



Full wwPDB EM Validation Report ⓘ

Oct 6, 2021 – 05:18 am BST

PDB ID : 7P5V
EMDB ID : EMD-13202
Title : Structure of homomeric LRRC8A Volume-Regulated Anion Channel in complex with synthetic nanobody Sb1
Authors : Deneka, D.; Rutz, S.; Sawicka, M.
Deposited on : 2021-07-15
Resolution : 3.06 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.0.dev97
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

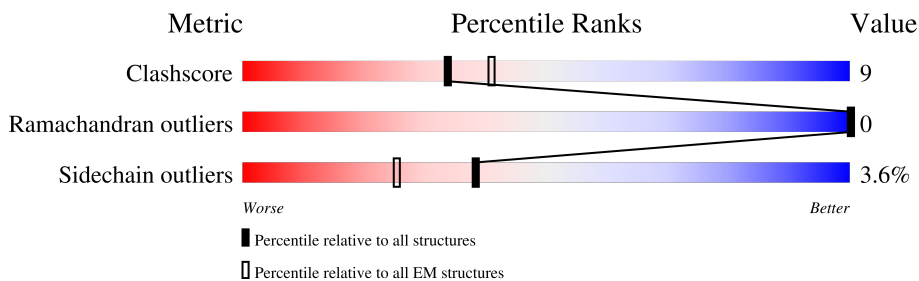
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.06 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	810	8% (poor fit), 65% (0 outliers), 23% (1 outlier), 11% (2+ outliers)
1	B	810	5% (poor fit), 68% (0 outliers), 21% (1 outlier), 10% (2+ outliers)
1	C	810	8% (poor fit), 66% (0 outliers), 20% (1 outlier), 11% (2+ outliers)
1	D	810	69% (0 outliers), 21% (1 outlier), 10% (2+ outliers)
1	E	810	7% (poor fit), 64% (0 outliers), 22% (1 outlier), 11% (2+ outliers)
1	F	810	5% (poor fit), 68% (0 outliers), 21% (1 outlier), 10% (2+ outliers)
2	G	144	39% (poor fit), 61% (0 outliers), 18% (1 outlier), 21% (2+ outliers)
2	H	144	32% (poor fit), 58% (0 outliers), 19% (1 outlier), 21% (2+ outliers)

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Mol	Chain	Length	Quality of chain
2	I	144	
2	J	144	
2	K	144	
2	L	144	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 41274 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
1	E	718	5922	3853	997	1047	25	0	0
1	F	732	6030	3916	1018	1071	25	0	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q80WG5
A	2	ILE	-	expression tag	UNP Q80WG5
A	3	PRO	-	expression tag	UNP Q80WG5
A	4	VAL	-	expression tag	UNP Q80WG5
A	5	THR	-	expression tag	UNP Q80WG5
A	6	GLU	-	expression tag	UNP Q80WG5
A	7	LEU	-	expression tag	UNP Q80WG5
A	8	ARG	-	expression tag	UNP Q80WG5
A	9	TYR	-	expression tag	UNP Q80WG5
A	10	PHE	-	expression tag	UNP Q80WG5
A	11	ALA	-	expression tag	UNP Q80WG5
A	12	ASP	-	expression tag	UNP Q80WG5
A	13	THR	-	expression tag	UNP Q80WG5
A	14	GLN	-	expression tag	UNP Q80WG5
A	809	GLN	-	expression tag	UNP Q80WG5
A	810	ALA	-	expression tag	UNP Q80WG5
B	1	MET	-	initiating methionine	UNP Q80WG5
B	2	ILE	-	expression tag	UNP Q80WG5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	3	PRO	-	expression tag	UNP Q80WG5
B	4	VAL	-	expression tag	UNP Q80WG5
B	5	THR	-	expression tag	UNP Q80WG5
B	6	GLU	-	expression tag	UNP Q80WG5
B	7	LEU	-	expression tag	UNP Q80WG5
B	8	ARG	-	expression tag	UNP Q80WG5
B	9	TYR	-	expression tag	UNP Q80WG5
B	10	PHE	-	expression tag	UNP Q80WG5
B	11	ALA	-	expression tag	UNP Q80WG5
B	12	ASP	-	expression tag	UNP Q80WG5
B	13	THR	-	expression tag	UNP Q80WG5
B	14	GLN	-	expression tag	UNP Q80WG5
B	809	GLN	-	expression tag	UNP Q80WG5
B	810	ALA	-	expression tag	UNP Q80WG5
C	1	MET	-	initiating methionine	UNP Q80WG5
C	2	ILE	-	expression tag	UNP Q80WG5
C	3	PRO	-	expression tag	UNP Q80WG5
C	4	VAL	-	expression tag	UNP Q80WG5
C	5	THR	-	expression tag	UNP Q80WG5
C	6	GLU	-	expression tag	UNP Q80WG5
C	7	LEU	-	expression tag	UNP Q80WG5
C	8	ARG	-	expression tag	UNP Q80WG5
C	9	TYR	-	expression tag	UNP Q80WG5
C	10	PHE	-	expression tag	UNP Q80WG5
C	11	ALA	-	expression tag	UNP Q80WG5
C	12	ASP	-	expression tag	UNP Q80WG5
C	13	THR	-	expression tag	UNP Q80WG5
C	14	GLN	-	expression tag	UNP Q80WG5
C	809	GLN	-	expression tag	UNP Q80WG5
C	810	ALA	-	expression tag	UNP Q80WG5
D	1	MET	-	initiating methionine	UNP Q80WG5
D	2	ILE	-	expression tag	UNP Q80WG5
D	3	PRO	-	expression tag	UNP Q80WG5
D	4	VAL	-	expression tag	UNP Q80WG5
D	5	THR	-	expression tag	UNP Q80WG5
D	6	GLU	-	expression tag	UNP Q80WG5
D	7	LEU	-	expression tag	UNP Q80WG5
D	8	ARG	-	expression tag	UNP Q80WG5
D	9	TYR	-	expression tag	UNP Q80WG5
D	10	PHE	-	expression tag	UNP Q80WG5
D	11	ALA	-	expression tag	UNP Q80WG5
D	12	ASP	-	expression tag	UNP Q80WG5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	13	THR	-	expression tag	UNP Q80WG5
D	14	GLN	-	expression tag	UNP Q80WG5
D	809	GLN	-	expression tag	UNP Q80WG5
D	810	ALA	-	expression tag	UNP Q80WG5
E	1	MET	-	initiating methionine	UNP Q80WG5
E	2	ILE	-	expression tag	UNP Q80WG5
E	3	PRO	-	expression tag	UNP Q80WG5
E	4	VAL	-	expression tag	UNP Q80WG5
E	5	THR	-	expression tag	UNP Q80WG5
E	6	GLU	-	expression tag	UNP Q80WG5
E	7	LEU	-	expression tag	UNP Q80WG5
E	8	ARG	-	expression tag	UNP Q80WG5
E	9	TYR	-	expression tag	UNP Q80WG5
E	10	PHE	-	expression tag	UNP Q80WG5
E	11	ALA	-	expression tag	UNP Q80WG5
E	12	ASP	-	expression tag	UNP Q80WG5
E	13	THR	-	expression tag	UNP Q80WG5
E	14	GLN	-	expression tag	UNP Q80WG5
E	809	GLN	-	expression tag	UNP Q80WG5
E	810	ALA	-	expression tag	UNP Q80WG5
F	1	MET	-	initiating methionine	UNP Q80WG5
F	2	ILE	-	expression tag	UNP Q80WG5
F	3	PRO	-	expression tag	UNP Q80WG5
F	4	VAL	-	expression tag	UNP Q80WG5
F	5	THR	-	expression tag	UNP Q80WG5
F	6	GLU	-	expression tag	UNP Q80WG5
F	7	LEU	-	expression tag	UNP Q80WG5
F	8	ARG	-	expression tag	UNP Q80WG5
F	9	TYR	-	expression tag	UNP Q80WG5
F	10	PHE	-	expression tag	UNP Q80WG5
F	11	ALA	-	expression tag	UNP Q80WG5
F	12	ASP	-	expression tag	UNP Q80WG5
F	13	THR	-	expression tag	UNP Q80WG5
F	14	GLN	-	expression tag	UNP Q80WG5
F	809	GLN	-	expression tag	UNP Q80WG5
F	810	ALA	-	expression tag	UNP Q80WG5

- Molecule 2 is a protein called Synthetic nanobody Sb1.

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

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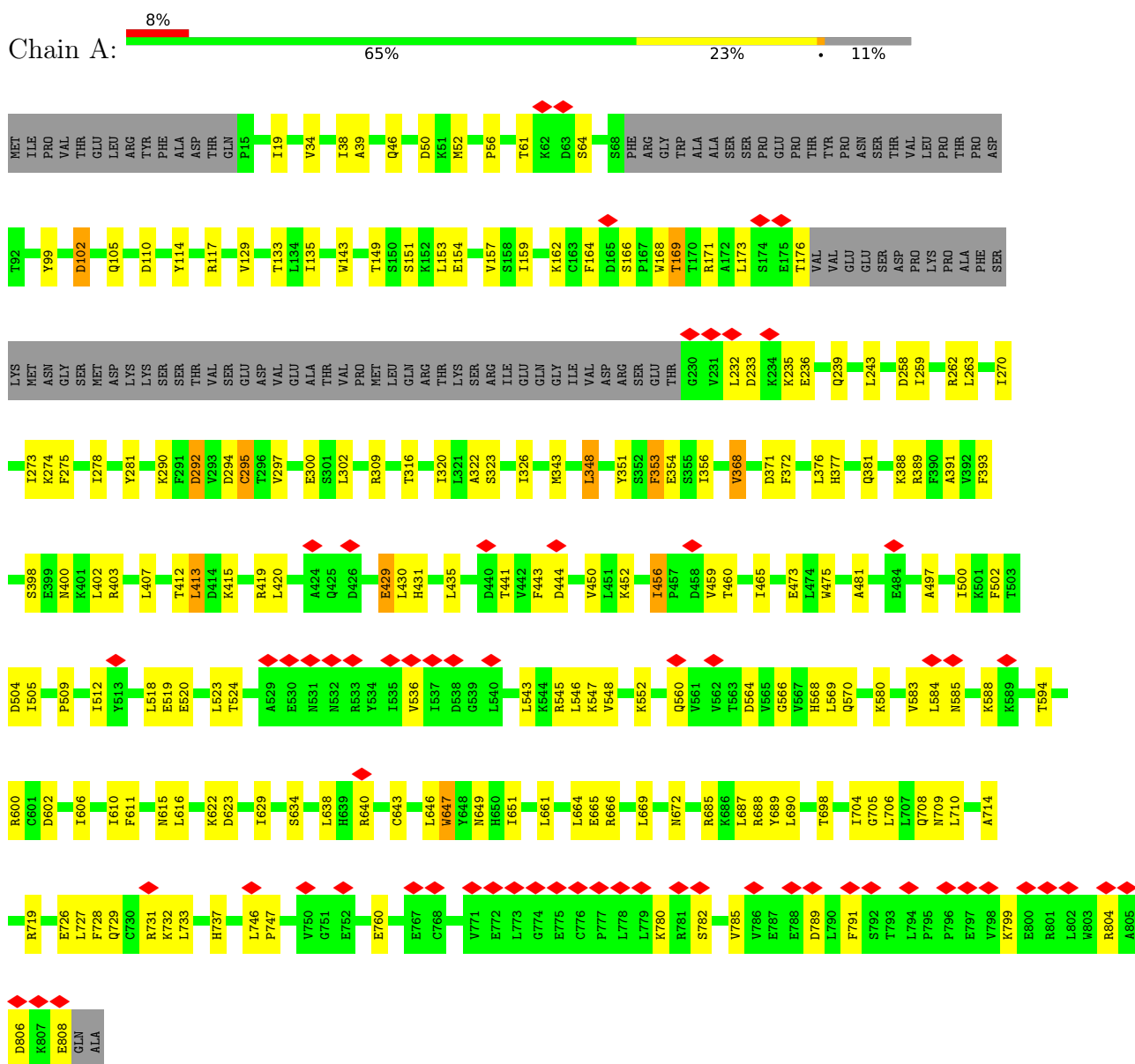
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	114	Total 903	C 575	N 152	O 172	S 4	0	0
2	I	114	Total 903	C 575	N 152	O 172	S 4	0	0
2	J	114	Total 903	C 575	N 152	O 172	S 4	0	0
2	K	114	Total 903	C 575	N 152	O 172	S 4	0	0
2	L	114	Total 903	C 575	N 152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

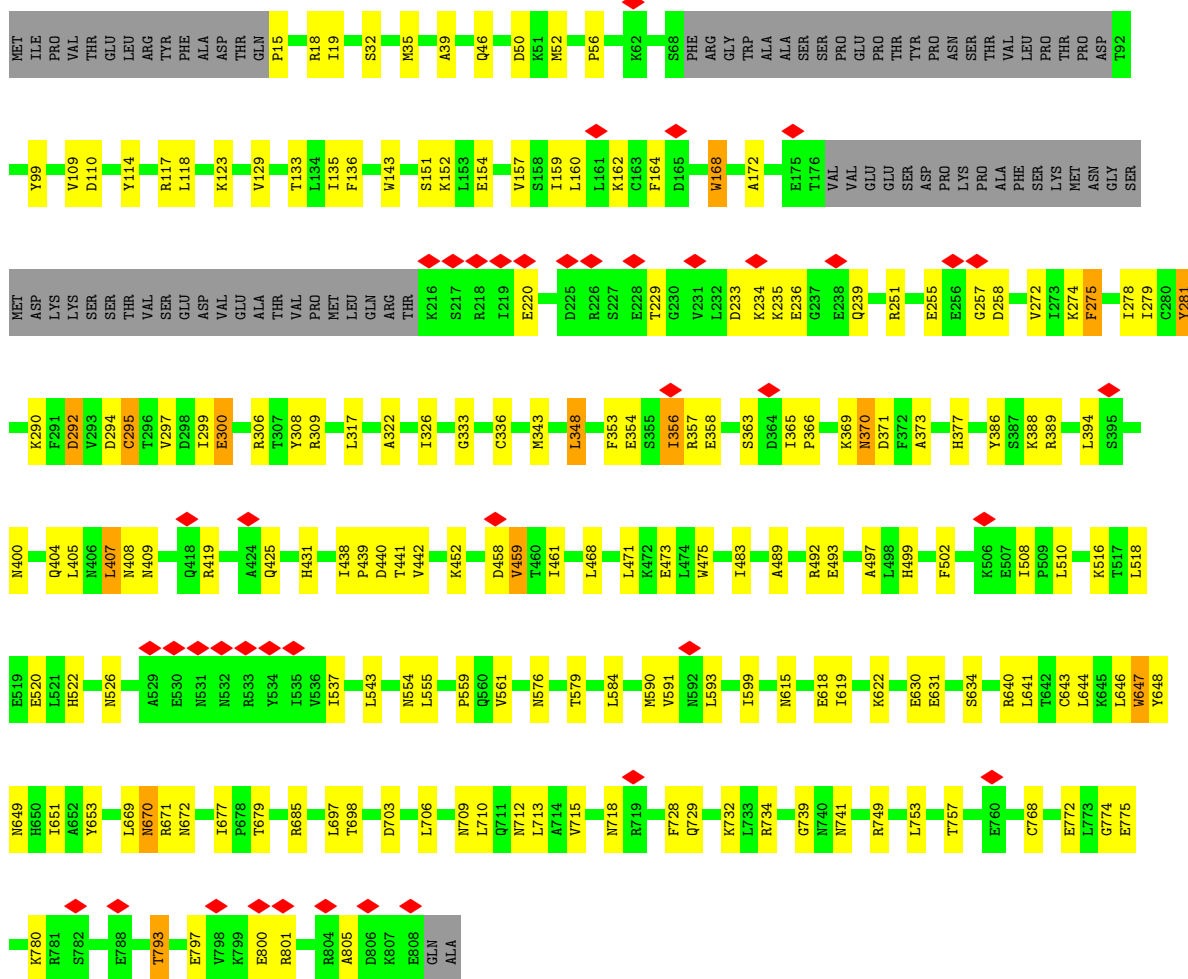
3 Residue-property plots

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.

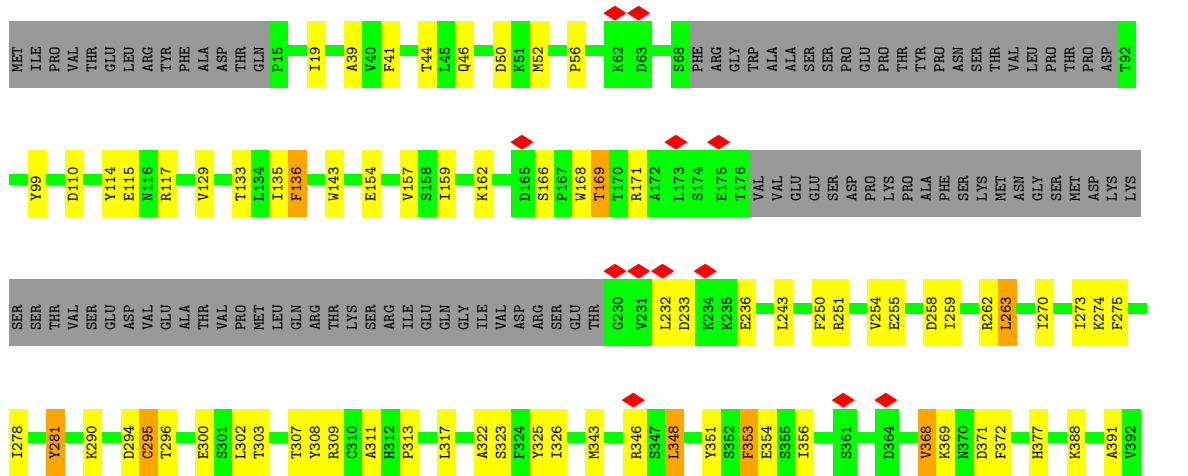
- Molecule 1: Volume-regulated anion channel subunit LRRC8A

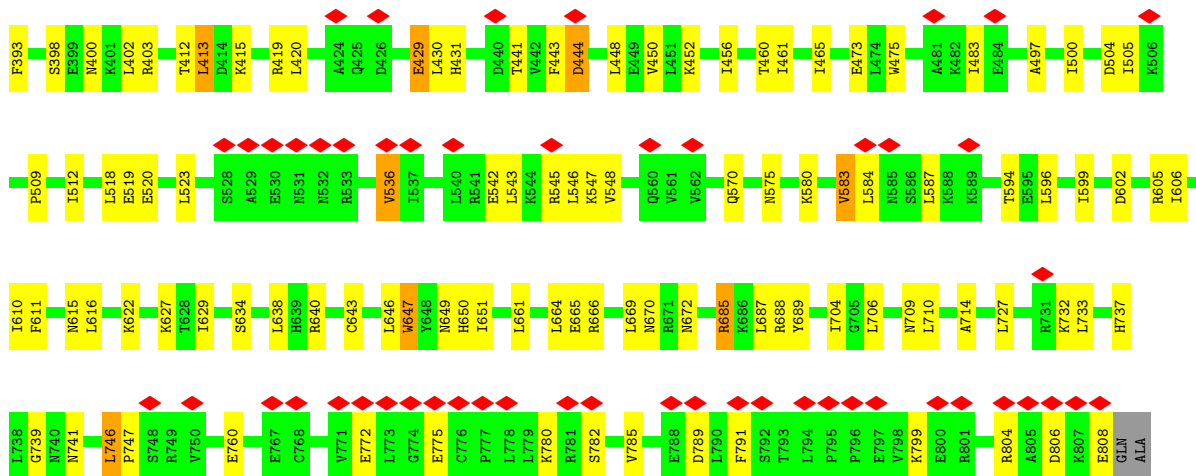


- Molecule 1: Volume-regulated anion channel subunit LRRC8A

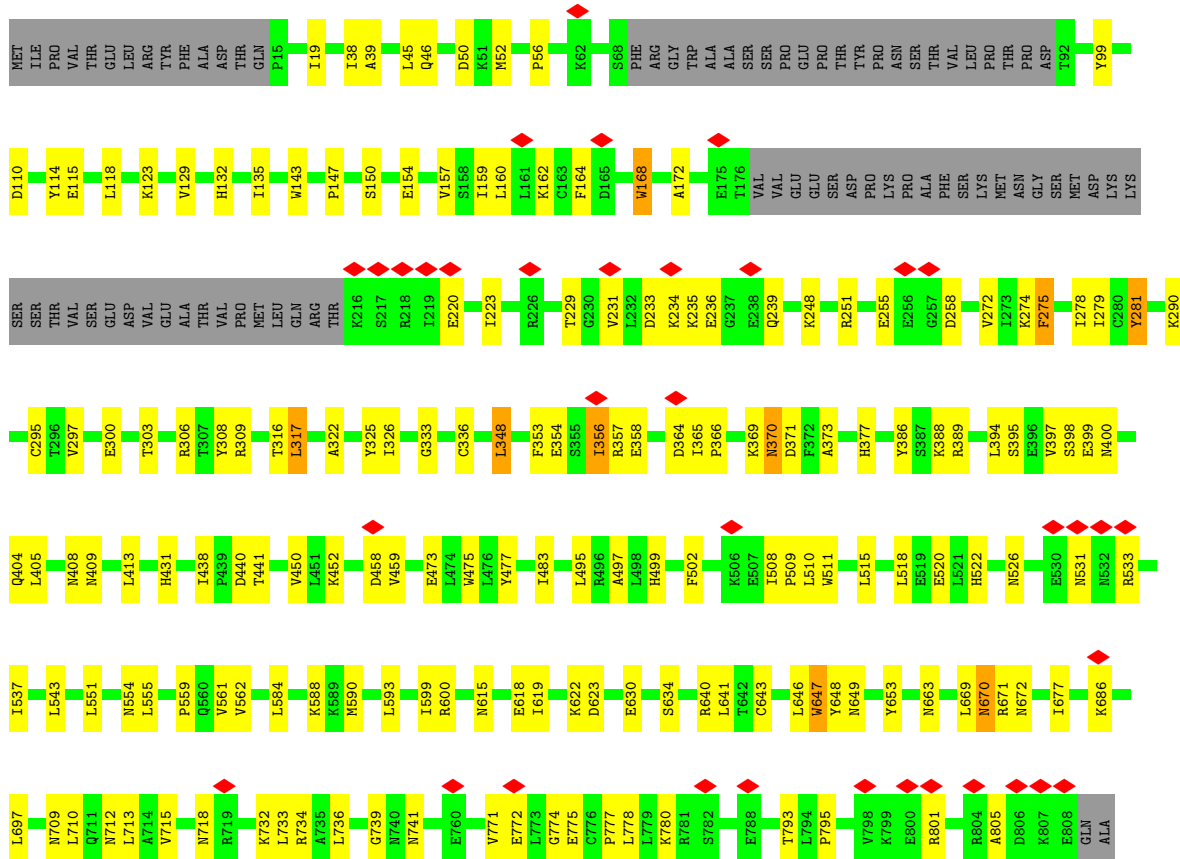


• Molecule 1: Volume-regulated anion channel subunit LRRC8A



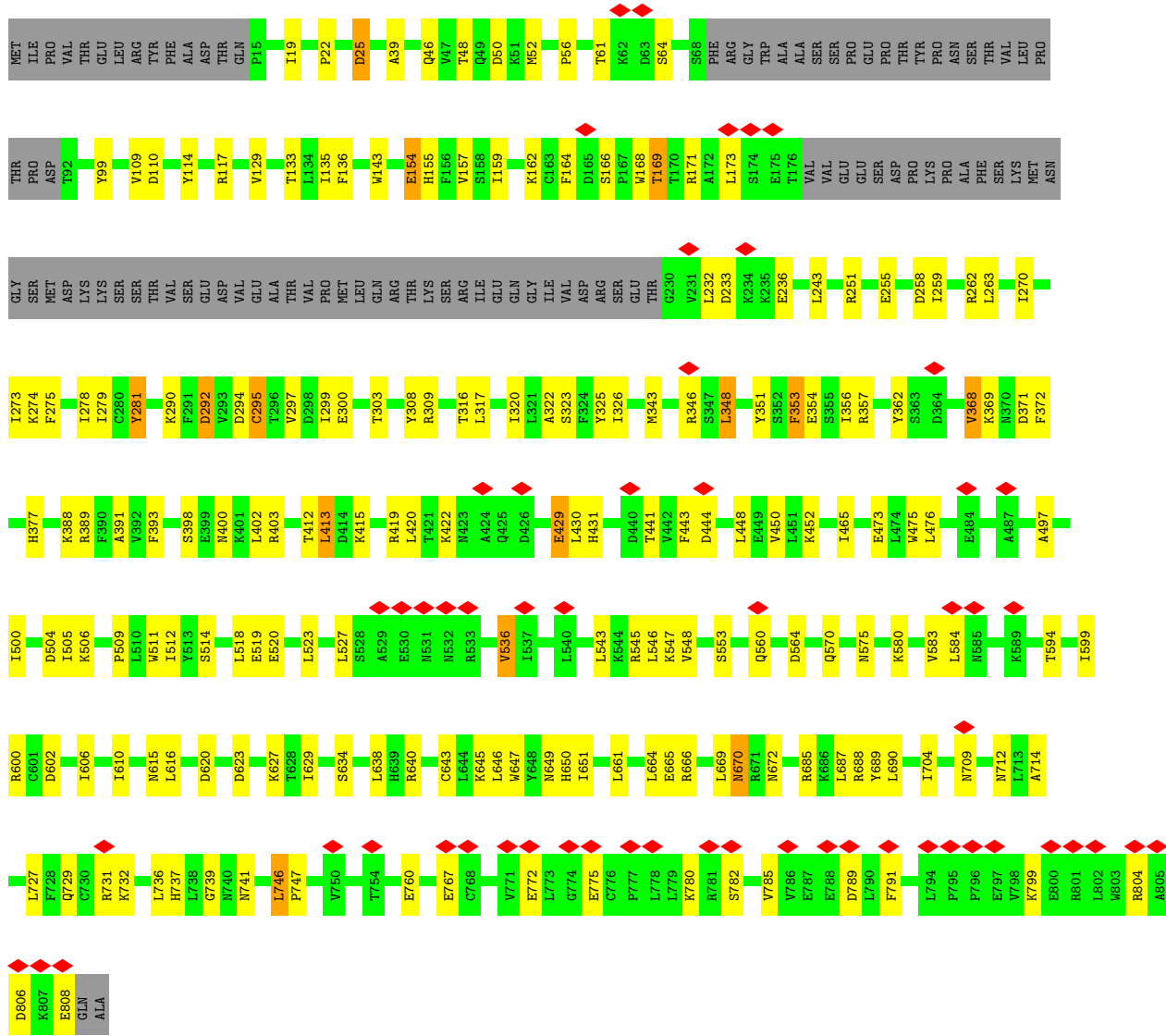


• Molecule 1: Volume-regulated anion channel subunit LRRC8A

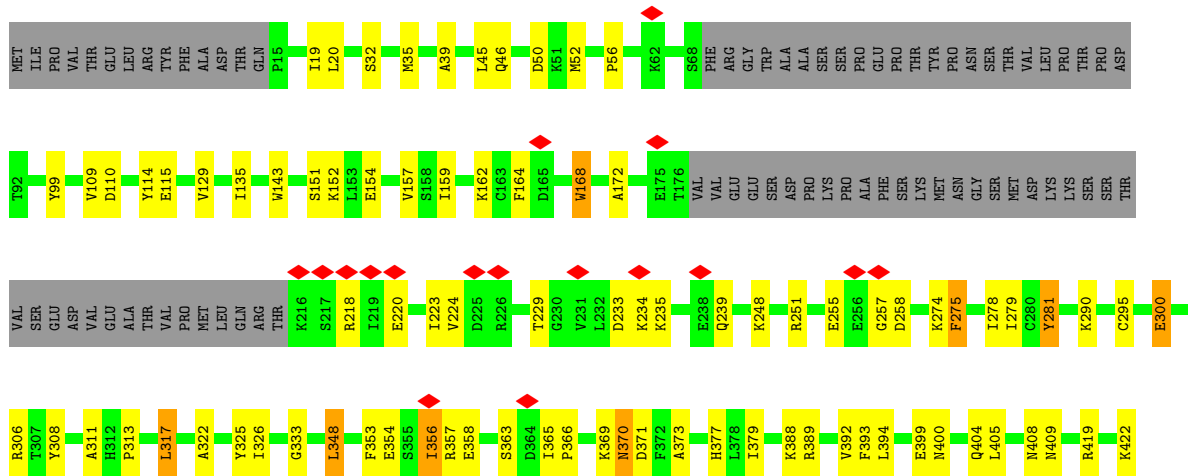


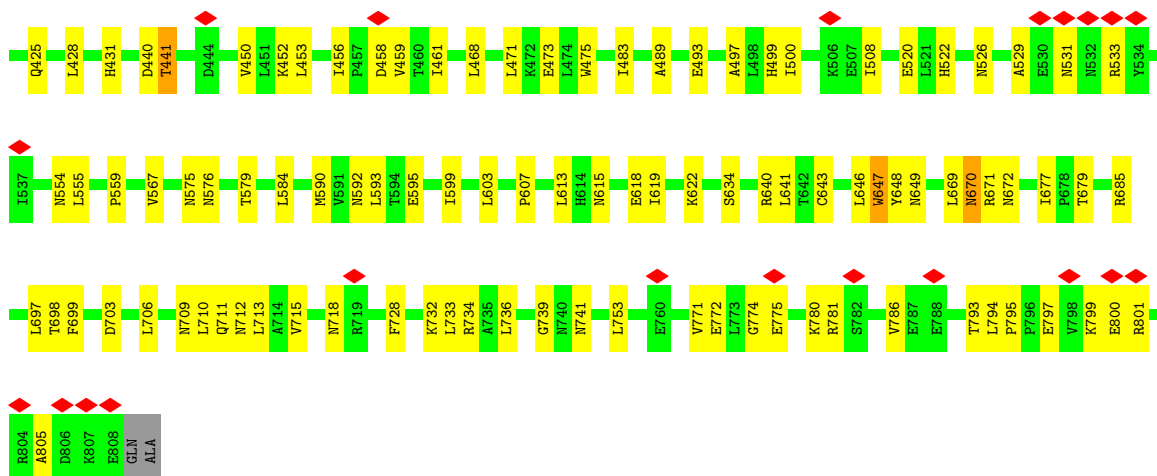
• Molecule 1: Volume-regulated anion channel subunit LRRC8A



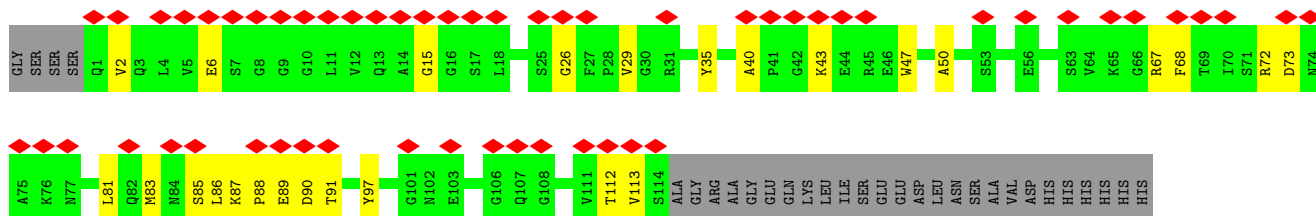
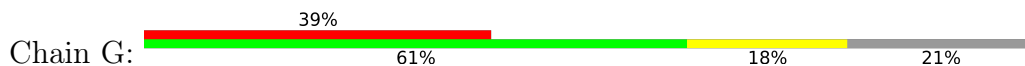


• Molecule 1: Volume-regulated anion channel subunit LRRC8A

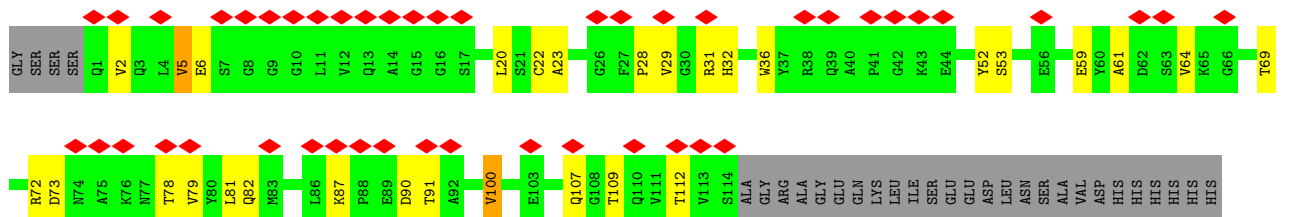




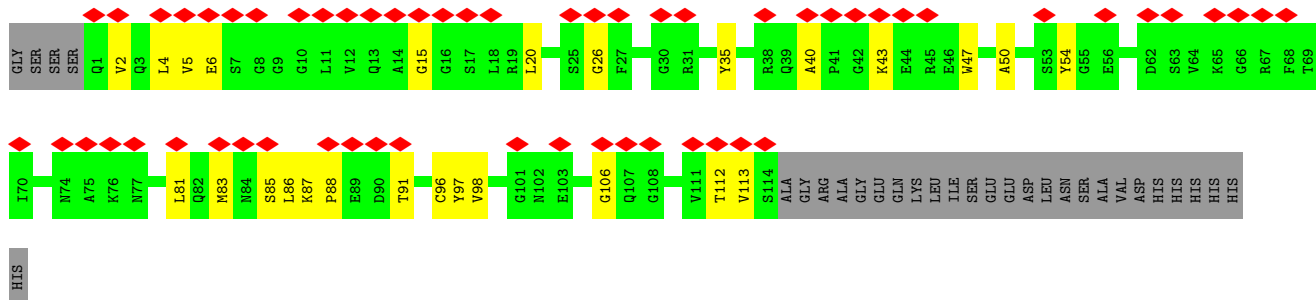
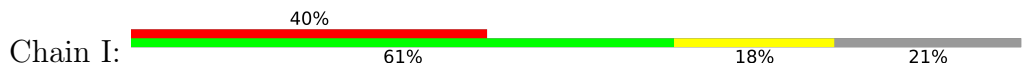
• Molecule 2: Synthetic nanobody Sb1



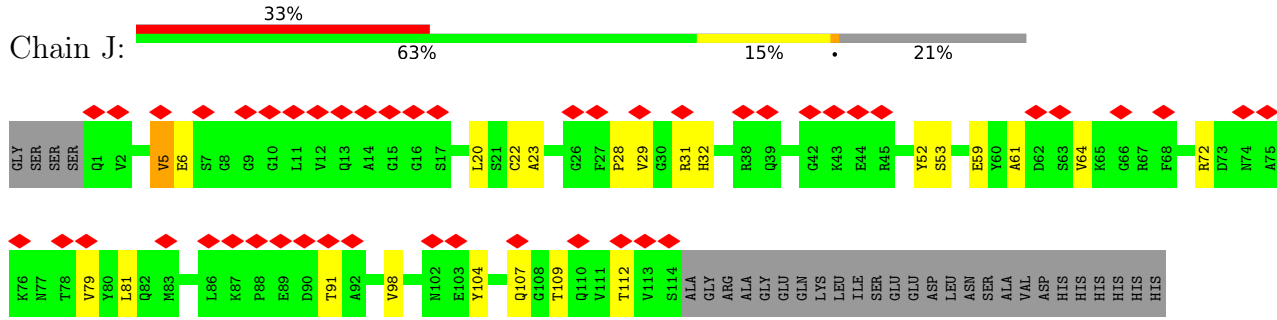
• Molecule 2: Synthetic nanobody Sb1



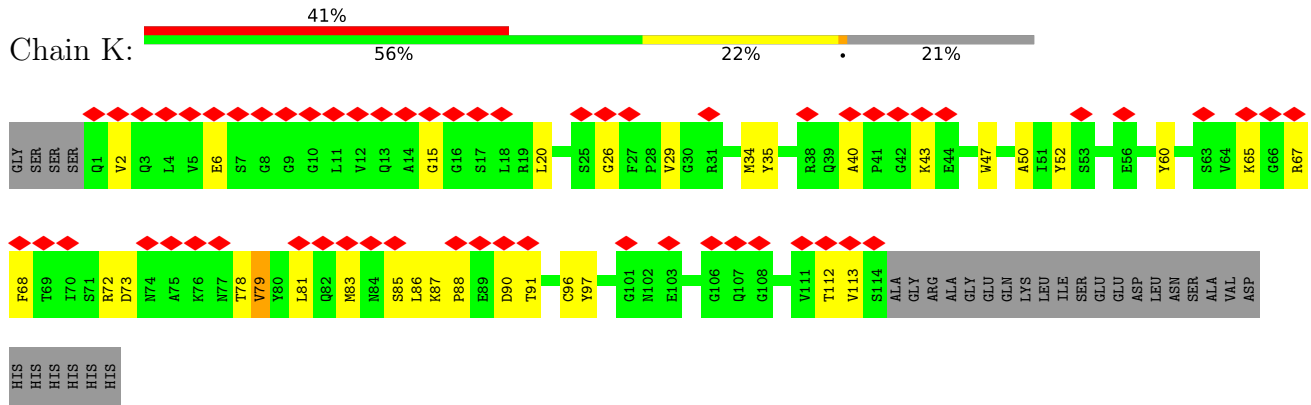
• Molecule 2: Synthetic nanobody Sb1



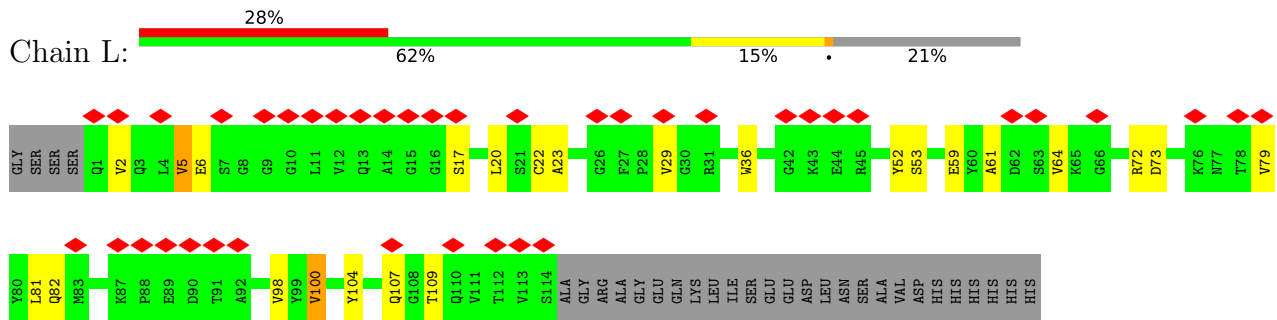
• Molecule 2: Synthetic nanobody Sb1



• Molecule 2: Synthetic nanobody Sb1



• Molecule 2: Synthetic nanobody Sb1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59962	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	67	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.257	Depositor
Minimum map value	-0.105	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	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	0.29	0/6055	0.48	0/8207
1	B	0.29	0/6163	0.48	0/8352
1	C	0.29	0/6055	0.48	0/8207
1	D	0.29	0/6163	0.49	0/8352
1	E	0.29	0/6055	0.48	0/8207
1	F	0.28	0/6163	0.48	0/8352
2	G	0.26	0/927	0.47	0/1258
2	H	0.26	0/927	0.49	0/1258
2	I	0.26	0/927	0.48	0/1258
2	J	0.26	0/927	0.49	0/1258
2	K	0.26	0/927	0.48	0/1258
2	L	0.26	0/927	0.49	0/1258
All	All	0.28	0/42216	0.48	0/57225

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	117	0
1	B	6030	0	6184	109	0
1	C	5922	0	6081	109	0
1	D	6030	0	6184	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	5922	0	6081	114	0
1	F	6030	0	6184	108	0
2	G	903	0	852	16	0
2	H	903	0	852	22	0
2	I	903	0	852	15	0
2	J	903	0	852	15	0
2	K	903	0	852	21	0
2	L	903	0	852	17	0
All	All	41274	0	41907	747	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 (747) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:634:SER:HG	2:K:52:TYR:HH	1.26	0.82
2:G:83:MET:HB3	2:G:86:LEU:HD21	1.62	0.81
2:K:83:MET:HB3	2:K:86:LEU:HD21	1.61	0.80
1:C:351:TYR:HB3	1:C:368:VAL:HG23	1.69	0.73
1:C:643:CYS:SG	1:C:666:ARG:NH1	2.62	0.73
1:E:643:CYS:SG	1:E:666:ARG:NH1	2.62	0.73
1:E:429:GLU:HG3	1:E:452:LYS:HE3	1.71	0.73
1:B:164:PHE:O	1:B:389:ARG:NH1	2.21	0.72
1:B:405:LEU:O	1:B:409:ASN:ND2	2.23	0.72
1:E:419:ARG:NH1	1:E:431:HIS:O	2.23	0.72
1:E:473:GLU:HG2	1:E:497:ALA:HB3	1.72	0.72
1:D:164:PHE:O	1:D:389:ARG:NH1	2.24	0.71
2:I:83:MET:HB3	2:I:86:LEU:HD21	1.71	0.70
1:F:164:PHE:O	1:F:389:ARG:NH1	2.24	0.69
1:D:258:ASP:H	1:D:371:ASP:HB2	1.57	0.69
1:A:343:MET:HA	1:A:348:LEU:HD11	1.76	0.68
1:A:643:CYS:SG	1:A:666:ARG:NH1	2.66	0.68
1:D:618:GLU:HG3	1:D:643:CYS:HB3	1.74	0.68
1:A:429:GLU:HG3	1:A:452:LYS:HE3	1.75	0.68
1:C:294:ASP:OD1	1:C:309:ARG:NH1	2.27	0.68
2:J:52:TYR:O	2:J:72:ARG:NH2	2.26	0.68
1:E:351:TYR:HB3	1:E:368:VAL:HG23	1.75	0.68
2:I:2:VAL:HA	2:I:26:GLY:HA3	1.76	0.67
1:A:294:ASP:OD1	1:A:309:ARG:NH1	2.28	0.67
2:L:52:TYR:O	2:L:72:ARG:NH2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:GLU:HG2	1:C:497:ALA:HB3	1.77	0.66
1:F:255:GLU:HG3	1:F:369:LYS:HB2	1.78	0.66
2:G:2:VAL:HA	2:G:26:GLY:HA3	1.77	0.66
1:C:135:ILE:HG12	1:C:274:LYS:HZ3	1.59	0.66
1:C:429:GLU:HG3	1:C:452:LYS:HE3	1.77	0.66
1:C:419:ARG:NH1	1:C:431:HIS:O	2.28	0.66
2:H:20:LEU:HB2	2:H:81:LEU:HB3	1.79	0.65
1:A:729:GLN:OE1	1:A:731:ARG:NH2	2.30	0.65
1:E:615:ASN:HA	1:E:640:ARG:HE	1.61	0.65
1:A:473:GLU:HG2	1:A:497:ALA:HB3	1.77	0.65
1:B:300:GLU:OE2	1:B:306:ARG:NH1	2.29	0.64
1:C:343:MET:HA	1:C:348:LEU:HD11	1.79	0.64
1:F:300:GLU:OE2	1:F:306:ARG:NH1	2.30	0.64
1:F:619:ILE:HG22	1:F:641:LEU:HD11	1.80	0.64
1:D:118:LEU:HD23	1:D:123:LYS:HG3	1.80	0.64
1:E:343:MET:HA	1:E:348:LEU:HD11	1.79	0.64
2:H:52:TYR:O	2:H:72:ARG:NH2	2.30	0.64
1:B:618:GLU:HG3	1:B:643:CYS:HB3	1.78	0.64
1:B:438:ILE:HG13	1:B:459:VAL:HG21	1.79	0.63
1:F:357:ARG:NH1	1:F:365:ILE:O	2.31	0.63
1:B:619:ILE:HG22	1:B:641:LEU:HD11	1.80	0.63
1:F:618:GLU:HG3	1:F:643:CYS:HB3	1.81	0.63
1:B:373:ALA:O	1:B:377:HIS:ND1	2.32	0.63
1:F:452:LYS:HA	1:F:475:TRP:HB2	1.81	0.62
1:A:292:ASP:OD1	1:A:292:ASP:N	2.32	0.62
1:B:255:GLU:HG3	1:B:369:LYS:HB2	1.80	0.62
1:D:373:ALA:O	1:D:377:HIS:ND1	2.30	0.62
1:F:405:LEU:O	1:F:409:ASN:ND2	2.27	0.62
1:A:705:GLY:O	1:A:708:GLN:NE2	2.33	0.62
1:B:258:ASP:H	1:B:371:ASP:HB2	1.65	0.62
1:B:357:ARG:NH1	1:B:365:ILE:O	2.33	0.62
1:E:429:GLU:HB2	1:E:450:VAL:HB	1.82	0.61
1:B:292:ASP:OD1	1:B:292:ASP:N	2.33	0.61
1:C:259:ILE:N	1:C:371:ASP:OD2	2.30	0.61
1:A:669:LEU:O	1:A:672:ASN:ND2	2.33	0.61
1:F:774:GLY:O	1:F:801:ARG:NH2	2.32	0.61
1:B:712:ASN:OD1	1:B:734:ARG:NH2	2.32	0.61
2:J:5:VAL:HG13	2:J:23:ALA:HB3	1.82	0.61
2:J:29:VAL:O	2:J:72:ARG:NH1	2.34	0.61
1:B:408:ASN:ND2	1:B:440:ASP:OD2	2.30	0.61
1:D:438:ILE:HG13	1:D:459:VAL:HG21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ASP:OD1	1:A:105:GLN:NE2	2.20	0.61
1:E:135:ILE:HG12	1:E:274:LYS:HZ3	1.64	0.61
1:E:412:THR:HG23	1:E:415:LYS:H	1.66	0.61
2:H:20:LEU:HD22	2:H:81:LEU:HD23	1.81	0.61
1:A:258:ASP:O	1:A:262:ARG:NH1	2.34	0.60
1:A:135:ILE:HG12	1:A:274:LYS:HZ2	1.66	0.60
1:D:473:GLU:HG2	1:D:497:ALA:HB3	1.83	0.60
2:H:29:VAL:HG22	2:H:72:ARG:HD2	1.84	0.60
1:A:52:MET:HG3	1:A:114:TYR:HD2	1.66	0.60
1:D:615:ASN:OD1	1:D:640:ARG:NH2	2.35	0.60
1:A:351:TYR:HB3	1:A:368:VAL:HG23	1.84	0.60
1:B:739:GLY:O	1:B:741:ASN:ND2	2.34	0.60
1:E:258:ASP:H	1:E:371:ASP:HB2	1.67	0.60
1:F:712:ASN:OD1	1:F:734:ARG:NH2	2.33	0.60
2:K:67:ARG:NH2	2:K:90:ASP:OD2	2.35	0.60
1:C:429:GLU:HB2	1:C:450:VAL:HB	1.82	0.60
1:F:373:ALA:O	1:F:377:HIS:ND1	2.33	0.60
2:L:5:VAL:HG13	2:L:23:ALA:HB3	1.84	0.60
1:C:709:ASN:HA	1:C:732:LYS:HD2	1.83	0.60
1:D:45:LEU:HD21	1:D:317:LEU:HD13	1.84	0.60
1:C:412:THR:HG23	1:C:415:LYS:H	1.67	0.60
1:D:39:ALA:HB2	1:D:129:VAL:HG12	1.84	0.60
1:E:452:LYS:HA	1:E:475:TRP:HB2	1.84	0.59
1:F:739:GLY:O	1:F:741:ASN:ND2	2.35	0.59
1:B:39:ALA:HB2	1:B:129:VAL:HG12	1.82	0.59
1:D:255:GLU:HG3	1:D:369:LYS:HB2	1.82	0.59
1:C:504:ASP:OD1	1:C:505:ILE:N	2.35	0.59
1:F:251:ARG:HD2	1:F:394:LEU:HD11	1.84	0.59
2:J:53:SER:HA	2:J:72:ARG:HH22	1.67	0.59
1:A:419:ARG:NH1	1:A:431:HIS:O	2.34	0.59
1:B:461:ILE:HB	1:B:483:ILE:HG13	1.85	0.59
1:C:615:ASN:HA	1:C:640:ARG:HE	1.66	0.59
2:H:29:VAL:O	2:H:72:ARG:NH1	2.36	0.59
1:D:357:ARG:NH1	1:D:365:ILE:O	2.35	0.59
1:F:39:ALA:HB2	1:F:129:VAL:HG12	1.85	0.59
1:C:669:LEU:O	1:C:672:ASN:ND2	2.36	0.59
1:E:669:LEU:O	1:E:672:ASN:ND2	2.36	0.59
2:J:61:ALA:HB3	2:J:64:VAL:HG22	1.85	0.59
2:K:91:THR:HG23	2:K:112:THR:HA	1.85	0.59
1:D:677:ILE:HD11	1:D:697:LEU:HD13	1.85	0.58
1:F:45:LEU:HD21	1:F:317:LEU:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:408:ASN:ND2	1:D:440:ASP:OD2	2.36	0.58
1:E:117:ARG:HG2	1:E:295:CYS:HA	1.86	0.58
2:I:35:TYR:HB2	2:I:97:TYR:HB3	1.85	0.58
1:A:560:GLN:NE2	1:A:564:ASP:OD2	2.37	0.58
1:C:46:GLN:O	1:C:50:ASP:HB3	2.03	0.58
1:D:46:GLN:O	1:D:50:ASP:HB3	2.03	0.58
1:F:258:ASP:H	1:F:371:ASP:HB2	1.68	0.58
2:H:61:ALA:HB3	2:H:64:VAL:HG22	1.85	0.58
1:B:370:ASN:OD1	1:B:370:ASN:N	2.32	0.58
1:B:590:MET:HE3	1:B:593:LEU:HD22	1.86	0.58
1:F:370:ASN:OD1	1:F:370:ASN:N	2.36	0.58
1:B:46:GLN:O	1:B:50:ASP:HB3	2.04	0.58
2:L:6:GLU:O	2:L:107:GLN:NE2	2.37	0.58
2:H:5:VAL:HG13	2:H:23:ALA:HB3	1.86	0.57
2:L:20:LEU:HB2	2:L:81:LEU:HB3	1.87	0.57
1:A:629:ILE:HD13	1:A:651:ILE:HD13	1.86	0.57
1:C:646:LEU:O	1:C:649:ASN:ND2	2.35	0.57
1:D:52:MET:HG3	1:D:114:TYR:HD2	1.68	0.57
1:F:473:GLU:HG2	1:F:497:ALA:HB3	1.86	0.57
1:D:303:THR:HG1	1:D:308:TYR:HH	1.52	0.57
1:F:258:ASP:HB2	1:F:370:ASN:HD22	1.68	0.57
1:A:435:LEU:HB2	1:A:456:ILE:HD13	1.86	0.57
1:D:405:LEU:O	1:D:409:ASN:ND2	2.29	0.57
1:D:739:GLY:O	1:D:741:ASN:ND2	2.37	0.57
1:E:560:GLN:NE2	1:E:564:ASP:OD2	2.37	0.57
2:J:20:LEU:HB2	2:J:81:LEU:HB3	1.85	0.57
2:J:32:HIS:O	2:J:72:ARG:NH1	2.37	0.57
2:L:20:LEU:HD22	2:L:81:LEU:HD23	1.86	0.57
1:E:255:GLU:HG2	1:E:369:LYS:HB2	1.86	0.57
2:L:61:ALA:HB3	2:L:64:VAL:HG22	1.85	0.57
1:A:412:THR:HG23	1:A:415:LYS:H	1.70	0.57
2:I:20:LEU:HD12	2:I:81:LEU:HD23	1.87	0.56
1:D:258:ASP:HB2	1:D:370:ASN:HD22	1.69	0.56
1:D:619:ILE:HG22	1:D:641:LEU:HD11	1.86	0.56
1:E:519:GLU:HG2	1:E:545:ARG:HG3	1.86	0.56
1:A:615:ASN:HA	1:A:640:ARG:HE	1.71	0.56
1:C:19:ILE:HD11	1:C:157:VAL:HG23	1.87	0.56
1:C:509:PRO:HB2	1:C:512:ILE:HG23	1.87	0.56
1:F:567:VAL:O	1:F:592:ASN:ND2	2.38	0.56
2:H:2:VAL:HG21	2:H:100:VAL:HG21	1.88	0.56
2:H:53:SER:HA	2:H:72:ARG:HH22	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ILE:HD11	1:A:157:VAL:HG23	1.87	0.56
1:A:169:THR:HG23	1:A:393:PHE:HE1	1.70	0.56
1:D:630:GLU:OE2	1:D:653:TYR:OH	2.19	0.56
1:E:714:ALA:HA	1:E:737:HIS:HB2	1.86	0.56
2:K:85:SER:O	2:K:87:LYS:NZ	2.38	0.56
1:D:452:LYS:HA	1:D:475:TRP:HB2	1.88	0.56
1:E:509:PRO:HB2	1:E:512:ILE:HG23	1.88	0.56
1:F:615:ASN:OD1	1:F:640:ARG:NH2	2.39	0.56
1:F:646:LEU:O	1:F:649:ASN:ND2	2.39	0.56
1:E:804:ARG:HH12	1:E:808:GLU:HB3	1.71	0.56
1:B:630:GLU:OE2	1:B:653:TYR:OH	2.18	0.55
1:C:629:ILE:HD13	1:C:651:ILE:HD13	1.87	0.55
1:C:714:ALA:HA	1:C:737:HIS:HB2	1.88	0.55
1:F:46:GLN:O	1:F:50:ASP:HB3	2.06	0.55
1:E:19:ILE:HD11	1:E:157:VAL:HG23	1.88	0.55
1:A:714:ALA:HA	1:A:737:HIS:HB2	1.89	0.55
1:C:166:SER:O	1:C:169:THR:OG1	2.24	0.55
1:C:760:GLU:HA	1:C:785:VAL:HB	1.87	0.55
2:L:29:VAL:HG22	2:L:72:ARG:HD2	1.89	0.55
1:A:166:SER:O	1:A:169:THR:OG1	2.23	0.55
1:B:322:ALA:O	1:B:326:ILE:HG23	2.06	0.55
1:E:129:VAL:O	1:E:133:THR:HG23	2.06	0.55
2:H:22:CYS:HB3	2:H:79:VAL:HB	1.88	0.55
1:A:789:ASP:N	1:A:789:ASP:OD1	2.39	0.55
2:H:6:GLU:O	2:H:107:GLN:NE2	2.40	0.55
1:A:117:ARG:HG2	1:A:295:CYS:HA	1.89	0.55
2:G:35:TYR:HB2	2:G:97:TYR:HB3	1.88	0.55
1:E:258:ASP:O	1:E:262:ARG:NH1	2.39	0.55
1:F:251:ARG:HH22	1:F:366:PRO:HG2	1.72	0.55
1:A:39:ALA:HB2	1:A:129:VAL:HG12	1.88	0.54
1:E:162:LYS:HG3	1:E:243:LEU:HD11	1.90	0.54
1:E:164:PHE:O	1:E:389:ARG:NH1	2.40	0.54
1:B:32:SER:HA	1:B:35:MET:HE2	1.88	0.54
1:B:576:ASN:HB3	1:B:579:THR:HB	1.88	0.54
1:D:322:ALA:O	1:D:326:ILE:HG23	2.07	0.54
1:D:710:LEU:HD21	1:D:713:LEU:HB2	1.89	0.54
1:C:452:LYS:HA	1:C:475:TRP:HB2	1.89	0.54
1:B:251:ARG:HH22	1:B:366:PRO:HG2	1.72	0.54
1:D:251:ARG:HD2	1:D:394:LEU:HD11	1.88	0.54
1:E:629:ILE:HD13	1:E:651:ILE:HD13	1.90	0.54
1:E:729:GLN:OE1	1:E:731:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:2:VAL:HA	2:K:26:GLY:HA3	1.90	0.54
1:A:429:GLU:HB2	1:A:450:VAL:HB	1.90	0.54
1:E:606:ILE:HG23	1:E:610:ILE:HD12	1.90	0.54
1:B:258:ASP:HB2	1:B:370:ASN:HD22	1.73	0.53
1:C:258:ASP:H	1:C:371:ASP:HB2	1.70	0.53
1:E:166:SER:O	1:E:169:THR:OG1	2.26	0.53
1:F:709:ASN:HA	1:F:732:LYS:HD2	1.89	0.53
2:I:88:PRO:HA	2:I:113:VAL:HB	1.89	0.53
1:C:258:ASP:O	1:C:262:ARG:NH1	2.41	0.53
1:F:576:ASN:HB3	1:F:579:THR:HB	1.91	0.53
1:A:259:ILE:N	1:A:371:ASP:OD2	2.32	0.53
1:C:804:ARG:HH12	1:C:808:GLU:HB3	1.72	0.53
1:D:712:ASN:OD1	1:D:734:ARG:NH2	2.41	0.53
1:E:168:TRP:HH2	1:E:398:SER:HB2	1.73	0.53
1:F:419:ARG:NH1	1:F:431:HIS:O	2.40	0.53
1:A:316:THR:OG1	1:F:115:GLU:OE2	2.26	0.53
1:C:162:LYS:HG3	1:C:243:LEU:HD11	1.91	0.53
1:D:370:ASN:OD1	1:D:370:ASN:N	2.33	0.53
1:A:162:LYS:HG3	1:A:243:LEU:HD11	1.91	0.53
1:D:599:ILE:HG13	1:D:622:LYS:HB3	1.89	0.53
1:A:258:ASP:H	1:A:371:ASP:HB2	1.74	0.53
1:D:356:ILE:HD12	1:D:388:LYS:HG2	1.90	0.53
1:D:646:LEU:O	1:D:649:ASN:ND2	2.42	0.53
2:I:85:SER:O	2:I:87:LYS:NZ	2.41	0.53
1:A:102:ASP:OD1	1:A:102:ASP:N	2.38	0.52
1:A:400:ASN:OD1	1:A:403:ARG:NH1	2.40	0.52
1:E:789:ASP:OD1	1:E:789:ASP:N	2.41	0.52
1:B:452:LYS:HA	1:B:475:TRP:HB2	1.91	0.52
1:B:709:ASN:HA	1:B:732:LYS:HD2	1.90	0.52
1:C:39:ALA:HB2	1:C:129:VAL:HG12	1.90	0.52
1:E:580:LYS:HA	1:E:602:ASP:HB3	1.92	0.52
1:F:322:ALA:O	1:F:326:ILE:HG23	2.09	0.52
1:A:168:TRP:HH2	1:A:398:SER:HB2	1.75	0.52
1:B:647:TRP:HE3	1:B:670:ASN:HD21	1.57	0.52
1:E:46:GLN:O	1:E:50:ASP:HB3	2.10	0.52
1:B:670:ASN:OD1	1:B:670:ASN:N	2.33	0.52
1:C:519:GLU:HG2	1:C:545:ARG:HG3	1.90	0.52
1:D:251:ARG:HH12	1:D:366:PRO:HG2	1.74	0.52
1:F:677:ILE:HD11	1:F:697:LEU:HD13	1.91	0.52
1:F:647:TRP:HE3	1:F:670:ASN:HD21	1.58	0.52
2:G:91:THR:HG23	2:G:112:THR:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:646:LEU:O	1:B:649:ASN:ND2	2.42	0.52
1:C:129:VAL:O	1:C:133:THR:HG23	2.10	0.52
1:E:520:GLU:HG2	1:E:548:VAL:HB	1.92	0.52
1:A:61:THR:O	1:A:64:SER:OG	2.26	0.51
1:C:168:TRP:HH2	1:C:398:SER:HB2	1.75	0.51
1:E:292:ASP:OD1	1:E:292:ASP:N	2.41	0.51
1:E:616:LEU:HB3	1:E:638:LEU:HD23	1.93	0.51
1:C:420:LEU:HD12	1:C:430:LEU:HD13	1.93	0.51
1:E:39:ALA:HB2	1:E:129:VAL:HG12	1.92	0.51
1:E:322:ALA:O	1:E:326:ILE:HG23	2.10	0.51
1:E:413:LEU:HD11	1:E:444:ASP:HB3	1.93	0.51
1:E:767:GLU:OE2	1:F:732:LYS:NZ	2.41	0.51
1:E:400:ASN:OD1	1:E:403:ARG:NH1	2.39	0.51
2:J:28:PRO:HB2	2:J:31:ARG:HD3	1.92	0.51
1:E:61:THR:O	1:E:64:SER:OG	2.23	0.51
1:E:168:TRP:CH2	1:E:398:SER:HB2	2.46	0.51
1:F:408:ASN:ND2	1:F:440:ASP:OD2	2.43	0.51
1:C:594:THR:HA	1:C:616:LEU:HA	1.92	0.50
1:D:777:PRO:HB2	1:D:778:LEU:HD12	1.92	0.50
1:F:235:LYS:O	1:F:239:GLN:HG2	2.11	0.50
1:A:520:GLU:HG2	1:A:548:VAL:HB	1.93	0.50
1:C:171:ARG:HE	1:C:232:LEU:HD11	1.76	0.50
1:C:278:ILE:HA	1:C:281:TYR:CD2	2.47	0.50
1:D:647:TRP:HE3	1:D:670:ASN:HD21	1.57	0.50
1:A:646:LEU:O	1:A:649:ASN:ND2	2.37	0.50
1:A:616:LEU:HB3	1:A:638:LEU:HD23	1.94	0.50
1:F:634:SER:OG	2:L:59:GLU:OE2	2.25	0.50
1:A:46:GLN:O	1:A:50:ASP:HB3	2.11	0.50
1:A:583:VAL:HG23	1:A:584:LEU:H	1.77	0.50
1:E:518:LEU:HB3	1:E:543:LEU:HD22	1.94	0.50
1:F:400:ASN:O	1:F:404:GLN:HG2	2.12	0.50
1:A:600:ARG:HG2	1:A:623:ASP:HB3	1.93	0.50
1:C:789:ASP:OD1	1:C:789:ASP:N	2.43	0.50
1:B:634:SER:OG	2:H:59:GLU:OE2	2.23	0.50
1:A:505:ILE:HD12	1:A:536:VAL:HG11	1.94	0.49
1:B:251:ARG:HD2	1:B:394:LEU:HD11	1.94	0.49
1:B:526:ASN:OD1	1:B:554:ASN:ND2	2.45	0.49
1:C:580:LYS:HA	1:C:602:ASP:HB3	1.93	0.49
1:D:452:LYS:HG2	1:D:475:TRP:CG	2.46	0.49
1:A:760:GLU:HA	1:A:785:VAL:HB	1.93	0.49
1:B:135:ILE:HG12	1:B:274:LYS:HZ2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ALA:O	1:A:326:ILE:HG23	2.12	0.49
1:B:400:ASN:O	1:B:404:GLN:HG2	2.12	0.49
1:B:473:GLU:HG2	1:B:497:ALA:HB3	1.93	0.49
1:C:117:ARG:HG2	1:C:295:CYS:HA	1.94	0.49
1:D:251:ARG:HH22	1:D:366:PRO:HG2	1.77	0.49
1:E:52:MET:HG3	1:E:114:TYR:HD2	1.78	0.49
1:A:509:PRO:HB2	1:A:512:ILE:HG23	1.94	0.49
1:A:804:ARG:HH12	1:A:808:GLU:HB3	1.77	0.49
1:D:518:LEU:HD23	1:D:543:LEU:HD13	1.93	0.49
1:E:22:PRO:HD2	1:E:25:ASP:HB2	1.94	0.49
2:G:85:SER:O	2:G:87:LYS:NZ	2.45	0.49
1:B:677:ILE:HD11	1:B:697:LEU:HD13	1.94	0.49
1:D:526:ASN:OD1	1:D:554:ASN:ND2	2.44	0.49
1:E:746:LEU:HD23	1:E:747:PRO:HD2	1.95	0.49
2:I:91:THR:HG23	2:I:112:THR:HA	1.94	0.49
2:K:20:LEU:HD12	2:K:81:LEU:HD23	1.93	0.49
1:E:171:ARG:HE	1:E:232:LEU:HD11	1.77	0.49
1:F:647:TRP:O	1:F:649:ASN:ND2	2.45	0.49
1:A:666:ARG:HG2	1:A:689:TYR:HB2	1.94	0.49
1:B:647:TRP:O	1:B:649:ASN:ND2	2.46	0.49
1:D:154:GLU:HA	1:D:157:VAL:HG12	1.95	0.49
2:J:22:CYS:HB3	2:J:79:VAL:HB	1.94	0.49
1:E:450:VAL:HG22	1:E:473:GLU:HB2	1.95	0.49
1:A:171:ARG:HE	1:A:232:LEU:HD11	1.78	0.49
1:A:356:ILE:HD12	1:A:388:LYS:HA	1.95	0.49
1:E:666:ARG:HG2	1:E:689:TYR:HB2	1.94	0.49
1:F:154:GLU:HA	1:F:157:VAL:HG12	1.95	0.49
2:G:68:PHE:HB3	2:G:81:LEU:HD11	1.94	0.49
1:A:353:PHE:CE1	1:A:391:ALA:HB2	2.47	0.48
1:D:348:LEU:HD23	1:D:348:LEU:H	1.77	0.48
1:E:583:VAL:HG23	1:E:584:LEU:H	1.78	0.48
2:K:29:VAL:O	2:K:72:ARG:NH1	2.46	0.48
1:A:726:GLU:OE1	1:A:726:GLU:N	2.40	0.48
1:B:343:MET:HG3	1:B:348:LEU:HD21	1.95	0.48
1:E:760:GLU:HA	1:E:785:VAL:HB	1.94	0.48
1:A:278:ILE:HA	1:A:281:TYR:CD2	2.49	0.48
1:A:709:ASN:HA	1:A:732:LYS:HD2	1.94	0.48
1:B:295:CYS:HB2	1:B:297:VAL:HG13	1.95	0.48
1:C:413:LEU:HD11	1:C:444:ASP:HB3	1.95	0.48
1:C:606:ILE:HG23	1:C:610:ILE:HD12	1.95	0.48
1:D:303:THR:OG1	1:D:308:TYR:OH	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:LYS:HA	1:A:475:TRP:HB2	1.94	0.48
1:A:606:ILE:HG23	1:A:610:ILE:HD12	1.96	0.48
1:B:407:LEU:HD11	1:B:439:PRO:HG3	1.95	0.48
1:C:168:TRP:CH2	1:C:398:SER:HB2	2.47	0.48
1:C:450:VAL:HG22	1:C:473:GLU:HB2	1.96	0.48
1:C:547:LYS:HD2	1:C:570:GLN:HG3	1.94	0.48
1:F:590:MET:HE3	1:F:593:LEU:HD22	1.96	0.48
2:G:15:GLY:N	2:G:86:LEU:O	2.41	0.48
2:J:29:VAL:HG22	2:J:72:ARG:HD2	1.94	0.48
1:A:519:GLU:HA	1:A:546:LEU:HA	1.95	0.48
1:B:251:ARG:HH12	1:B:366:PRO:HG2	1.78	0.48
2:L:98:VAL:HG12	2:L:104:TYR:HB2	1.95	0.48
1:A:323:SER:O	1:A:326:ILE:HG12	2.14	0.48
1:B:555:LEU:O	1:B:576:ASN:ND2	2.47	0.48
1:C:169:THR:HG23	1:C:393:PHE:HE2	1.79	0.48
1:E:348:LEU:HB3	1:E:377:HIS:ND1	2.29	0.48
1:E:504:ASP:OD1	1:E:505:ILE:N	2.44	0.48
1:B:475:TRP:HA	1:B:499:HIS:HB2	1.96	0.48
2:K:60:TYR:HB2	2:K:65:LYS:HG3	1.96	0.48
1:B:15:PRO:O	1:B:18:ARG:NH1	2.46	0.48
1:B:118:LEU:HD23	1:B:123:LYS:HG3	1.96	0.48
1:B:520:GLU:OE2	1:B:522:HIS:NE2	2.45	0.48
1:D:400:ASN:O	1:D:404:GLN:HG2	2.14	0.48
1:C:518:LEU:HB3	1:C:543:LEU:HD22	1.95	0.48
1:F:526:ASN:OD1	1:F:554:ASN:ND2	2.47	0.48
1:F:599:ILE:HG13	1:F:622:LYS:HB3	1.95	0.48
2:G:29:VAL:O	2:G:72:ARG:NH1	2.47	0.48
2:G:47:TRP:HE1	2:G:50:ALA:HB2	1.79	0.48
2:J:20:LEU:HD22	2:J:81:LEU:HD23	1.95	0.48
1:B:357:ARG:HD2	1:B:363:SER:HA	1.95	0.48
1:D:135:ILE:HG12	1:D:274:LYS:HZ3	1.79	0.48
1:D:475:TRP:HA	1:D:499:HIS:HB2	1.96	0.48
1:D:475:TRP:HZ3	1:D:477:TYR:HH	1.62	0.48
1:E:353:PHE:CE1	1:E:391:ALA:HB2	2.49	0.48
2:I:6:GLU:OE1	2:I:6:GLU:N	2.46	0.48
1:B:774:GLY:O	1:B:801:ARG:NH2	2.47	0.47
1:F:278:ILE:HA	1:F:281:TYR:CD2	2.48	0.47
1:B:599:ILE:HG13	1:B:622:LYS:HB3	1.96	0.47
1:B:615:ASN:OD1	1:B:640:ARG:NH2	2.47	0.47
1:C:670:ASN:OD1	1:C:670:ASN:N	2.42	0.47
1:D:647:TRP:O	1:D:649:ASN:ND2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:504:ASP:OD2	1:E:506:LYS:NZ	2.45	0.47
1:E:646:LEU:O	1:E:649:ASN:ND2	2.38	0.47
2:J:6:GLU:O	2:J:107:GLN:NE2	2.47	0.47
1:A:168:TRP:CH2	1:A:398:SER:HB2	2.49	0.47
1:C:346:ARG:HB3	1:C:348:LEU:HG	1.97	0.47
1:F:19:ILE:HD11	1:F:157:VAL:HG23	1.95	0.47
1:F:32:SER:HA	1:F:35:MET:HE2	1.95	0.47
1:A:151:SER:O	1:A:154:GLU:HG3	2.15	0.47
1:A:459:VAL:HG23	1:A:481:ALA:HA	1.96	0.47
1:A:665:GLU:HA	1:A:687:LEU:HA	1.96	0.47
1:B:555:LEU:HD13	1:B:559:PRO:HD3	1.96	0.47
1:C:661:LEU:HB3	1:C:664:LEU:HG	1.96	0.47
1:D:272:VAL:HG22	1:D:336:CYS:HB3	1.96	0.47
1:E:169:THR:HG23	1:E:393:PHE:CE2	2.49	0.47
1:E:505:ILE:HD12	1:E:536:VAL:HG11	1.97	0.47
1:F:698:THR:HG23	1:F:699:PHE:HD1	1.79	0.47
1:A:169:THR:HG23	1:A:393:PHE:CE1	2.48	0.47
1:C:233:ASP:O	1:C:236:GLU:HG3	2.14	0.47
1:C:323:SER:O	1:C:326:ILE:HG12	2.14	0.47
1:C:746:LEU:HD23	1:C:747:PRO:HD2	1.97	0.47
1:D:450:VAL:HG22	1:D:473:GLU:HB2	1.95	0.47
1:A:519:GLU:HG2	1:A:545:ARG:HG3	1.97	0.47
1:A:524:THR:HG23	1:A:552:LYS:HD3	1.97	0.47
1:B:272:VAL:HG22	1:B:336:CYS:HB3	1.97	0.47
1:C:505:ILE:HD12	1:C:536:VAL:HG11	1.95	0.47
1:C:666:ARG:HG2	1:C:689:TYR:HB2	1.97	0.47
1:C:782:SER:N	1:C:806:ASP:OD2	2.37	0.47
1:D:19:ILE:HD11	1:D:157:VAL:HG23	1.95	0.47
1:D:431:HIS:HA	1:D:452:LYS:HB2	1.96	0.47
1:E:547:LYS:HD2	1:E:570:GLN:HG3	1.96	0.47
1:E:687:LEU:HD21	1:E:690:LEU:HD13	1.96	0.47
1:F:356:ILE:HD12	1:F:388:LYS:HG2	1.96	0.47
1:F:450:VAL:HG22	1:F:473:GLU:HB2	1.96	0.47
1:F:555:LEU:HD13	1:F:559:PRO:HD3	1.96	0.47
1:F:711:GLN:OE1	1:F:734:ARG:NE	2.38	0.47
2:G:6:GLU:OE1	2:G:6:GLU:N	2.48	0.47
2:L:29:VAL:O	2:L:72:ARG:NH1	2.48	0.47
1:C:739:GLY:O	1:C:741:ASN:ND2	2.48	0.47
1:D:278:ILE:HA	1:D:281:TYR:CD2	2.50	0.47
1:E:661:LEU:HB3	1:E:664:LEU:HG	1.97	0.47
1:C:136:PHE:CE1	1:C:274:LYS:HE3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:278:ILE:HA	1:E:281:TYR:CD2	2.49	0.47
1:E:346:ARG:HB3	1:E:348:LEU:HG	1.97	0.47
2:G:67:ARG:NH2	2:G:90:ASP:OD2	2.47	0.47
1:F:218:ARG:HG2	1:F:223:ILE:HB	1.97	0.47
1:F:290:LYS:HB2	1:F:290:LYS:HE3	1.70	0.47
1:F:733:LEU:HD21	1:F:736:LEU:HD21	1.97	0.47
2:K:35:TYR:HB2	2:K:97:TYR:HB3	1.97	0.47
1:A:129:VAL:O	1:A:133:THR:HG23	2.15	0.46
1:A:368:VAL:HG21	1:A:376:LEU:HD12	1.96	0.46
1:A:450:VAL:HG22	1:A:473:GLU:HB2	1.97	0.46
1:B:591:VAL:O	1:B:615:ASN:ND2	2.39	0.46
1:E:154:GLU:HA	1:E:157:VAL:HG12	1.97	0.46
1:E:356:ILE:HD13	1:E:391:ALA:HB3	1.97	0.46
1:E:665:GLU:OE1	1:E:688:ARG:NE	2.37	0.46
1:F:772:GLU:O	1:F:775:GLU:HG2	2.15	0.46
2:H:32:HIS:O	2:H:72:ARG:NH1	2.48	0.46
1:C:665:GLU:HA	1:C:687:LEU:HA	1.96	0.46
1:D:709:ASN:HA	1:D:732:LYS:HD2	1.96	0.46
1:F:452:LYS:HG2	1:F:475:TRP:CG	2.50	0.46
1:F:771:VAL:HG23	1:F:795:PRO:HG2	1.97	0.46
2:K:68:PHE:HB3	2:K:81:LEU:HD11	1.97	0.46
1:C:685:ARG:HE	1:C:706:LEU:HB3	1.80	0.46
1:D:38:ILE:HD11	1:D:325:TYR:HD1	1.81	0.46
1:F:168:TRP:CZ3	1:F:172:ALA:HB2	2.50	0.46
2:H:91:THR:HG23	2:H:112:THR:HA	1.98	0.46
2:I:4:LEU:HD11	2:I:98:VAL:HG12	1.97	0.46
1:A:661:LEU:HB3	1:A:664:LEU:HG	1.97	0.46
1:B:154:GLU:HA	1:B:157:VAL:HG12	1.98	0.46
2:I:15:GLY:HA2	2:I:85:SER:HA	1.97	0.46
1:A:580:LYS:HA	1:A:602:ASP:HB3	1.98	0.46
1:A:594:THR:HA	1:A:616:LEU:HA	1.97	0.46
1:A:622:LYS:HB2	1:A:647:TRP:NE1	2.30	0.46
1:D:159:ILE:HA	1:D:162:LYS:HG2	1.98	0.46
1:E:739:GLY:O	1:E:741:ASN:ND2	2.49	0.46
2:K:15:GLY:HA2	2:K:85:SER:HA	1.97	0.46
1:A:233:ASP:O	1:A:236:GLU:HG3	2.16	0.46
1:B:19:ILE:HD11	1:B:157:VAL:HG23	1.96	0.46
1:B:56:PRO:HG2	1:B:99:TYR:CD1	2.51	0.46
1:D:168:TRP:CZ3	1:D:172:ALA:HB2	2.51	0.46
1:E:294:ASP:OD1	1:E:309:ARG:NH1	2.47	0.46
2:K:47:TRP:HE1	2:K:50:ALA:HB2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:73:ASP:OD1	2:L:73:ASP:N	2.48	0.46
1:A:566:GLY:HA2	1:A:569:LEU:HD12	1.97	0.46
1:A:782:SER:N	1:A:806:ASP:OD2	2.47	0.46
1:C:583:VAL:HG23	1:C:584:LEU:H	1.81	0.46
1:C:627:LYS:HG2	1:C:650:HIS:HB2	1.98	0.46
2:K:73:ASP:OD1	2:K:78:THR:OG1	2.28	0.46
1:B:46:GLN:NE2	1:B:114:TYR:OH	2.48	0.46
2:I:96:CYS:O	2:I:106:GLY:N	2.48	0.46
2:K:6:GLU:OE2	2:K:96:CYS:N	2.43	0.46
1:E:357:ARG:HB2	1:E:362:TYR:O	2.16	0.46
1:F:489:ALA:O	1:F:493:GLU:HG2	2.16	0.46
2:I:47:TRP:HE1	2:I:50:ALA:HB2	1.81	0.46
1:B:168:TRP:CZ3	1:B:172:ALA:HB2	2.51	0.46
1:D:537:ILE:HG13	1:D:561:VAL:HG11	1.98	0.46
1:F:520:GLU:OE2	1:F:522:HIS:NE2	2.46	0.46
1:F:595:GLU:HG2	1:F:618:GLU:HB2	1.97	0.46
2:J:98:VAL:HG12	2:J:104:TYR:HB2	1.98	0.46
2:K:6:GLU:N	2:K:6:GLU:OE1	2.48	0.46
1:B:152:LYS:NZ	1:B:257:GLY:HA3	2.30	0.45
1:B:729:GLN:OE1	1:B:749:ARG:NH2	2.41	0.45
1:C:243:LEU:HD23	1:C:393:PHE:CZ	2.52	0.45
1:C:251:ARG:O	1:C:255:GLU:HB2	2.15	0.45
1:E:159:ILE:O	1:E:162:LYS:HG2	2.17	0.45
2:K:88:PRO:HA	2:K:113:VAL:HB	1.97	0.45
1:E:243:LEU:HD23	1:E:393:PHE:CZ	2.50	0.45
1:E:323:SER:O	1:E:326:ILE:HG12	2.14	0.45
1:A:56:PRO:HG2	1:A:99:TYR:CD1	2.51	0.45
1:B:278:ILE:HA	1:B:281:TYR:CD2	2.51	0.45
1:E:233:ASP:O	1:E:236:GLU:HG3	2.15	0.45
1:A:504:ASP:OD1	1:A:505:ILE:N	2.45	0.45
1:D:634:SER:OG	2:J:59:GLU:OE2	2.25	0.45
1:E:511:TRP:O	1:E:514:SER:OG	2.29	0.45
1:F:461:ILE:HB	1:F:483:ILE:HG13	1.98	0.45
1:A:173:LEU:O	1:A:176:THR:OG1	2.34	0.45
1:A:611:PHE:CE1	1:A:634:SER:HB2	2.52	0.45
1:B:537:ILE:HG13	1:B:561:VAL:HG11	1.98	0.45
1:B:710:LEU:HD21	1:B:713:LEU:HB2	1.99	0.45
1:D:290:LYS:HB2	1:D:290:LYS:HE3	1.68	0.45
1:D:395:SER:HG	1:D:398:SER:HG	1.65	0.45
1:D:555:LEU:HD13	1:D:559:PRO:HD3	1.97	0.45
1:E:154:GLU:HG3	1:E:155:HIS:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:543:LEU:HD13	1:C:546:LEU:HD13	1.98	0.45
1:C:780:LYS:HD2	1:C:806:ASP:HA	1.98	0.45
1:A:159:ILE:O	1:A:162:LYS:HG2	2.17	0.45
1:A:546:LEU:HB3	1:A:568:HIS:HE1	1.82	0.45
1:B:499:HIS:NE2	1:B:522:HIS:HD2	2.14	0.45
1:C:356:ILE:HD12	1:C:388:LYS:HA	1.99	0.45
1:F:248:LYS:NZ	1:F:399:GLU:OE2	2.36	0.45
1:F:669:LEU:O	1:F:672:ASN:ND2	2.50	0.45
1:A:543:LEU:HD13	1:A:546:LEU:HD13	1.99	0.45
1:A:547:LYS:HD2	1:A:570:GLN:HG3	1.99	0.45
1:F:431:HIS:HA	1:F:452:LYS:HB2	1.99	0.45
1:B:159:ILE:HA	1:B:162:LYS:HG2	1.99	0.45
1:B:772:GLU:O	1:B:775:GLU:HG2	2.17	0.45
1:B:492:ARG:NH2	1:B:516:LYS:HD2	2.32	0.45
1:C:500:ILE:HB	1:C:523:LEU:HD23	1.98	0.45
1:C:605:ARG:HD2	2:I:54:TYR:CZ	2.52	0.45
1:D:495:LEU:HD23	1:D:515:LEU:HD13	1.97	0.45
1:D:590:MET:HE3	1:D:593:LEU:HD22	1.99	0.45
1:D:715:VAL:O	1:D:718:ASN:ND2	2.50	0.45
2:L:53:SER:HA	2:L:72:ARG:HH2	1.82	0.45
1:A:348:LEU:HB3	1:A:377:HIS:ND1	2.32	0.44
1:C:772:GLU:O	1:C:775:GLU:HG2	2.17	0.44
1:D:771:VAL:HG23	1:D:795:PRO:HG2	1.99	0.44
1:E:782:SER:N	1:E:806:ASP:OD2	2.42	0.44
2:I:40:ALA:HB3	2:I:43:LYS:HD2	1.99	0.44
1:C:290:LYS:HE3	1:C:290:LYS:HB2	1.69	0.44
1:C:461:ILE:HB	1:C:483:ILE:HG13	1.99	0.44
1:D:772:GLU:O	1:D:775:GLU:HG2	2.17	0.44
1:F:159:ILE:HA	1:F:162:LYS:HG2	1.99	0.44
1:F:425:GLN:N	1:F:425:GLN:OE1	2.50	0.44
2:G:88:PRO:HA	2:G:113:VAL:HB	2.00	0.44
2:H:87:LYS:N	2:H:90:ASP:OD2	2.39	0.44
1:E:169:THR:HG23	1:E:393:PHE:HE2	1.83	0.44
1:F:152:LYS:NZ	1:F:257:GLY:HA3	2.33	0.44
2:K:15:GLY:N	2:K:86:LEU:O	2.49	0.44
1:A:704:ILE:HD13	1:A:727:LEU:HD13	2.00	0.44
1:A:746:LEU:HD23	1:A:747:PRO:HD2	1.99	0.44
1:B:354:GLU:O	1:B:358:GLU:HB2	2.18	0.44
1:E:627:LYS:HG2	1:E:650:HIS:HB2	2.00	0.44
1:F:135:ILE:HG12	1:F:274:LYS:HZ3	1.82	0.44
1:C:56:PRO:HG2	1:C:99:TYR:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:PHE:CE1	1:C:465:ILE:HG22	2.53	0.44
1:D:669:LEU:O	1:D:672:ASN:ND2	2.50	0.44
1:E:791:PHE:CE2	1:E:799:LYS:HE3	2.52	0.44
2:H:73:ASP:N	2:H:73:ASP:OD1	2.50	0.44
2:H:73:ASP:OD1	2:H:78:THR:OG1	2.30	0.44
1:A:518:LEU:HB3	1:A:543:LEU:HD22	2.00	0.44
1:F:593:LEU:HD23	1:F:613:LEU:HD13	1.99	0.44
1:F:603:LEU:HD13	1:F:607:PRO:HD3	2.00	0.44
1:A:413:LEU:HD11	1:A:444:ASP:HB3	1.98	0.44
1:B:109:VAL:HG21	1:B:308:TYR:CE2	2.52	0.44
1:B:502:PHE:CE1	1:B:508:ILE:HD11	2.52	0.44
1:B:728:PHE:HA	1:B:753:LEU:HD21	1.99	0.44
1:D:663:ASN:HA	1:D:686:LYS:HD2	1.99	0.44
1:E:56:PRO:HG2	1:E:99:TYR:CD1	2.53	0.44
1:F:19:ILE:HD12	1:F:379:ILE:HD11	1.98	0.44
1:B:135:ILE:HG23	1:B:274:LYS:NZ	2.33	0.44
1:E:620:ASP:HA	1:E:645:LYS:HB2	1.99	0.44
1:A:154:GLU:HA	1:A:157:VAL:HG12	2.00	0.44
1:A:500:ILE:HB	1:A:523:LEU:HD23	1.99	0.44
1:A:622:LYS:HB2	1:A:647:TRP:HE1	1.83	0.44
1:B:425:GLN:N	1:B:425:GLN:OE1	2.51	0.44
1:C:353:PHE:CE1	1:C:391:ALA:HB2	2.53	0.44
1:C:791:PHE:CE2	1:C:799:LYS:HE3	2.53	0.44
1:D:780:LYS:HG2	1:D:805:ALA:HB1	1.99	0.44
2:H:5:VAL:HG23	2:H:107:GLN:HG2	1.99	0.44
2:L:36:TRP:CE2	2:L:81:LEU:HB2	2.52	0.44
1:A:356:ILE:HD13	1:A:391:ALA:HB3	2.00	0.43
1:A:728:PHE:O	1:A:731:ARG:NH1	2.50	0.43
1:E:356:ILE:HD12	1:E:388:LYS:HA	2.00	0.43
1:F:251:ARG:HH12	1:F:366:PRO:HG2	1.82	0.43
2:G:15:GLY:HA2	2:G:85:SER:HA	2.00	0.43
1:F:56:PRO:HG2	1:F:99:TYR:CD1	2.54	0.43
1:F:468:LEU:HB3	1:F:471:LEU:HB2	1.99	0.43
1:F:475:TRP:HA	1:F:499:HIS:HB2	1.99	0.43
1:F:781:ARG:HH12	1:F:786:VAL:HG12	1.83	0.43
2:L:22:CYS:HB2	2:L:36:TRP:CH2	2.52	0.43
1:C:322:ALA:O	1:C:326:ILE:HG23	2.17	0.43
1:C:587:LEU:HD21	1:C:596:LEU:HD21	2.00	0.43
1:D:647:TRP:CD1	1:D:647:TRP:N	2.85	0.43
2:L:2:VAL:HG21	2:L:100:VAL:HG21	2.00	0.43
1:C:52:MET:HG3	1:C:114:TYR:HD2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:LEU:HB3	1:C:377:HIS:ND1	2.34	0.43
1:D:56:PRO:HG2	1:D:99:TYR:CD1	2.53	0.43
1:D:248:LYS:NZ	1:D:399:GLU:OE2	2.39	0.43
1:F:647:TRP:N	1:F:647:TRP:CD1	2.85	0.43
1:B:685:ARG:HH21	1:B:706:LEU:HD13	1.83	0.43
1:B:800:GLU:OE1	1:C:688:ARG:NH1	2.49	0.43
1:D:135:ILE:HD13	1:D:274:LYS:HD3	2.00	0.43
1:D:235:LYS:O	1:D:239:GLN:HG2	2.19	0.43
1:F:129:VAL:HG13	1:F:325:TYR:CE1	2.53	0.43
2:H:69:THR:HB	2:H:82:GLN:HB3	2.00	0.43
1:B:160:LEU:HD11	1:B:386:TYR:HB3	2.01	0.43
1:B:734:ARG:O	1:B:757:THR:N	2.44	0.43
1:E:780:LYS:HD2	1:E:806:ASP:HA	2.00	0.43
1:B:647:TRP:CD1	1:B:647:TRP:N	2.86	0.43
1:B:797:GLU:HG2	1:C:688:ARG:HD3	2.01	0.43
1:C:296:THR:HG23	1:C:307:THR:HG22	2.00	0.43
1:C:452:LYS:HE2	1:C:475:TRP:CZ3	2.54	0.43
1:C:520:GLU:HG2	1:C:548:VAL:HB	1.99	0.43
1:D:115:GLU:OE2	1:E:316:THR:OG1	2.32	0.43
1:D:510:LEU:HD12	1:D:510:LEU:HA	1.83	0.43
1:E:129:VAL:HG13	1:E:325:TYR:CE1	2.54	0.43
1:F:728:PHE:HA	1:F:753:LEU:HD21	2.00	0.43
1:B:679:THR:OG1	1:B:703:ASP:OD2	2.31	0.43
1:B:780:LYS:HG2	1:B:805:ALA:HB1	1.99	0.43
1:D:670:ASN:OD1	1:D:670:ASN:N	2.34	0.43
1:B:290:LYS:HE3	1:B:290:LYS:HB2	1.76	0.43
1:B:419:ARG:NH1	1:B:431:HIS:O	2.51	0.43
1:F:685:ARG:HH21	1:F:706:LEU:HD13	1.84	0.43
1:A:698:THR:HG22	1:A:719:ARG:HB2	2.01	0.42
1:C:400:ASN:OD1	1:C:403:ARG:NH1	2.52	0.42
1:C:519:GLU:HA	1:C:546:LEU:HA	2.01	0.42
2:G:87:LYS:HB3	2:G:89:GLU:OE1	2.19	0.42
1:A:173:LEU:HD13	1:A:173:LEU:HA	1.89	0.42
1:A:235:LYS:O	1:A:239:GLN:HG2	2.19	0.42
1:B:348:LEU:H	1:B:348:LEU:HD23	1.83	0.42
1:B:499:HIS:CE1	1:B:522:HIS:HD2	2.37	0.42
1:C:169:THR:HG23	1:C:393:PHE:CE2	2.53	0.42
1:C:302:LEU:HD11	1:D:309:ARG:HD3	2.01	0.42
1:C:616:LEU:HB3	1:C:638:LEU:HD23	2.00	0.42
1:D:132:HIS:HA	1:D:135:ILE:HG22	2.01	0.42
1:D:223:ILE:HA	1:D:483:ILE:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:PHE:CE1	1:D:333:GLY:HA3	2.54	0.42
1:F:348:LEU:HD23	1:F:348:LEU:H	1.84	0.42
1:F:679:THR:OG1	1:F:703:ASP:OD2	2.33	0.42
1:B:35:MET:HE3	1:B:133:THR:HG22	2.01	0.42
1:B:669:LEU:O	1:B:672:ASN:ND2	2.53	0.42
1:F:278:ILE:HA	1:F:281:TYR:HD2	1.84	0.42
1:F:422:LYS:HG2	1:F:428:LEU:HD23	2.01	0.42
1:B:117:ARG:HG2	1:B:295:CYS:HA	2.00	0.42
1:B:235:LYS:O	1:B:239:GLN:HG2	2.20	0.42
1:B:275:PHE:CE1	1:B:333:GLY:HA3	2.54	0.42
1:B:768:CYS:HB2	1:B:793:THR:HG21	2.01	0.42
1:C:430:LEU:HB3	1:C:448:LEU:HD21	2.02	0.42
1:C:450:VAL:HG13	1:C:473:GLU:HB2	2.01	0.42
1:F:715:VAL:O	1:F:718:ASN:ND2	2.50	0.42
1:A:270:ILE:O	1:A:273:ILE:HG13	2.19	0.42
1:A:443:PHE:CE1	1:A:465:ILE:HG22	2.55	0.42
1:B:510:LEU:HD12	1:B:510:LEU:HA	1.82	0.42
1:C:710:LEU:HG	1:C:733:LEU:HD13	2.02	0.42
1:D:531:ASN:H	1:D:533:ARG:NH2	2.16	0.42
1:E:109:VAL:HG21	1:E:308:TYR:CE2	2.54	0.42
2:H:28:PRO:HG2	2:H:31:ARG:HB2	2.01	0.42
1:A:407:LEU:HD12	1:A:407:LEU:HA	1.87	0.42
1:C:115:GLU:OE2	1:D:316:THR:OG1	2.38	0.42
1:D:135:ILE:HG23	1:D:274:LYS:NZ	2.34	0.42
1:E:243:LEU:HD12	1:E:243:LEU:HA	1.85	0.42
1:E:297:VAL:HG23	1:E:299:ILE:HG12	2.01	0.42
1:E:709:ASN:HA	1:E:732:LYS:HD2	2.01	0.42
1:D:520:GLU:OE2	1:D:522:HIS:NE2	2.34	0.42
1:D:733:LEU:HD21	1:D:736:LEU:HD21	2.00	0.42
1:E:136:PHE:CE1	1:E:274:LYS:HE3	2.55	0.42
1:E:259:ILE:N	1:E:371:ASP:OD2	2.38	0.42
1:E:420:LEU:HD12	1:E:430:LEU:HD13	2.00	0.42
1:E:575:ASN:HA	1:E:599:ILE:O	2.20	0.42
1:F:441:THR:O	1:F:441:THR:OG1	2.38	0.42
1:B:452:LYS:HG2	1:B:475:TRP:CG	2.54	0.42
1:C:431:HIS:HA	1:C:452:LYS:HB2	2.01	0.42
1:D:147:PRO:HA	1:D:150:SER:HB3	2.00	0.42
1:D:774:GLY:O	1:D:801:ARG:NH2	2.53	0.42
1:E:303:THR:OG1	1:E:308:TYR:OH	2.30	0.42
1:F:648:TYR:CE2	1:F:671:ARG:HG3	2.55	0.42
1:A:149:THR:O	1:A:153:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:600:ARG:HG2	1:E:623:ASP:HB3	2.02	0.42
1:B:52:MET:HG3	1:B:114:TYR:HD2	1.84	0.42
1:D:600:ARG:HG2	1:D:623:ASP:CB	2.50	0.42
1:F:275:PHE:CE1	1:F:333:GLY:HA3	2.55	0.42
1:F:500:ILE:HG21	1:F:508:ILE:HG12	2.02	0.42
2:J:91:THR:HG23	2:J:112:THR:HA	2.02	0.42
1:A:585:ASN:OD1	1:A:588:LYS:NZ	2.31	0.41
1:C:154:GLU:HA	1:C:157:VAL:HG12	2.01	0.41
1:F:135:ILE:HG23	1:F:274:LYS:NZ	2.35	0.41
1:F:311:ALA:O	1:F:313:PRO:HD3	2.20	0.41
1:F:780:LYS:HG2	1:F:805:ALA:HB1	2.02	0.41
2:G:73:ASP:OD1	2:G:73:ASP:N	2.53	0.41
1:A:290:LYS:HE3	1:A:290:LYS:HB2	1.66	0.41
1:A:791:PHE:CE2	1:A:799:LYS:HE3	2.54	0.41
1:B:715:VAL:O	1:B:718:ASN:ND2	2.53	0.41
1:D:233:ASP:OD1	1:D:234:LYS:N	2.54	0.41
1:E:443:PHE:CE1	1:E:465:ILE:HG22	2.55	0.41
1:F:531:ASN:H	1:F:533:ARG:NH2	2.19	0.41
2:L:22:CYS:HB3	2:L:79:VAL:HB	2.01	0.41
1:C:41:PHE:O	1:C:44:THR:HG22	2.20	0.41
1:C:311:ALA:O	1:C:313:PRO:HD3	2.20	0.41
1:E:476:LEU:HB2	1:E:500:ILE:HD13	2.01	0.41
1:A:316:THR:O	1:A:320:ILE:HG12	2.20	0.41
1:A:780:LYS:HD2	1:A:806:ASP:HA	2.02	0.41
1:B:648:TYR:CE2	1:B:671:ARG:HG3	2.56	0.41
1:C:159:ILE:O	1:C:162:LYS:HG2	2.20	0.41
1:C:575:ASN:HA	1:C:599:ILE:O	2.20	0.41
1:E:290:LYS:HB2	1:E:290:LYS:HE3	1.68	0.41
1:E:430:LEU:HB3	1:E:448:LEU:HD21	2.02	0.41
1:E:527:LEU:HG	1:E:553:SER:HB3	2.02	0.41
1:F:19:ILE:HG13	1:F:20:LEU:HD22	2.02	0.41
2:G:40:ALA:HB3	2:G:43:LYS:HD2	2.03	0.41
1:A:34:VAL:O	1:A:38:ILE:HG23	2.20	0.41
1:A:500:ILE:HG22	1:A:502:PHE:HD1	1.85	0.41
1:B:439:PRO:HB2	1:B:442:VAL:HG13	2.03	0.41
1:E:173:LEU:HD13	1:E:173:LEU:HA	1.89	0.41
1:E:251:ARG:O	1:E:255:GLU:HB2	2.21	0.41
1:E:270:ILE:O	1:E:273:ILE:HG13	2.20	0.41
1:F:529:ALA:O	1:F:533:ARG:HB3	2.20	0.41
2:H:36:TRP:CE2	2:H:81:LEU:HB2	2.55	0.41
1:A:302:LEU:HD11	1:B:309:ARG:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:GLU:OE2	1:D:306:ARG:NH1	2.52	0.41
1:D:509:PRO:HB3	1:D:511:TRP:NE1	2.35	0.41
1:E:736:LEU:HD23	1:E:736:LEU:HA	1.90	0.41
1:F:710:LEU:HD21	1:F:713:LEU:HB2	2.02	0.41
1:A:710:LEU:HG	1:A:733:LEU:HD13	2.03	0.41
1:B:297:VAL:HG23	1:B:299:ILE:HG12	2.03	0.41
1:C:243:LEU:HD12	1:C:243:LEU:HA	1.86	0.41
1:C:255:GLU:HG2	1:C:369:LYS:HB2	2.02	0.41
1:F:109:VAL:HG21	1:F:308:TYR:CE2	2.55	0.41
1:F:151:SER:O	1:F:154:GLU:HG3	2.20	0.41
1:A:164:PHE:O	1:A:389:ARG:NH1	2.53	0.41
1:A:611:PHE:CD1	1:A:634:SER:HB2	2.56	0.41
1:A:687:LEU:HD21	1:A:690:LEU:HD13	2.02	0.41
1:D:364:ASP:HB2	1:D:397:VAL:HG23	2.03	0.41
1:B:468:LEU:HB3	1:B:471:LEU:HB2	2.03	0.41
1:B:489:ALA:O	1:B:493:GLU:HG2	2.21	0.41
1:B:649:ASN:HB2	1:B:651:ILE:HG13	2.03	0.41
1:C:704:ILE:HD13	1:C:727:LEU:HD13	2.02	0.41
1:D:413:LEU:HD12	1:D:413:LEU:HA	1.91	0.41
1:D:588:LYS:HE2	1:D:588:LYS:HB3	1.96	0.41
1:D:648:TYR:CE1	1:D:671:ARG:HG3	2.56	0.41
1:E:500:ILE:HB	1:E:523:LEU:HD23	2.02	0.41
1:E:594:THR:HA	1:E:616:LEU:HA	2.02	0.41
1:E:772:GLU:O	1:E:775:GLU:HG2	2.20	0.41
1:F:233:ASP:OD1	1:F:234:LYS:N	2.54	0.41
1:F:354:GLU:O	1:F:358:GLU:HB2	2.21	0.41
1:F:357:ARG:HD2	1:F:363:SER:HA	2.01	0.41
2:L:17:SER:HB3	2:L:82:GLN:NE2	2.36	0.41
1:A:685:ARG:HE	1:A:706:LEU:HB3	1.84	0.41
1:B:233:ASP:OD1	1:B:234:LYS:N	2.54	0.41
1:B:518:LEU:HD23	1:B:543:LEU:HD13	2.02	0.41
1:D:502:PHE:CE1	1:D:508:ILE:HD11	2.56	0.40
2:K:40:ALA:HB3	2:K:43:LYS:HB3	2.03	0.40
1:A:377:HIS:O	1:A:381:GLN:HG2	2.21	0.40
1:A:420:LEU:HD12	1:A:430:LEU:HD13	2.03	0.40
1:A:688:ARG:HD3	1:F:797:GLU:HG2	2.03	0.40
1:C:263:LEU:HD23	1:C:263:LEU:HA	1.85	0.40
1:C:270:ILE:O	1:C:273:ILE:HG13	2.21	0.40
1:E:422:LYS:HE2	1:E:422:LYS:HB3	1.85	0.40
1:E:519:GLU:HA	1:E:546:LEU:HA	2.02	0.40
1:F:135:ILE:HD13	1:F:274:LYS:HD3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:575:ASN:HA	1:F:599:ILE:O	2.20	0.40
2:K:34:MET:HG3	2:K:79:VAL:HG21	2.02	0.40
1:B:294:ASP:OD1	1:B:309:ARG:NH1	2.54	0.40
1:D:129:VAL:HG13	1:D:325:TYR:CE1	2.56	0.40
1:D:354:GLU:O	1:D:358:GLU:HB2	2.21	0.40
1:E:316:THR:O	1:E:320:ILE:HG12	2.21	0.40
1:F:453:LEU:HD22	1:F:456:ILE:HD12	2.02	0.40
2:K:40:ALA:HB3	2:K:43:LYS:HD2	2.04	0.40
1:B:151:SER:O	1:B:154:GLU:HG3	2.20	0.40
1:C:250:PHE:CZ	1:C:254:VAL:HG21	2.57	0.40
1:C:303:THR:HG1	1:C:308:TYR:HH	1.63	0.40
1:C:611:PHE:CE1	1:C:634:SER:HB2	2.56	0.40
1:D:551:LEU:HD11	1:D:562:VAL:HG21	2.02	0.40
1:E:670:ASN:OD1	1:E:670:ASN:N	2.40	0.40
1:E:704:ILE:HD13	1:E:727:LEU:HD13	2.03	0.40
1:F:52:MET:HG3	1:F:114:TYR:HB2	2.04	0.40
1:F:223:ILE:HA	1:F:483:ILE:O	2.20	0.40
1:A:688:ARG:NH1	1:F:800:GLU:OE1	2.55	0.40
1:B:356:ILE:HD12	1:B:388:LYS:HG2	2.03	0.40
1:B:631:GLU:HG3	2:H:52:TYR:CE2	2.57	0.40
1:C:129:VAL:HG13	1:C:325:TYR:CE1	2.56	0.40
1:C:622:LYS:HB2	1:C:647:TRP:NE1	2.36	0.40
1:D:160:LEU:HD11	1:D:386:TYR:HB3	2.04	0.40
1:F:794:LEU:O	1:F:799:LYS:NZ	2.55	0.40
2:I:15:GLY:N	2:I:86:LEU:O	2.52	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	712/810 (88%)	687 (96%)	25 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	726/810 (90%)	699 (96%)	27 (4%)	0	100	100
1	C	712/810 (88%)	685 (96%)	27 (4%)	0	100	100
1	D	726/810 (90%)	700 (96%)	26 (4%)	0	100	100
1	E	712/810 (88%)	687 (96%)	25 (4%)	0	100	100
1	F	726/810 (90%)	699 (96%)	27 (4%)	0	100	100
2	G	112/144 (78%)	111 (99%)	1 (1%)	0	100	100
2	H	112/144 (78%)	109 (97%)	3 (3%)	0	100	100
2	I	112/144 (78%)	109 (97%)	3 (3%)	0	100	100
2	J	112/144 (78%)	110 (98%)	2 (2%)	0	100	100
2	K	112/144 (78%)	109 (97%)	3 (3%)	0	100	100
2	L	112/144 (78%)	110 (98%)	2 (2%)	0	100	100
All	All	4986/5724 (87%)	4815 (97%)	171 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	666/749 (89%)	644 (97%)	22 (3%)	38	67
1	B	678/749 (90%)	650 (96%)	28 (4%)	30	61
1	C	666/749 (89%)	638 (96%)	28 (4%)	30	60
1	D	678/749 (90%)	655 (97%)	23 (3%)	37	67
1	E	666/749 (89%)	637 (96%)	29 (4%)	28	58
1	F	678/749 (90%)	653 (96%)	25 (4%)	34	64
2	G	92/116 (79%)	92 (100%)	0	100	100
2	H	92/116 (79%)	89 (97%)	3 (3%)	38	67
2	I	92/116 (79%)	91 (99%)	1 (1%)	73	88
2	J	92/116 (79%)	90 (98%)	2 (2%)	52	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	92/116 (79%)	91 (99%)	1 (1%)	73	88
2	L	92/116 (79%)	89 (97%)	3 (3%)	38	67
All	All	4584/5190 (88%)	4419 (96%)	165 (4%)	38	65

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	ASP
1	A	110	ASP
1	A	143	TRP
1	A	169	THR
1	A	263	LEU
1	A	275	PHE
1	A	292	ASP
1	A	295	CYS
1	A	297	VAL
1	A	300	GLU
1	A	348	LEU
1	A	353	PHE
1	A	354	GLU
1	A	368	VAL
1	A	372	PHE
1	A	402	LEU
1	A	413	LEU
1	A	429	GLU
1	A	441	THR
1	A	456	ILE
1	A	460	THR
1	A	647	TRP
1	B	110	ASP
1	B	136	PHE
1	B	143	TRP
1	B	168	TRP
1	B	220	GLU
1	B	229	THR
1	B	236	GLU
1	B	275	PHE
1	B	279	ILE
1	B	281	TYR
1	B	292	ASP
1	B	295	CYS

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Mol	Chain	Res	Type
1	B	300	GLU
1	B	317	LEU
1	B	348	LEU
1	B	353	PHE
1	B	356	ILE
1	B	370	ASN
1	B	407	LEU
1	B	441	THR
1	B	458	ASP
1	B	459	VAL
1	B	584	LEU
1	B	644	LEU
1	B	647	TRP
1	B	670	ASN
1	B	698	THR
1	B	793	THR
1	C	110	ASP
1	C	136	PHE
1	C	143	TRP
1	C	169	THR
1	C	263	LEU
1	C	275	PHE
1	C	281	TYR
1	C	295	CYS
1	C	300	GLU
1	C	317	LEU
1	C	348	LEU
1	C	353	PHE
1	C	354	GLU
1	C	368	VAL
1	C	372	PHE
1	C	402	LEU
1	C	413	LEU
1	C	429	GLU
1	C	441	THR
1	C	444	ASP
1	C	456	ILE
1	C	460	THR
1	C	536	VAL
1	C	542	GLU
1	C	583	VAL
1	C	647	TRP

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Mol	Chain	Res	Type
1	C	685	ARG
1	C	746	LEU
1	D	110	ASP
1	D	143	TRP
1	D	168	TRP
1	D	220	GLU
1	D	229	THR
1	D	231	VAL
1	D	236	GLU
1	D	275	PHE
1	D	279	ILE
1	D	281	TYR
1	D	295	CYS
1	D	297	VAL
1	D	317	LEU
1	D	348	LEU
1	D	353	PHE
1	D	356	ILE
1	D	370	ASN
1	D	441	THR
1	D	458	ASP
1	D	584	LEU
1	D	647	TRP
1	D	670	ASN
1	D	793	THR
1	E	25	ASP
1	E	48	THR
1	E	110	ASP
1	E	143	TRP
1	E	154	GLU
1	E	169	THR
1	E	263	LEU
1	E	275	PHE
1	E	279	ILE
1	E	281	TYR
1	E	292	ASP
1	E	295	CYS
1	E	300	GLU
1	E	317	LEU
1	E	348	LEU
1	E	353	PHE
1	E	354	GLU

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Mol	Chain	Res	Type
1	E	368	VAL
1	E	372	PHE
1	E	402	LEU
1	E	413	LEU
1	E	429	GLU
1	E	441	THR
1	E	536	VAL
1	E	647	TRP
1	E	670	ASN
1	E	685	ARG
1	E	712	ASN
1	E	746	LEU
1	F	110	ASP
1	F	143	TRP
1	F	168	TRP
1	F	220	GLU
1	F	224	VAL
1	F	229	THR
1	F	275	PHE
1	F	279	ILE
1	F	281	TYR
1	F	295	CYS
1	F	300	GLU
1	F	317	LEU
1	F	348	LEU
1	F	353	PHE
1	F	356	ILE
1	F	370	ASN
1	F	392	VAL
1	F	393	PHE
1	F	441	THR
1	F	458	ASP
1	F	459	VAL
1	F	584	LEU
1	F	647	TRP
1	F	670	ASN
1	F	793	THR
2	H	5	VAL
2	H	100	VAL
2	H	109	THR
2	I	5	VAL
2	J	5	VAL

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Mol	Chain	Res	Type
2	J	109	THR
2	K	79	VAL
2	L	5	VAL
2	L	100	VAL
2	L	109	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	708	GLN
1	B	554	ASN
1	C	287	HIS
1	C	288	ASN
1	C	381	GLN
1	F	554	ASN
2	L	110	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 monosaccharides 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

There are no chain breaks in this entry.

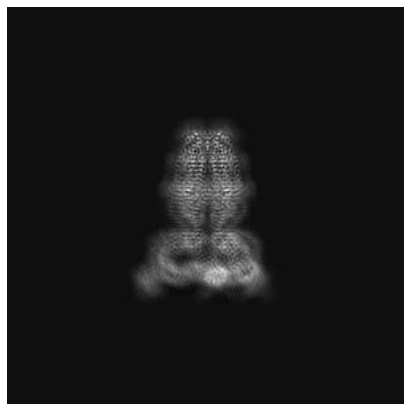
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13202. These allow visual inspection of the internal detail of the map and identification of artifacts.

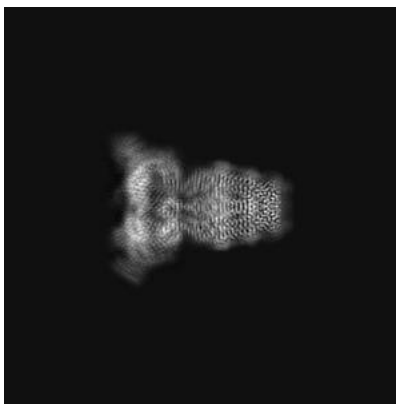
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

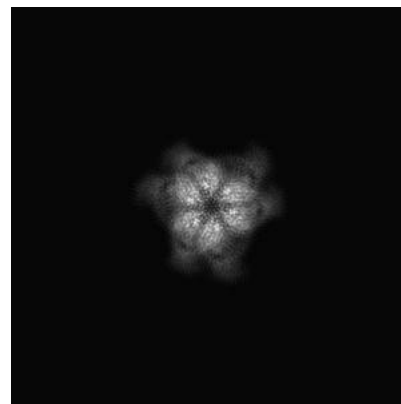
6.1.1 Primary map



X

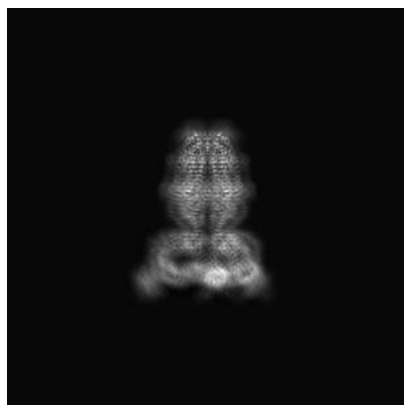


Y

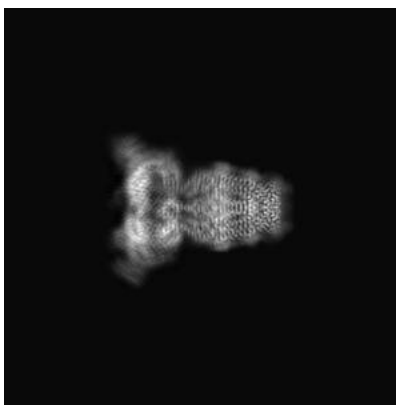


Z

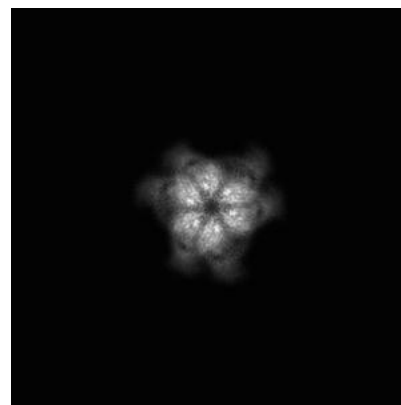
6.1.2 Raw map



X



Y



Z

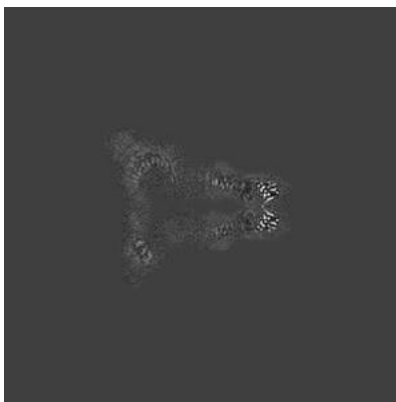
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

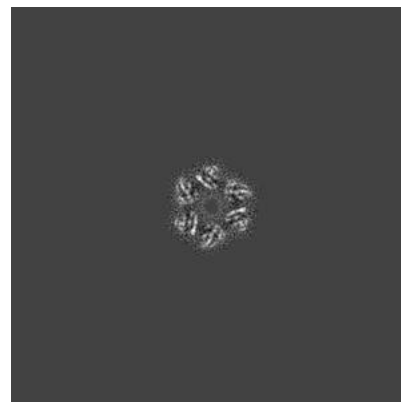
6.2.1 Primary map



X Index: 168



Y Index: 168

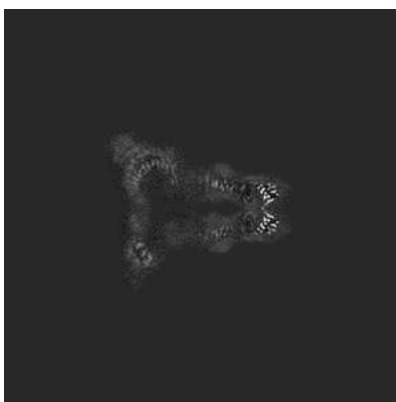


Z Index: 168

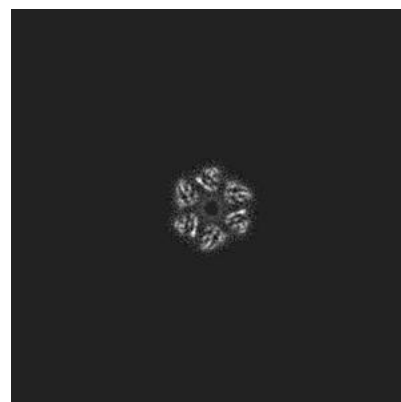
6.2.2 Raw map



X Index: 168



Y Index: 168



Z Index: 168

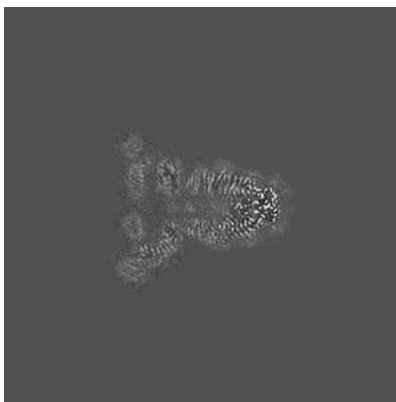
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

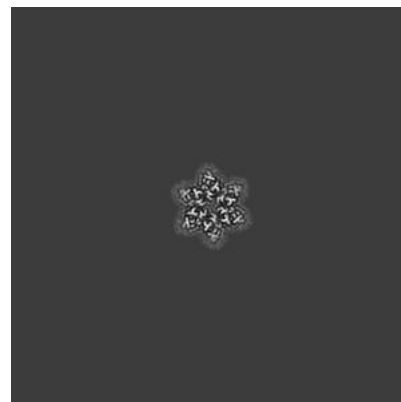
6.3.1 Primary map



X Index: 168



Y Index: 181

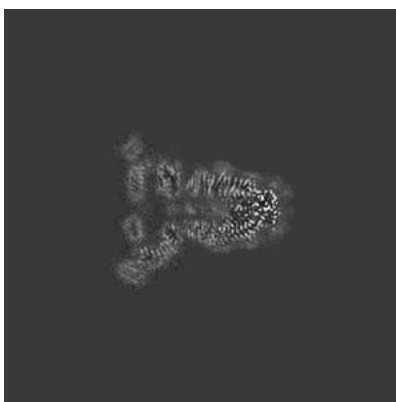


Z Index: 206

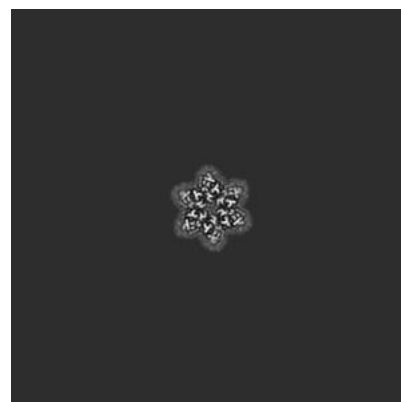
6.3.2 Raw map



X Index: 168



Y Index: 181

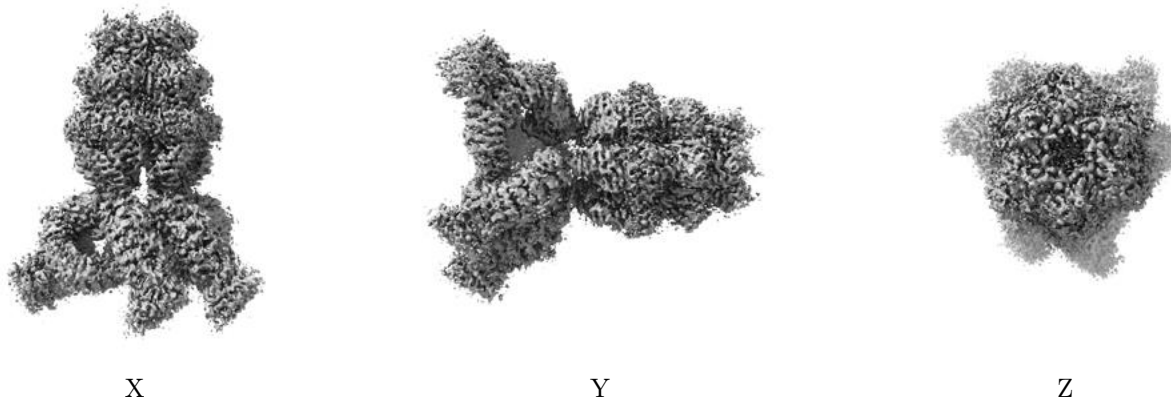


Z Index: 206

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

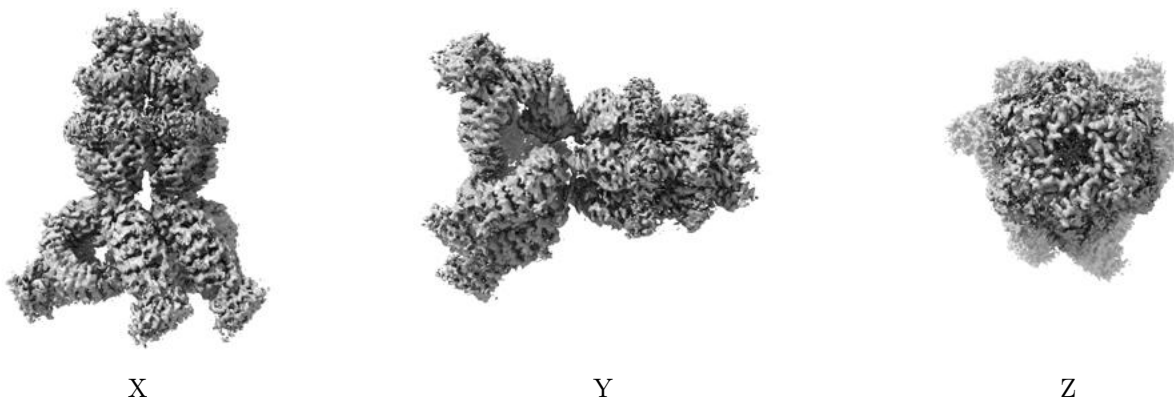
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

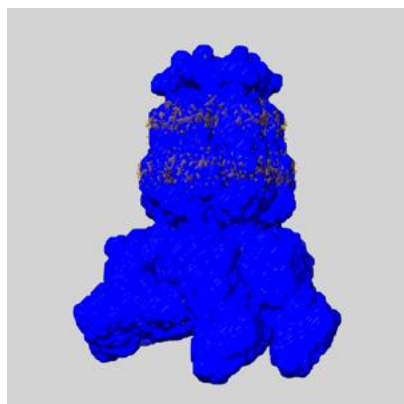
6.5 Mask visualisation [i](#)

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

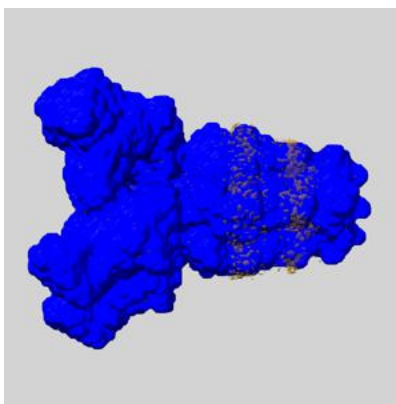
A mask typically either:

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

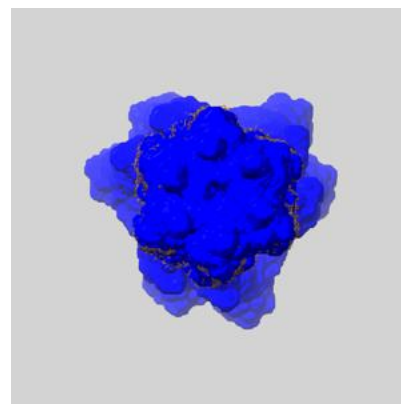
6.5.1 emd_13202_msk_1.map [i](#)



X



Y

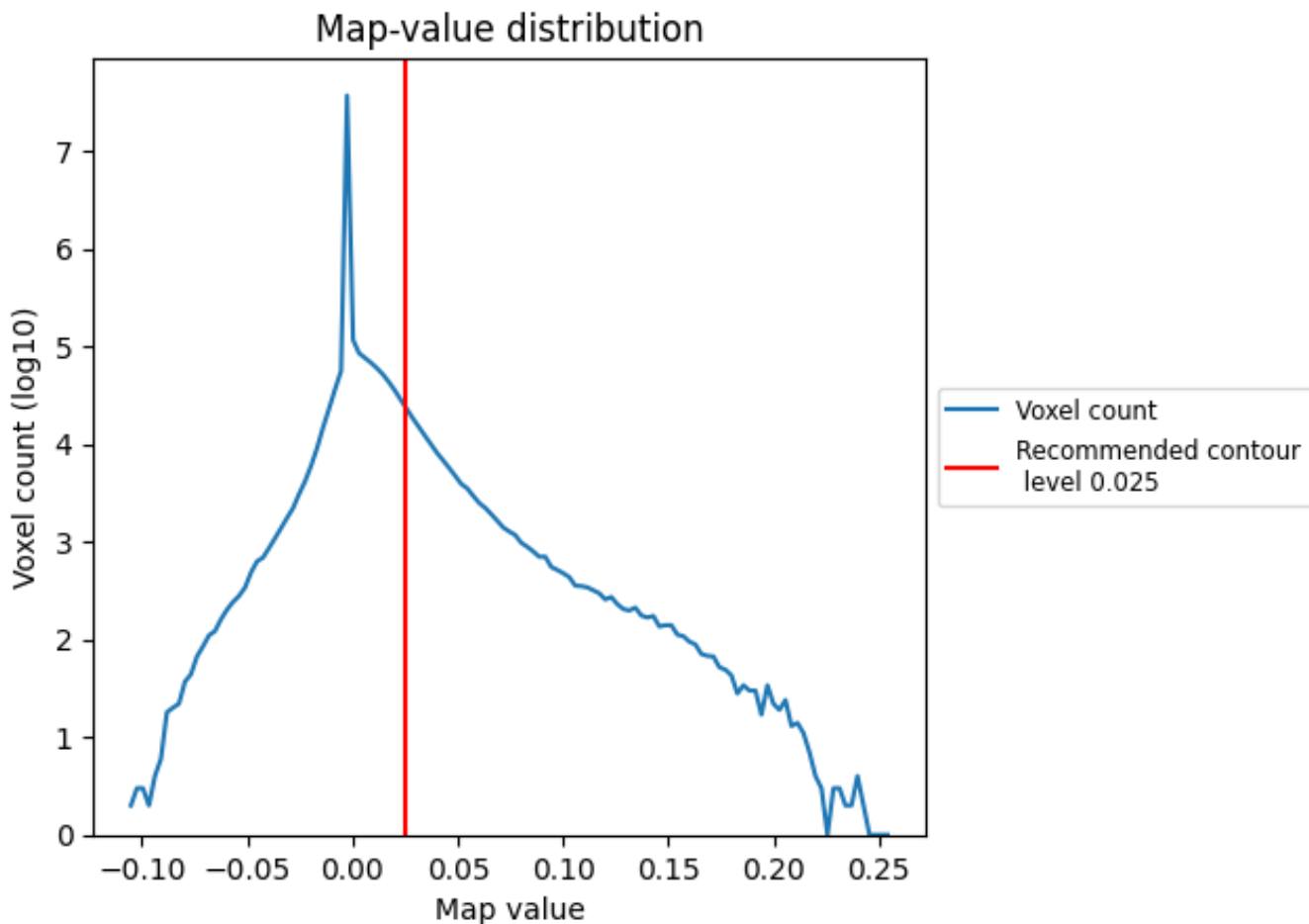


Z

7 Map analysis [i](#)

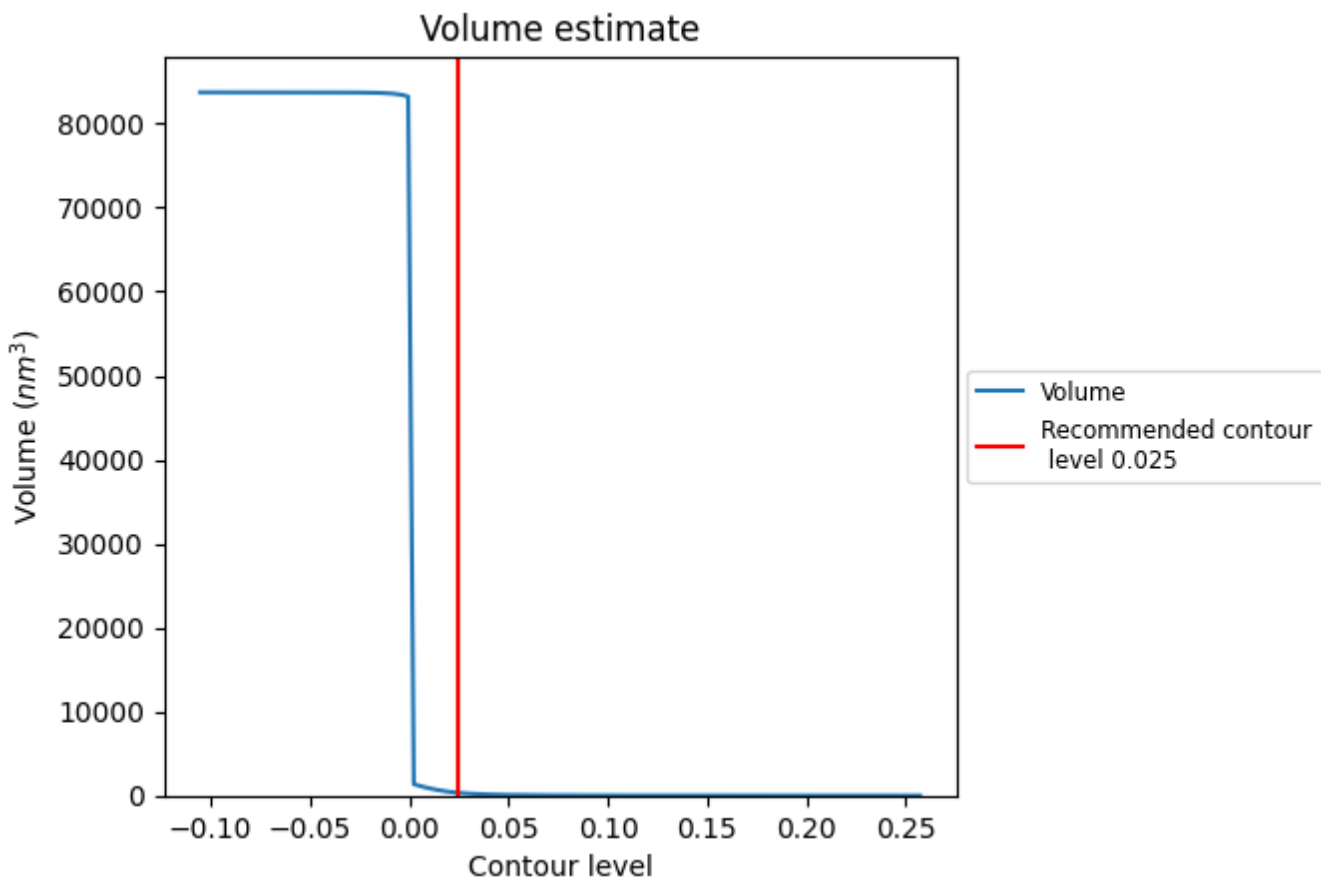
This section contains the results of statistical analysis of the map.

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.

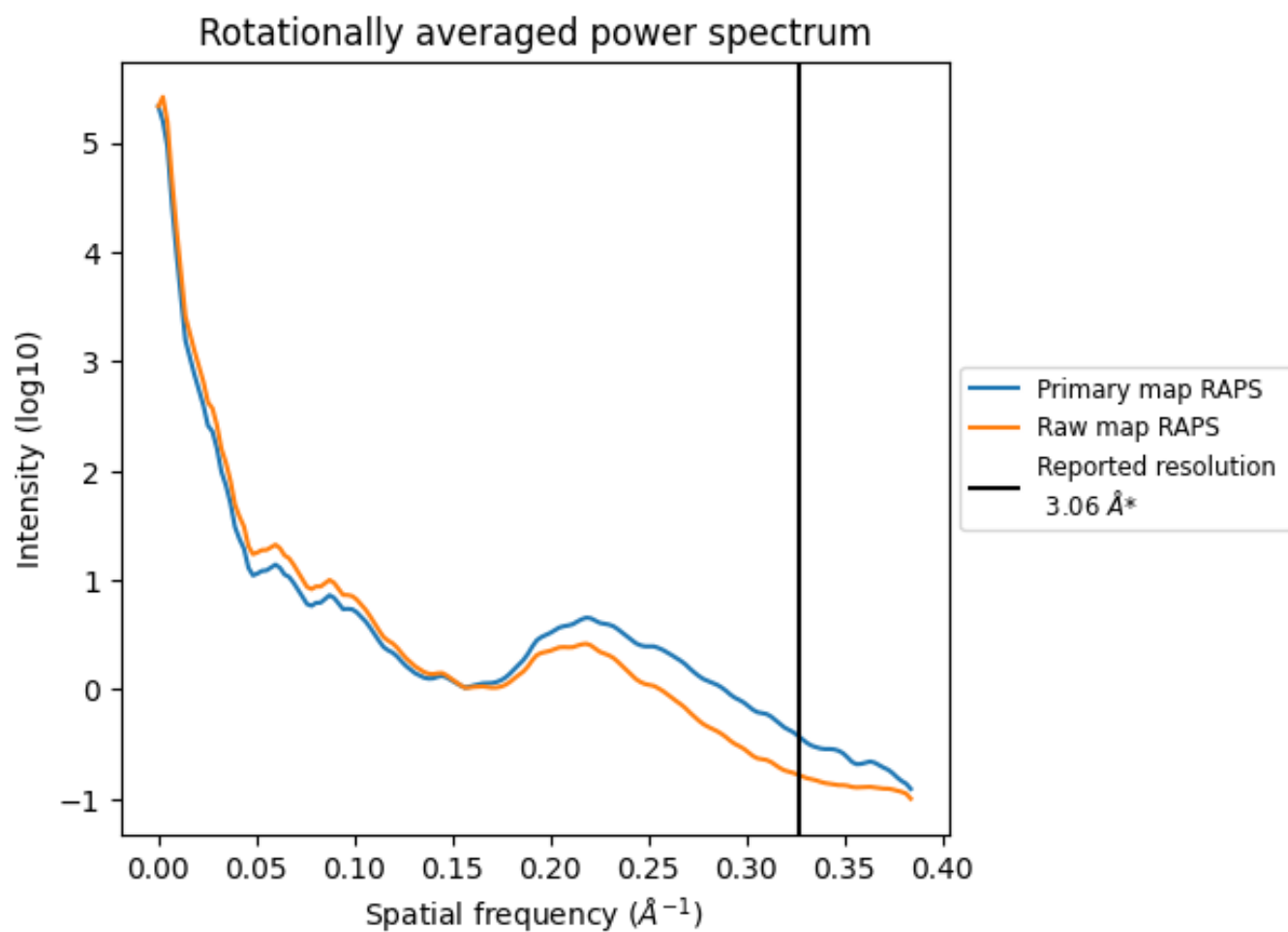
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 322 nm³; this corresponds to an approximate mass of 291 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

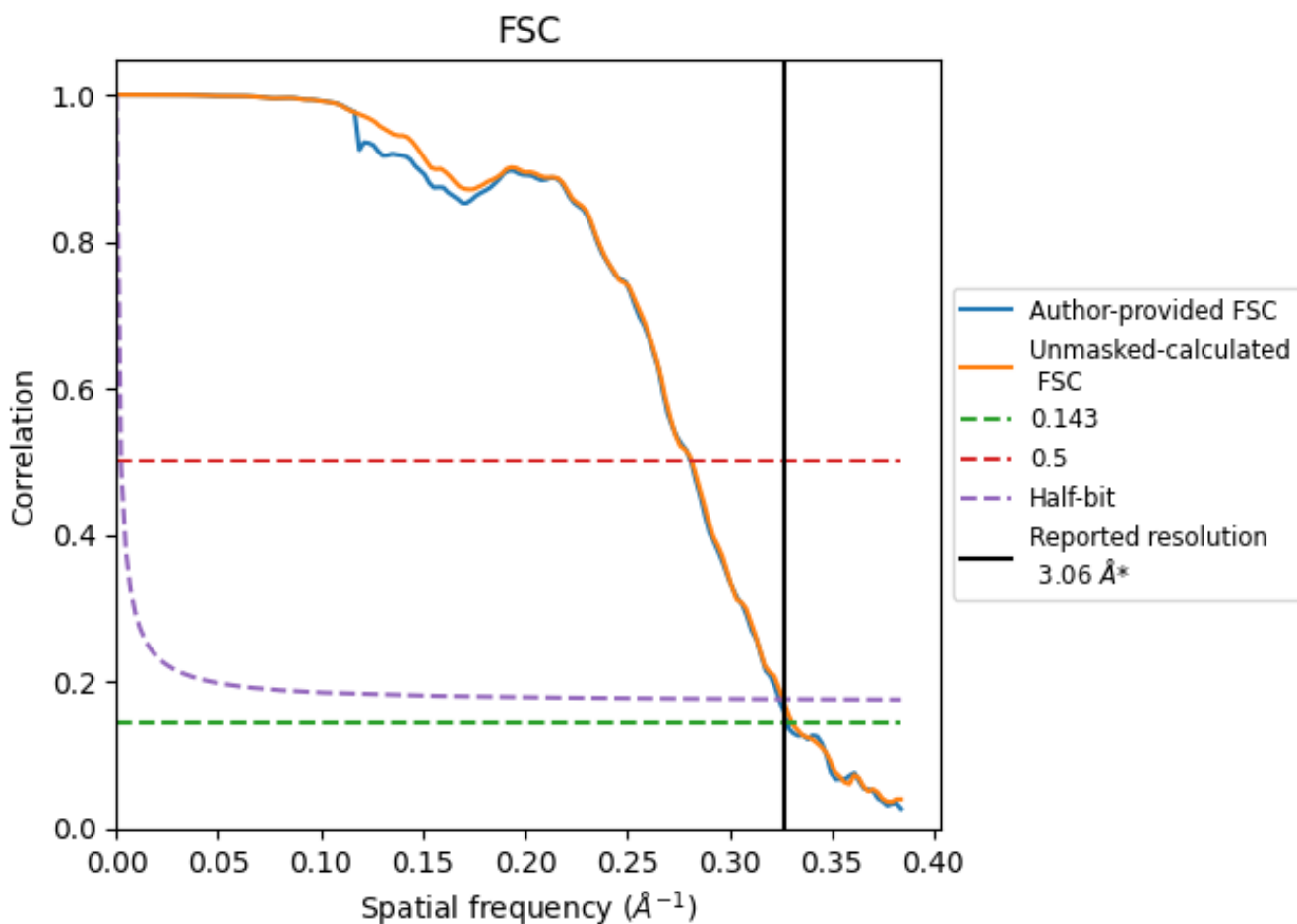


*Reported resolution corresponds to spatial frequency of 0.327 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.327 Å⁻¹

8.2 Resolution estimates [i](#)

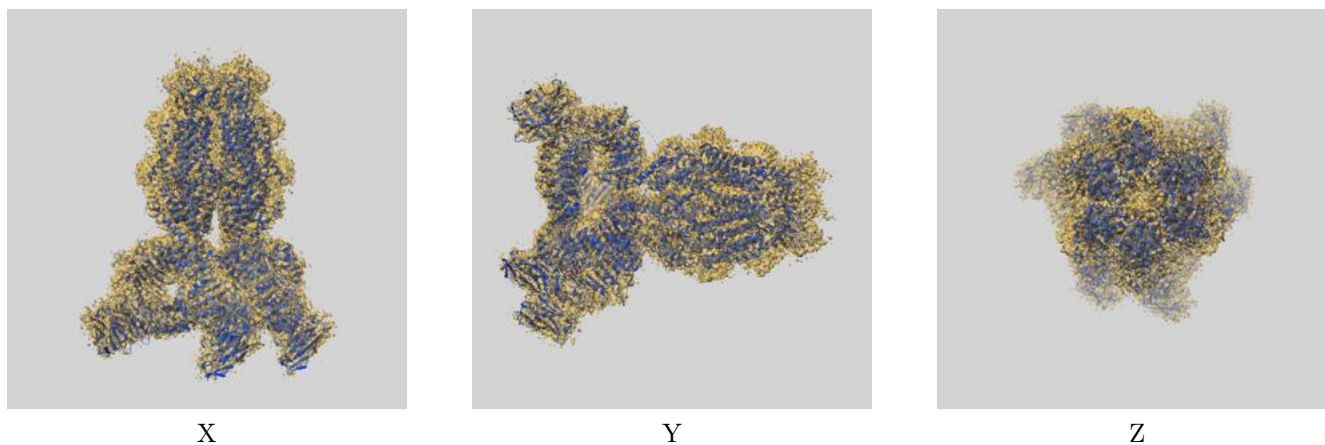
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.06	-	-
Author-provided FSC curve	3.05	3.56	3.08
Unmasked-calculated*	3.02	3.55	3.06

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

9 Map-model fit [i](#)

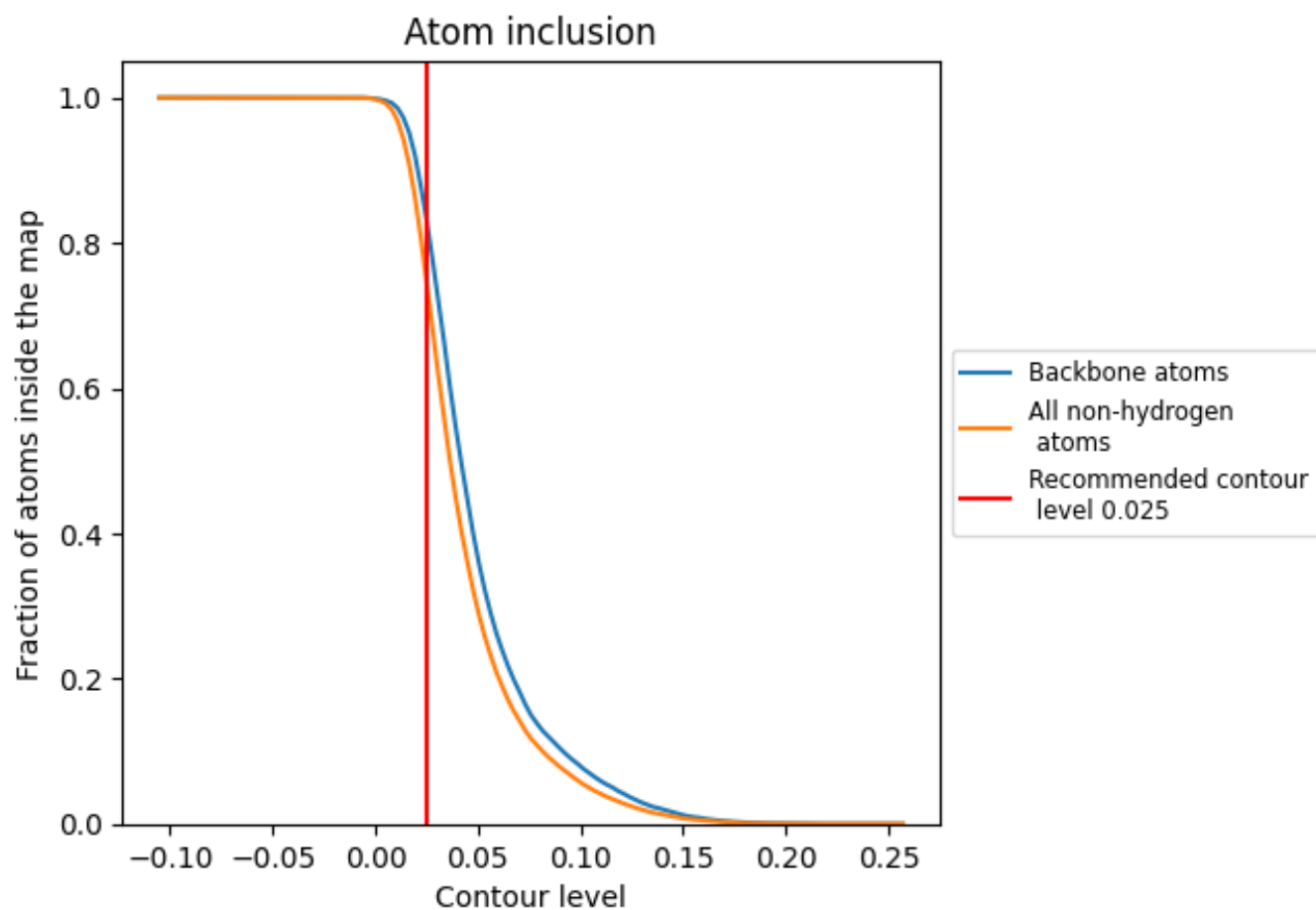
This section contains information regarding the fit between EMDB map EMD-13202 and PDB model 7P5V. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.025 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 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.