



Full wwPDB EM Validation Report ⓘ

Mar 15, 2026 – 07:19 AM UTC

PDB ID : 8B41 / pdb_00008b41
EMDB ID : EMD-15836
Title : Structure of heteromeric LRRC8A/C (1:1 co-transfected) Volume-Regulated Anion Channel in complex with synthetic nanobody Sb1
Authors : Sawicka, M.; Dutzler, R.
Deposited on : 2022-09-19
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

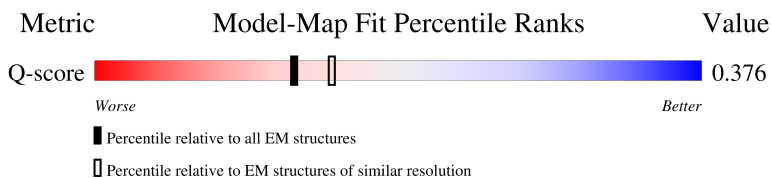
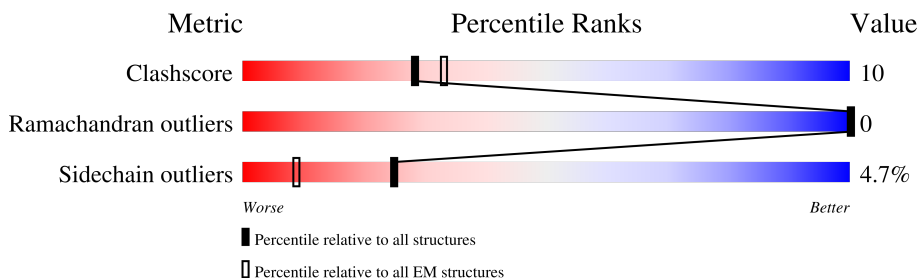
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	811	8%25%••69%
2	F	811	5%18%5%•76%
3	G	118	25%66%31%•
3	H	118	22%61%34%••
3	I	118	72%63%33%••
3	J	118	88%70%25%••

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 31259 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	732	Total	C	N	O	S	0	0
			6030	3916	1018	1071	25		
1	C	718	Total	C	N	O	S	0	0
			5922	3853	997	1047	25		
1	D	732	Total	C	N	O	S	0	0
			6030	3916	1018	1071	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

Continued on next page...

Continued from previous page...

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	254	Total	C	N	O	S	0	0
			2125	1415	332	357	21		
2	F	195	Total	C	N	O	S	0	0
			1618	1083	247	270	18		

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

- Molecule 3 is a protein called Synthetic nanobody Sb1.

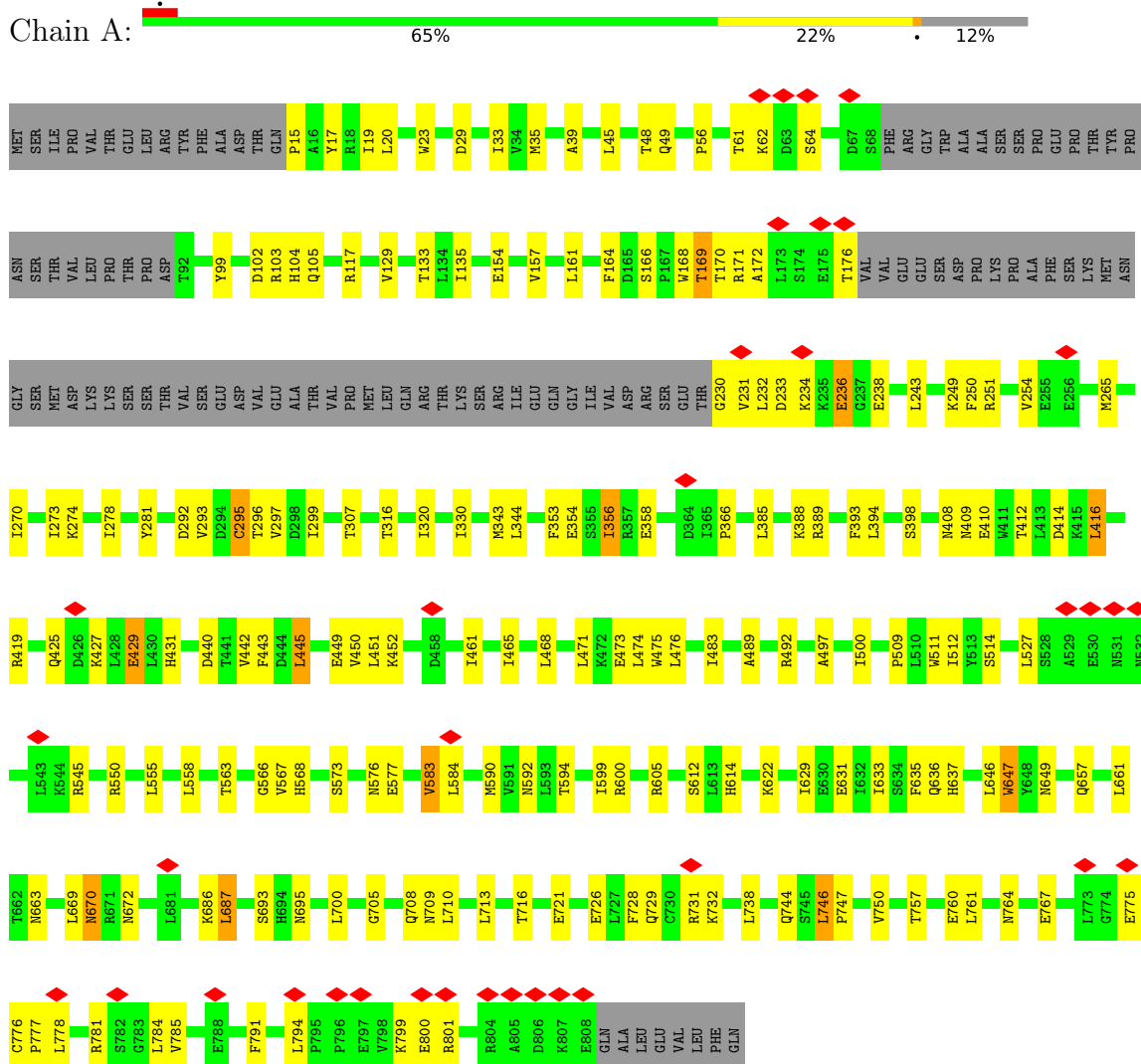
Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	114	Total 903	C 575	N 152	O 172	S 4	0	0
3	H	114	Total 903	C 575	N 152	O 172	S 4	0	0
3	I	114	Total 903	C 575	N 152	O 172	S 4	0	0
3	J	114	Total 903	C 575	N 152	O 172	S 4	0	0

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

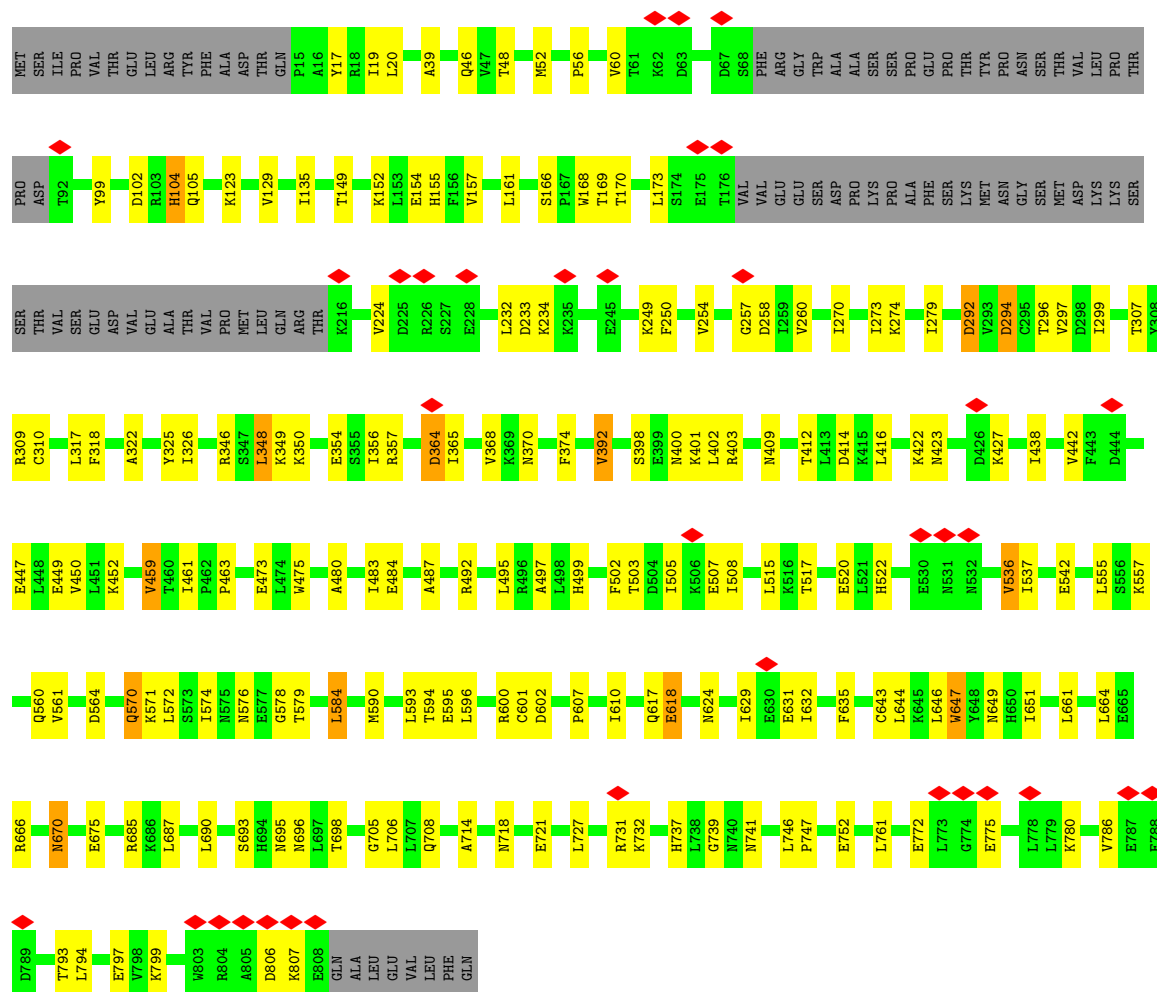
Chain A:



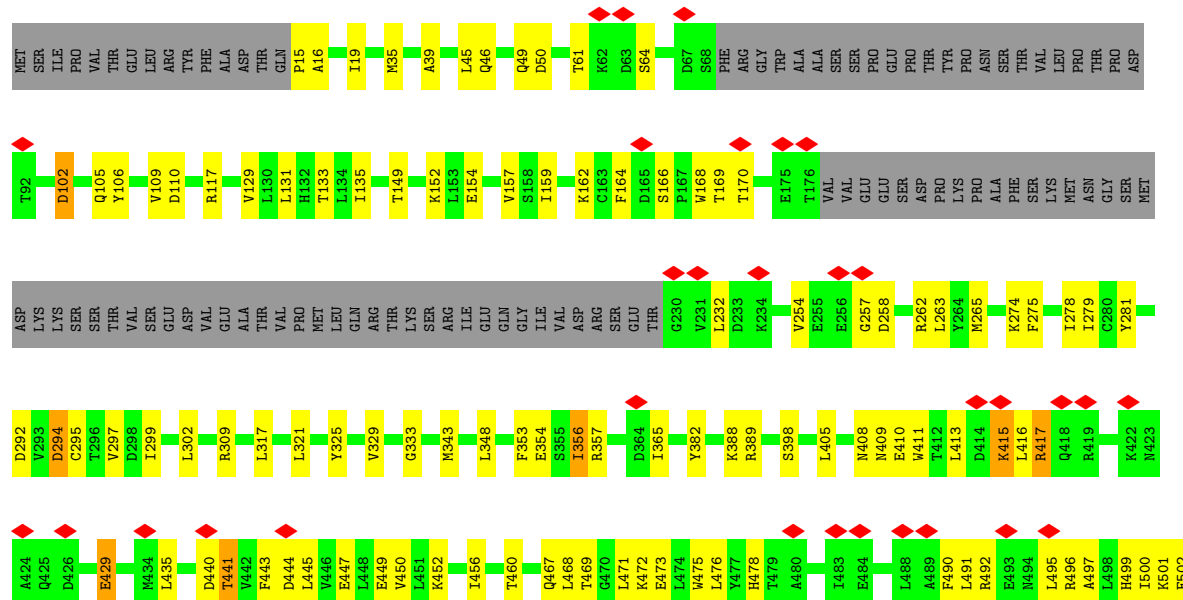
• Molecule 1: Volume-regulated anion channel subunit LRRC8A

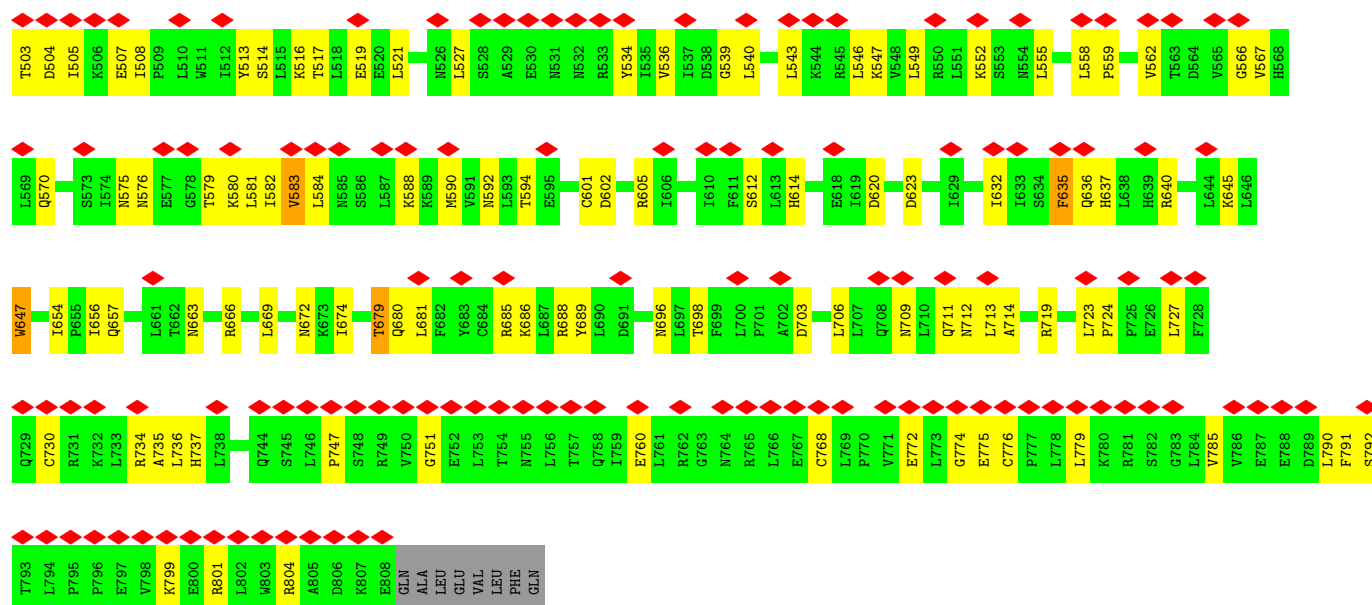
Chain B:



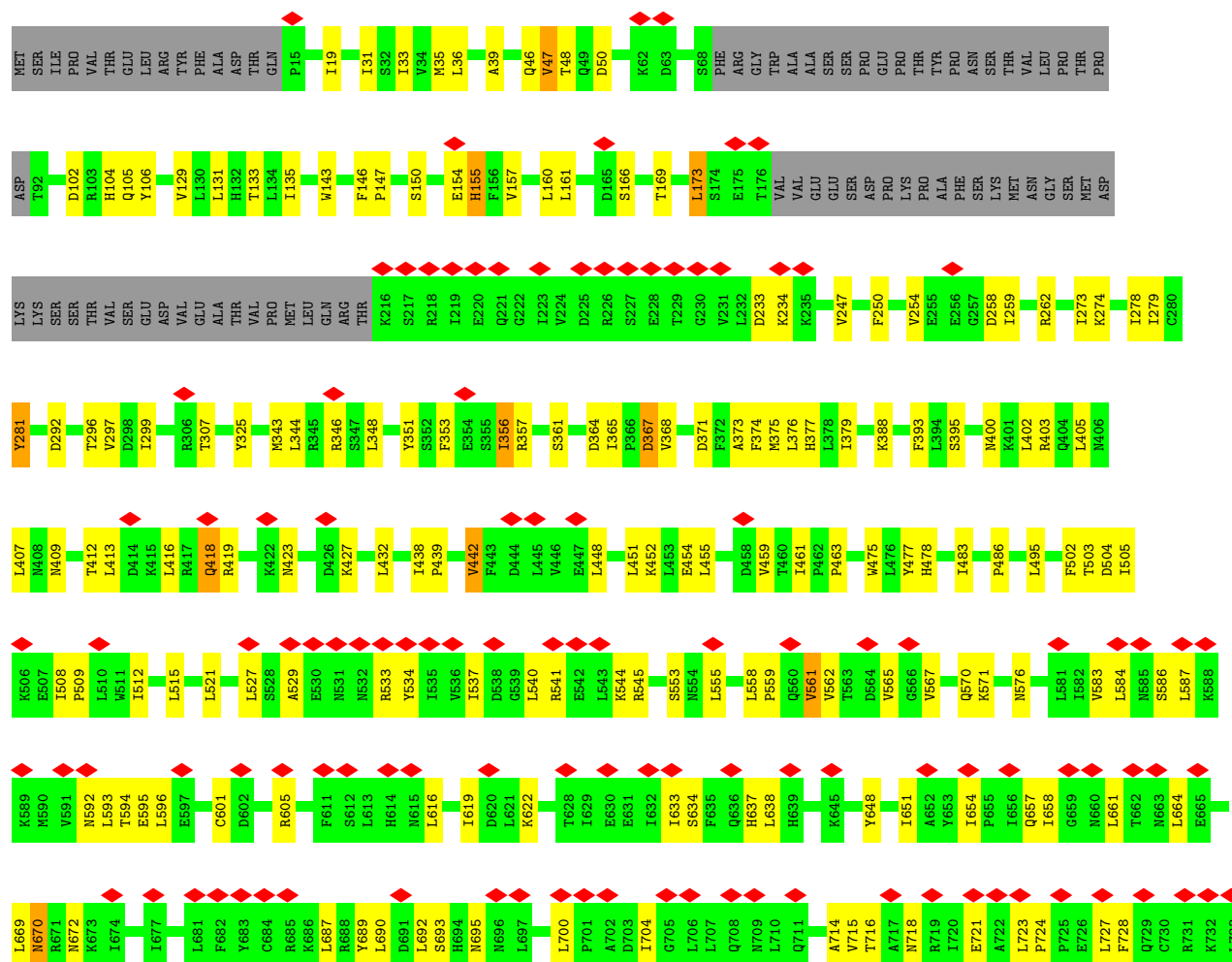


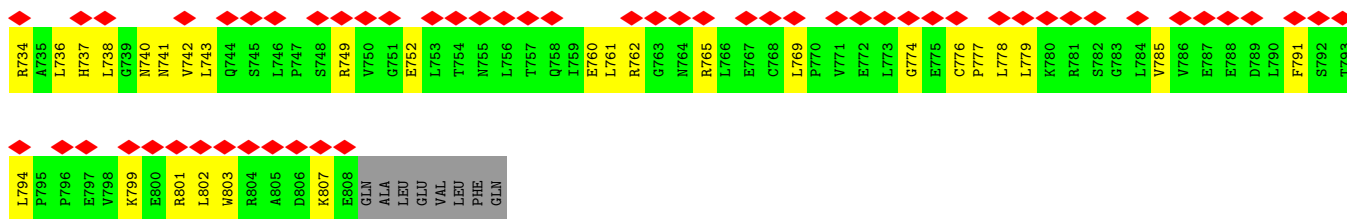
• Molecule 1: Volume-regulated anion channel subunit LRRC8A



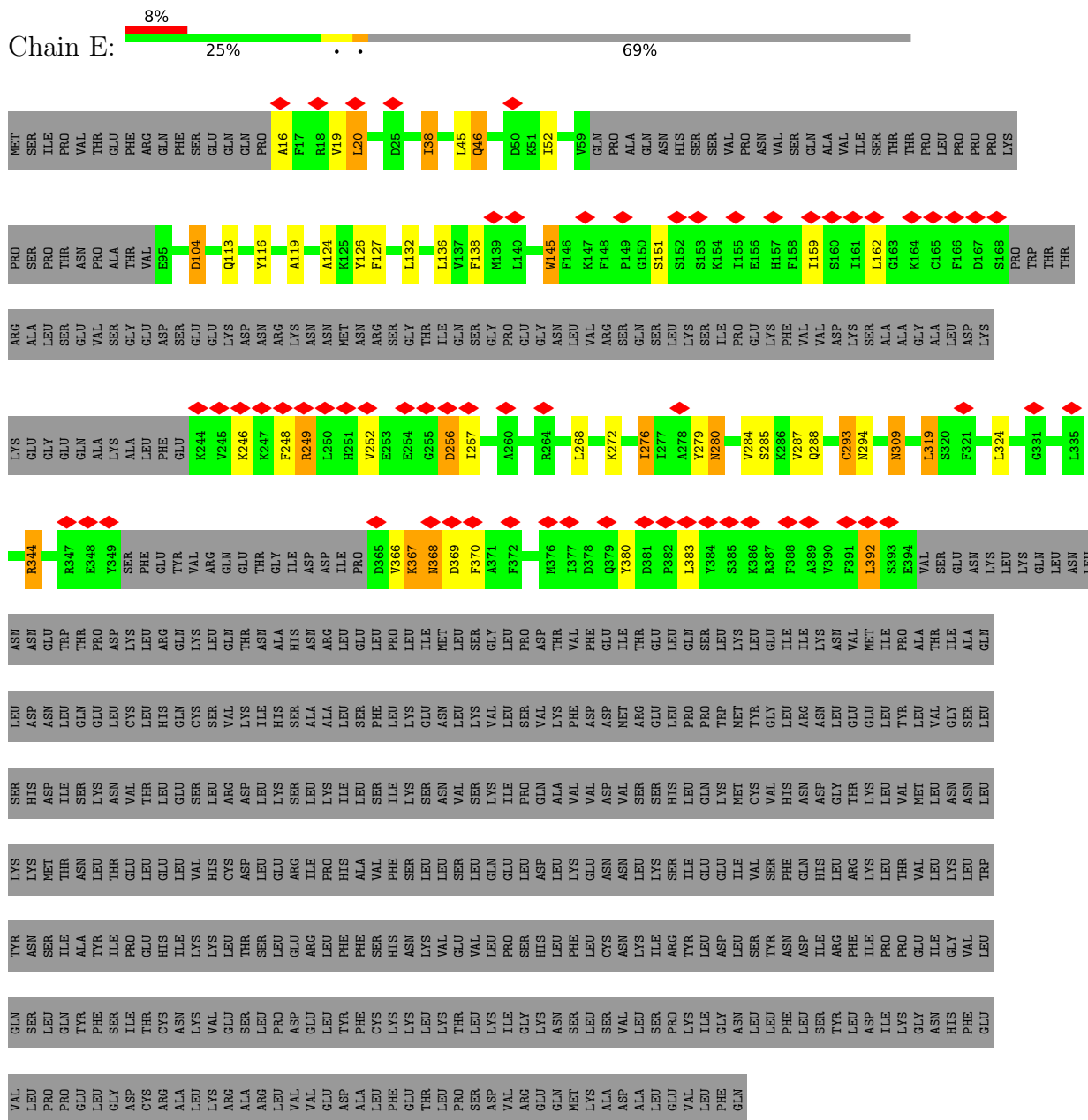


• Molecule 1: Volume-regulated anion channel subunit LRRC8A



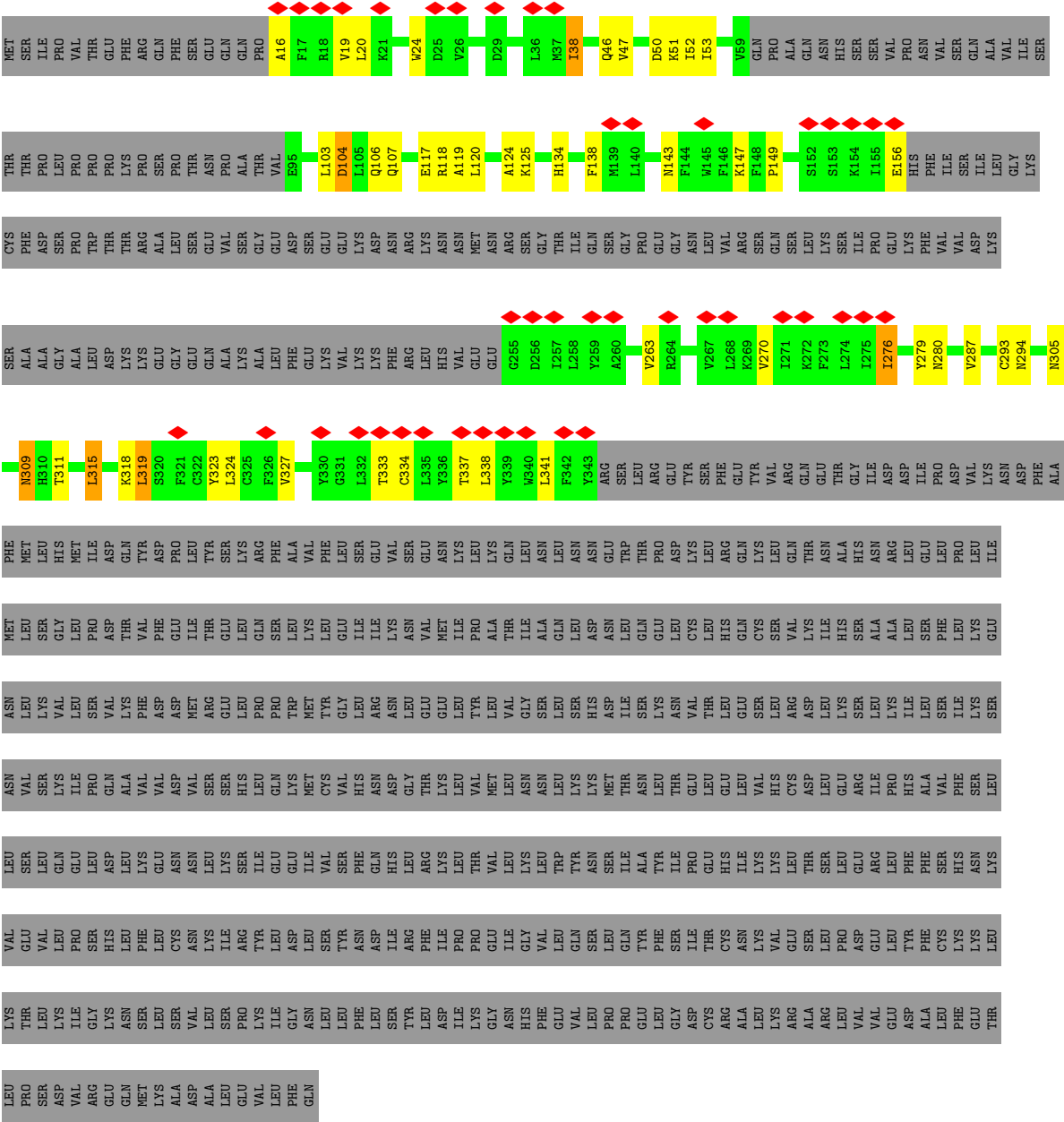


• Molecule 2: Volume-regulated anion channel subunit LRRC8C

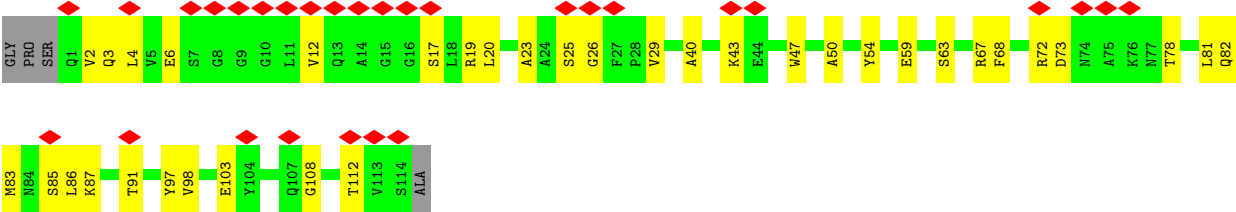


• Molecule 2: Volume-regulated anion channel subunit LRRC8C

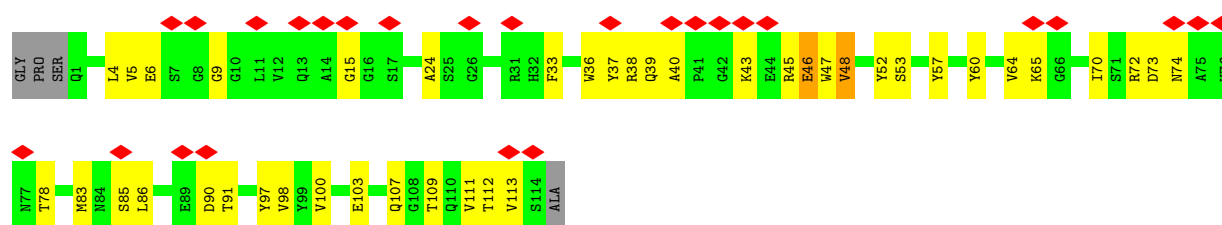




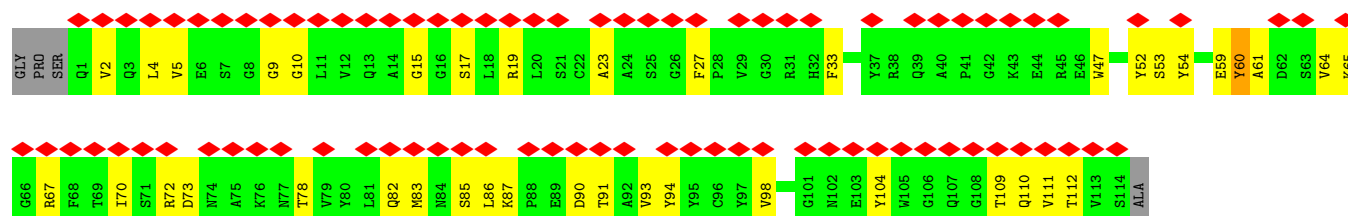
● Molecule 3: Synthetic nanobody Sb1



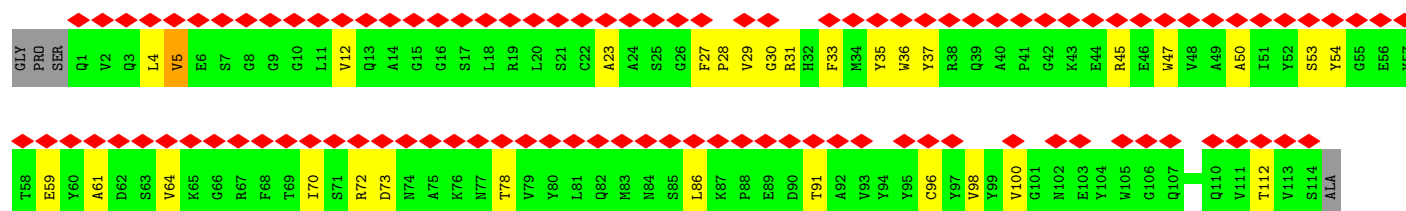
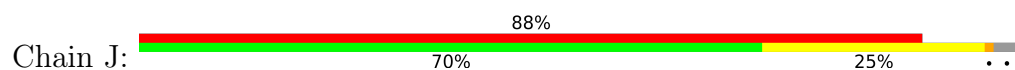
● Molecule 3: Synthetic nanobody Sb1



• Molecule 3: Synthetic nanobody Sb1



• Molecule 3: Synthetic nanobody Sb1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	329716	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 ($e^-/\text{\AA}^2$)	60	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	0.121	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.02	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	0.12	0/6055	0.28	0/8207
1	B	0.13	0/6163	0.29	0/8352
1	C	0.13	0/6055	0.29	0/8207
1	D	0.11	0/6163	0.28	0/8352
2	E	0.11	0/2184	0.28	0/2946
2	F	0.13	0/1664	0.31	0/2252
3	G	0.10	0/927	0.28	0/1258
3	H	0.10	0/927	0.29	0/1258
3	I	0.10	0/927	0.31	0/1258
3	J	0.10	0/927	0.29	0/1258
All	All	0.12	0/31992	0.29	0/43348

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	109	0
1	B	6030	0	6184	113	0
1	C	5922	0	6081	124	0
1	D	6030	0	6184	122	0
2	E	2125	0	2122	32	0
2	F	1618	0	1621	29	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	903	0	852	20	0
3	H	903	0	852	24	0
3	I	903	0	852	26	0
3	J	903	0	852	19	0
All	All	31259	0	31681	599	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (599) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:17:SER:HA	3:I:83:MET:O	1.71	0.91
1:D:258:ASP:H	1:D:371:ASP:HB2	1.46	0.80
1:C:413:LEU:HD22	1:C:417:ARG:HH12	1.48	0.78
2:E:256:ASP:H	2:E:369:ASP:HB2	1.49	0.77
1:C:135:ILE:HG23	1:C:274:LYS:HZ2	1.50	0.77
1:A:48:THR:HG23	1:A:49:GLN:HG3	1.64	0.76
2:E:119:ALA:HB2	2:E:293:CYS:HB3	1.67	0.76
1:A:171:ARG:HH21	1:A:230:GLY:HA3	1.51	0.75
1:A:429:GLU:HG3	1:A:452:LYS:HE3	1.69	0.74
1:A:251:ARG:HH12	1:A:366:PRO:HG2	1.52	0.72
1:B:258:ASP:HB2	1:B:370:ASN:HD22	1.55	0.72
1:A:419:ARG:NH1	1:A:431:HIS:O	2.23	0.71
1:C:232:LEU:O	1:C:409:ASN:ND2	2.24	0.71
2:E:113:GLN:NE2	2:F:309:ASN:OD1	2.23	0.70
1:A:555:LEU:O	1:A:576:ASN:ND2	2.25	0.70
1:A:781:ARG:NH1	1:A:784:LEU:O	2.25	0.70
1:A:49:GLN:NE2	2:F:47:VAL:O	2.25	0.69
1:B:675:GLU:HA	1:B:696:ASN:HB2	1.73	0.69
1:D:461:ILE:HB	1:D:483:ILE:HG13	1.74	0.69
2:E:256:ASP:HB2	2:E:368:ASN:HB2	1.73	0.69
1:B:135:ILE:HG23	1:B:274:LYS:HZ2	1.56	0.68
1:A:777:PRO:HB2	1:A:778:LEU:HD12	1.75	0.68
1:D:794:LEU:O	1:D:799:LYS:NZ	2.27	0.68
3:G:17:SER:HA	3:G:83:MET:O	1.94	0.68
3:I:91:THR:HG23	3:I:112:THR:HA	1.76	0.67
1:D:760:GLU:HA	1:D:785:VAL:HB	1.75	0.67
1:D:135:ILE:HG23	1:D:274:LYS:HZ2	1.60	0.67
1:C:768:CYS:HA	1:C:790:LEU:HD11	1.74	0.67
1:B:794:LEU:O	1:B:799:LYS:NZ	2.27	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:469:THR:HA	1:C:490:PHE:HZ	1.61	0.66
1:B:438:ILE:HG13	1:B:459:VAL:HG21	1.75	0.66
1:C:449:GLU:HA	1:C:471:LEU:HA	1.77	0.66
1:A:473:GLU:HG2	1:A:497:ALA:HB3	1.76	0.66
3:G:83:MET:HB3	3:G:86:LEU:HD21	1.78	0.66
1:C:452:LYS:HA	1:C:475:TRP:HB2	1.76	0.66
1:D:721:GLU:HA	1:D:743:LEU:HA	1.78	0.65
1:B:452:LYS:HA	1:B:475:TRP:HB2	1.77	0.65
1:C:472:LYS:HD2	1:C:496:ARG:HG2	1.77	0.65
3:I:19:ARG:HH11	3:I:82:GLN:HB2	1.62	0.65
1:C:567:VAL:O	1:C:592:ASN:ND2	2.30	0.64
1:C:576:ASN:HB3	1:C:579:THR:HB	1.79	0.64
1:C:168:TRP:HH2	1:C:398:SER:HB2	1.62	0.64
1:C:492:ARG:HH21	1:C:514:SER:HB2	1.61	0.64
1:B:102:ASP:OD1	1:B:105:GLN:NE2	2.29	0.64
2:E:249:ARG:HH22	2:E:392:LEU:HD11	1.62	0.64
3:G:2:VAL:HA	3:G:26:GLY:HA3	1.80	0.64
1:C:443:PHE:O	1:C:467:GLN:NE2	2.31	0.63
2:F:104:ASP:OD1	2:F:104:ASP:N	2.28	0.63
1:A:461:ILE:HB	1:A:483:ILE:HG13	1.79	0.63
1:A:103:ARG:NH1	2:F:106:GLN:OE1	2.31	0.63
1:C:441:THR:O	1:C:444:ASP:HB2	1.97	0.63
3:I:83:MET:HB3	3:I:86:LEU:HD21	1.79	0.63
1:A:416:LEU:HD11	1:A:442:VAL:HG12	1.80	0.63
1:A:669:LEU:O	1:A:672:ASN:ND2	2.32	0.63
1:C:669:LEU:O	1:C:672:ASN:ND2	2.31	0.63
1:D:704:ILE:HD13	1:D:727:LEU:HA	1.80	0.63
1:B:555:LEU:O	1:B:576:ASN:ND2	2.32	0.62
2:E:366:VAL:HB	2:E:370:PHE:HB3	1.81	0.62
1:A:166:SER:O	1:A:169:THR:OG1	2.17	0.62
1:D:454:GLU:HA	1:D:477:TYR:HB2	1.81	0.62
3:J:29:VAL:HG22	3:J:72:ARG:HD2	1.81	0.62
1:A:550:ARG:NH1	1:A:573:SER:OG	2.33	0.62
1:C:102:ASP:OD1	1:C:102:ASP:N	2.27	0.62
1:D:258:ASP:O	1:D:262:ARG:NH1	2.33	0.61
3:G:68:PHE:HB3	3:G:81:LEU:HD11	1.82	0.61
1:B:19:ILE:HD11	1:B:157:VAL:HG23	1.82	0.61
1:A:567:VAL:O	1:A:592:ASN:ND2	2.34	0.61
1:C:714:ALA:HA	1:C:737:HIS:HB2	1.81	0.61
3:G:40:ALA:HB3	3:G:43:LYS:HB3	1.81	0.61
1:D:774:GLY:O	1:D:801:ARG:NH2	2.29	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:64:VAL:HA	3:I:67:ARG:HD3	1.82	0.61
1:A:452:LYS:HA	1:A:475:TRP:HB2	1.84	0.60
1:B:576:ASN:HB3	1:B:579:THR:HB	1.83	0.60
1:B:629:ILE:HD13	1:B:651:ILE:HD13	1.83	0.60
3:H:6:GLU:O	3:H:107:GLN:NE2	2.35	0.60
1:C:519:GLU:HA	1:C:546:LEU:HA	1.82	0.60
1:C:774:GLY:O	1:C:801:ARG:NH2	2.32	0.60
1:D:689:TYR:OH	1:D:734:ARG:NH2	2.35	0.60
1:D:452:LYS:HA	1:D:475:TRP:HB2	1.84	0.60
1:B:463:PRO:HA	1:B:487:ALA:HB2	1.84	0.60
1:A:599:ILE:HG22	1:A:600:ARG:HG3	1.85	0.59
1:B:46:GLN:NE2	1:B:123:LYS:O	2.35	0.59
1:C:723:LEU:HB2	1:C:747:PRO:HG2	1.83	0.59
1:C:688:ARG:NH1	1:C:711:GLN:OE1	2.35	0.59
1:C:698:THR:HG22	1:C:719:ARG:HB2	1.84	0.59
1:A:295:CYS:HB2	1:A:297:VAL:HG13	1.84	0.59
1:A:693:SER:O	1:A:695:ASN:ND2	2.35	0.59
1:D:622:LYS:HG3	1:D:648:TYR:HB2	1.82	0.59
1:B:661:LEU:HB3	1:B:664:LEU:HG	1.83	0.59
1:D:405:LEU:O	1:D:409:ASN:ND2	2.36	0.59
1:B:102:ASP:OD1	1:B:102:ASP:N	2.36	0.59
1:B:647:TRP:O	1:B:649:ASN:ND2	2.36	0.58
3:H:83:MET:HE1	3:H:111:VAL:HG11	1.85	0.58
1:A:577:GLU:HA	1:A:600:ARG:HH21	1.68	0.58
1:A:164:PHE:O	1:A:389:ARG:NH1	2.36	0.58
1:C:408:ASN:HD21	1:C:440:ASP:H	1.48	0.58
1:D:357:ARG:NH1	1:D:365:ILE:O	2.36	0.58
1:D:740:ASN:N	1:D:762:ARG:O	2.36	0.58
1:B:400:ASN:OD1	1:B:403:ARG:NH2	2.37	0.58
1:D:534:TYR:HB3	1:D:559:PRO:HB3	1.85	0.58
1:D:39:ALA:HB2	1:D:129:VAL:HG12	1.86	0.58
1:D:669:LEU:HB2	1:D:692:LEU:HD22	1.85	0.58
2:F:134:HIS:NE2	2:F:279:TYR:OH	2.37	0.58
1:A:670:ASN:OD1	1:A:670:ASN:N	2.37	0.57
1:B:357:ARG:NH1	1:B:365:ILE:O	2.36	0.57
1:D:348:LEU:HD23	1:D:348:LEU:H	1.69	0.57
3:G:63:SER:O	3:G:67:ARG:NH1	2.37	0.57
1:B:632:ILE:O	1:B:635:PHE:HB2	2.04	0.57
1:D:356:ILE:HD13	1:D:388:LYS:HG2	1.85	0.57
1:A:663:ASN:OD1	1:A:686:LYS:NZ	2.37	0.57
1:D:160:LEU:HD21	1:D:379:ILE:HG21	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:29:VAL:O	3:G:72:ARG:NH1	2.37	0.57
3:H:52:TYR:O	3:H:72:ARG:NH2	2.37	0.57
1:D:367:ASP:OD1	1:D:367:ASP:N	2.36	0.57
1:A:568:HIS:HA	1:A:592:ASN:HD22	1.69	0.56
1:B:232:LEU:O	1:B:409:ASN:ND2	2.33	0.56
1:A:721:GLU:OE1	1:A:744:GLN:NE2	2.39	0.56
1:B:557:LYS:HG3	1:B:584:LEU:HD21	1.88	0.56
1:C:258:ASP:O	1:C:262:ARG:NH1	2.38	0.56
1:C:620:ASP:HA	1:C:645:LYS:HB2	1.86	0.56
3:G:6:GLU:OE1	3:G:108:GLY:N	2.30	0.56
1:D:567:VAL:O	1:D:592:ASN:ND2	2.38	0.56
1:C:504:ASP:OD1	1:C:505:ILE:N	2.38	0.56
3:J:50:ALA:HB3	3:J:59:GLU:HB2	1.87	0.56
1:C:35:MET:HE2	1:C:133:THR:HG22	1.87	0.56
1:C:647:TRP:CD1	1:C:647:TRP:H	2.23	0.56
1:C:685:ARG:HH21	1:C:706:LEU:HD13	1.70	0.56
3:H:15:GLY:HA2	3:H:85:SER:HA	1.86	0.56
1:C:166:SER:O	1:C:169:THR:OG1	2.23	0.56
1:D:400:ASN:OD1	1:D:403:ARG:NH2	2.38	0.56
3:J:5:VAL:HG13	3:J:23:ALA:HB3	1.87	0.56
1:A:760:GLU:HA	1:A:785:VAL:HB	1.86	0.56
2:E:104:ASP:OD1	2:E:104:ASP:N	2.40	0.56
3:G:19:ARG:HH11	3:G:82:GLN:HB2	1.69	0.56
3:G:85:SER:O	3:G:87:LYS:NZ	2.38	0.55
1:A:647:TRP:O	1:A:649:ASN:ND2	2.40	0.55
1:B:46:GLN:HB2	1:B:318:PHE:HZ	1.70	0.55
2:F:270:VAL:HG21	2:F:338:LEU:HD22	1.88	0.55
1:C:46:GLN:HA	1:C:50:ASP:HB2	1.88	0.55
1:C:435:LEU:H	1:C:456:ILE:HG12	1.71	0.55
1:A:705:GLY:O	1:A:708:GLN:NE2	2.40	0.55
3:I:9:GLY:HA3	3:I:109:THR:HB	1.89	0.55
1:A:61:THR:O	1:A:64:SER:OG	2.23	0.55
1:C:570:GLN:O	1:C:594:THR:OG1	2.25	0.55
1:D:693:SER:O	1:D:695:ASN:ND2	2.40	0.55
1:C:580:LYS:HA	1:C:602:ASP:HB3	1.88	0.55
1:C:679:THR:OG1	1:C:703:ASP:OD2	2.20	0.55
1:D:571:LYS:HG3	1:D:595:GLU:HB2	1.88	0.55
1:A:728:PHE:O	1:A:731:ARG:NH1	2.40	0.55
1:B:473:GLU:HG2	1:B:497:ALA:HB3	1.89	0.55
1:C:491:LEU:HD22	1:C:495:LEU:HD22	1.89	0.55
3:I:61:ALA:HB3	3:I:64:VAL:HG22	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ASP:N	1:A:102:ASP:OD1	2.36	0.54
1:C:558:LEU:HD22	1:C:583:VAL:HG12	1.89	0.54
2:F:52:ILE:HD11	2:F:120:LEU:HD22	1.89	0.54
1:C:354:GLU:HA	1:C:357:ARG:HG2	1.89	0.54
1:C:473:GLU:HA	1:C:497:ALA:HB3	1.88	0.54
1:D:233:ASP:OD1	1:D:234:LYS:N	2.41	0.54
3:H:40:ALA:HB3	3:H:43:LYS:HB3	1.90	0.54
3:I:53:SER:HA	3:I:72:ARG:HH12	1.73	0.54
1:A:243:LEU:HB3	1:A:393:PHE:HE2	1.71	0.54
1:C:429:GLU:HB2	1:C:450:VAL:HB	1.88	0.54
3:H:4:LEU:HD23	3:H:24:ALA:HB2	1.90	0.54
1:B:461:ILE:HB	1:B:483:ILE:HG13	1.89	0.54
1:D:495:LEU:HD23	1:D:515:LEU:HD13	1.90	0.54
2:F:19:VAL:HG23	2:F:20:LEU:HD22	1.88	0.54
3:I:93:VAL:HA	3:I:110:GLN:HA	1.89	0.54
1:A:15:PRO:HB2	1:A:17:TYR:HD1	1.73	0.53
1:A:232:LEU:O	1:A:409:ASN:ND2	2.41	0.53
1:C:321:LEU:O	1:C:325:TYR:N	2.42	0.53
2:E:344:ARG:HE	2:E:344:ARG:HA	1.74	0.53
1:C:547:LYS:HD2	1:C:570:GLN:HG3	1.90	0.53
2:F:24:TRP:CD1	2:F:337:THR:HG1	2.25	0.53
1:C:792:SER:HA	1:C:799:LYS:HD2	1.91	0.53
2:E:309:ASN:N	2:E:309:ASN:OD1	2.41	0.53
2:F:119:ALA:HB2	2:F:293:CYS:HB3	1.91	0.53
1:C:329:VAL:O	1:C:333:GLY:N	2.42	0.53
1:C:540:LEU:HD12	1:C:543:LEU:HD12	1.91	0.53
3:G:47:TRP:HE1	3:G:50:ALA:HB2	1.73	0.53
1:A:489:ALA:HA	1:A:492:ARG:HD2	1.90	0.53
1:D:147:PRO:HA	1:D:150:SER:HB3	1.88	0.53
1:A:102:ASP:OD1	1:A:105:GLN:NE2	2.29	0.53
3:G:20:LEU:HD12	3:G:81:LEU:HD23	1.91	0.53
1:A:636:GLN:HG3	1:A:637:HIS:HD2	1.74	0.53
1:B:705:GLY:O	1:B:708:GLN:NE2	2.42	0.53
1:A:169:THR:HG23	1:A:393:PHE:HE1	1.74	0.53
1:D:658:ILE:HA	1:D:661:LEU:HD13	1.90	0.52
1:B:296:THR:HG23	1:B:307:THR:HG22	1.91	0.52
3:I:60:TYR:HE2	3:I:70:ILE:HG22	1.73	0.52
3:I:98:VAL:HG12	3:I:104:TYR:HB2	1.90	0.52
1:A:19:ILE:HD11	1:A:157:VAL:HG23	1.91	0.52
1:B:39:ALA:HB2	1:B:129:VAL:HG12	1.91	0.52
1:B:412:THR:OG1	1:B:414:ASP:OD1	2.27	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:ILE:HA	1:D:281:TYR:CD1	2.45	0.52
1:D:438:ILE:HG13	1:D:459:VAL:HG21	1.90	0.52
1:C:475:TRP:HA	1:C:499:HIS:HB2	1.92	0.52
1:D:736:LEU:HD13	1:D:738:LEU:HD11	1.91	0.52
2:F:117:GLU:OE1	2:F:118:ARG:NE	2.42	0.52
1:A:296:THR:HG23	1:A:307:THR:HG22	1.90	0.52
1:B:618:GLU:HG3	1:B:643:CYS:HB3	1.92	0.52
1:D:670:ASN:OD1	1:D:670:ASN:N	2.35	0.52
1:D:661:LEU:HB3	1:D:664:LEU:HG	1.91	0.52
1:A:39:ALA:HB2	1:A:129:VAL:HG12	1.92	0.52
1:D:562:VAL:HA	1:D:565:VAL:HG12	1.91	0.52
1:D:278:ILE:HA	1:D:281:TYR:HD1	1.74	0.52
1:D:292:ASP:OD1	1:D:292:ASP:N	2.42	0.52
2:F:134:HIS:CG	2:F:276:ILE:HD11	2.45	0.52
3:H:36:TRP:HD1	3:H:70:ILE:HD12	1.75	0.52
1:C:39:ALA:HB2	1:C:129:VAL:HG12	1.92	0.52
2:E:276:ILE:O	2:E:280:ASN:HB2	2.10	0.52
2:E:285:SER:O	2:E:288:GLN:NE2	2.42	0.52
2:F:16:ALA:HA	2:F:20:LEU:HD23	1.93	0.51
2:F:294:ASN:OD1	2:F:305:ASN:ND2	2.43	0.51
3:H:73:ASP:OD1	3:H:78:THR:OG1	2.26	0.51
1:A:509:PRO:HB2	1:A:512:ILE:HG23	1.92	0.51
1:A:709:ASN:HA	1:A:732:LYS:HD2	1.92	0.51
3:I:67:ARG:NH2	3:I:90:ASP:OD2	2.42	0.51
1:B:570:GLN:HE21	1:B:571:LYS:HB2	1.75	0.51
3:J:53:SER:HA	3:J:72:ARG:HH22	1.76	0.51
1:B:297:VAL:HG23	1:B:299:ILE:HG12	1.91	0.51
1:B:685:ARG:HH21	1:B:706:LEU:HD13	1.73	0.51
1:C:472:LYS:HB3	1:C:496:ARG:HB2	1.91	0.51
1:C:581:LEU:HB3	1:C:601:CYS:HB3	1.93	0.51
1:D:155:HIS:HB3	1:D:250:PHE:HE1	1.75	0.51
1:D:463:PRO:HB3	1:D:486:PRO:HB2	1.92	0.51
1:A:605:ARG:HD2	3:G:54:TYR:CZ	2.45	0.51
1:C:117:ARG:HG2	1:C:295:CYS:HA	1.92	0.51
1:D:478:HIS:CD2	1:D:503:THR:HG23	2.45	0.51
1:D:364:ASP:O	1:D:395:SER:HA	2.10	0.51
2:E:367:LYS:HG3	2:E:368:ASN:H	1.76	0.51
1:B:233:ASP:OD1	1:B:234:LYS:N	2.44	0.51
1:D:721:GLU:HB3	1:D:742:VAL:HG23	1.92	0.51
3:I:15:GLY:N	3:I:86:LEU:O	2.41	0.51
1:D:407:LEU:HD11	1:D:439:PRO:HG3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:593:LEU:HD21	1:D:596:LEU:HB2	1.93	0.51
3:G:3:GLN:HB2	3:G:25:SER:HB2	1.93	0.51
1:B:168:TRP:CZ3	1:B:398:SER:HB2	2.46	0.51
1:B:292:ASP:OD1	1:B:292:ASP:N	2.41	0.51
3:J:47:TRP:HE1	3:J:50:ALA:HB2	1.76	0.51
1:A:449:GLU:HA	1:A:471:LEU:HA	1.93	0.50
1:D:343:MET:HG3	1:D:348:LEU:HD21	1.93	0.50
1:D:777:PRO:HB2	1:D:778:LEU:HD12	1.92	0.50
1:D:373:ALA:O	1:D:377:HIS:ND1	2.27	0.50
2:E:145:TRP:O	2:E:151:SER:OG	2.24	0.50
2:E:280:ASN:HB3	2:E:324:LEU:HD21	1.93	0.50
3:I:61:ALA:O	3:I:65:LYS:N	2.45	0.50
1:C:102:ASP:OD2	1:D:106:TYR:OH	2.24	0.50
1:D:297:VAL:HG23	1:D:299:ILE:HG12	1.93	0.50
1:C:408:ASN:ND2	1:C:440:ASP:H	2.09	0.50
1:D:728:PHE:HB3	1:D:752:GLU:HB2	1.94	0.50
1:A:35:MET:HE2	1:A:133:THR:HG22	1.94	0.50
1:A:800:GLU:HA	1:C:804:ARG:HH21	1.77	0.50
1:D:146:PHE:HD1	1:D:147:PRO:HD2	1.76	0.50
3:H:97:TYR:HE1	3:H:103:GLU:HB3	1.76	0.50
1:B:294:ASP:OD1	1:B:309:ARG:NH1	2.45	0.50
1:D:634:SER:O	1:D:637:HIS:ND1	2.33	0.50
3:H:53:SER:HA	3:H:72:ARG:HH22	1.75	0.50
3:J:28:PRO:HG2	3:J:31:ARG:HB2	1.93	0.50
1:A:135:ILE:HG12	1:A:274:LYS:HZ2	1.77	0.50
1:D:423:ASN:OD1	1:D:427:LYS:N	2.38	0.50
1:C:429:GLU:HG3	1:C:452:LYS:HE3	1.93	0.49
1:D:47:VAL:HG12	1:D:48:THR:HG23	1.94	0.49
1:D:19:ILE:HD11	1:D:157:VAL:HG23	1.94	0.49
1:B:571:LYS:HG3	1:B:595:GLU:HB2	1.93	0.49
1:B:731:ARG:CZ	1:B:752:GLU:HB3	2.41	0.49
1:C:356:ILE:HD12	1:C:388:LYS:HG2	1.95	0.49
1:A:427:LYS:NZ	1:A:473:GLU:OE2	2.33	0.49
1:D:803:TRP:O	1:D:807:LYS:HG2	2.12	0.49
1:B:670:ASN:OD1	1:B:670:ASN:N	2.37	0.49
1:D:102:ASP:N	1:D:105:GLN:OE1	2.36	0.49
1:D:761:LEU:N	1:D:785:VAL:O	2.38	0.49
2:E:52:ILE:HD12	2:E:116:TYR:HA	1.93	0.49
3:I:60:TYR:HB2	3:I:65:LYS:HG3	1.93	0.49
1:A:746:LEU:HD23	1:A:747:PRO:HD2	1.94	0.49
1:B:675:GLU:HG2	1:B:696:ASN:HD22	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:46:GLN:HA	2:F:50:ASP:HB2	1.94	0.49
1:B:450:VAL:HG22	1:B:473:GLU:HB2	1.95	0.49
1:B:520:GLU:OE2	1:B:522:HIS:NE2	2.46	0.49
1:B:780:LYS:HD2	1:B:806:ASP:HA	1.95	0.49
1:D:357:ARG:O	1:D:361:SER:N	2.45	0.49
3:I:94:TYR:HE1	3:I:111:VAL:HB	1.78	0.49
2:E:284:VAL:HG21	2:E:324:LEU:HD11	1.95	0.49
1:A:450:VAL:HG13	1:A:473:GLU:HB2	1.94	0.48
1:B:155:HIS:HB3	1:B:250:PHE:HE1	1.78	0.48
1:B:452:LYS:HE2	1:B:475:TRP:CE2	2.48	0.48
1:C:632:ILE:O	1:C:635:PHE:HB2	2.13	0.48
1:A:629:ILE:HG21	1:A:646:LEU:HD13	1.95	0.48
1:B:714:ALA:HA	1:B:737:HIS:HB2	1.95	0.48
1:B:772:GLU:O	1:B:775:GLU:HG2	2.14	0.48
1:C:131:LEU:O	1:C:135:ILE:HG22	2.13	0.48
1:A:429:GLU:HB2	1:A:450:VAL:HB	1.95	0.48
1:C:688:ARG:HG2	1:C:709:ASN:HB3	1.94	0.48
1:B:364:ASP:OD1	1:B:364:ASP:N	2.47	0.48
1:A:776:CYS:O	1:A:801:ARG:NH2	2.47	0.48
1:C:751:GLY:HA3	1:C:772:GLU:HB3	1.96	0.48
2:F:38:ILE:HG23	2:F:319:LEU:HD11	1.95	0.48
1:A:635:PHE:HD2	1:A:661:LEU:HD21	1.79	0.48
1:B:495:LEU:HD23	1:B:515:LEU:HD13	1.94	0.48
1:C:555:LEU:O	1:C:576:ASN:ND2	2.47	0.48
1:C:566:GLY:HA3	1:C:590:MET:HG2	1.95	0.48
1:A:631:GLU:OE1	1:A:631:GLU:N	2.43	0.48
1:B:560:GLN:NE2	1:B:564:ASP:OD1	2.47	0.48
1:C:513:TYR:OH	1:C:536:VAL:O	2.17	0.48
1:D:737:HIS:HA	1:D:760:GLU:HB3	1.96	0.48
1:A:633:ILE:HD13	1:A:657:GLN:HB3	1.96	0.48
1:A:636:GLN:NE2	3:G:59:GLU:OE1	2.39	0.48
1:C:712:ASN:HA	1:C:735:ALA:HB3	1.96	0.48
1:D:541:ARG:O	1:D:544:LYS:NZ	2.41	0.48
1:D:605:ARG:HD3	3:J:54:TYR:CZ	2.49	0.48
1:C:516:LYS:HG3	1:C:517:THR:HG23	1.96	0.47
1:D:716:THR:O	1:D:718:ASN:ND2	2.47	0.47
1:A:172:ALA:O	1:A:176:THR:N	2.47	0.47
1:B:594:THR:O	1:B:617:GLN:N	2.41	0.47
1:C:417:ARG:CZ	1:C:445:LEU:HD21	2.44	0.47
1:C:582:ILE:HG23	1:C:584:LEU:HG	1.96	0.47
1:D:687:LEU:HD21	1:D:690:LEU:HD13	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:33:PHE:CD2	3:I:52:TYR:HA	2.48	0.47
1:D:250:PHE:CZ	1:D:254:VAL:HG21	2.49	0.47
1:A:249:LYS:NZ	1:B:173:LEU:O	2.40	0.47
1:A:425:GLN:N	1:A:425:GLN:OE1	2.47	0.47
1:B:416:LEU:HD13	1:B:442:VAL:HG12	1.97	0.47
1:D:166:SER:O	1:D:169:THR:OG1	2.33	0.47
1:D:715:VAL:O	1:D:741:ASN:ND2	2.38	0.47
2:E:38:ILE:HG23	2:E:319:LEU:HD11	1.97	0.47
3:J:12:VAL:HG11	3:J:86:LEU:HD22	1.96	0.47
1:A:278:ILE:HA	1:A:281:TYR:CD2	2.49	0.47
1:B:644:LEU:HD21	1:B:646:LEU:HG	1.96	0.47
1:C:495:LEU:O	1:C:496:ARG:NH1	2.43	0.47
1:D:46:GLN:HA	1:D:50:ASP:HB2	1.96	0.47
1:D:716:THR:HG23	1:D:740:ASN:HD22	1.79	0.47
1:D:742:VAL:HA	1:D:765:ARG:HD3	1.96	0.47
1:D:776:CYS:HB2	1:D:779:LEU:HB2	1.96	0.47
2:E:16:ALA:HA	2:E:159:ILE:HG13	1.96	0.47
2:F:263:VAL:HG22	2:F:341:LEU:HD13	1.97	0.47
1:A:710:LEU:HD21	1:A:713:LEU:HB2	1.97	0.47
1:D:296:THR:HG23	1:D:307:THR:HG22	1.96	0.47
1:B:503:THR:OG1	1:B:507:GLU:OE2	2.29	0.47
1:C:154:GLU:HA	1:C:157:VAL:HG12	1.97	0.47
3:I:73:ASP:OD1	3:I:73:ASP:N	2.48	0.47
1:A:408:ASN:HD21	1:A:440:ASP:HB2	1.80	0.47
1:A:726:GLU:HA	1:A:729:GLN:HG2	1.97	0.47
1:C:168:TRP:CH2	1:C:398:SER:HB2	2.46	0.46
1:A:265:MET:HA	1:A:343:MET:HE1	1.96	0.46
1:B:149:THR:HB	1:B:260:VAL:HG22	1.98	0.46
2:E:124:ALA:HB2	2:E:287:VAL:HG12	1.97	0.46
3:H:91:THR:HG23	3:H:112:THR:HA	1.97	0.46
2:F:124:ALA:HB2	2:F:287:VAL:HG12	1.96	0.46
2:F:280:ASN:HB3	2:F:324:LEU:HD21	1.96	0.46
3:I:5:VAL:HG23	3:I:23:ALA:HB3	1.97	0.46
1:D:258:ASP:N	1:D:371:ASP:HB2	2.24	0.46
3:G:4:LEU:HD11	3:G:98:VAL:HG12	1.97	0.46
3:H:91:THR:HG23	3:H:112:THR:HG22	1.98	0.46
1:B:166:SER:HB3	1:B:169:THR:HG23	1.97	0.46
1:B:590:MET:HE3	1:B:593:LEU:HD22	1.98	0.46
1:B:463:PRO:HD3	1:B:484:GLU:CD	2.41	0.46
1:C:713:LEU:HB3	1:C:736:LEU:HD23	1.98	0.46
3:H:38:ARG:NE	3:H:46:GLU:OE1	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:MET:HA	1:C:343:MET:HE1	1.96	0.46
1:C:292:ASP:OD1	1:C:292:ASP:N	2.49	0.46
1:C:513:TYR:CG	1:C:539:GLY:HA3	2.51	0.46
1:B:258:ASP:OD2	1:B:349:LYS:NZ	2.35	0.46
1:B:423:ASN:HD21	1:B:427:LYS:HB2	1.80	0.46
1:B:350:LYS:HE3	1:B:350:LYS:HB3	1.81	0.46
1:B:739:GLY:O	1:B:741:ASN:ND2	2.48	0.46
1:D:155:HIS:HB3	1:D:250:PHE:CE1	2.51	0.46
1:D:454:GLU:HG2	1:D:455:LEU:HG	1.98	0.46
1:D:723:LEU:HD21	1:D:743:LEU:HD11	1.96	0.46
1:D:779:LEU:HG	1:D:802:LEU:HD21	1.98	0.46
1:C:61:THR:O	1:C:64:SER:OG	2.24	0.46
1:C:500:ILE:HG22	1:C:502:PHE:HD1	1.81	0.46
2:E:45:LEU:HD23	2:E:45:LEU:HA	1.75	0.46
3:I:4:LEU:HD11	3:I:98:VAL:HG12	1.96	0.46
1:B:687:LEU:HD21	1:B:690:LEU:HD13	1.97	0.45
1:C:447:GLU:OE1	1:C:447:GLU:N	2.45	0.45
2:F:46:GLN:NE2	2:F:125:LYS:O	2.49	0.45
1:C:297:VAL:HG23	1:C:299:ILE:HG12	1.98	0.45
3:I:2:VAL:HG13	3:I:27:PHE:CD1	2.51	0.45
1:D:413:LEU:H	1:D:413:LEU:HD12	1.81	0.45
3:J:4:LEU:HD11	3:J:98:VAL:HG12	1.98	0.45
3:J:36:TRP:HD1	3:J:70:ILE:HD12	1.81	0.45
1:A:45:LEU:HD12	1:A:45:LEU:HA	1.77	0.45
1:A:274:LYS:HE2	1:A:274:LYS:HB3	1.77	0.45
1:B:152:LYS:NZ	1:B:257:GLY:HA3	2.32	0.45
1:A:234:LYS:O	1:A:238:GLU:HG2	2.17	0.45
1:B:346:ARG:HG2	1:B:348:LEU:HB3	1.99	0.45
1:C:159:ILE:O	1:C:162:LYS:HG2	2.17	0.45
3:J:61:ALA:HB3	3:J:64:VAL:HG22	1.98	0.45
1:A:117:ARG:HB2	1:A:295:CYS:HB3	1.99	0.45
1:A:738:LEU:O	1:A:764:ASN:ND2	2.47	0.45
1:A:738:LEU:HB2	1:A:761:LEU:HD23	1.97	0.45
1:B:601:CYS:HB2	1:B:624:ASN:HD21	1.82	0.45
1:C:295:CYS:HB2	1:C:297:VAL:HG13	1.98	0.45
2:E:19:VAL:HG23	2:E:20:LEU:HD22	1.99	0.45
2:F:143:ASN:O	2:F:147:LYS:HG2	2.17	0.45
1:B:499:HIS:HA	1:B:522:HIS:HB2	1.99	0.45
1:C:166:SER:HB3	1:C:169:THR:HG23	1.98	0.45
1:B:578:GLY:N	1:B:600:ARG:HB3	2.32	0.45
1:A:233:ASP:O	1:A:236:GLU:HG3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:272:LYS:HB3	2:E:272:LYS:HE2	1.82	0.44
3:H:48:VAL:HG12	3:H:64:VAL:HG21	1.99	0.44
3:J:23:ALA:HA	3:J:78:THR:HG22	1.98	0.44
1:A:385:LEU:HA	1:A:388:LYS:HE3	1.98	0.44
1:C:654:ILE:HD11	1:C:674:ILE:HD13	1.99	0.44
1:D:400:ASN:HA	1:D:403:ARG:HH21	1.82	0.44
1:D:576:ASN:HB2	1:D:601:CYS:HA	1.99	0.44
1:A:23:TRP:HA	2:F:149:PRO:HG2	1.99	0.44
1:A:270:ILE:O	1:A:273:ILE:HG13	2.17	0.44
1:B:761:LEU:HB2	1:B:786:VAL:HG23	1.99	0.44
2:E:46:GLN:HE21	2:E:46:GLN:HB2	1.54	0.44
3:H:9:GLY:HA3	3:H:109:THR:HB	1.98	0.44
1:C:478:HIS:CE1	1:C:501:LYS:HG2	2.53	0.44
1:D:616:LEU:HB3	1:D:638:LEU:HD21	2.00	0.44
3:G:73:ASP:OD1	3:G:73:ASP:N	2.48	0.44
1:B:322:ALA:O	1:B:326:ILE:HG23	2.18	0.44
1:B:631:GLU:OE1	1:B:631:GLU:N	2.46	0.44
2:E:127:PHE:HE2	2:E:319:LEU:HD12	1.83	0.44
1:C:452:LYS:HE2	1:C:475:TRP:CE2	2.52	0.44
1:D:273:ILE:HG13	1:D:274:LYS:N	2.32	0.44
3:J:33:PHE:O	3:J:98:VAL:HG23	2.17	0.44
1:A:243:LEU:HB3	1:A:393:PHE:CE2	2.52	0.44
1:A:356:ILE:HD12	1:A:388:LYS:HG2	2.00	0.44
1:C:637:HIS:NE2	3:I:59:GLU:OE1	2.50	0.44
1:D:274:LYS:HB3	1:D:274:LYS:HE2	1.77	0.44
1:D:651:ILE:O	1:D:672:ASN:HB3	2.18	0.44
2:E:248:PHE:CZ	2:E:252:VAL:HG21	2.53	0.44
1:A:354:GLU:O	1:A:358:GLU:HB2	2.17	0.44
1:C:534:TYR:HE1	1:C:555:LEU:HD22	1.82	0.44
1:C:623:ASP:OD2	1:D:545:ARG:NH1	2.51	0.44
3:H:52:TYR:CG	3:H:57:TYR:HB2	2.53	0.44
1:A:451:LEU:HB3	1:A:474:LEU:HD12	1.99	0.43
1:A:583:VAL:HG23	1:A:584:LEU:H	1.82	0.43
1:C:129:VAL:HG13	1:C:325:TYR:CE1	2.53	0.43
1:D:173:LEU:HD13	1:D:173:LEU:HA	1.90	0.43
1:B:270:ILE:O	1:B:273:ILE:HG13	2.18	0.43
1:B:354:GLU:OE1	1:B:354:GLU:N	2.50	0.43
1:B:693:SER:HA	1:B:718:ASN:HD21	1.83	0.43
1:C:636:GLN:HE22	3:I:47:TRP:HH2	1.67	0.43
1:D:129:VAL:HG13	1:D:325:TYR:CE1	2.53	0.43
1:D:509:PRO:HB2	1:D:512:ILE:HG23	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:ASN:HA	1:A:686:LYS:HD2	1.99	0.43
1:B:250:PHE:CZ	1:B:254:VAL:HG21	2.52	0.43
1:D:537:ILE:HG13	1:D:561:VAL:HG11	1.99	0.43
1:D:714:ALA:HA	1:D:737:HIS:HB2	2.01	0.43
1:A:767:GLU:OE2	1:B:732:LYS:NZ	2.46	0.43
1:D:448:LEU:HD21	1:D:451:LEU:HD13	1.99	0.43
2:E:126:TYR:OH	2:F:318:LYS:HG3	2.18	0.43
3:H:33:PHE:CD2	3:H:52:TYR:HA	2.53	0.43
1:A:251:ARG:HD2	1:A:394:LEU:HD11	2.01	0.43
1:B:797:GLU:H	1:B:797:GLU:HG3	1.62	0.43
1:C:614:HIS:O	1:C:640:ARG:NH2	2.42	0.43
1:D:35:MET:HE2	1:D:133:THR:HG22	2.00	0.43
1:D:47:VAL:HG22	2:E:45:LEU:HD21	2.00	0.43
1:D:693:SER:HA	1:D:718:ASN:HD21	1.83	0.43
1:B:348:LEU:HD12	1:B:374:PHE:HA	2.00	0.43
1:B:502:PHE:CZ	1:B:508:ILE:HD11	2.54	0.43
1:C:772:GLU:O	1:C:775:GLU:HG2	2.18	0.43
1:D:700:LEU:HD12	1:D:724:PRO:HD2	2.00	0.43
2:F:53:ILE:HB	2:F:309:ASN:HD21	1.84	0.43
3:J:73:ASP:OD1	3:J:73:ASP:N	2.51	0.43
3:J:91:THR:HG23	3:J:112:THR:HA	2.00	0.43
1:A:171:ARG:HD2	1:A:232:LEU:HD21	1.99	0.43
1:A:412:THR:OG1	1:A:414:ASP:OD1	2.27	0.43
1:B:807:LYS:HD3	1:B:807:LYS:HA	1.88	0.43
3:G:91:THR:HG23	3:G:112:THR:HG22	2.01	0.43
3:H:38:ARG:NH1	3:H:90:ASP:HA	2.34	0.43
1:C:15:PRO:HB2	1:C:16:ALA:H	1.69	0.43
1:A:250:PHE:CZ	1:A:254:VAL:HG21	2.53	0.43
1:A:612:SER:O	1:A:614:HIS:ND1	2.39	0.43
1:B:129:VAL:HG13	1:B:325:TYR:CE1	2.54	0.43
1:B:746:LEU:HD23	1:B:747:PRO:HD2	2.01	0.43
1:C:711:GLN:O	1:C:734:ARG:N	2.52	0.43
1:D:633:ILE:HD13	1:D:657:GLN:HB3	2.01	0.43
1:A:316:THR:O	1:A:320:ILE:HG12	2.19	0.42
1:B:154:GLU:HA	1:B:157:VAL:HG12	2.01	0.42
1:B:249:LYS:HD3	1:B:249:LYS:HA	1.88	0.42
1:C:760:GLU:HA	1:C:785:VAL:HB	2.01	0.42
1:D:346:ARG:HG3	1:D:348:LEU:HB3	2.01	0.42
1:D:555:LEU:H	1:D:576:ASN:HD22	1.67	0.42
1:A:416:LEU:HD13	1:A:445:LEU:HD11	2.01	0.42
1:B:168:TRP:NE1	1:B:402:LEU:HD23	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:731:ARG:HA	1:B:731:ARG:HD3	1.86	0.42
1:D:376:LEU:HD23	1:D:376:LEU:HA	1.86	0.42
1:B:173:LEU:HD21	1:B:392:VAL:HG21	2.00	0.42
1:A:647:TRP:H	1:A:647:TRP:CD1	2.36	0.42
1:C:152:LYS:NZ	1:C:257:GLY:HA3	2.35	0.42
1:D:154:GLU:HA	1:D:157:VAL:HG12	2.01	0.42
1:D:419:ARG:HH12	1:D:432:LEU:HD23	1.85	0.42
3:I:85:SER:O	3:I:87:LYS:NZ	2.52	0.42
3:H:73:ASP:OD1	3:H:73:ASP:N	2.52	0.42
1:A:443:PHE:CE1	1:A:465:ILE:HG22	2.55	0.42
1:B:52:MET:HE2	1:B:310:CYS:HB2	2.02	0.42
1:B:447:GLU:OE1	1:B:447:GLU:N	2.37	0.42
3:G:23:ALA:HA	3:G:78:THR:HG22	2.02	0.42
1:B:17:TYR:HA	1:B:20:LEU:HD23	2.02	0.42
1:B:166:SER:O	1:B:169:THR:OG1	2.30	0.42
1:B:505:ILE:HD12	1:B:536:VAL:HG11	2.00	0.42
1:B:607:PRO:HG2	1:B:610:ILE:HG13	2.02	0.42
3:I:10:GLY:O	3:I:111:VAL:HA	2.19	0.42
3:J:35:TYR:O	3:J:96:CYS:HA	2.20	0.42
1:A:700:LEU:HD23	1:A:700:LEU:HA	1.94	0.42
1:B:492:ARG:O	1:B:517:THR:OG1	2.34	0.42
1:C:19:ILE:HG22	1:C:382:TYR:CE2	2.54	0.42
1:C:656:ILE:HB	1:C:680:GLN:HB2	2.01	0.42
1:D:504:ASP:OD1	1:D:505:ILE:N	2.52	0.42
1:D:769:LEU:HD12	1:D:791:PHE:HA	2.02	0.42
3:J:27:PHE:CZ	3:J:98:VAL:HG21	2.54	0.42
3:J:30:GLY:HA2	3:J:72:ARG:CZ	2.50	0.42
1:B:593:LEU:HD21	1:B:596:LEU:HB2	2.01	0.42
1:D:131:LEU:O	1:D:135:ILE:HG22	2.20	0.42
1:D:502:PHE:CZ	1:D:508:ILE:HD11	2.55	0.42
1:B:502:PHE:HB2	1:B:507:GLU:HB2	2.02	0.42
1:C:149:THR:HG21	1:C:263:LEU:HD12	2.02	0.42
1:C:278:ILE:HA	1:C:281:TYR:CD1	2.55	0.42
1:A:168:TRP:HH2	1:A:398:SER:HB2	1.85	0.41
1:C:117:ARG:HB2	1:C:295:CYS:HB3	2.01	0.41
1:C:294:ASP:OD1	1:C:309:ARG:NH1	2.53	0.41
1:C:724:PRO:HG2	1:C:727:LEU:HB2	2.02	0.41
1:D:716:THR:HG23	1:D:740:ASN:HB2	2.02	0.41
1:A:791:PHE:CD1	1:A:794:LEU:HD12	2.54	0.41
1:B:542:GLU:N	1:B:542:GLU:OE1	2.54	0.41
1:C:411:TRP:HZ3	1:C:415:LYS:HZ3	1.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:588:LYS:HB2	1:C:612:SER:HB3	2.01	0.41
1:D:416:LEU:HD13	1:D:442:VAL:HA	2.01	0.41
1:B:572:LEU:HD21	1:B:574:ILE:HD11	2.02	0.41
1:B:578:GLY:H	1:B:600:ARG:HB3	1.85	0.41
1:C:274:LYS:HB3	1:C:274:LYS:HE2	1.83	0.41
1:D:529:ALA:O	1:D:533:ARG:HB3	2.21	0.41
1:B:427:LYS:HB3	1:B:449:GLU:HG2	2.02	0.41
1:C:503:THR:N	1:C:507:GLU:OE1	2.49	0.41
1:C:552:LYS:HA	1:C:575:ASN:O	2.20	0.41
1:C:559:PRO:HB2	1:C:562:VAL:HG23	2.03	0.41
1:C:776:CYS:HB2	1:C:779:LEU:HB2	2.02	0.41
1:D:348:LEU:HD12	1:D:374:PHE:HA	2.02	0.41
3:H:86:LEU:HB3	3:H:113:VAL:HG21	2.02	0.41
1:A:292:ASP:OD1	1:A:292:ASP:N	2.53	0.41
2:E:368:ASN:OD1	2:E:368:ASN:N	2.52	0.41
2:F:315:LEU:O	2:F:319:LEU:N	2.53	0.41
2:F:323:TYR:O	2:F:327:VAL:HG23	2.21	0.41
3:H:60:TYR:HB2	3:H:65:LYS:HD2	2.01	0.41
1:A:687:LEU:HD12	1:A:687:LEU:HA	1.78	0.41
1:D:143:TRP:CD1	1:D:143:TRP:H	2.38	0.41
1:D:351:TYR:HD1	1:D:377:HIS:CE1	2.39	0.41
1:D:418:GLN:HE21	1:D:418:GLN:HB3	1.55	0.41
1:A:61:THR:HB	1:A:62:LYS:HE2	2.02	0.41
1:A:622:LYS:HB2	1:A:647:TRP:HE1	1.86	0.41
1:C:663:ASN:OD1	1:C:686:LYS:NZ	2.53	0.41
1:D:540:LEU:HD23	1:D:540:LEU:HA	1.93	0.41
1:D:570:GLN:OE1	1:D:594:THR:OG1	2.37	0.41
3:H:37:TYR:CZ	3:H:47:TRP:HB2	2.55	0.41
1:A:511:TRP:O	1:A:514:SER:OG	2.24	0.41
1:A:791:PHE:CE2	1:A:799:LYS:HE3	2.55	0.41
1:B:422:LYS:HA	1:B:427:LYS:O	2.21	0.41
1:C:105:GLN:NE2	1:C:302:LEU:O	2.54	0.41
1:C:106:TYR:HA	1:C:109:VAL:HG12	2.03	0.41
1:C:657:GLN:OE1	1:C:657:GLN:N	2.46	0.41
2:F:104:ASP:OD1	2:F:107:GLN:NE2	2.54	0.41
1:A:56:PRO:HG2	1:A:99:TYR:CD1	2.56	0.41
1:B:152:LYS:HZ3	1:B:257:GLY:HA3	1.85	0.41
1:B:370:ASN:OD1	1:B:370:ASN:N	2.54	0.41
1:B:480:ALA:HB2	1:B:507:GLU:HA	2.03	0.41
1:C:505:ILE:HD11	1:C:527:LEU:HA	2.02	0.41
1:C:605:ARG:HD2	3:I:54:TYR:CE1	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:558:LEU:HD12	1:D:559:PRO:HD2	2.03	0.41
2:E:272:LYS:O	2:E:276:ILE:HG12	2.20	0.41
2:F:134:HIS:CD2	2:F:276:ILE:HD11	2.56	0.41
2:F:309:ASN:HD22	2:F:309:ASN:N	2.19	0.41
3:H:39:GLN:OE1	3:H:45:ARG:NH2	2.54	0.41
3:J:37:TYR:HB3	3:J:45:ARG:HG2	2.02	0.41
1:A:558:LEU:HD22	1:A:583:VAL:HG12	2.03	0.41
1:C:666:ARG:HA	1:C:689:TYR:HB2	2.02	0.41
1:D:521:LEU:HD23	1:D:540:LEU:HD21	2.03	0.41
1:D:583:VAL:O	1:D:586:SER:OG	2.27	0.41
2:E:19:VAL:HG12	2:E:380:TYR:CE2	2.56	0.41
3:G:97:TYR:HE1	3:G:103:GLU:HB3	1.84	0.41
1:A:476:LEU:HB2	1:A:500:ILE:HD13	2.03	0.40
1:B:537:ILE:HG13	1:B:561:VAL:HG11	2.03	0.40
1:B:646:LEU:O	1:B:649:ASN:ND2	2.47	0.40
3:H:4:LEU:HD11	3:H:98:VAL:HG12	2.03	0.40
1:B:693:SER:O	1:B:695:ASN:ND2	2.54	0.40
1:C:35:MET:HE3	1:C:325:TYR:HE1	1.85	0.40
1:D:247:VAL:HG21	1:D:393:PHE:HD2	1.86	0.40
2:E:246:LYS:HE2	2:E:246:LYS:HB3	1.92	0.40
1:A:443:PHE:HA	1:A:468:LEU:HD11	2.03	0.40
1:A:566:GLY:HA3	1:A:590:MET:HG2	2.03	0.40
1:B:48:THR:HA	1:C:49:GLN:OE1	2.21	0.40
1:B:56:PRO:HG2	1:B:99:TYR:CD1	2.57	0.40
1:B:423:ASN:OD1	1:B:427:LYS:N	2.42	0.40
1:C:502:PHE:CZ	1:C:508:ILE:HD11	2.57	0.40
1:C:521:LEU:HD23	1:C:549:LEU:HD13	2.03	0.40
1:D:749:ARG:NH2	1:D:752:GLU:OE1	2.53	0.40
1:C:164:PHE:CD1	1:C:389:ARG:HG3	2.56	0.40
1:D:375:MET:O	1:D:379:ILE:HG12	2.22	0.40
1:A:117:ARG:CB	1:A:295:CYS:HB3	2.51	0.40
1:B:104:HIS:NE2	1:C:110:ASP:OD2	2.53	0.40
1:B:643:CYS:SG	1:B:666:ARG:NH2	2.92	0.40
1:C:357:ARG:HB3	1:C:365:ILE:HD12	2.04	0.40
1:C:476:LEU:HB2	1:C:500:ILE:HD13	2.03	0.40
1:C:791:PHE:CE2	1:C:799:LYS:HE3	2.57	0.40
2:E:136:LEU:HD23	2:E:136:LEU:HA	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	682 (96%)	30 (4%)	0	100	100
1	B	726/817 (89%)	699 (96%)	27 (4%)	0	100	100
1	C	712/817 (87%)	684 (96%)	28 (4%)	0	100	100
1	D	726/817 (89%)	698 (96%)	28 (4%)	0	100	100
2	E	246/811 (30%)	238 (97%)	8 (3%)	0	100	100
2	F	189/811 (23%)	185 (98%)	4 (2%)	0	100	100
3	G	112/118 (95%)	111 (99%)	1 (1%)	0	100	100
3	H	112/118 (95%)	109 (97%)	3 (3%)	0	100	100
3	I	112/118 (95%)	110 (98%)	2 (2%)	0	100	100
3	J	112/118 (95%)	109 (97%)	3 (3%)	0	100	100
All	All	3759/5362 (70%)	3625 (96%)	134 (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%)	632 (95%)	34 (5%)	21	46
1	B	678/756 (90%)	651 (96%)	27 (4%)	28	52
1	C	666/756 (88%)	639 (96%)	27 (4%)	27	51
1	D	678/756 (90%)	650 (96%)	28 (4%)	27	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	236/755 (31%)	212 (90%)	24 (10%)	7	27
2	F	180/755 (24%)	167 (93%)	13 (7%)	13	39
3	G	92/94 (98%)	91 (99%)	1 (1%)	65	73
3	H	92/94 (98%)	87 (95%)	5 (5%)	20	45
3	I	92/94 (98%)	90 (98%)	2 (2%)	45	63
3	J	92/94 (98%)	90 (98%)	2 (2%)	45	63
All	All	3472/4910 (71%)	3309 (95%)	163 (5%)	25	48

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	29	ASP
1	A	33	ILE
1	A	104	HIS
1	A	154	GLU
1	A	161	LEU
1	A	169	THR
1	A	170	THR
1	A	231	VAL
1	A	236	GLU
1	A	293	VAL
1	A	295	CYS
1	A	299	ILE
1	A	330	ILE
1	A	344	LEU
1	A	353	PHE
1	A	356	ILE
1	A	410	GLU
1	A	416	LEU
1	A	429	GLU
1	A	445	LEU
1	A	527	LEU
1	A	545	ARG
1	A	563	THR
1	A	583	VAL
1	A	594	THR
1	A	647	TRP
1	A	670	ASN
1	A	687	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	716	THR
1	A	746	LEU
1	A	750	VAL
1	A	757	THR
1	A	775	GLU
1	B	60	VAL
1	B	104	HIS
1	B	161	LEU
1	B	170	THR
1	B	224	VAL
1	B	279	ILE
1	B	292	ASP
1	B	294	ASP
1	B	317	LEU
1	B	348	LEU
1	B	356	ILE
1	B	364	ASP
1	B	368	VAL
1	B	392	VAL
1	B	401	LYS
1	B	459	VAL
1	B	536	VAL
1	B	570	GLN
1	B	584	LEU
1	B	602	ASP
1	B	618	GLU
1	B	647	TRP
1	B	670	ASN
1	B	698	THR
1	B	721	GLU
1	B	727	LEU
1	B	793	THR
1	C	45	LEU
1	C	102	ASP
1	C	170	THR
1	C	254	VAL
1	C	275	PHE
1	C	279	ILE
1	C	294	ASP
1	C	317	LEU
1	C	348	LEU
1	C	353	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	356	ILE
1	C	405	LEU
1	C	410	GLU
1	C	415	LYS
1	C	416	LEU
1	C	417	ARG
1	C	429	GLU
1	C	441	THR
1	C	460	THR
1	C	468	LEU
1	C	583	VAL
1	C	635	PHE
1	C	647	TRP
1	C	679	THR
1	C	681	LEU
1	C	696	ASN
1	C	730	CYS
1	D	31	ILE
1	D	33	ILE
1	D	36	LEU
1	D	47	VAL
1	D	104	HIS
1	D	155	HIS
1	D	161	LEU
1	D	173	LEU
1	D	259	ILE
1	D	279	ILE
1	D	281	TYR
1	D	344	LEU
1	D	353	PHE
1	D	356	ILE
1	D	367	ASP
1	D	368	VAL
1	D	402	LEU
1	D	412	THR
1	D	418	GLN
1	D	442	VAL
1	D	527	LEU
1	D	553	SER
1	D	561	VAL
1	D	584	LEU
1	D	587	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	619	ILE
1	D	654	ILE
1	D	670	ASN
2	E	20	LEU
2	E	38	ILE
2	E	46	GLN
2	E	104	ASP
2	E	132	LEU
2	E	138	PHE
2	E	145	TRP
2	E	162	LEU
2	E	249	ARG
2	E	256	ASP
2	E	257	ILE
2	E	268	LEU
2	E	276	ILE
2	E	279	TYR
2	E	280	ASN
2	E	293	CYS
2	E	294	ASN
2	E	309	ASN
2	E	319	LEU
2	E	344	ARG
2	E	367	LYS
2	E	368	ASN
2	E	383	LEU
2	E	392	LEU
2	F	38	ILE
2	F	51	LYS
2	F	103	LEU
2	F	104	ASP
2	F	138	PHE
2	F	156	GLU
2	F	276	ILE
2	F	309	ASN
2	F	311	THR
2	F	315	LEU
2	F	319	LEU
2	F	333	THR
2	F	334	CYS
3	G	12	VAL
3	H	5	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	46	GLU
3	H	48	VAL
3	H	74	ASN
3	H	100	VAL
3	I	60	TYR
3	I	78	THR
3	J	5	VAL
3	J	100	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	406	ASN
1	A	467	GLN
1	A	568	HIS
1	A	592	ASN
1	A	709	ASN
1	B	105	GLN
1	B	406	ASN
1	B	494	ASN
1	B	570	GLN
1	B	592	ASN
1	B	624	ASN
1	B	639	HIS
1	B	696	ASN
1	B	718	ASN
1	B	741	ASN
1	C	105	GLN
1	C	408	ASN
1	C	494	ASN
1	C	709	ASN
1	C	712	ASN
1	D	267	GLN
1	D	418	GLN
1	D	467	GLN
1	D	499	HIS
1	D	526	ASN
1	D	532	ASN
1	D	592	ASN
1	D	615	ASN
1	D	624	ASN
1	D	650	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	718	ASN
1	D	740	ASN
2	E	46	GLN
2	E	375	HIS
2	E	379	GLN
2	F	49	GLN
2	F	305	ASN
3	H	82	GLN
3	H	110	GLN
3	I	82	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.

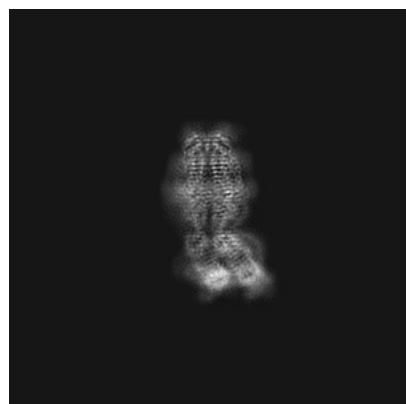
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15836. These allow visual inspection of the internal detail of the map and identification of artifacts.

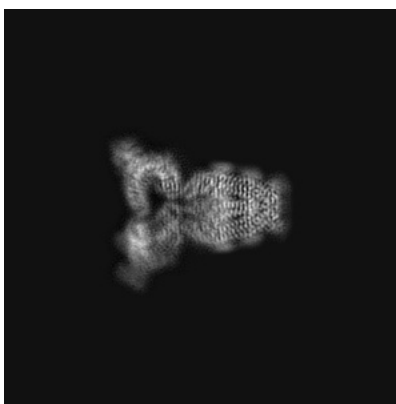
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

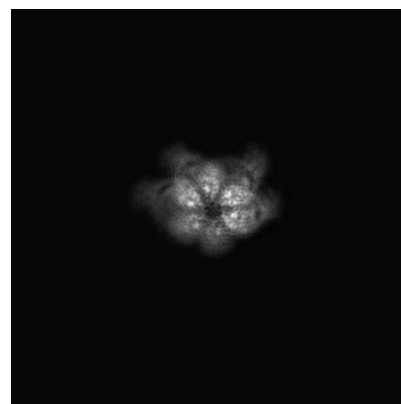
6.1.1 Primary map



X

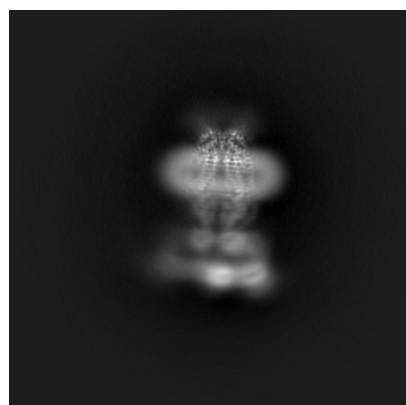


Y

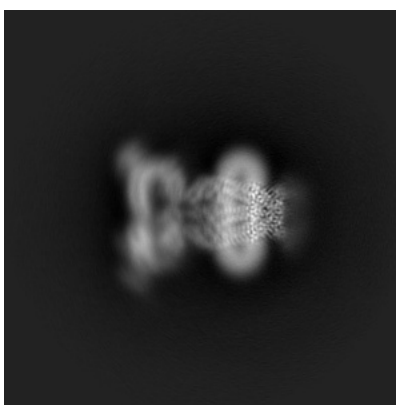


Z

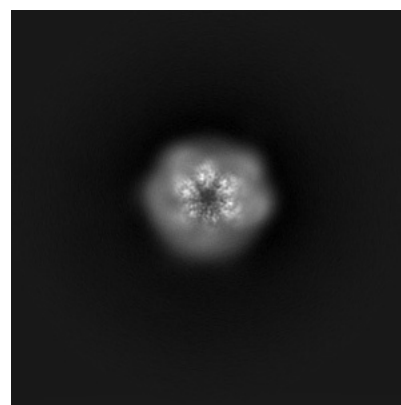
6.1.2 Raw map



X



Y

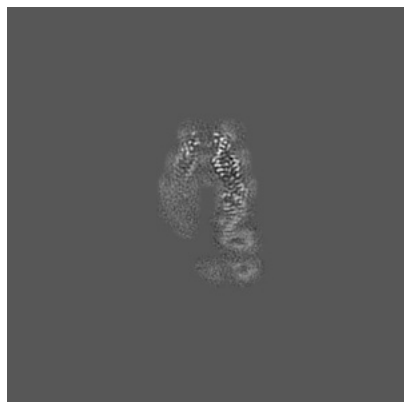


Z

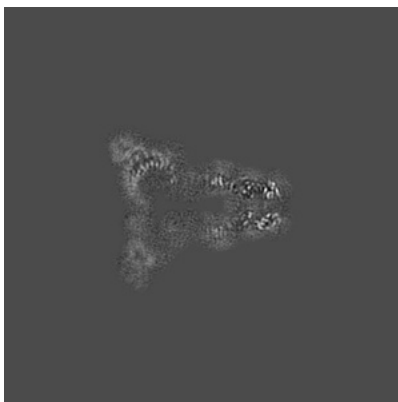
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

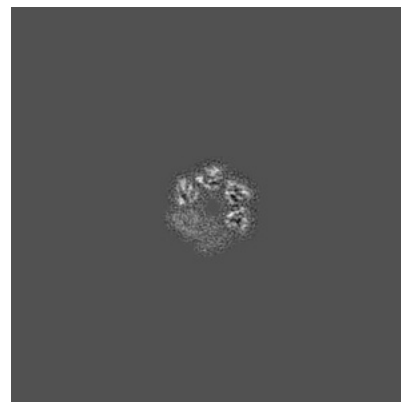
6.2.1 Primary map



X Index: 168



Y Index: 168

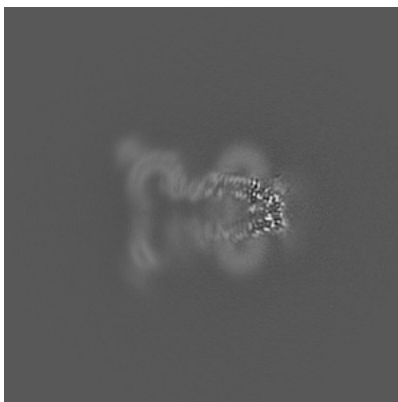


Z Index: 168

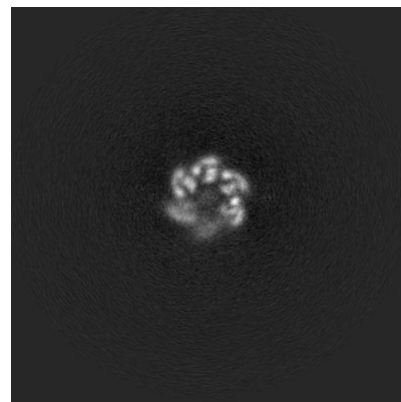
6.2.2 Raw map



X Index: 168



Y Index: 168

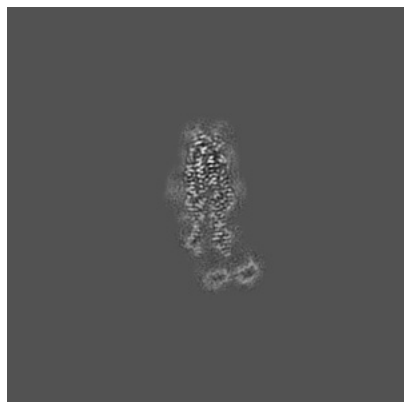


Z Index: 168

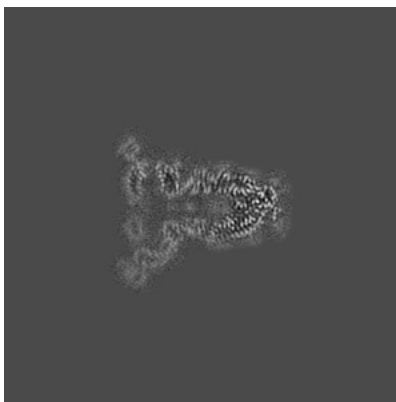
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

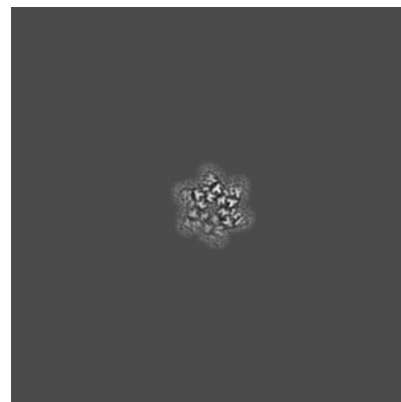
6.3.1 Primary map



X Index: 185

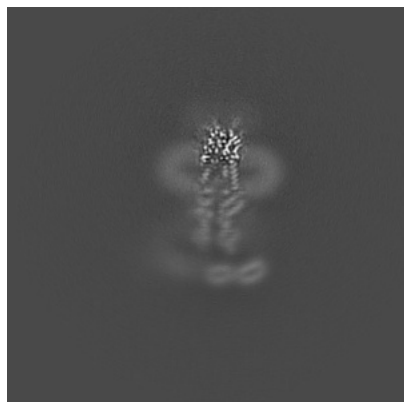


Y Index: 179

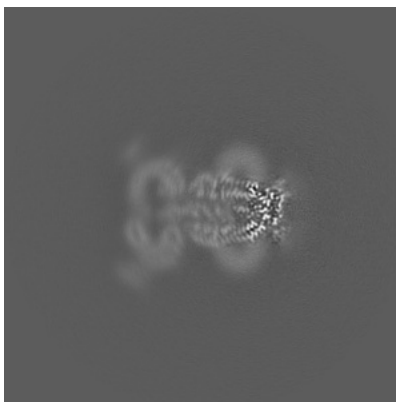


Z Index: 206

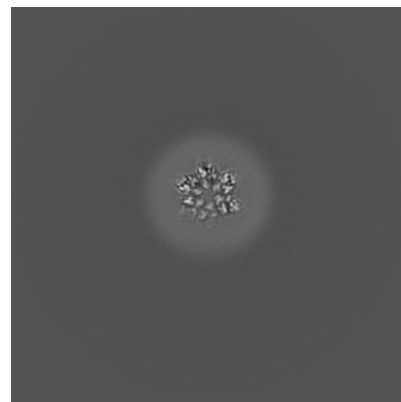
6.3.2 Raw map



X Index: 179



Y Index: 190

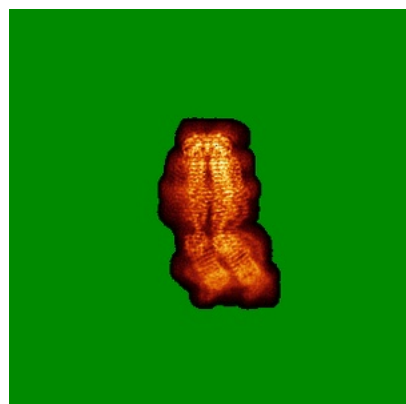


Z Index: 209

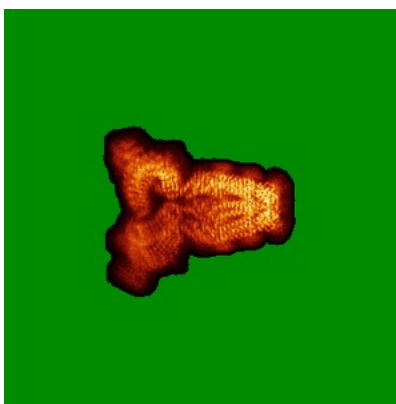
The images above show the largest variance slices of the map in three orthogonal directions.

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

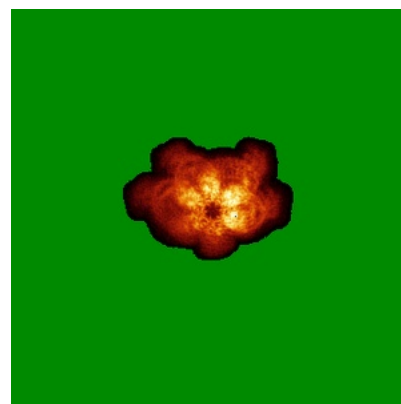
6.4.1 Primary map



X

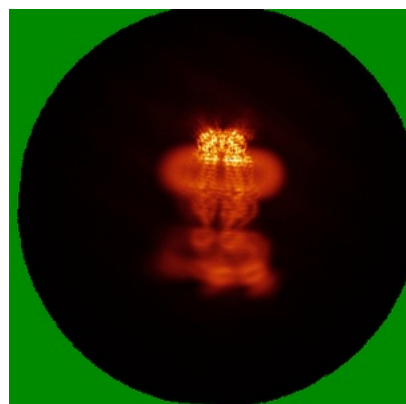


Y

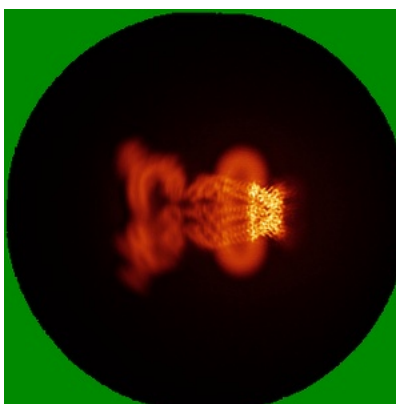


Z

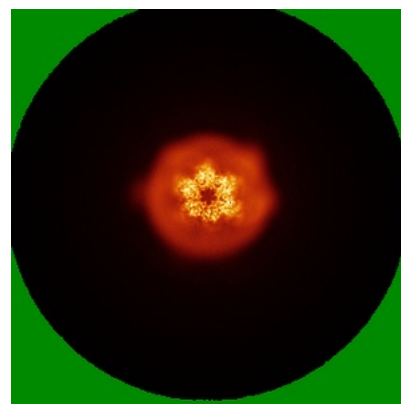
6.4.2 Raw map



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](#)

This section was not generated.

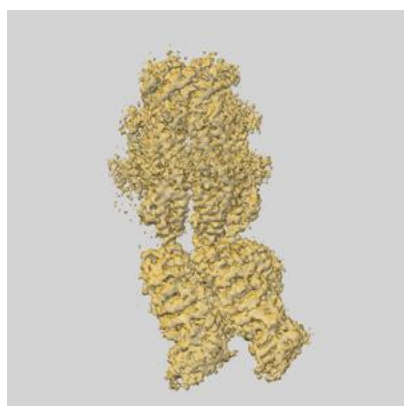
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

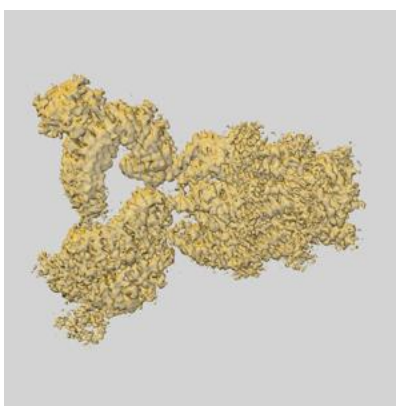
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

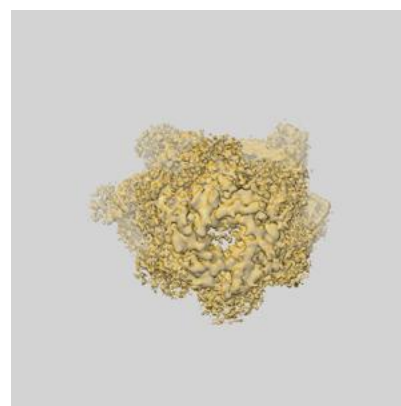
6.6.1 emd_15836_msk_1.map [i](#)



X



Y

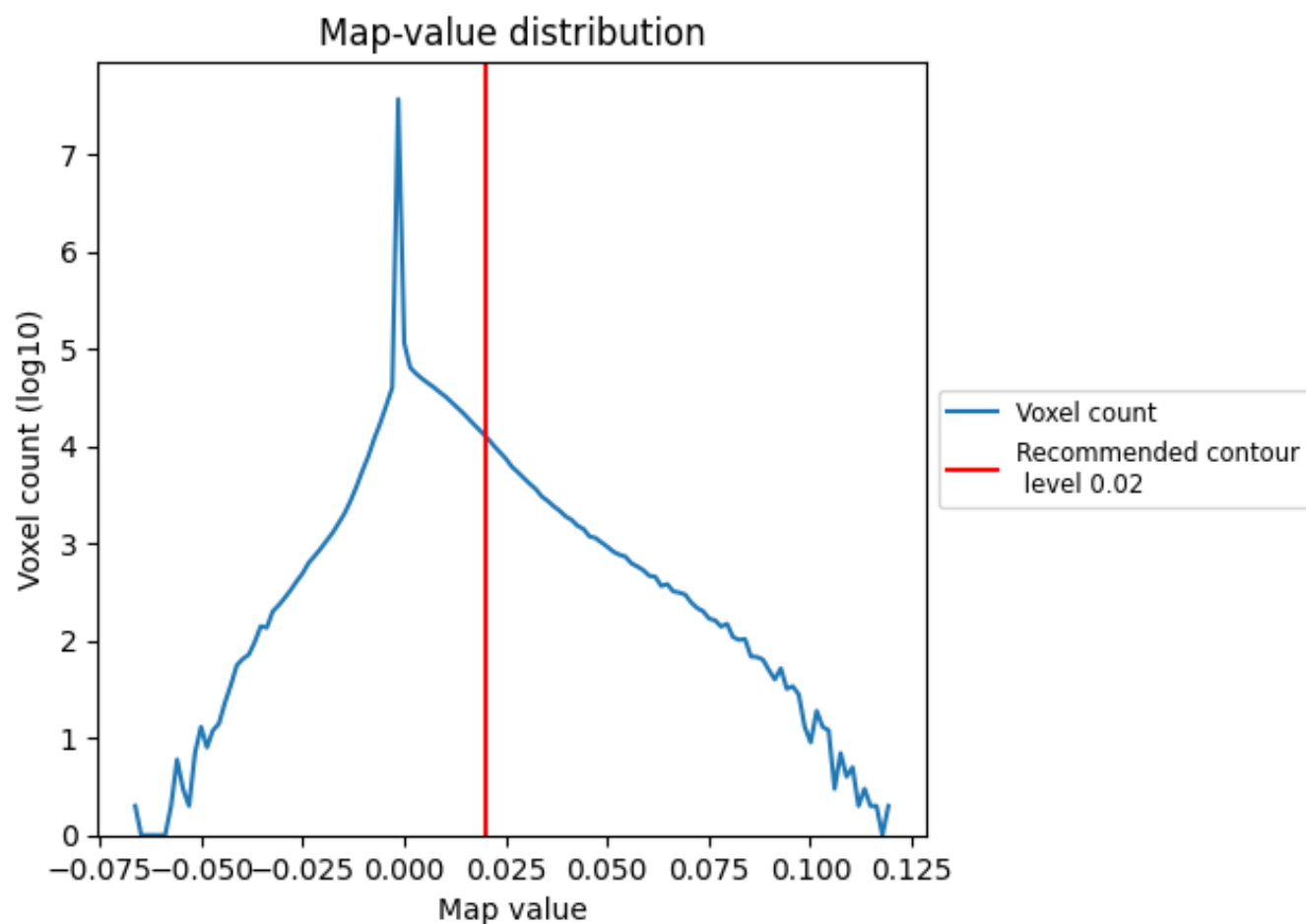


Z

7 Map analysis [i](#)

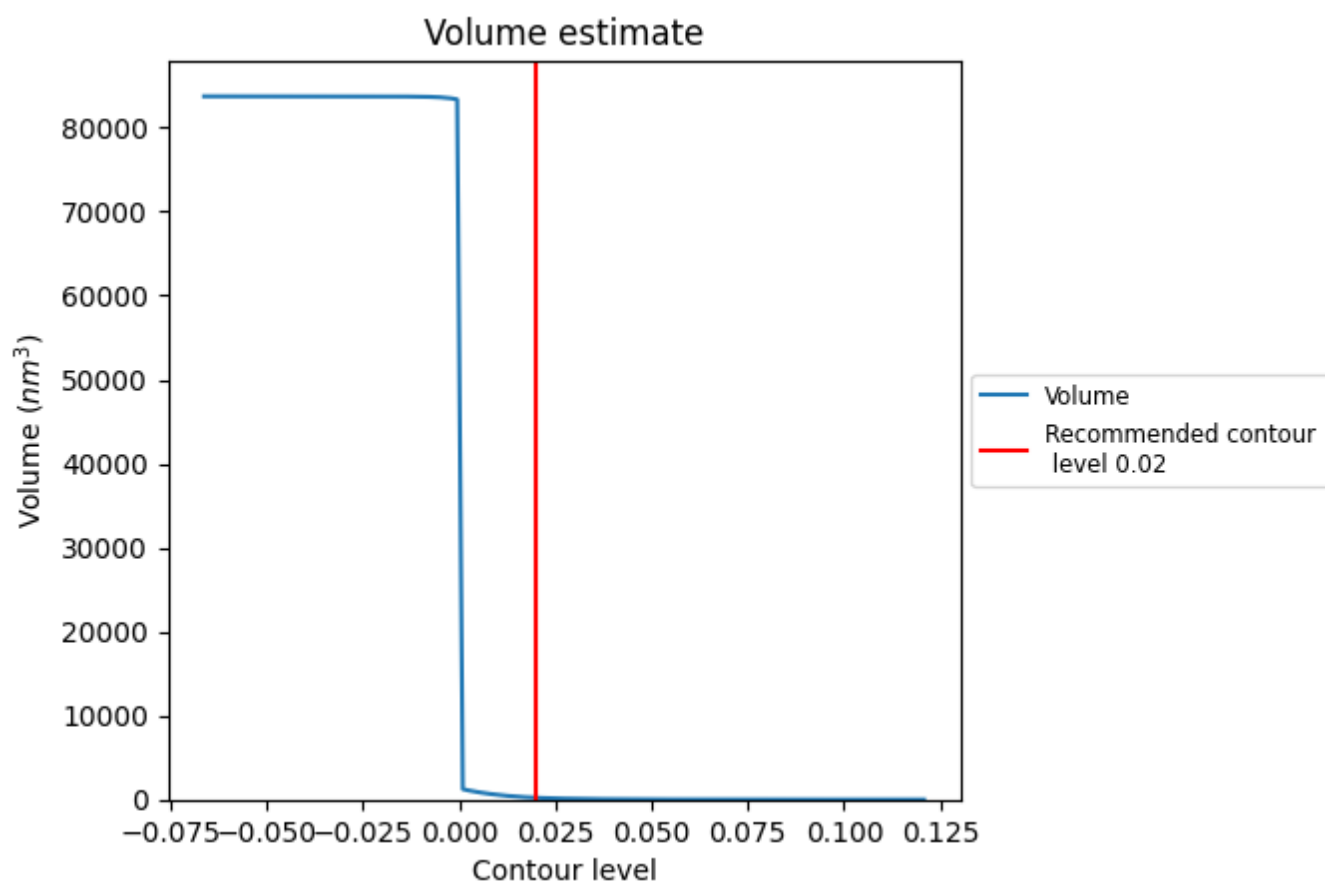
This section contains the results of statistical analysis of the map.

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.

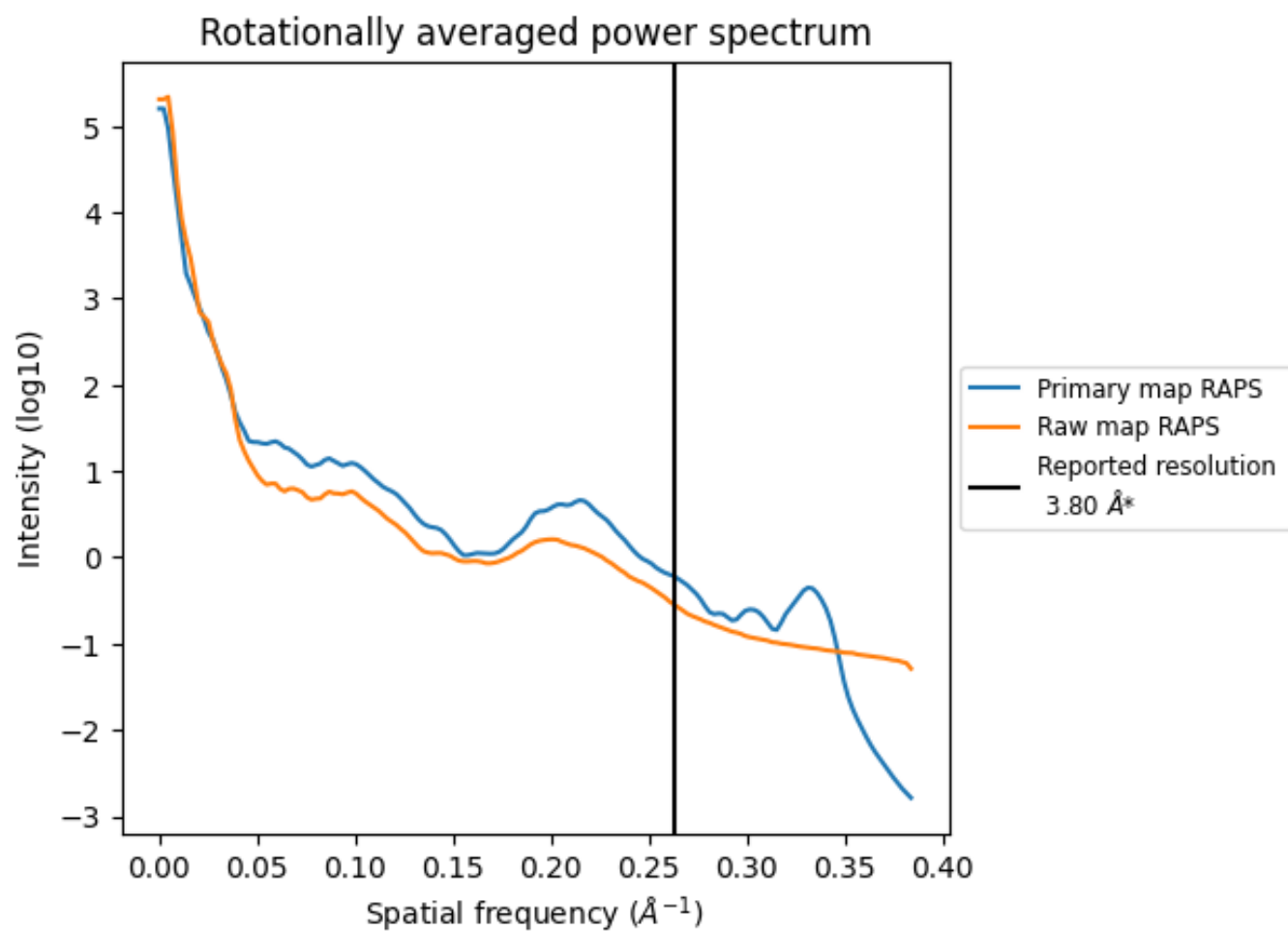
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 216 nm³; this corresponds to an approximate mass of 195 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 ⓘ

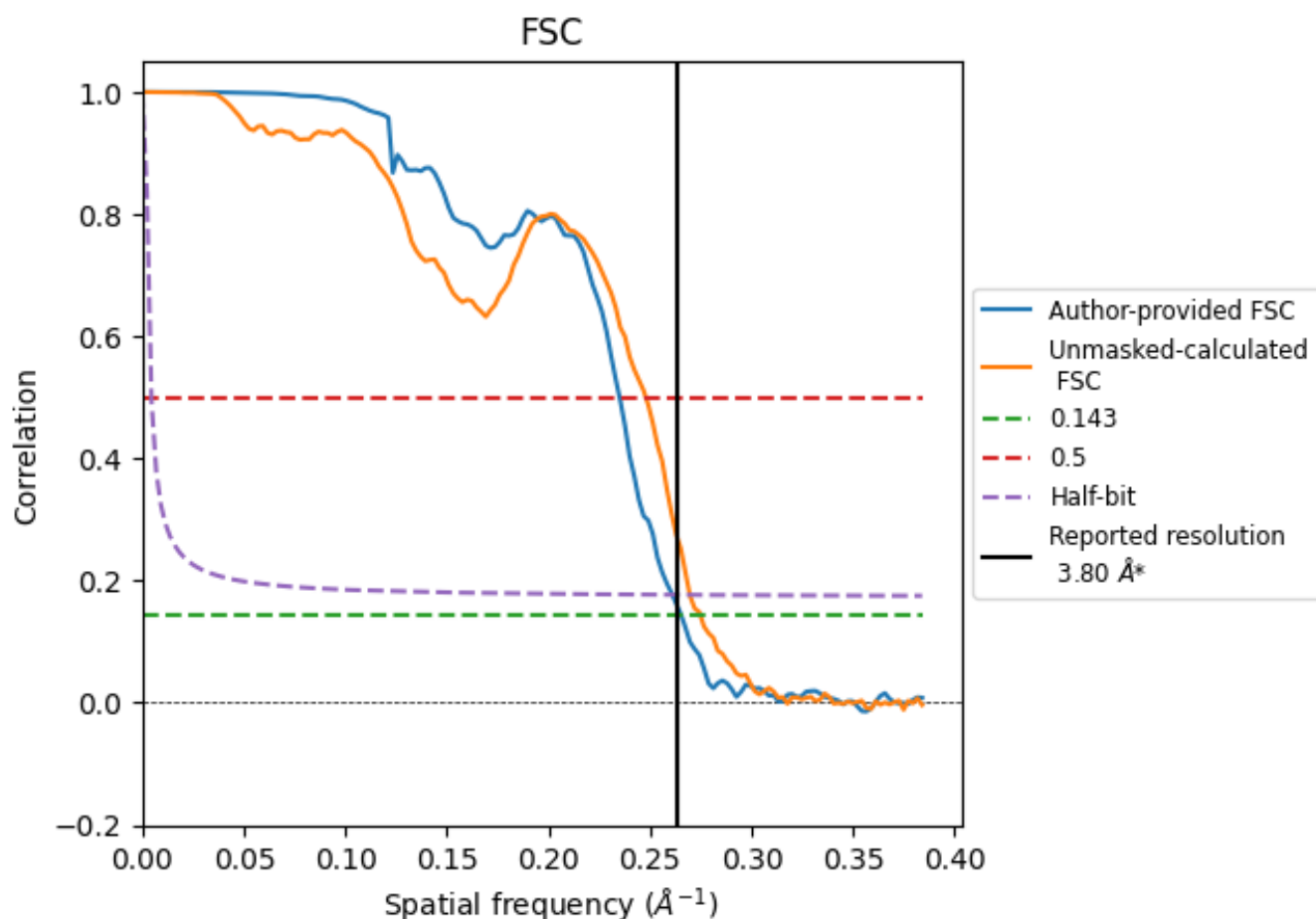


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 $0.263 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

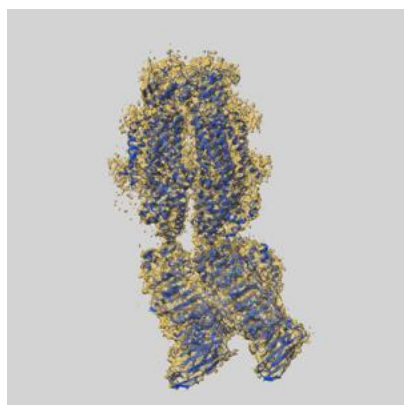
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.77	4.25	3.83
Unmasked-calculated*	3.64	4.03	3.71

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

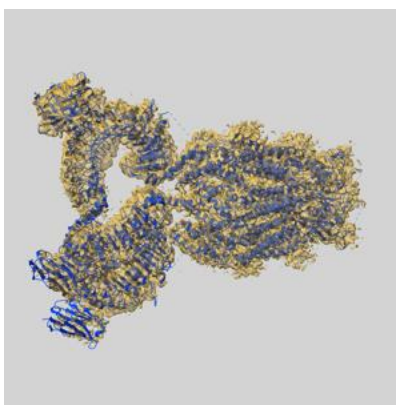
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15836 and PDB model 8B41. Per-residue inclusion information can be found in section [3](#) on page [7](#).

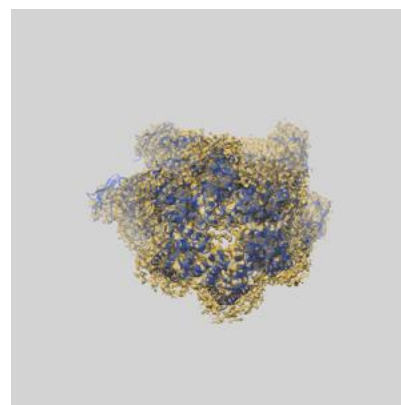
9.1 Map-model overlay [i](#)



X



Y



Z

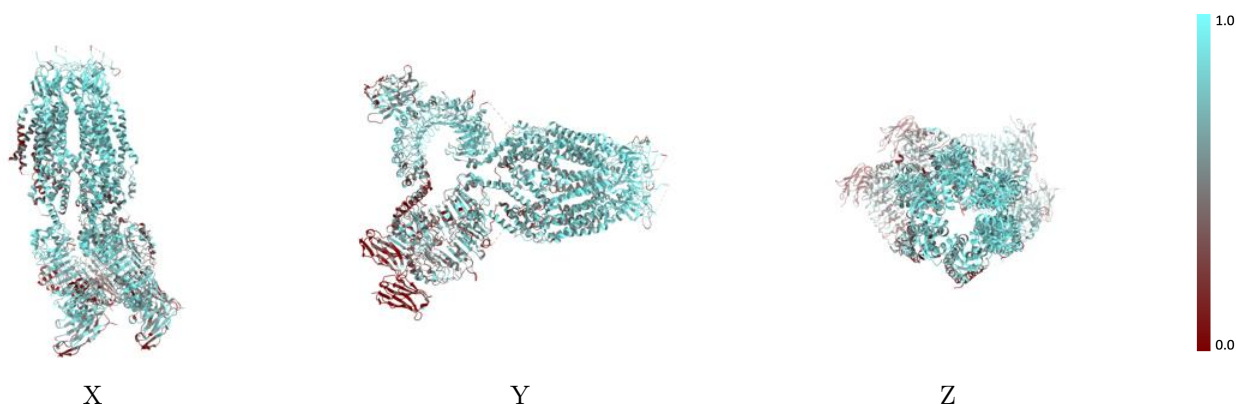
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



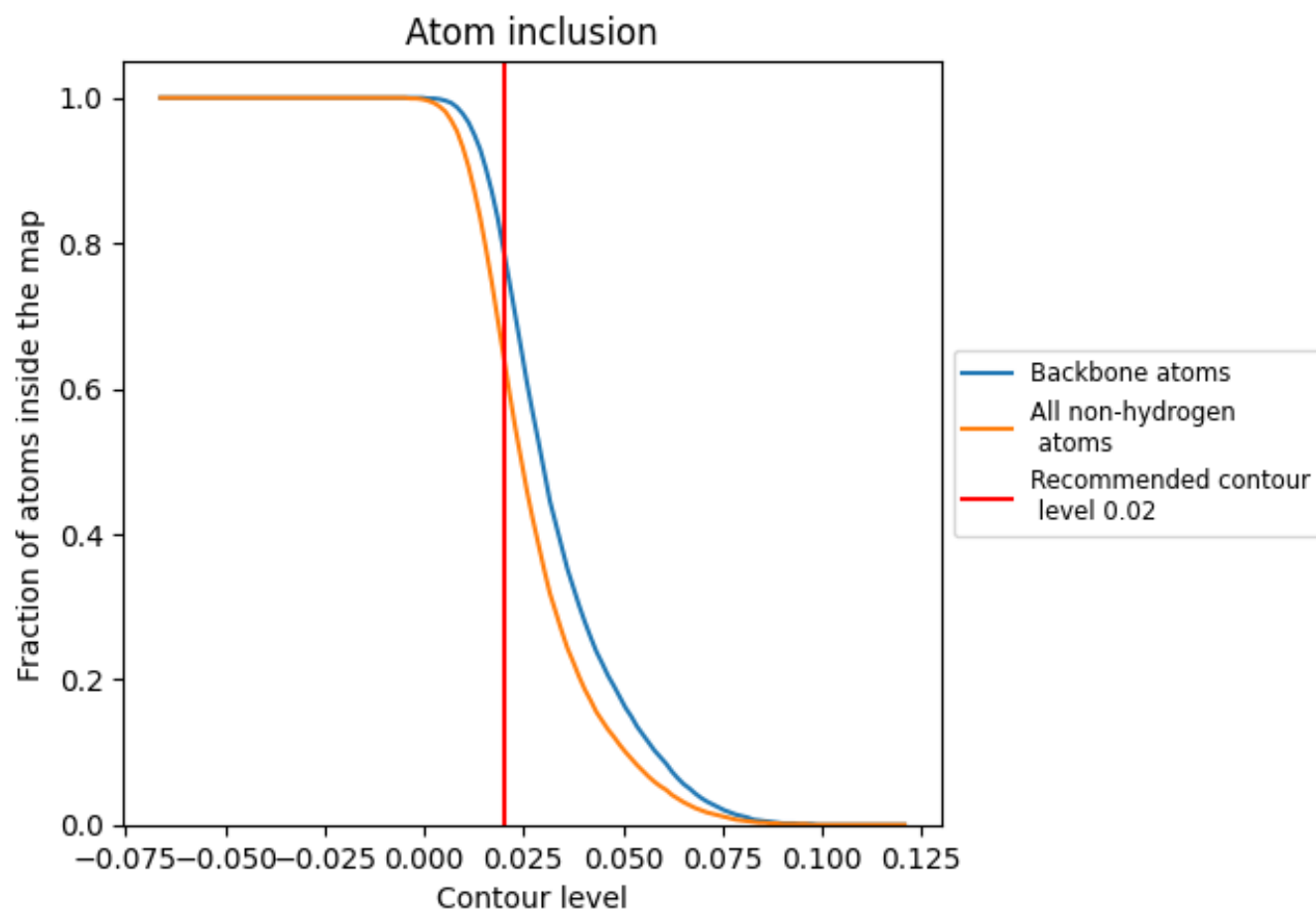
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 64% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6450	0.3760
A	0.7570	0.4240
B	0.7730	0.4380
C	0.6310	0.3660
D	0.6060	0.3570
E	0.5970	0.3640
F	0.6060	0.3850
G	0.5770	0.2930
H	0.5820	0.3100
I	0.2600	0.2060
J	0.1070	0.1780

1.0

0.0

<0.0