2	3:E:808:ASN:HD21	1.75	0.51
1:D:162:LYS:HG3	1:D:243:LEU:HD11	1.92	0.51
3:F:662:GLU:HG2	3:F:687:CYS:HB3	1.93	0.51
1:D:232:LEU:HD23	1:D:405:LEU:HG	1.93	0.51
3:F:194:GLU:HA	3:F:197:VAL:HG12	1.93	0.51
1:A:343:MET:HG3	1:A:348:LEU:HD22	1.93	0.51
1:B:39:ALA:HB2	1:B:129:VAL:HG12	1.93	0.51
1:C:614:HIS:HA	1:C:638:LEU:HG	1.92	0.51
3:F:624:LYS:HA	3:F:646:GLU:HB3	1.93	0.51
3:E:707:ASN:HA	3:E:730:LYS:HD2	1.92	0.51
2:I:5:VAL:HG23	2:I:23:ALA:HB3	1.93	0.51
2:I:48:VAL:HG13	2:I:64:VAL:HG21	1.91	0.51
3:F:599:LEU:HD23	3:F:599:LEU:H	1.76	0.51
1:A:322:ALA:O	1:A:326:ILE:HG23	2.11	0.50
1:B:322:ALA:O	1:B:326:ILE:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:ARG:HG2	1:C:295:CYS:HA	1.94	0.50
2:G:98:VAL:HG12	2:G:104:TYR:HB2	1.93	0.50
3:E:494:VAL:HG22	3:E:517:GLU:HB3	1.92	0.50
1:A:102:ASP:H	1:A:105:GLN:NE2	2.09	0.50
1:A:431:HIS:HA	1:A:452:LYS:HB2	1.93	0.50
1:D:278:ILE:HA	1:D:281:TYR:CD2	2.46	0.50
3:F:733:CYS:HA	3:F:756:HIS:HB2	1.94	0.50
1:B:501:LYS:HA	1:B:524:THR:HB	1.93	0.50
1:A:463:PRO:HB3	1:A:486:PRO:HB2	1.94	0.50
1:D:522:HIS:HA	1:D:550:ARG:HB3	1.94	0.50
2:J:40:ALA:HB3	2:J:43:LYS:HB3	1.93	0.50
3:E:410:PRO:HG2	3:E:438:LEU:HD12	1.93	0.50
1:B:46:GLN:O	1:B:50:ASP:HB3	2.11	0.50
1:B:460:THR:HA	1:B:482:LYS:O	2.12	0.50
1:D:473:GLU:HG2	1:D:497:ALA:HB3	1.93	0.50
3:E:186:TYR:HD1	3:E:187:PRO:HD2	1.75	0.50
3:F:451:LEU:HD12	3:F:483:PRO:HG3	1.93	0.50
1:C:477:TYR:HA	1:C:501:LYS:HB2	1.94	0.50
1:C:617:GLN:HA	1:C:641:LEU:HA	1.93	0.50
1:B:635:PHE:HB3	1:B:661:LEU:HD21	1.94	0.50
1:A:39:ALA:HB2	1:A:129:VAL:HG12	1.94	0.49
1:D:574:ILE:HG21	1:D:581:LEU:HD22	1.94	0.49
3:F:58:LEU:HB3	3:F:59:PRO:HD2	1.94	0.49
3:E:640:LEU:HD22	3:E:657:LEU:HD11	1.94	0.49
3:E:708:LEU:H	3:E:708:LEU:HD23	1.78	0.49
3:F:568:ILE:HA	3:F:596:LYS:HB3	1.94	0.49
1:A:131:LEU:O	1:A:135:ILE:HG23	2.13	0.49
1:B:343:MET:HG3	1:B:348:LEU:HD21	1.94	0.49
1:C:443:PHE:HE1	1:C:465:ILE:HG22	1.77	0.49
1:D:117:ARG:HG2	1:D:295:CYS:HA	1.94	0.49
3:E:58:LEU:HB3	3:E:59:PRO:HD2	1.94	0.49
3:F:345:HIS:CD2	3:F:346:LEU:HD13	2.48	0.49
3:F:487:PHE:CZ	3:F:506:PRO:HD2	2.47	0.49
1:A:461:ILE:HB	1:A:483:ILE:HG13	1.94	0.49
1:A:704:ILE:HD13	1:A:727:LEU:HB2	1.93	0.49
1:D:527:LEU:H	1:D:553:SER:HB2	1.77	0.49
2:I:83:MET:HE2	2:I:86:LEU:HD21	1.95	0.49
1:C:413:LEU:HD21	1:C:417:ARG:HH22	1.77	0.49
1:C:450:VAL:HA	1:C:473:GLU:HB2	1.93	0.49
1:D:635:PHE:HB3	1:D:661:LEU:HD21	1.93	0.49
2:H:6:GLU:H	2:H:107:GLN:HE21	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:506:PRO:HA	3:E:528:GLU:HB2	1.93	0.49
3:E:560:LYS:HG3	3:E:588:ARG:HB2	1.94	0.49
3:F:144:GLN:HA	3:F:147:VAL:HG22	1.93	0.49
3:F:708:LEU:HD13	3:F:711:LEU:HD21	1.94	0.49
1:A:255:GLU:HG2	1:A:369:LYS:HB2	1.93	0.49
1:A:615:ASN:HA	1:A:640:ARG:HH21	1.78	0.49
3:E:676:ILE:HG13	3:E:679:PHE:HD2	1.78	0.49
1:C:736:LEU:HD22	1:C:738:LEU:HD21	1.95	0.49
1:D:226:ARG:HH12	1:D:463:PRO:HG3	1.78	0.49
2:H:12:VAL:HG11	2:H:86:LEU:HD22	1.94	0.49
3:F:24:TRP:CD1	3:F:383:THR:HG1	2.31	0.49
1:C:356:ILE:HD12	1:C:388:LYS:HG3	1.94	0.48
1:C:611:PHE:HA	1:C:638:LEU:HD11	1.95	0.48
1:A:772:GLU:O	1:A:775:GLU:HG2	2.14	0.48
1:D:226:ARG:HH22	1:D:463:PRO:HG3	1.77	0.48
3:E:662:GLU:HG2	3:E:687:CYS:HB3	1.95	0.48
3:E:587:LEU:HD13	3:E:590:LEU:HD22	1.95	0.48
1:A:632:ILE:O	1:A:635:PHE:HB2	2.14	0.48
1:C:728:PHE:HA	1:C:753:LEU:HD21	1.96	0.48
2:H:50:ALA:HB3	2:H:59:GLU:HG2	1.94	0.48
3:F:330:VAL:HG23	3:F:366:LEU:HD23	1.94	0.48
1:C:154:GLU:HA	1:C:157:VAL:HG12	1.95	0.48
1:C:685:ARG:HE	1:C:706:LEU:HB3	1.78	0.48
3:F:390:ILE:HG13	3:F:391:PRO:HD2	1.95	0.48
2:J:91:THR:HG23	2:J:112:THR:HA	1.95	0.48
3:E:25:ASP:HA	3:E:28:MET:HG2	1.95	0.48
3:E:339:CYS:SG	3:E:341:PRO:HD3	2.54	0.48
1:A:258:ASP:H	1:A:371:ASP:HB2	1.77	0.48
1:C:263:LEU:HA	1:C:263:LEU:HD23	1.75	0.48
1:C:540:LEU:HD12	1:C:543:LEU:HD12	1.96	0.48
3:E:651:PRO:HG2	3:E:654:ILE:HG13	1.95	0.48
1:B:171:ARG:HH22	1:B:230:GLY:HA3	1.79	0.48
3:F:504:LYS:HG3	3:F:506:PRO:HD3	1.95	0.48
3:F:578:MET:HB3	3:F:581:LEU:HD11	1.95	0.48
3:F:755:GLN:HG2	3:F:776:LYS:HB3	1.95	0.48
1:C:176:THR:HG23	1:C:360:SER:HA	1.95	0.48
1:D:245:GLU:HA	1:D:248:LYS:HD2	1.96	0.48
1:D:490:PHE:O	1:D:494:ASN:HB2	2.14	0.48
3:E:148:PHE:HE2	3:E:343:VAL:HG11	1.79	0.48
1:C:322:ALA:O	1:C:326:ILE:HG23	2.14	0.48
1:C:429:GLU:HG3	1:C:452:LYS:HE3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:200:LEU:HD21	3:E:423:VAL:HG11	1.95	0.48
3:F:301:SER:O	3:F:415:ASP:HB2	2.14	0.48
2:J:29:VAL:HG22	2:J:72:ARG:HD2	1.95	0.47
3:E:208:TRP:NE1	3:E:446:LEU:HD23	2.29	0.47
1:C:420:LEU:HA	1:C:430:LEU:HD13	1.96	0.47
1:A:590:MET:HB3	1:A:593:LEU:HD13	1.96	0.47
1:B:372:PHE:HZ	1:B:390:PHE:HE2	1.61	0.47
1:D:416:LEU:HD11	1:D:441:THR:HG23	1.96	0.47
1:D:250:PHE:CZ	1:D:254:VAL:HG21	2.50	0.47
3:E:673:ILE:HG21	3:E:690:LEU:HD13	1.97	0.47
1:B:772:GLU:O	1:B:775:GLU:HG2	2.15	0.47
2:H:5:VAL:HG13	2:H:23:ALA:HB3	1.95	0.47
3:F:203:CYS:SG	3:F:434:PHE:HA	2.54	0.47
3:F:783:GLY:HA2	3:F:808:ASN:HD21	1.80	0.47
1:B:235:LYS:O	1:B:239:GLN:HG2	2.15	0.47
1:D:164:PHE:CD1	1:D:389:ARG:HG3	2.50	0.47
1:D:550:ARG:HH21	1:D:552:LYS:HD2	1.79	0.47
3:E:36:LEU:HB2	3:E:173:THR:HG21	1.97	0.47
3:E:330:VAL:HG23	3:E:366:LEU:HD23	1.97	0.47
3:F:587:LEU:HD23	3:F:590:LEU:HD13	1.97	0.47
2:J:94:TYR:O	2:J:108:GLY:CA	2.60	0.47
3:E:767:LEU:HB2	3:E:791:PRO:HG2	1.96	0.47
3:F:629:ASN:HA	3:F:632:LYS:HE2	1.97	0.47
1:B:45:LEU:HD21	1:B:317:LEU:HD13	1.97	0.47
1:B:46:GLN:HB2	1:B:318:PHE:HZ	1.79	0.47
2:H:29:VAL:HG21	2:H:79:VAL:HG22	1.97	0.47
3:E:464:VAL:HG22	3:E:474:LEU:HB2	1.96	0.47
1:A:728:PHE:HA	1:A:753:LEU:HD21	1.96	0.46
1:D:788:GLU:HB3	3:E:612:HIS:HA	1.98	0.46
3:F:186:TYR:CE2	3:F:188:LYS:HB2	2.50	0.46
1:A:154:GLU:HA	1:A:157:VAL:HG12	1.97	0.46
1:B:278:ILE:HA	1:B:281:TYR:CD2	2.50	0.46
1:B:629:ILE:HD13	1:B:651:ILE:HD13	1.97	0.46
1:B:685:ARG:HH21	1:B:706:LEU:HB3	1.80	0.46
1:C:449:GLU:HA	1:C:471:LEU:HA	1.97	0.46
1:C:714:ALA:HB2	1:C:737:HIS:HD2	1.79	0.46
1:D:416:LEU:HD13	1:D:442:VAL:HA	1.97	0.46
1:A:720:ILE:HB	1:A:741:ASN:HD22	1.81	0.46
3:F:746:ILE:HA	3:F:770:GLN:NE2	2.30	0.46
1:A:739:GLY:HA2	1:A:764:ASN:HD21	1.80	0.46
1:C:416:LEU:HD11	1:C:442:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:633:ILE:HD13	1:C:657:GLN:HB3	1.98	0.46
3:E:609:VAL:HG12	3:E:612:HIS:HE1	1.80	0.46
1:A:258:ASP:HA	1:A:371:ASP:HB2	1.97	0.46
1:D:717:ALA:H	1:D:740:ASN:HB2	1.80	0.46
1:D:776:CYS:HB2	1:D:779:LEU:HB3	1.97	0.46
1:C:385:LEU:O	1:C:389:ARG:HG2	2.15	0.46
1:D:168:TRP:HH2	1:D:398:SER:HB2	1.79	0.46
3:E:549:VAL:HG21	3:E:580:GLY:HA3	1.98	0.46
3:E:650:ILE:HG23	3:E:654:ILE:HD12	1.98	0.46
1:B:34:VAL:O	1:B:38:ILE:HG23	2.16	0.46
1:B:131:LEU:O	1:B:135:ILE:HG12	2.16	0.46
1:C:611:PHE:HZ	1:C:631:GLU:HB3	1.79	0.46
2:I:68:PHE:HB3	2:I:81:LEU:HD11	1.97	0.46
3:E:587:LEU:HB3	3:E:590:LEU:HB2	1.96	0.46
3:E:691:TRP:HA	3:E:716:ASN:HD21	1.81	0.46
1:A:235:LYS:O	1:A:239:GLN:HG2	2.15	0.46
3:E:59:PRO:HD3	3:F:134:PRO:HG2	1.97	0.46
3:F:505:ILE:HB	3:F:527:VAL:HG12	1.97	0.46
3:E:767:LEU:HD11	3:E:787:ILE:HD13	1.97	0.46
1:A:505:ILE:HD11	1:A:527:LEU:HA	1.98	0.45
1:C:129:VAL:HG13	1:C:325:TYR:CE1	2.50	0.45
1:C:258:ASP:HA	1:C:371:ASP:HB2	1.99	0.45
2:I:60:TYR:HB2	2:I:65:LYS:HG3	1.97	0.45
3:E:703:THR:HB	3:E:724:ALA:HB1	1.98	0.45
3:F:208:TRP:NE1	3:F:446:LEU:HD23	2.31	0.45
1:B:721:GLU:HA	1:B:743:LEU:HA	1.98	0.45
1:C:235:LYS:O	1:C:239:GLN:HG2	2.16	0.45
1:C:538:ASP:HA	1:C:561:VAL:HG21	1.99	0.45
3:E:216:THR:HG21	3:E:405:SER:HB2	1.97	0.45
3:F:295:ARG:HH11	3:F:438:LEU:HD12	1.80	0.45
3:F:564:GLU:HG2	3:F:592:ILE:HB	1.97	0.45
1:A:635:PHE:HB2	1:A:661:LEU:HD21	1.97	0.45
2:J:60:TYR:CE1	2:J:70:ILE:HG22	2.52	0.45
1:B:164:PHE:CD1	1:B:389:ARG:HG3	2.51	0.45
1:B:769:LEU:HD12	1:B:794:LEU:HG	1.98	0.45
1:D:129:VAL:HG13	1:D:325:TYR:CE1	2.51	0.45
2:H:52:TYR:CG	2:H:57:TYR:HB2	2.52	0.45
1:C:46:GLN:O	1:C:50:ASP:HB3	2.16	0.45
1:C:665:GLU:HG2	1:C:686:LYS:HB3	1.99	0.45
3:F:454:GLU:HG3	3:F:455:TRP:HD1	1.82	0.45
1:A:15:PRO:HB2	1:A:16:ALA:H	1.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:PHE:CZ	1:B:254:VAL:HG21	2.52	0.45
1:C:34:VAL:O	1:C:38:ILE:HG23	2.17	0.45
1:D:450:VAL:HG13	1:D:473:GLU:HB2	1.99	0.45
1:D:682:PHE:HA	1:D:707:LEU:HD21	1.98	0.45
1:D:761:LEU:HB2	1:D:786:VAL:HG23	1.98	0.45
2:I:110:GLN:HG3	2:I:112:THR:HG23	1.99	0.45
1:B:129:VAL:HG13	1:B:325:TYR:CE1	2.52	0.45
1:D:278:ILE:HA	1:D:281:TYR:HD2	1.80	0.45
3:E:138:LYS:C	3:E:140:ASN:H	2.25	0.45
3:E:710:SER:HA	3:E:733:CYS:HB3	1.99	0.45
3:F:395:TYR:HB2	3:F:417:ALA:HA	1.98	0.45
3:F:401:ARG:HE	3:F:409:ILE:HG22	1.82	0.45
1:A:278:ILE:HA	1:A:281:TYR:CD2	2.52	0.45
1:A:354:GLU:HA	1:A:357:ARG:HG2	1.99	0.45
1:D:546:LEU:HG	1:D:569:LEU:HD21	1.98	0.45
1:A:19:ILE:HG13	1:A:20:LEU:HD22	1.99	0.45
1:B:577:GLU:HA	1:B:600:ARG:CZ	2.46	0.45
1:C:566:GLY:HA3	1:C:590:MET:HG2	1.99	0.45
1:D:168:TRP:CH2	1:D:398:SER:HB2	2.52	0.45
3:E:203:CYS:SG	3:E:434:PHE:HA	2.57	0.45
1:B:129:VAL:O	1:B:133:THR:HG23	2.16	0.44
1:B:622:LYS:HB2	1:B:647:TRP:HE1	1.82	0.44
1:C:243:LEU:HA	1:C:246:LYS:HD2	1.99	0.44
2:G:60:TYR:CE2	2:G:70:ILE:HG22	2.53	0.44
1:A:296:THR:HG23	1:A:307:THR:HG22	2.00	0.44
1:A:433:PHE:HE1	1:A:455:LEU:HD12	1.81	0.44
1:B:385:LEU:O	1:B:389:ARG:HG2	2.17	0.44
1:A:109:VAL:HG21	1:A:308:TYR:CE2	2.51	0.44
1:B:413:LEU:HD13	1:B:444:ASP:HB2	2.00	0.44
1:B:670:ASN:HD22	1:B:671:ARG:HG2	1.83	0.44
1:B:788:GLU:HA	1:B:791:PHE:HB3	1.99	0.44
1:C:578:GLY:H	1:C:600:ARG:HB3	1.82	0.44
2:H:33:PHE:CD2	2:H:52:TYR:HA	2.52	0.44
3:E:180:SER:HA	3:E:311:GLN:NE2	2.33	0.44
3:F:358:MET:HE3	3:F:362:LEU:HD13	1.98	0.44
1:A:591:VAL:HA	1:A:613:LEU:HD22	1.99	0.44
1:D:538:ASP:HA	1:D:561:VAL:HG21	1.98	0.44
3:F:148:PHE:HE1	3:F:343:VAL:HG11	1.82	0.44
1:A:685:ARG:HH21	1:A:706:LEU:HD13	1.83	0.44
1:C:547:LYS:HD2	1:C:570:GLN:HG3	1.98	0.44
3:E:345:HIS:CD2	3:E:346:LEU:HD13	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:673:ILE:HD13	3:E:695:ILE:HD13	1.99	0.44
1:C:354:GLU:HA	1:C:357:ARG:HG2	2.00	0.44
1:C:431:HIS:CE1	1:C:433:PHE:HB2	2.53	0.44
1:C:685:ARG:HH21	1:C:706:LEU:HB3	1.83	0.44
1:C:622:LYS:HB2	1:C:647:TRP:HE1	1.83	0.44
1:C:769:LEU:HD12	1:C:791:PHE:HA	2.00	0.44
1:D:601:CYS:HB2	1:D:624:ASN:HD21	1.83	0.44
3:F:828:LEU:HD22	3:F:846:LEU:HD13	1.99	0.44
1:C:278:ILE:HA	1:C:281:TYR:CD2	2.53	0.44
3:E:617:VAL:HG13	3:E:641:GLU:HB2	2.00	0.44
1:B:736:LEU:HD13	1:B:738:LEU:HD11	2.00	0.44
1:D:746:LEU:HD23	1:D:747:PRO:HD2	1.99	0.44
3:E:749:GLY:HA3	3:E:770:GLN:HB3	2.00	0.44
3:F:158:LEU:HD23	3:F:158:LEU:HA	1.79	0.44
1:A:746:LEU:HB3	1:A:770:PRO:HG3	2.00	0.43
2:I:15:GLY:HA2	2:I:85:SER:HA	2.00	0.43
2:I:97:TYR:HE1	2:I:103:GLU:HB3	1.83	0.43
3:F:490:THR:HA	3:F:512[A]:MET:HA	1.99	0.43
1:A:250:PHE:CE1	1:A:254:VAL:HG21	2.53	0.43
1:A:365:ILE:HD13	1:A:391:ALA:HB1	2.00	0.43
1:D:348:LEU:HD23	1:D:348:LEU:H	1.83	0.43
3:E:175:ILE:HG21	3:E:318:LYS:NZ	2.32	0.43
3:E:384:LEU:HD23	3:E:384:LEU:HA	1.78	0.43
3:E:797:LEU:HB3	3:E:800:LEU:HB2	2.00	0.43
3:F:339:CYS:SG	3:F:341:PRO:HD3	2.57	0.43
1:D:243:LEU:HB3	1:D:393:PHE:CE1	2.53	0.43
1:D:548:VAL:HG13	1:D:571:LYS:HD3	2.00	0.43
3:E:54:CYS:HA	3:E:354:CYS:HA	2.00	0.43
3:E:559:LEU:O	3:E:587:LEU:HD23	2.18	0.43
1:A:648:TYR:HA	1:A:671:ARG:HB2	2.00	0.43
1:A:729:GLN:NE2	1:A:749:ARG:HH22	2.16	0.43
1:C:117:ARG:HB3	1:C:295:CYS:HB3	2.00	0.43
1:C:250:PHE:HA	1:C:253:HIS:CD2	2.53	0.43
1:D:385:LEU:O	1:D:389:ARG:HG2	2.18	0.43
1:D:772:GLU:O	1:D:775:GLU:HG2	2.18	0.43
3:E:490:THR:HA	3:E:512[A]:MET:HA	1.99	0.43
2:I:27:PHE:CZ	2:I:98:VAL:HG21	2.54	0.43
2:J:30:GLY:HA2	2:J:72:ARG:CZ	2.49	0.43
3:E:299:GLU:HB2	3:E:413:LYS:HG3	1.99	0.43
1:A:492:ARG:HG2	1:A:515:LEU:HA	2.01	0.43
1:B:258:ASP:H	1:B:371:ASP:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:21:LYS:HE2	3:E:21:LYS:HB3	1.84	0.43
3:E:192:LYS:HB2	3:E:304:ILE:HD11	1.99	0.43
3:E:629:ASN:HA	3:E:632:LYS:HE2	2.00	0.43
3:F:138:LYS:C	3:F:140:ASN:H	2.26	0.43
1:A:413:LEU:HD21	1:A:417:ARG:HH12	1.83	0.43
1:A:500:ILE:HB	1:A:523:LEU:HD23	2.00	0.43
1:C:407:LEU:HD12	1:C:411:TRP:HD1	1.83	0.43
1:C:420:LEU:HD11	1:C:428:LEU:HG	2.01	0.43
1:D:295:CYS:HB2	1:D:297:VAL:HG13	2.01	0.43
3:E:187:PRO:HA	3:E:190:CYS:HB3	2.00	0.43
3:F:19:ILE:HD11	3:F:423:VAL:HG22	2.01	0.43
3:F:631:LEU:HD11	3:F:657:LEU:HD11	2.01	0.43
1:C:149:THR:HG22	1:C:259:ILE:HG23	2.00	0.43
1:C:721:GLU:HA	1:C:742:VAL:HG23	2.00	0.43
1:D:769:LEU:HD12	1:D:791:PHE:HA	2.01	0.43
2:G:35:TYR:HB3	2:G:37:TYR:HE1	1.84	0.43
2:J:20:LEU:HD13	2:J:81:LEU:HD23	2.01	0.43
3:F:158:LEU:HB3	3:F:163:LYS:HD2	2.01	0.43
1:B:605:ARG:HD3	2:H:54:TYR:CZ	2.53	0.43
1:D:648:TYR:CE2	1:D:671:ARG:HG3	2.54	0.43
2:I:4:LEU:HD11	2:I:98:VAL:HB	2.00	0.43
1:A:233:ASP:O	1:A:236:GLU:HG3	2.19	0.43
1:D:459:VAL:HG13	1:D:481:ALA:HA	2.00	0.43
3:E:406:PHE:HE2	3:E:442:SER:HB3	1.83	0.43
1:A:45:LEU:HD21	1:A:317:LEU:HD13	2.00	0.42
1:A:709:ASN:HD22	1:A:732:LYS:NZ	2.17	0.42
1:D:771:VAL:HG23	1:D:795:PRO:HG2	1.99	0.42
2:H:32:HIS:CE1	2:H:100:VAL:HG12	2.54	0.42
3:E:392:LEU:HD12	3:E:418:PHE:HA	2.01	0.42
3:E:800:LEU:HD22	3:E:823:LEU:HD22	2.01	0.42
3:F:603:PRO:HB2	3:F:605:ASN:OD1	2.19	0.42
3:F:781:ASN:HA	3:F:804:GLU:HB3	2.01	0.42
1:B:24:TRP:CG	1:B:339:THR:HG1	2.37	0.42
1:B:590:MET:HE3	1:B:593:LEU:HD22	2.01	0.42
1:D:16:ALA:O	1:D:19:ILE:HG12	2.19	0.42
1:D:407:LEU:HG	1:D:411:TRP:CD1	2.55	0.42
1:C:642:THR:HA	1:C:664:LEU:HA	2.00	0.42
1:D:411:TRP:O	1:D:441:THR:HG21	2.20	0.42
1:D:478:HIS:CD2	1:D:501:LYS:HG2	2.54	0.42
3:E:17:TYR:O	3:E:21:LYS:HG2	2.18	0.42
3:E:813:LEU:HB3	3:E:817:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:THR:HG23	1:B:307:THR:HG22	2.02	0.42
3:F:322:ILE:O	3:F:326:THR:HG23	2.19	0.42
3:F:392:LEU:HD12	3:F:418:PHE:HD1	1.83	0.42
3:F:416:PHE:HD1	3:F:416:PHE:HA	1.70	0.42
3:F:721:LEU:HB2	3:F:745:PRO:HG2	2.01	0.42
3:F:755:GLN:HA	3:F:777:LEU:HA	2.02	0.42
3:F:768:PRO:HG2	3:F:771:LEU:HB2	2.02	0.42
1:B:572:LEU:HD22	1:B:590:MET:HE1	2.02	0.42
1:C:412:THR:HG23	1:C:415:LYS:H	1.85	0.42
1:C:505:ILE:HD12	1:C:536:VAL:HG11	2.02	0.42
1:D:427:LYS:HB3	1:D:449:GLU:HB3	2.01	0.42
3:E:812:ARG:HB3	3:F:732:ARG:NH1	2.33	0.42
1:B:803:TRP:O	1:B:807:LYS:HG2	2.19	0.42
3:F:57:VAL:HG22	3:F:351:VAL:O	2.19	0.42
3:F:149:ILE:HD13	3:F:149:ILE:HA	1.84	0.42
3:F:322:ILE:HG13	3:F:323:LEU:N	2.35	0.42
1:A:553:SER:HB2	1:A:555:LEU:HG	2.02	0.42
1:C:578:GLY:N	1:C:600:ARG:HB3	2.34	0.42
1:C:698:THR:HG22	1:C:719:ARG:HB2	2.02	0.42
1:D:452:LYS:HG2	1:D:475:TRP:CD1	2.55	0.42
1:D:578:GLY:N	1:D:600:ARG:HB3	2.32	0.42
2:H:83:MET:HE1	2:H:111:VAL:HG11	2.00	0.42
1:A:348:LEU:HD23	1:A:374:PHE:CD1	2.55	0.42
1:B:427:LYS:HB3	1:B:449:GLU:HG2	2.01	0.42
1:C:24:TRP:CD1	1:C:339:THR:HG1	2.38	0.42
1:C:452:LYS:HG2	1:C:475:TRP:CG	2.55	0.42
1:D:149:THR:HG21	1:D:263:LEU:HD12	2.02	0.42
1:D:488:LEU:HD13	1:D:511:TRP:HB2	2.02	0.42
3:E:42:ALA:HB1	3:E:166:PRO:HG3	2.00	0.42
3:E:365:LEU:HD12	3:E:365:LEU:HA	1.89	0.42
3:F:596:LYS:HD2	3:F:619:HIS:O	2.20	0.42
1:B:168:TRP:CZ3	1:B:398:SER:HB2	2.55	0.42
1:B:270:ILE:O	1:B:273:ILE:HG13	2.20	0.42
1:B:350:LYS:HE3	1:B:350:LYS:HB3	1.83	0.42
1:B:776:CYS:HB2	1:B:779:LEU:HB3	2.01	0.42
1:D:419:ARG:NH1	1:D:432:LEU:HD23	2.35	0.42
2:G:20:LEU:HB2	2:G:81:LEU:HB3	2.00	0.42
3:E:149:ILE:HD13	3:E:149:ILE:HA	1.78	0.42
3:E:767:LEU:HB3	3:E:771:LEU:HD21	2.01	0.42
3:F:390:ILE:HD12	3:F:390:ILE:HA	1.92	0.42
1:A:164:PHE:CD1	1:A:389:ARG:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:LEU:HD13	1:A:173:LEU:HA	1.88	0.42
1:B:369:LYS:HE3	1:B:369:LYS:HB3	1.95	0.42
1:B:461:ILE:HB	1:B:483:ILE:HG13	2.02	0.42
1:C:534:TYR:CE1	1:C:559:PRO:HG3	2.55	0.42
1:C:725:PRO:HA	1:C:728:PHE:HD2	1.85	0.42
1:C:726:GLU:O	1:C:729:GLN:HB2	2.20	0.42
1:C:734:ARG:HG2	1:C:755:ASN:HB3	2.01	0.42
1:D:450:VAL:HG22	1:D:473:GLU:HB2	2.02	0.42
3:E:603:PRO:HB2	3:E:605:ASN:OD1	2.20	0.42
1:A:102:ASP:H	1:A:105:GLN:HE21	1.66	0.41
1:A:121:PHE:HZ	1:A:282:THR:HG23	1.85	0.41
1:A:149:THR:HG21	1:A:263:LEU:HD12	2.02	0.41
1:B:719:ARG:HH12	1:B:742:VAL:HG13	1.85	0.41
1:D:598:LEU:HB2	1:D:621:LEU:HD23	2.02	0.41
1:D:728:PHE:HA	1:D:753:LEU:HD21	2.01	0.41
2:G:30:GLY:HA3	2:G:74:ASN:HD21	1.85	0.41
2:H:93:VAL:HA	2:H:110:GLN:HA	2.01	0.41
1:B:232:LEU:HD13	1:B:232:LEU:HA	1.89	0.41
1:C:121:PHE:HZ	1:C:282:THR:HG23	1.85	0.41
1:C:243:LEU:HD23	1:C:393:PHE:CE2	2.55	0.41
1:D:570:GLN:HA	1:D:593:LEU:HA	2.02	0.41
3:E:340:LYS:HG2	3:E:351:VAL:HG22	2.01	0.41
3:F:183:TRP:HB2	3:F:307:LEU:HD23	2.01	0.41
1:B:22:PRO:HD2	1:B:25:ASP:HB2	2.01	0.41
1:B:721:GLU:HB3	1:B:742:VAL:HG23	2.01	0.41
3:E:155:HIS:HB3	3:F:360:TYR:HE2	1.85	0.41
1:A:635:PHE:HA	1:A:638:LEU:HD13	2.03	0.41
1:B:278:ILE:HA	1:B:281:TYR:HD2	1.85	0.41
1:C:598:LEU:HB2	1:C:621:LEU:HD23	2.03	0.41
2:G:12:VAL:O	2:G:113:VAL:HA	2.21	0.41
2:I:83:MET:HB3	2:I:86:LEU:HD21	2.01	0.41
3:E:439:SER:OG	3:E:441:VAL:HG13	2.21	0.41
1:A:159:ILE:HG22	1:A:390:PHE:HE1	1.84	0.41
1:A:563:THR:HG21	1:A:589:LYS:HE2	2.02	0.41
1:B:219:ILE:H	1:B:219:ILE:HG13	1.59	0.41
1:B:534:TYR:HB3	1:B:559:PRO:HB3	2.01	0.41
1:C:719:ARG:NH1	1:D:640:ARG:HB3	2.36	0.41
3:F:732:ARG:HA	3:F:754:LEU:HA	2.03	0.41
1:A:510:LEU:HD12	1:A:513:TYR:HE2	1.85	0.41
1:A:520:GLU:HG2	1:A:548:VAL:HB	2.01	0.41
1:A:622:LYS:HB2	1:A:647:TRP:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ARG:HG3	1:B:363:SER:HA	2.02	0.41
1:B:405:LEU:HD13	1:B:405:LEU:HA	1.96	0.41
1:D:429:GLU:OE2	1:D:431:HIS:HB2	2.20	0.41
3:E:744:ILE:HD11	3:E:759:ILE:HD13	2.03	0.41
3:F:409:ILE:HD12	3:F:409:ILE:HA	1.91	0.41
1:C:265:MET:HE2	1:C:265:MET:HB2	1.98	0.41
1:C:383:ASP:HA	1:C:384:PRO:HD3	1.94	0.41
1:C:772:GLU:O	1:C:775:GLU:HG2	2.21	0.41
1:D:520:GLU:HA	1:D:548:VAL:HB	2.02	0.41
3:E:723:THR:HG23	3:E:747:GLU:HG2	2.02	0.41
3:F:450:SER:O	3:F:454:GLU:HG2	2.21	0.41
3:F:719:GLU:HG2	3:F:740:ASN:HB3	2.03	0.41
1:B:420:LEU:HD11	1:B:445:LEU:HD23	2.02	0.41
1:C:233:ASP:OD2	1:C:235:LYS:HB2	2.21	0.41
1:C:648:TYR:CE2	1:C:671:ARG:HG3	2.56	0.41
1:C:656:ILE:HD11	2:I:37:TYR:CE2	2.56	0.41
1:D:15:PRO:HB2	1:D:16:ALA:H	1.63	0.41
3:E:155:HIS:HD2	3:F:360:TYR:HD2	1.69	0.41
3:F:613:LEU:HD23	3:F:634:MET:HE2	2.02	0.41
1:A:433:PHE:CE1	1:A:455:LEU:HD12	2.56	0.41
1:A:647:TRP:CD1	1:A:647:TRP:H	2.39	0.41
1:A:663:ASN:HA	1:A:686:LYS:HD2	2.02	0.41
1:B:365:ILE:HG22	1:B:394:LEU:HB3	2.03	0.41
1:B:605:ARG:HD3	2:H:54:TYR:OH	2.21	0.41
1:C:19:ILE:HG13	1:C:20:LEU:HD22	2.03	0.41
1:C:232:LEU:HB3	1:C:236:GLU:OE2	2.20	0.41
1:C:431:HIS:HA	1:C:452:LYS:HB2	2.03	0.41
1:C:617:GLN:HG2	1:C:640:ARG:HB3	2.02	0.41
1:C:647:TRP:CD1	1:C:647:TRP:H	2.38	0.41
1:D:243:LEU:HA	1:D:243:LEU:HD12	1.82	0.41
1:D:419:ARG:HH12	1:D:431:HIS:C	2.29	0.41
1:D:566:GLY:HA2	1:D:569:LEU:HD12	2.03	0.41
1:D:630:GLU:O	1:D:633:ILE:HG22	2.20	0.41
2:G:110:GLN:HG3	2:G:112:THR:HG23	2.03	0.41
2:H:40:ALA:HB3	2:H:43:LYS:HB3	2.02	0.41
3:F:19:ILE:HD13	3:F:20:LEU:HD22	2.02	0.41
3:F:599:LEU:HD13	3:F:603:PRO:HD3	2.03	0.41
1:B:630:GLU:O	1:B:633:ILE:HG22	2.21	0.41
1:C:146:PHE:CD1	1:C:147:PRO:HD2	2.56	0.41
1:C:665:GLU:HA	1:C:687:LEU:HA	2.02	0.41
3:F:386:TRP:HD1	3:F:389:ARG:NH2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:629:ILE:HG13	1:C:655:PRO:HG2	2.03	0.40
1:C:666:ARG:HG2	1:C:689:TYR:HB2	2.03	0.40
1:D:31:ILE:O	1:D:35:MET:HG3	2.21	0.40
1:D:428:LEU:HD23	1:D:428:LEU:HA	1.94	0.40
1:D:736:LEU:HD13	1:D:738:LEU:HD11	2.03	0.40
3:E:28:MET:HB2	3:E:376:TYR:CE2	2.56	0.40
3:E:401:ARG:HE	3:E:409:ILE:HB	1.86	0.40
3:F:15:PRO:HB3	3:F:18:ARG:HH12	1.87	0.40
3:F:392:LEU:HD13	3:F:421:HIS:ND1	2.36	0.40
3:F:794:ILE:HD12	3:F:797:LEU:HD12	2.03	0.40
1:B:353:PHE:HD1	1:B:353:PHE:HA	1.77	0.40
1:C:407:LEU:HD13	1:C:407:LEU:HA	1.89	0.40
1:C:416:LEU:HD11	1:C:442:VAL:HA	2.03	0.40
1:D:251:ARG:HH22	1:D:366:PRO:HG2	1.86	0.40
1:D:687:LEU:HD23	1:D:707:LEU:HD13	2.03	0.40
1:D:709:ASN:HA	1:D:732:LYS:HD2	2.03	0.40
3:E:544:VAL:HG12	3:E:546:PHE:HD1	1.87	0.40
1:B:431:HIS:CE1	1:B:433:PHE:HB2	2.56	0.40
1:B:733:LEU:HD21	1:B:736:LEU:HD21	2.03	0.40
3:E:183:TRP:HE1	3:E:304:ILE:HG23	1.86	0.40
3:E:500:ILE:HB	3:E:523:CYS:SG	2.61	0.40
3:F:189:THR:HG21	3:F:307:LEU:HD22	2.03	0.40
3:F:592:ILE:HG12	3:F:615:LYS:HB3	2.03	0.40
1:A:736:LEU:HD23	1:A:736:LEU:HA	1.87	0.40
1:B:585:ASN:OD1	1:B:588:LYS:HE3	2.22	0.40
1:D:115:GLU:HG3	3:E:360:TYR:CD2	2.57	0.40
1:D:147:PRO:HA	1:D:150:SER:HB3	2.04	0.40
1:D:509:PRO:HB2	1:D:512:ILE:HG23	2.04	0.40
1:D:607:PRO:HG2	1:D:610:ILE:HG13	2.02	0.40
3:F:795:SER:HB2	3:F:819:GLN:HG3	2.04	0.40
1:A:351:TYR:HB3	1:A:368:VAL:HG22	2.03	0.40
1:B:510:LEU:HD12	1:B:510:LEU:HA	1.92	0.40
1:C:166:SER:HB3	1:C:169:THR:HG23	2.02	0.40
1:D:435:LEU:H	1:D:456:ILE:HG12	1.86	0.40
3:E:457:PHE:O	3:E:461:ARG:HG2	2.22	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	712/818 (87%)	679 (95%)	33 (5%)	0	100	100
1	B	726/818 (89%)	690 (95%)	36 (5%)	0	100	100
1	C	712/818 (87%)	687 (96%)	25 (4%)	0	100	100
1	D	726/818 (89%)	699 (96%)	27 (4%)	0	100	100
2	G	112/118 (95%)	109 (97%)	3 (3%)	0	100	100
2	H	112/118 (95%)	109 (97%)	3 (3%)	0	100	100
2	I	112/118 (95%)	109 (97%)	3 (3%)	0	100	100
2	J	112/118 (95%)	110 (98%)	2 (2%)	0	100	100
3	E	697/924 (75%)	669 (96%)	27 (4%)	1 (0%)	48	79
3	F	697/924 (75%)	669 (96%)	27 (4%)	1 (0%)	48	79
All	All	4718/5592 (84%)	4530 (96%)	186 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	60	SER
3	F	60	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	666/756 (88%)	635 (95%)	31 (5%)	23	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	678/756 (90%)	646 (95%)	32 (5%)	23	56
1	C	666/756 (88%)	644 (97%)	22 (3%)	33	65
1	D	678/756 (90%)	660 (97%)	18 (3%)	39	70
2	G	92/94 (98%)	90 (98%)	2 (2%)	45	73
2	H	92/94 (98%)	87 (95%)	5 (5%)	20	52
2	I	92/94 (98%)	90 (98%)	2 (2%)	45	73
2	J	92/94 (98%)	90 (98%)	2 (2%)	45	73
3	E	655/842 (78%)	618 (94%)	37 (6%)	19	51
3	F	655/842 (78%)	621 (95%)	34 (5%)	21	53
All	All	4366/5084 (86%)	4181 (96%)	185 (4%)	28	59

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	53	ILE
1	A	98	LYS
1	A	104	HIS
1	A	135	ILE
1	A	279	ILE
1	A	292	ASP
1	A	293	VAL
1	A	295	CYS
1	A	297	VAL
1	A	317	LEU
1	A	344	LEU
1	A	348	LEU
1	A	353	PHE
1	A	354	GLU
1	A	356	ILE
1	A	358	GLU
1	A	394	LEU
1	A	402	LEU
1	A	412	THR
1	A	418	GLN
1	A	429	GLU
1	A	441	THR
1	A	460	THR
1	A	589	LYS

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Mol	Chain	Res	Type
1	A	647	TRP
1	A	681	LEU
1	A	684	CYS
1	A	721	GLU
1	A	727	LEU
1	A	750	VAL
1	B	49	GLN
1	B	104	HIS
1	B	135	ILE
1	B	161	LEU
1	B	170	THR
1	B	219	ILE
1	B	232	LEU
1	B	236	GLU
1	B	275	PHE
1	B	279	ILE
1	B	292	ASP
1	B	293	VAL
1	B	297	VAL
1	B	307	THR
1	B	317	LEU
1	B	344	LEU
1	B	345	ARG
1	B	350	LYS
1	B	353	PHE
1	B	354	GLU
1	B	365	ILE
1	B	392	VAL
1	B	394	LEU
1	B	429	GLU
1	B	441	THR
1	B	584	LEU
1	B	619	ILE
1	B	635	PHE
1	B	675	GLU
1	B	726	GLU
1	B	727	LEU
1	B	738	LEU
1	C	18	ARG
1	C	45	LEU
1	C	104	HIS
1	C	135	ILE

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Mol	Chain	Res	Type
1	C	233	ASP
1	C	254	VAL
1	C	274	LYS
1	C	279	ILE
1	C	290	LYS
1	C	307	THR
1	C	317	LEU
1	C	349	LYS
1	C	350	LYS
1	C	353	PHE
1	C	368	VAL
1	C	402	LEU
1	C	407	LEU
1	C	583	VAL
1	C	630	GLU
1	C	679	THR
1	C	681	LEU
1	C	746	LEU
1	D	115	GLU
1	D	275	PHE
1	D	293	VAL
1	D	295	CYS
1	D	317	LEU
1	D	353	PHE
1	D	354	GLU
1	D	368	VAL
1	D	372	PHE
1	D	383	ASP
1	D	392	VAL
1	D	418	GLN
1	D	459	VAL
1	D	584	LEU
1	D	628	THR
1	D	746	LEU
1	D	759	ILE
1	D	793	THR
2	G	11	LEU
2	G	12	VAL
2	H	5	VAL
2	H	46	GLU
2	H	59	GLU
2	H	79	VAL

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Mol	Chain	Res	Type
2	H	93	VAL
2	I	12	VAL
2	I	29	VAL
2	J	5	VAL
2	J	100	VAL
3	E	16	THR
3	E	17	TYR
3	E	19	ILE
3	E	25	ASP
3	E	49	LYS
3	E	54	CYS
3	E	55	LEU
3	E	60	SER
3	E	140	ASN
3	E	141	LEU
3	E	158	LEU
3	E	161	TYR
3	E	165	PHE
3	E	183	TRP
3	E	303	LEU
3	E	319	PHE
3	E	325	TYR
3	E	344	GLU
3	E	346	LEU
3	E	354	CYS
3	E	355	THR
3	E	384	LEU
3	E	392	LEU
3	E	397	PHE
3	E	414	ASN
3	E	420	LEU
3	E	421	HIS
3	E	441	VAL
3	E	456	THR
3	E	463	HIS
3	E	486	VAL
3	E	614	THR
3	E	704	HIS
3	E	725	VAL
3	E	810	LEU
3	E	817	LEU
3	E	829	VAL

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Mol	Chain	Res	Type
3	F	19	ILE
3	F	20	LEU
3	F	25	ASP
3	F	49	LYS
3	F	54	CYS
3	F	140	ASN
3	F	144	GLN
3	F	161	TYR
3	F	165	PHE
3	F	183	TRP
3	F	195	HIS
3	F	213	LEU
3	F	293	LYS
3	F	304	ILE
3	F	307	LEU
3	F	319	PHE
3	F	325	TYR
3	F	346	LEU
3	F	354	CYS
3	F	355	THR
3	F	362	LEU
3	F	366	LEU
3	F	387	LEU
3	F	390	ILE
3	F	392	LEU
3	F	397	PHE
3	F	416	PHE
3	F	419	LEU
3	F	420	LEU
3	F	425	GLN
3	F	451	LEU
3	F	459	LYS
3	F	698	ILE
3	F	725	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	HIS
1	A	105	GLN
1	A	377	HIS
1	A	406	ASN

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Mol	Chain	Res	Type
1	A	478	HIS
1	A	494	ASN
1	A	709	ASN
1	A	740	ASN
1	A	755	ASN
1	B	104	HIS
1	B	288	ASN
1	B	312	HIS
1	B	370	ASN
1	B	418	GLN
1	B	494	ASN
1	B	624	ASN
1	B	639	HIS
1	B	709	ASN
1	B	729	GLN
1	B	744	GLN
1	C	105	GLN
1	C	522	HIS
1	C	615	ASN
1	C	694	HIS
1	C	709	ASN
1	C	729	GLN
1	C	737	HIS
1	D	104	HIS
1	D	155	HIS
1	D	288	ASN
1	D	418	GLN
1	D	554	ASN
1	D	560	GLN
1	D	624	ASN
1	D	636	GLN
2	G	39	GLN
2	G	74	ASN
2	G	84	ASN
2	H	107	GLN
2	I	39	GLN
2	I	74	ASN
2	I	110	GLN
2	J	39	GLN
3	E	150	ASN
3	E	155	HIS
3	E	181	ASN

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Mol	Chain	Res	Type
3	E	337	HIS
3	E	511	GLN
3	E	612	HIS
3	E	629	ASN
3	E	692	HIS
3	E	781	ASN
3	E	819	GLN
3	E	847	ASN
3	F	140	ASN
3	F	145	GLN
3	F	297	HIS
3	F	345	HIS
3	F	425	GLN
3	F	462	GLN
3	F	511	GLN
3	F	538	HIS
3	F	629	ASN
3	F	636	ASN
3	F	659	ASN
3	F	752	GLN
3	F	770	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.

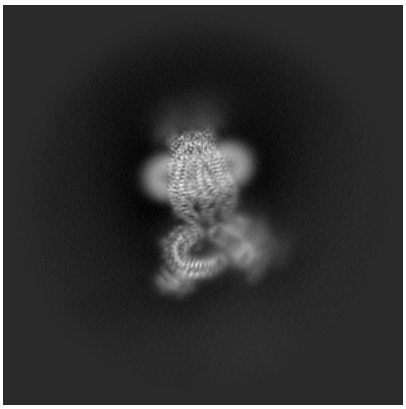
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-55590. These allow visual inspection of the internal detail of the map and identification of artifacts.

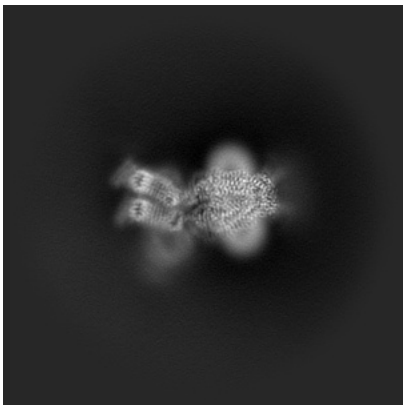
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

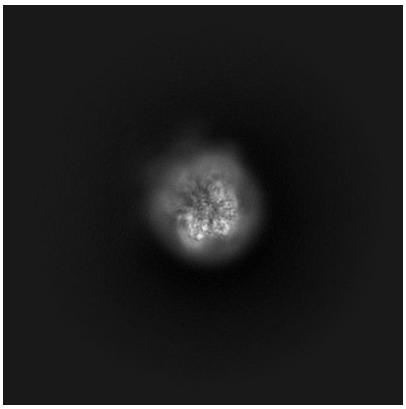
6.1.1 Primary map



X

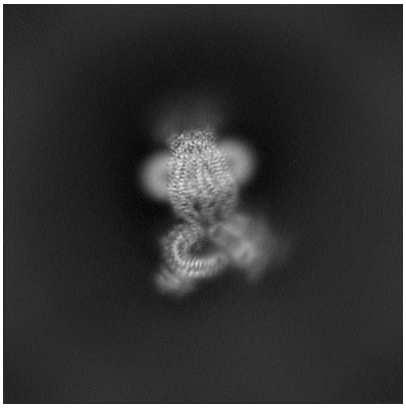


Y

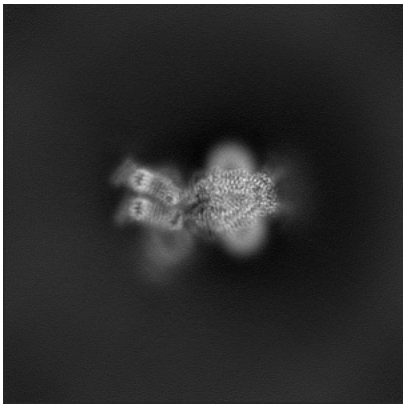


Z

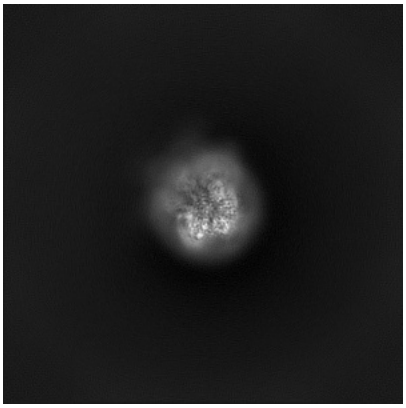
6.1.2 Raw map



X



Y



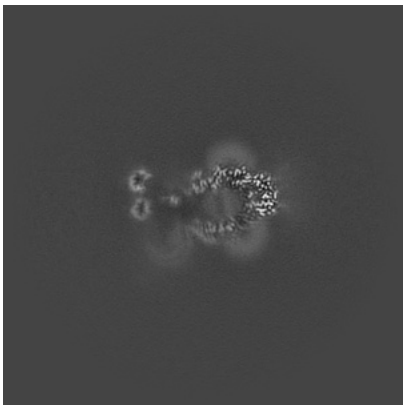
Z

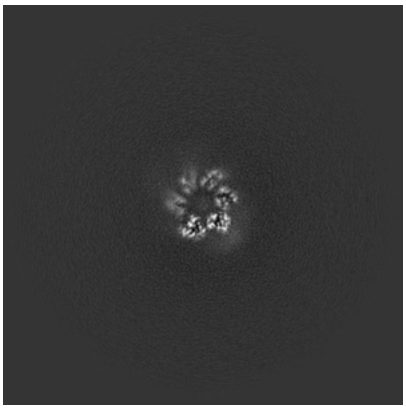
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

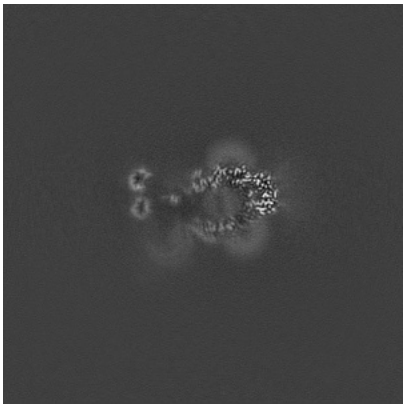
X Index: 183

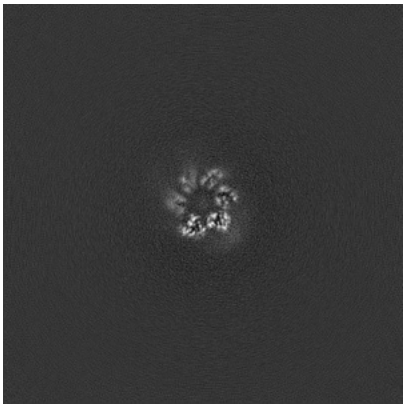

Y Index: 183


Z Index: 183

6.2.2 Raw map

X Index: 183


Y Index: 183

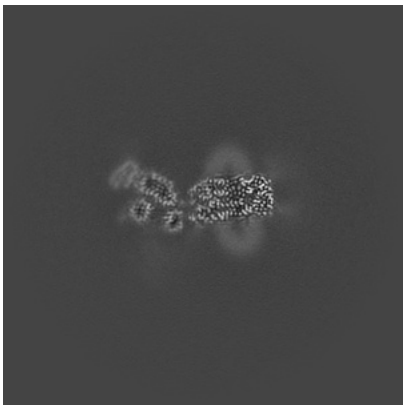

Z Index: 183

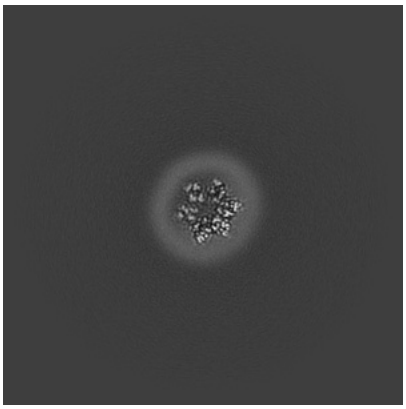
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

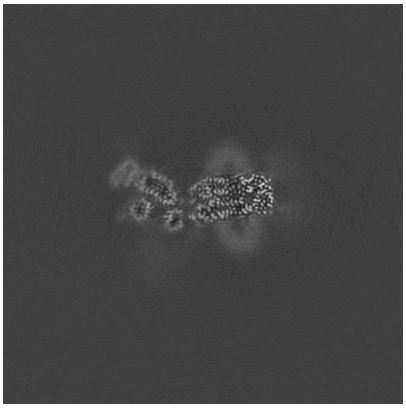
X Index: 199

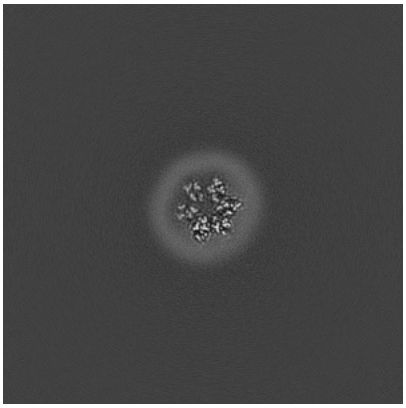

Y Index: 163


Z Index: 220

6.3.2 Raw map

X Index: 199

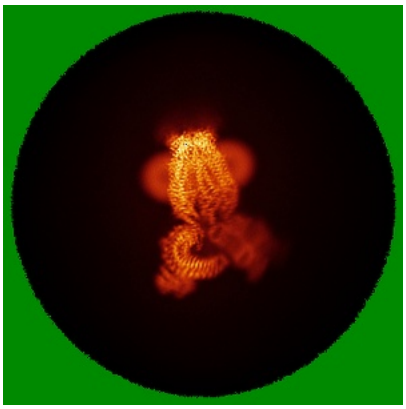

Y Index: 163

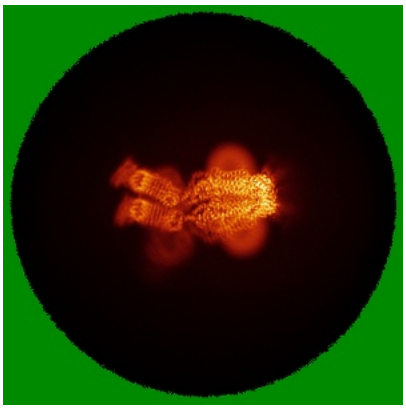

Z Index: 219

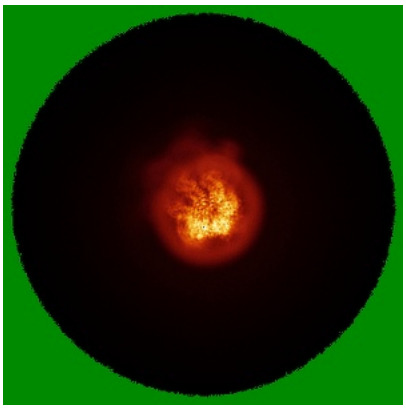
The images above show the largest variance slices of the map in three orthogonal directions.

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

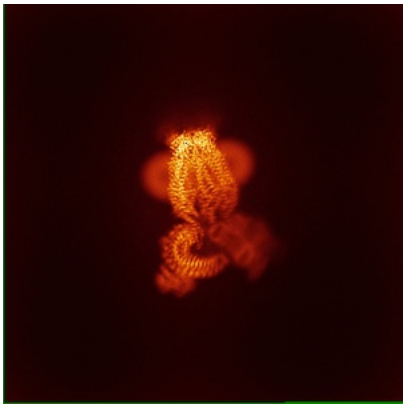
6.4.1 Primary map

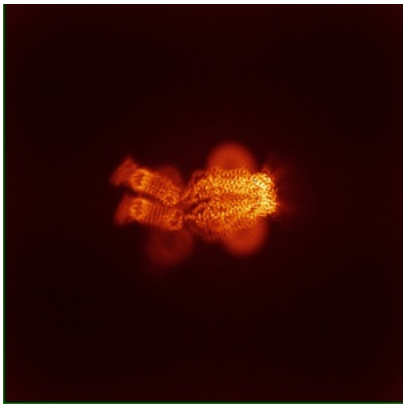

X

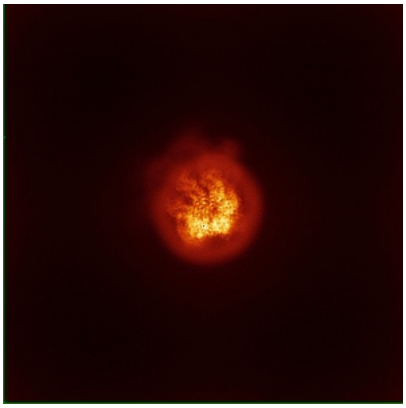

Y


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.

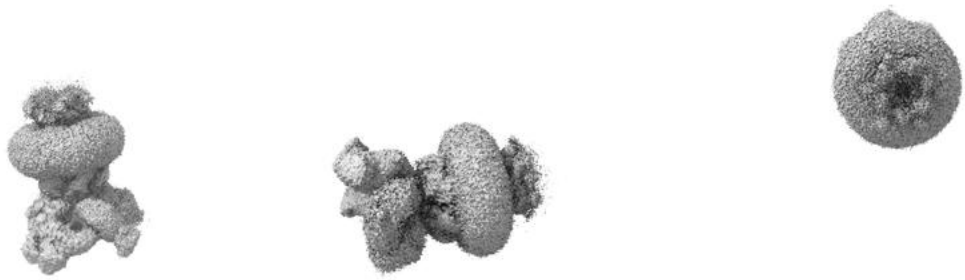
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0945. 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



X Y Z

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.

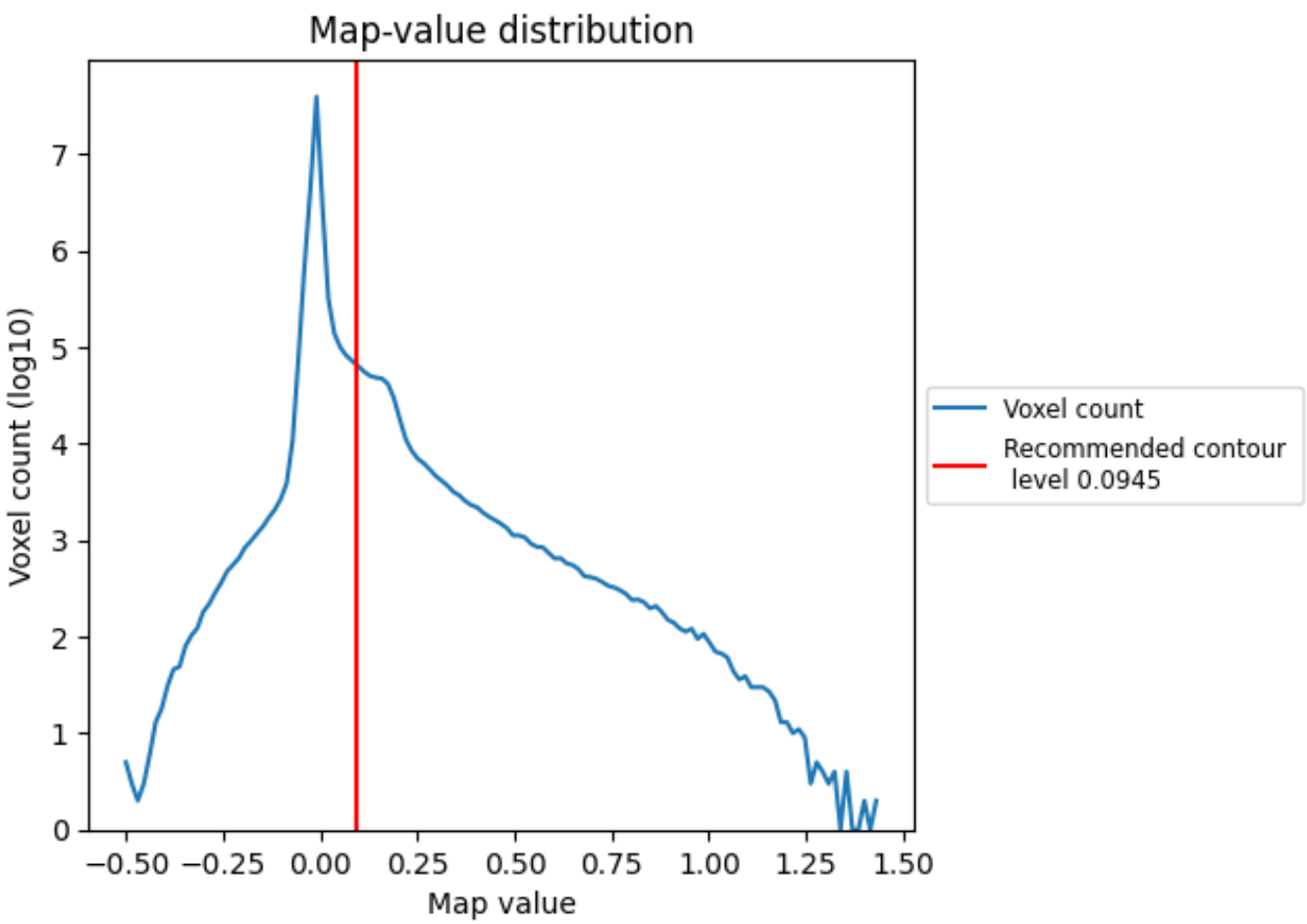
6.6 Mask visualisation (i)

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

7 Map analysis (i)

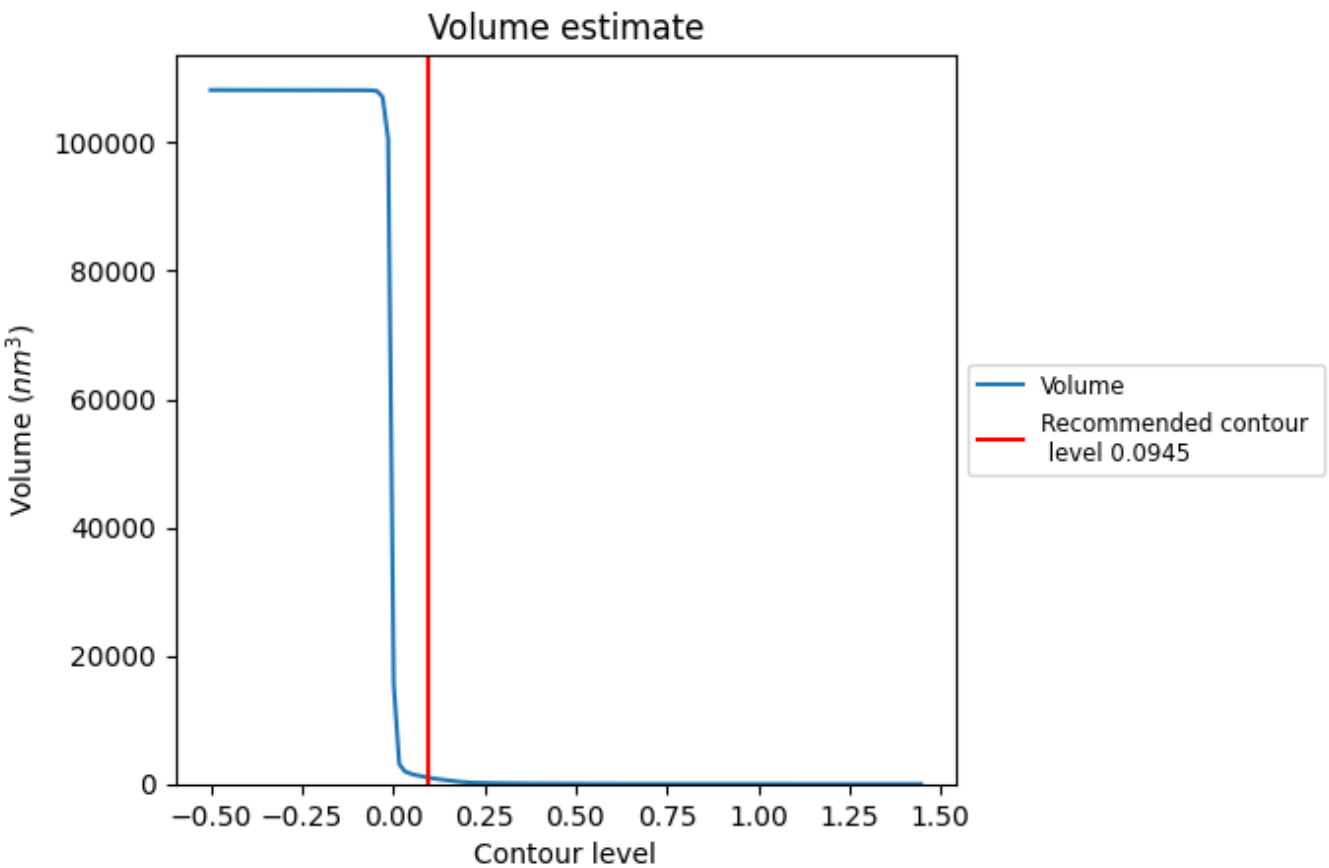
This section contains the results of statistical analysis of the map.

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.

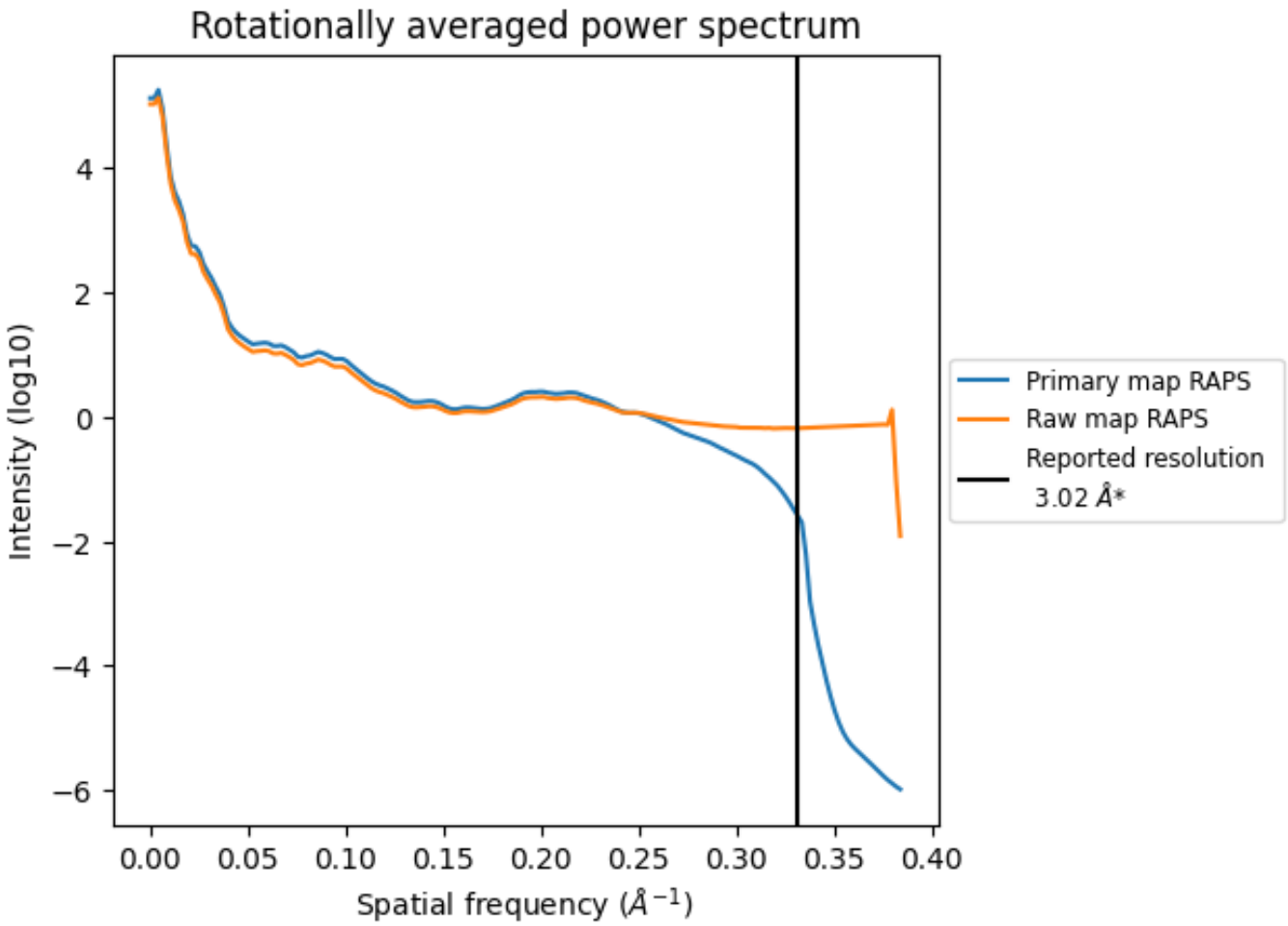
7.2 Volume estimate (i)



The volume at the recommended contour level is 1009 nm^3; this corresponds to an approximate mass of 911 kDa.

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

7.3 Rotationally averaged power spectrum (i)

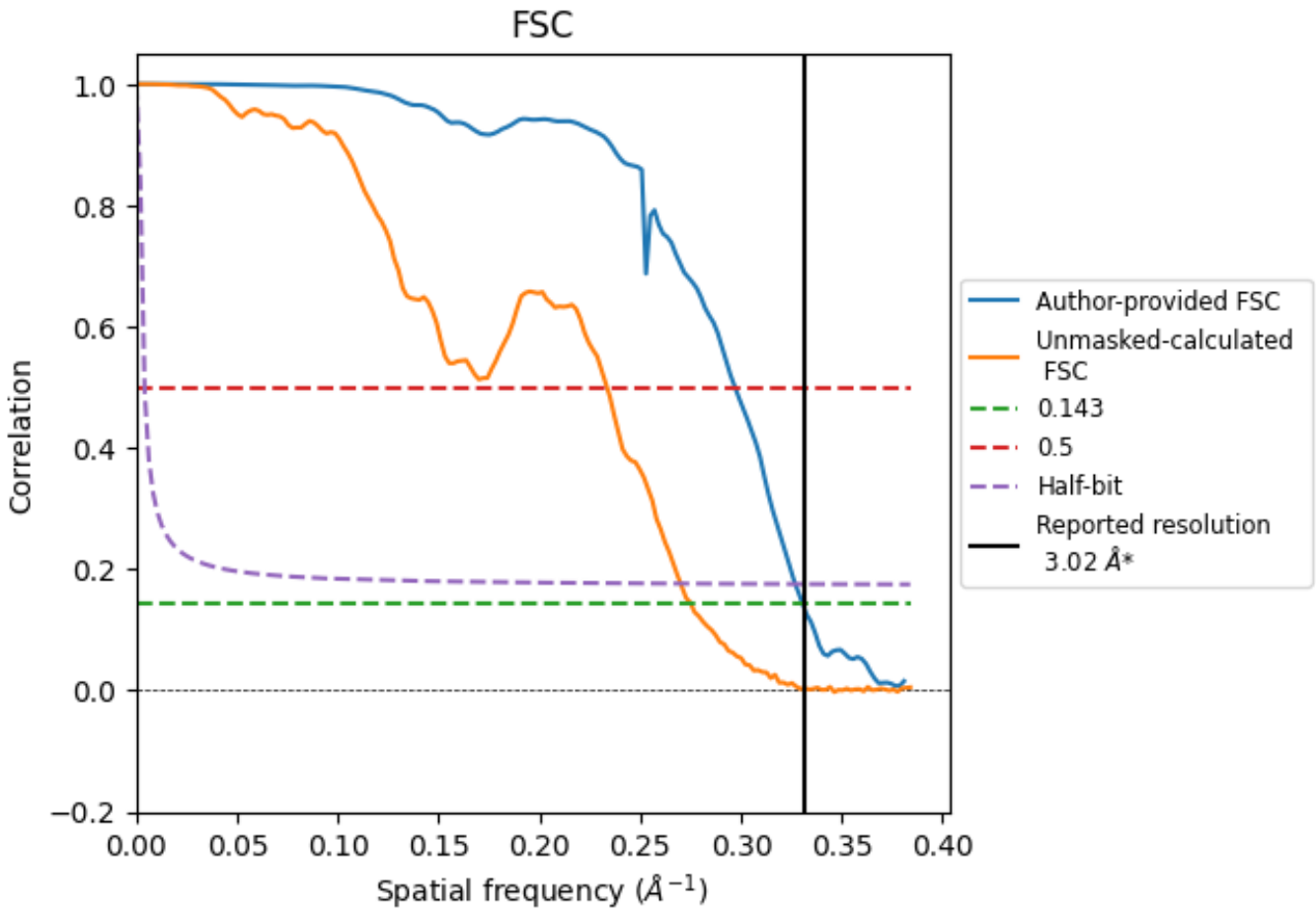


*Reported resolution corresponds to spatial frequency of 0.331 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.331 Å^{-1}

8.2 Resolution estimates (i)

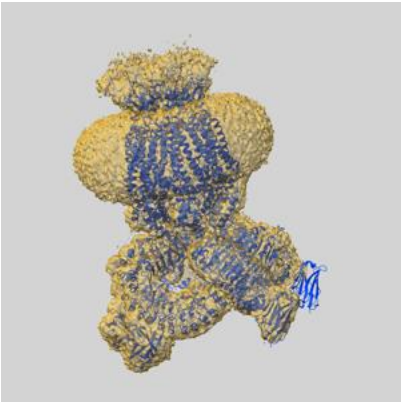
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.02	3.37	3.06
Unmasked-calculated*	3.64	4.28	3.70

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.64 differs from the reported value 3.02 by more than 10 %

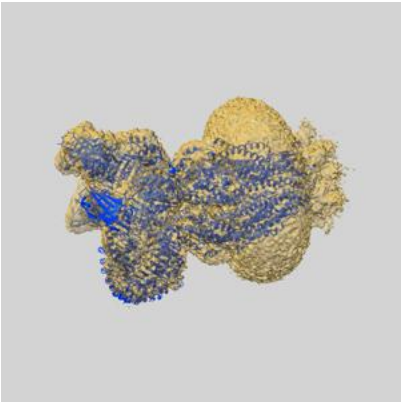
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-55590 and PDB model 9T5N. Per-residue inclusion information can be found in section 3 on page 10.

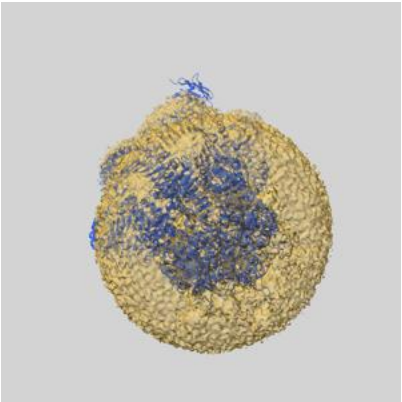
9.1 Map-model overlay (i)



X



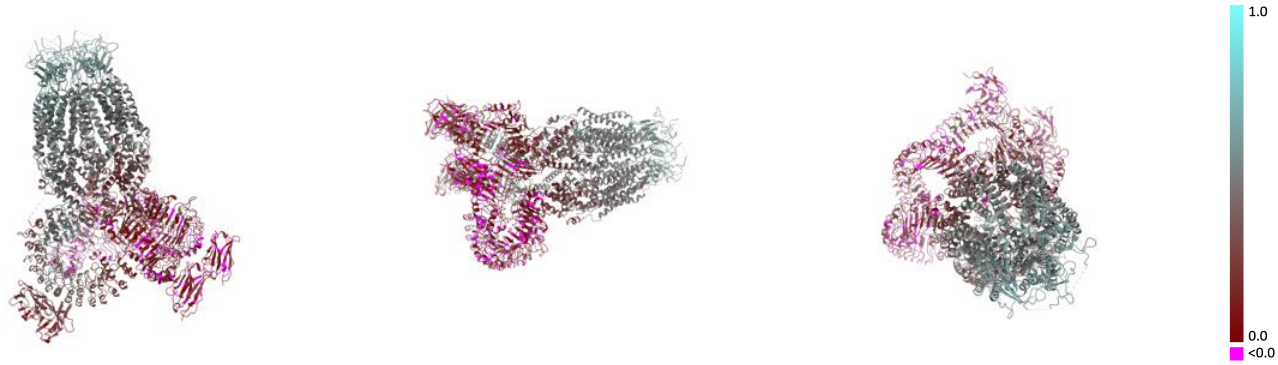
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0945 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

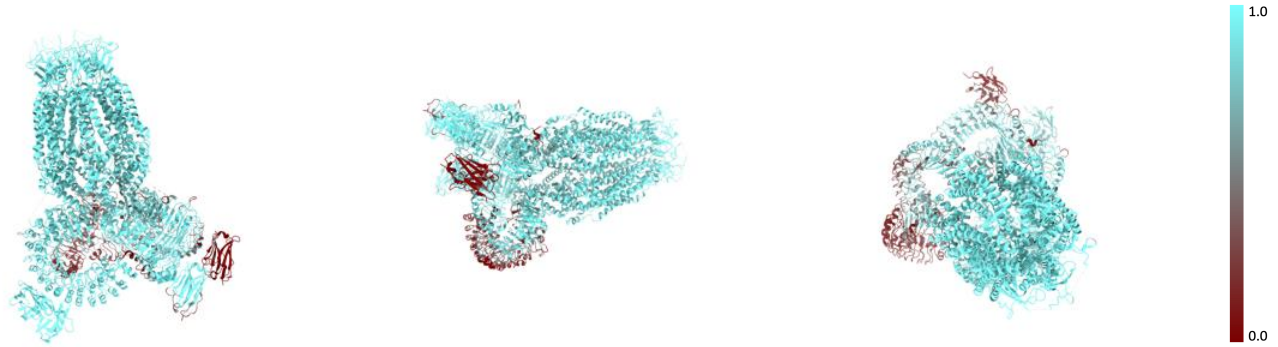
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

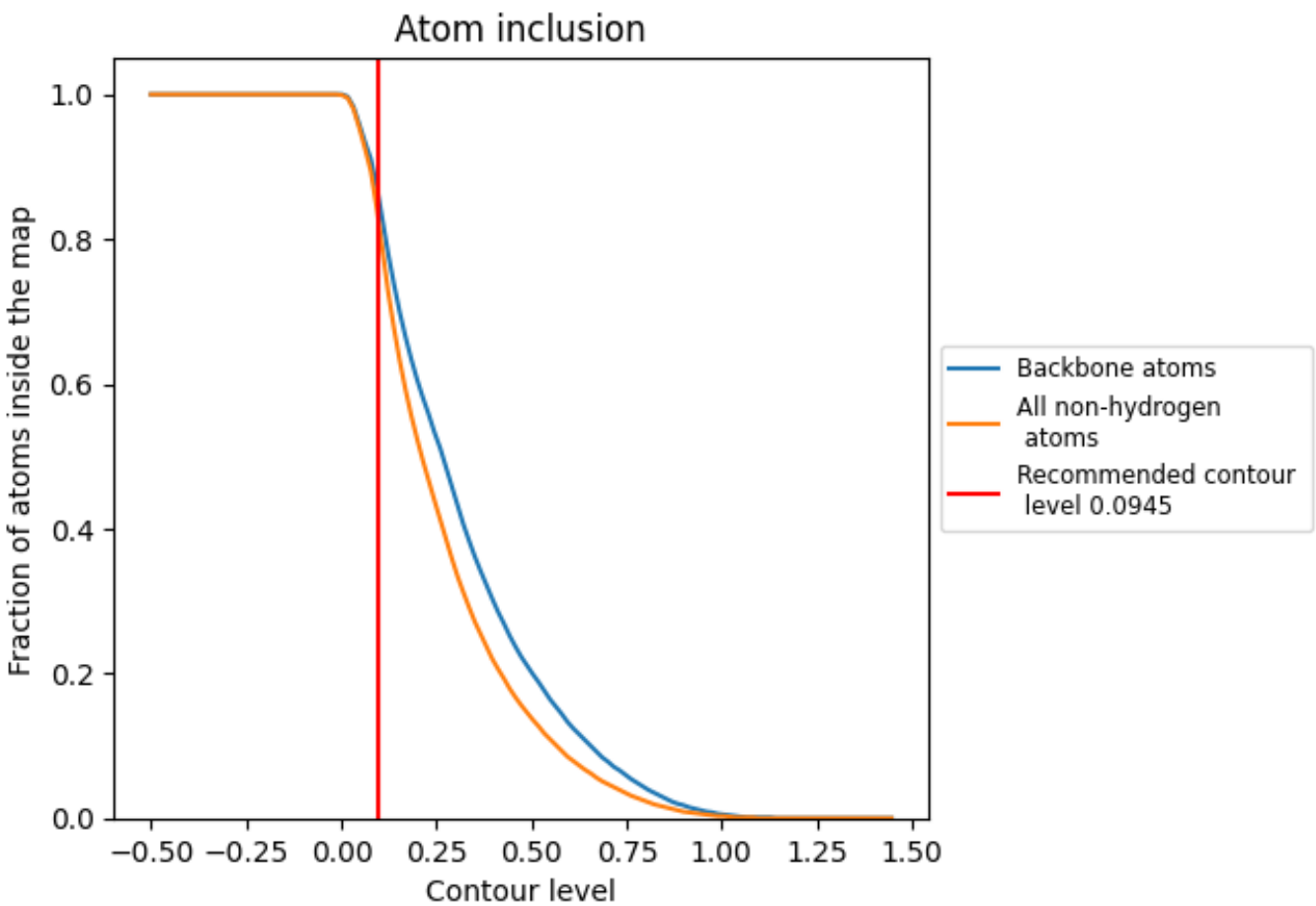
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0945).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0945) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8390	0.3130
A	0.9810	0.4480
B	0.9770	0.4510
C	0.9240	0.2920
D	0.8890	0.2790
E	0.7610	0.2450
F	0.5670	0.2420
G	0.9890	0.2510
H	0.9870	0.2570
I	0.8350	0.1240
J	0.0440	0.0620