WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report ⓘ

Aug 3, 2024 – 02:44 PM EDT

PDB ID	:	9ARI
EMDB ID	:	EMD-43783
Title	:	Rat GluN1-GluN2B NMDA receptor channel in complex with glutamate
Authors	:	Chou, T.-H.; Furukawa, H.
Deposited on	:	2024-02-23
Resolution	:	3.90 Å(reported)
Based on initial model	:	7SAA

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:

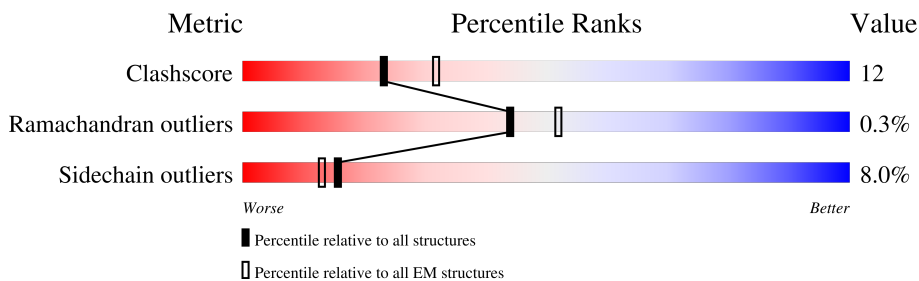|		
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.90 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	Percentile Ranks	Value
Clashscore		12
Ramachandran outliers		0.3%
Sidechain outliers		8.0%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

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 <=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	959	68% 12% · · 16%
1	C	959	68% 13% · · 16%
2	B	883	7% 74% 14% · 11%
2	D	883	7% 75% 13% · 11%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 20756 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 Isoform B of Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	801	Total	C	N	O	S	0	0
			5296	3417	885	974	20		
1	C	801	Total	C	N	O	S	0	0
			5296	3417	885	974	20		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	SER	CYS	conflict	UNP P35439
A	61	GLN	ASN	conflict	UNP P35439
A	260	ASP	ASN	conflict	UNP P35439
A	371	GLN	ASN	conflict	UNP P35439
A	492	GLN	ASN	conflict	UNP P35439
A	512	GLN	ASN	conflict	UNP P35439
A	615	GLN	GLU	conflict	UNP P35439
A	616	SER	GLU	conflict	UNP P35439
A	618	SER	GLU	conflict	UNP P35439
A	619	THR	GLU	conflict	UNP P35439
A	792	GLN	ASN	conflict	UNP P35439
A	831	CYS	PHE	conflict	UNP P35439
C	22	SER	CYS	conflict	UNP P35439
C	61	GLN	ASN	conflict	UNP P35439
C	260	ASP	ASN	conflict	UNP P35439
C	371	GLN	ASN	conflict	UNP P35439
C	492	GLN	ASN	conflict	UNP P35439
C	512	GLN	ASN	conflict	UNP P35439
C	615	GLN	GLU	conflict	UNP P35439
C	616	SER	GLU	conflict	UNP P35439
C	618	SER	GLU	conflict	UNP P35439
C	619	THR	GLU	conflict	UNP P35439
C	792	GLN	ASN	conflict	UNP P35439
C	831	CYS	PHE	conflict	UNP P35439

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	787	Total	C	N	O	S	0	0
			5072	3252	841	955	24		
2	D	787	Total	C	N	O	S	0	0
			5072	3252	841	955	24		

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-30	MET	-	initiating methionine	UNP Q00960
B	-29	GLY	-	expression tag	UNP Q00960
B	-28	THR	-	expression tag	UNP Q00960
B	-27	MET	-	expression tag	UNP Q00960
B	-26	ARG	-	expression tag	UNP Q00960
B	-25	LEU	-	expression tag	UNP Q00960
B	-24	PHE	-	expression tag	UNP Q00960
B	-23	LEU	-	expression tag	UNP Q00960
B	-22	LEU	-	expression tag	UNP Q00960
B	-21	ALA	-	expression tag	UNP Q00960
B	-20	VAL	-	expression tag	UNP Q00960
B	-19	LEU	-	expression tag	UNP Q00960
B	-18	PHE	-	expression tag	UNP Q00960
B	-17	LEU	-	expression tag	UNP Q00960
B	-16	PHE	-	expression tag	UNP Q00960
B	-15	SER	-	expression tag	UNP Q00960
B	-14	PHE	-	expression tag	UNP Q00960
B	-13	ALA	-	expression tag	UNP Q00960
B	-12	ARG	-	expression tag	UNP Q00960
B	-11	ALA	-	expression tag	UNP Q00960
B	-10	THR	-	expression tag	UNP Q00960
B	-9	GLY	-	expression tag	UNP Q00960
B	-8	TRP	-	expression tag	UNP Q00960
B	-7	SER	-	expression tag	UNP Q00960
B	-6	HIS	-	expression tag	UNP Q00960
B	-5	PRO	-	expression tag	UNP Q00960
B	-4	GLN	-	expression tag	UNP Q00960
B	-3	PHE	-	expression tag	UNP Q00960
B	-2	GLU	-	expression tag	UNP Q00960
B	-1	LYS	-	expression tag	UNP Q00960
B	0	GLY	-	expression tag	UNP Q00960
B	1	GLY	-	expression tag	UNP Q00960
B	2	GLY	-	expression tag	UNP Q00960
B	3	SER	-	expression tag	UNP Q00960
B	4	GLY	-	expression tag	UNP Q00960

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Chain	Residue	Modelled	Actual	Comment	Reference
B	5	GLY	-	expression tag	UNP Q00960
B	6	GLY	-	expression tag	UNP Q00960
B	7	SER	-	expression tag	UNP Q00960
B	8	GLY	-	expression tag	UNP Q00960
B	9	GLY	-	expression tag	UNP Q00960
B	10	SER	-	expression tag	UNP Q00960
B	11	ALA	-	expression tag	UNP Q00960
B	12	TRP	-	expression tag	UNP Q00960
B	13	SER	-	expression tag	UNP Q00960
B	14	HIS	-	expression tag	UNP Q00960
B	15	PRO	-	expression tag	UNP Q00960
B	16	GLN	-	expression tag	UNP Q00960
B	17	PHE	-	expression tag	UNP Q00960
B	18	GLU	-	expression tag	UNP Q00960
B	19	LYS	-	expression tag	UNP Q00960
B	20	GLY	-	expression tag	UNP Q00960
B	21	ALA	-	expression tag	UNP Q00960
B	22	LEU	-	expression tag	UNP Q00960
B	23	VAL	-	expression tag	UNP Q00960
B	24	PRO	-	expression tag	UNP Q00960
B	25	ARG	-	expression tag	UNP Q00960
B	26	GLY	-	expression tag	UNP Q00960
B	348	ASP	ASN	conflict	UNP Q00960
B	557	CYS	ASP	conflict	UNP Q00960
B	588	SER	CYS	conflict	UNP Q00960
B	838	SER	CYS	conflict	UNP Q00960
B	849	SER	CYS	conflict	UNP Q00960
D	-30	MET	-	initiating methionine	UNP Q00960
D	-29	GLY	-	expression tag	UNP Q00960
D	-28	THR	-	expression tag	UNP Q00960
D	-27	MET	-	expression tag	UNP Q00960
D	-26	ARG	-	expression tag	UNP Q00960
D	-25	LEU	-	expression tag	UNP Q00960
D	-24	PHE	-	expression tag	UNP Q00960
D	-23	LEU	-	expression tag	UNP Q00960
D	-22	LEU	-	expression tag	UNP Q00960
D	-21	ALA	-	expression tag	UNP Q00960
D	-20	VAL	-	expression tag	UNP Q00960
D	-19	LEU	-	expression tag	UNP Q00960
D	-18	PHE	-	expression tag	UNP Q00960
D	-17	LEU	-	expression tag	UNP Q00960
D	-16	PHE	-	expression tag	UNP Q00960

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	SER	-	expression tag	UNP Q00960
D	-14	PHE	-	expression tag	UNP Q00960
D	-13	ALA	-	expression tag	UNP Q00960
D	-12	ARG	-	expression tag	UNP Q00960
D	-11	ALA	-	expression tag	UNP Q00960
D	-10	THR	-	expression tag	UNP Q00960
D	-9	GLY	-	expression tag	UNP Q00960
D	-8	TRP	-	expression tag	UNP Q00960
D	-7	SER	-	expression tag	UNP Q00960
D	-6	HIS	-	expression tag	UNP Q00960
D	-5	PRO	-	expression tag	UNP Q00960
D	-4	GLN	-	expression tag	UNP Q00960
D	-3	PHE	-	expression tag	UNP Q00960
D	-2	GLU	-	expression tag	UNP Q00960
D	-1	LYS	-	expression tag	UNP Q00960
D	0	GLY	-	expression tag	UNP Q00960
D	1	GLY	-	expression tag	UNP Q00960
D	2	GLY	-	expression tag	UNP Q00960
D	3	SER	-	expression tag	UNP Q00960
D	4	GLY	-	expression tag	UNP Q00960
D	5	GLY	-	expression tag	UNP Q00960
D	6	GLY	-	expression tag	UNP Q00960
D	7	SER	-	expression tag	UNP Q00960
D	8	GLY	-	expression tag	UNP Q00960
D	9	GLY	-	expression tag	UNP Q00960
D	10	SER	-	expression tag	UNP Q00960
D	11	ALA	-	expression tag	UNP Q00960
D	12	TRP	-	expression tag	UNP Q00960
D	13	SER	-	expression tag	UNP Q00960
D	14	HIS	-	expression tag	UNP Q00960
D	15	PRO	-	expression tag	UNP Q00960
D	16	GLN	-	expression tag	UNP Q00960
D	17	PHE	-	expression tag	UNP Q00960
D	18	GLU	-	expression tag	UNP Q00960
D	19	LYS	-	expression tag	UNP Q00960
D	20	GLY	-	expression tag	UNP Q00960
D	21	ALA	-	expression tag	UNP Q00960
D	22	LEU	-	expression tag	UNP Q00960
D	23	VAL	-	expression tag	UNP Q00960
D	24	PRO	-	expression tag	UNP Q00960
D	25	ARG	-	expression tag	UNP Q00960
D	26	GLY	-	expression tag	UNP Q00960

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Chain	Residue	Modelled	Actual	Comment	Reference
D	348	ASP	ASN	conflict	UNP Q00960
D	557	CYS	ASP	conflict	UNP Q00960
D	588	SER	CYS	conflict	UNP Q00960
D	838	SER	CYS	conflict	UNP Q00960
D	849	SER	CYS	conflict	UNP Q00960

- Molecule 3 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	N	O	0
			10	5	1	4	
3	D	1	Total	C	N	O	0
			10	5	1	4	

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: Isoform B of Glutamate receptor ionotropic, NMDA 1

• Molecule 1: Isoform B of Glutamate receptor ionotropic, NMDA 1

• Molecule 2: Glutamate receptor ionotropic, NMDA 2B

Chain B:

7%

74% 14% · 11%

• Molecule 2: Glutamate receptor ionotropic, NMDA 2B

Chain D:

7%

75%   13% • 11%

MET GLY THR MET ARG LEU PHE LEU LEU ALA VAL LEU PHE LEU PHE SER PHE ALA ARG ALA THR GLY TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY SER GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS GLY ALA LEU VAL PRO ARG GLY ARG SER GLN

LYS SER PRO PRO S34 I35 G36 I37 A38 G43 T44 S45 D46 E47 V48 A49 I50 K51 D52 A53 H54 E55 K56 D57 D58 F59 H60 H61 L62 S63 V64 V65 E69 T76 V97 A100 T103 S116 I123 L124 G128 S131 S140 S141 M142 P148 G196

E200 L205 S208 D211 G212 I216 K221 I240 F241 E242 V243 A244 N245 T268 T275 T301 T302 A303 A304 S305 D306 N307 L308 S309 E310 H311 S319 R328 Q331 I340 N341 V342 T343 F344 E345 G346 R347 D348 L349 K361 L362 K380 S383

M394 CYS PRO GLU THR GLU GLU GLN GLU D403 L406 V409 T410 L411 V417 I418 V419 S426 G427 T428 C429 M430 T433 V434 P435 C436 I440 E443 N444 K445 T446 D447 E448 C456 C457 I464 L465 Y476 D477 L478 Y479 L480 H486 I498 V501

Y507 M508 A509 S512 L513 T514 I515 N516 E517 E521 D524 F525 T532 G533 I534 S535 V536 P553 F554 F563 L566 S581 PRO VAL GLY TYR ASN ARG SER LEU ALA ASP GLY ARG GLU PRO GLY GLY P598 L608 V613 F614 N615 N616 S617 V618 P619 T627

V634 A639 V640 I641 A644 A648 N649 L650 A651 A652 F653 M654 I655 Q656 V660 D661 Q662 V663 S664 S667 D668 K669 R673 P679 F683 G684 T685 T691 Y705 A728 F729 I730 Y731 D732 A733 L736 G741 V749 Y762 A765 R774 F784

A794 L795 W796 L797 T798 G799 I800 E804 Q812 L813 M824 I834 T835 W844 GLN PHE ARG HIS SER PHE MET GLY

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	230178	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	58.8	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.387	Depositor
Minimum map value	-0.909	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.0915	Depositor
Map size (Å)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.47	6/5406 (0.1%)	0.70	12/7457 (0.2%)
1	C	0.47	6/5406 (0.1%)	0.70	13/7457 (0.2%)
2	B	0.28	0/5163	0.50	4/7130 (0.1%)
2	D	0.28	0/5163	0.50	4/7130 (0.1%)
All	All	0.39	12/21138 (0.1%)	0.61	33/29174 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	669	THR	C-O	-6.26	1.11	1.23
1	A	669	THR	C-O	-6.24	1.11	1.23
1	A	671	ASN	C-O	-5.54	1.12	1.23
1	C	671	ASN	C-O	-5.54	1.12	1.23
1	A	796	SER	CA-CB	-5.43	1.44	1.52
1	C	796	SER	CA-CB	-5.42	1.44	1.52
1	A	632	TRP	C-O	-5.35	1.13	1.23
1	C	632	TRP	C-O	-5.35	1.13	1.23
1	A	645	PRO	N-CD	-5.18	1.40	1.47
1	C	645	PRO	N-CD	-5.17	1.40	1.47
1	C	670	ALA	C-O	-5.11	1.13	1.23
1	A	670	ALA	C-O	-5.09	1.13	1.23

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	479	PHE	CB-CA-C	-11.56	87.27	110.40
1	C	479	PHE	CB-CA-C	-11.55	87.29	110.40
2	B	615	ASN	CB-CA-C	7.30	125.00	110.40
2	D	615	ASN	CB-CA-C	7.29	124.98	110.40
1	C	493	PHE	CB-CA-C	-7.18	96.04	110.40
1	A	493	PHE	CB-CA-C	-7.17	96.06	110.40
2	B	563	PHE	CB-CA-C	-6.93	96.55	110.40
2	D	563	PHE	CB-CA-C	-6.92	96.55	110.40
1	C	792	GLN	CB-CA-C	-6.75	96.91	110.40
1	A	792	GLN	CB-CA-C	-6.73	96.93	110.40
1	A	669	THR	N-CA-CB	6.17	122.03	110.30
1	C	669	THR	N-CA-CB	6.15	121.99	110.30
2	D	525	PHE	CB-CA-C	-6.11	98.19	110.40
2	B	525	PHE	CB-CA-C	-6.10	98.20	110.40
1	C	675	PHE	CB-CA-C	6.08	122.55	110.40
1	A	675	PHE	CB-CA-C	6.06	122.53	110.40
1	C	455	VAL	CB-CA-C	-6.04	99.93	111.40
1	A	455	VAL	CB-CA-C	-6.03	99.94	111.40
1	C	635	LEU	C-N-CA	-5.90	106.94	121.70
1	C	801	HIS	CB-CA-C	-5.88	98.64	110.40
1	A	801	HIS	CB-CA-C	-5.87	98.65	110.40
1	A	573	ASP	CB-CA-C	-5.87	98.66	110.40
1	C	573	ASP	CB-CA-C	-5.84	98.72	110.40
1	C	473	PRO	N-CA-CB	-5.83	96.18	102.60
1	A	473	PRO	N-CA-CB	-5.81	96.21	102.60
2	B	512	SER	C-N-CA	-5.71	107.44	121.70
2	D	512	SER	C-N-CA	-5.70	107.46	121.70
1	C	569	ARG	CB-CA-C	5.36	121.12	110.40
1	A	569	ARG	CB-CA-C	5.36	121.12	110.40
1	C	797	ILE	N-CA-CB	5.35	123.10	110.80
1	A	797	ILE	N-CA-CB	5.34	123.09	110.80
1	A	670	ALA	N-CA-CB	5.16	117.32	110.10
1	C	670	ALA	N-CA-CB	5.13	117.29	110.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	830	THR	Mainchain
1	C	830	THR	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5296	0	4623	164	0
1	C	5296	0	4623	165	0
2	B	5072	0	4308	105	0
2	D	5072	0	4308	92	0
3	B	10	0	5	0	0
3	D	10	0	5	0	0
All	All	20756	0	17872	472	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 12.

All (472) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:513:LEU:O	2:B:514:THR:HG22	1.23	1.34
2:D:513:LEU:O	2:D:514:THR:HG22	1.23	1.29
2:D:513:LEU:O	2:D:514:THR:CG2	1.82	1.27
2:B:513:LEU:O	2:B:514:THR:CG2	1.82	1.26
1:A:429:PHE:CD1	1:A:479:PHE:HD2	1.62	1.18
1:C:429:PHE:CD1	1:C:479:PHE:HD2	1.62	1.17
2:B:644:ALA:HB1	1:C:669:THR:HG22	1.21	1.16
2:B:648:ALA:CB	1:C:673:ALA:HB2	1.84	1.08
1:A:598:LEU:HD21	1:A:653:LEU:HD23	1.37	1.06
1:C:598:LEU:HD21	1:C:653:LEU:HD23	1.37	1.06
1:A:456:ILE:HD13	1:A:456:ILE:H	1.20	1.05
2:B:648:ALA:HB1	1:C:673:ALA:HB2	1.38	1.04
1:A:598:LEU:CD2	1:A:653:LEU:HD23	1.87	1.04
1:C:456:ILE:HD13	1:C:456:ILE:H	1.20	1.03
1:A:459:GLY:O	1:A:461:ASN:N	1.89	1.03
2:B:644:ALA:CB	1:C:669:THR:HG22	1.88	1.03
1:C:459:GLY:O	1:C:461:ASN:N	1.89	1.03
1:C:598:LEU:CD2	1:C:653:LEU:HD23	1.87	1.03
1:A:429:PHE:CD1	1:A:479:PHE:CD2	2.50	1.00
1:C:572:LEU:CD1	1:C:675:PHE:CZ	2.46	0.99
1:A:572:LEU:CD1	1:A:675:PHE:CZ	2.46	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:LEU:CD1	1:C:493:PHE:CZ	2.47	0.98
1:C:429:PHE:HD1	1:C:479:PHE:HD2	1.00	0.98
1:A:601:LEU:HB3	1:A:649:SER:OG	1.65	0.97
1:C:429:PHE:CD1	1:C:479:PHE:CD2	2.50	0.97
1:A:419:LEU:CD1	1:A:493:PHE:CZ	2.47	0.96
1:C:419:LEU:HD11	1:C:493:PHE:CE1	2.01	0.96
1:C:830:THR:O	1:C:832:GLU:N	1.99	0.95
1:C:572:LEU:HD12	1:C:675:PHE:CZ	2.02	0.95
1:A:419:LEU:HD11	1:A:493:PHE:CE1	2.01	0.95
1:A:572:LEU:HD12	1:A:675:PHE:CZ	2.02	0.95
1:C:601:LEU:HB3	1:C:649:SER:OG	1.65	0.95
1:A:830:THR:O	1:A:832:GLU:N	1.99	0.94
1:A:429:PHE:HD1	1:A:479:PHE:HD2	1.00	0.94
2:B:649:ASN:OD1	1:C:676:LEU:HD21	1.67	0.93
1:A:419:LEU:HD11	1:A:493:PHE:CZ	2.07	0.90
1:C:638:SER:OG	1:C:639:GLY:N	1.96	0.89
1:A:638:SER:OG	1:A:639:GLY:N	1.96	0.88
1:C:419:LEU:HD11	1:C:493:PHE:CZ	2.07	0.88
1:C:572:LEU:HD12	1:C:675:PHE:HZ	1.38	0.87
1:A:457:CYS:HG	1:A:476:CYS:HG	1.17	0.87
1:A:572:LEU:HD12	1:A:675:PHE:HZ	1.38	0.85
1:A:419:LEU:HD12	1:A:493:PHE:CZ	2.12	0.84
2:B:648:ALA:CA	1:C:673:ALA:HB2	2.06	0.83
2:B:649:ASN:OD1	1:C:676:LEU:CD2	2.26	0.83
1:C:419:LEU:HD12	1:C:493:PHE:CZ	2.12	0.82
1:A:429:PHE:CE1	1:A:479:PHE:CD2	2.67	0.82
1:C:429:PHE:CE1	1:C:479:PHE:CD2	2.67	0.82
2:B:517:GLU:HG3	1:C:795:LEU:HD13	1.62	0.82
1:A:654:GLY:O	1:A:657:TRP:N	2.13	0.82
1:A:829:LEU:CD2	2:D:649:ASN:OD1	2.28	0.81
1:A:429:PHE:HD1	1:A:479:PHE:CD2	1.90	0.81
1:C:429:PHE:HD1	1:C:479:PHE:CD2	1.90	0.80
1:C:654:GLY:O	1:C:657:TRP:N	2.13	0.80
2:D:513:LEU:C	2:D:514:THR:HG22	2.02	0.80
1:C:598:LEU:CG	1:C:653:LEU:HD23	2.12	0.79
2:B:513:LEU:C	2:B:514:THR:HG22	2.02	0.79
1:A:795:LEU:HD12	1:A:795:LEU:O	1.84	0.78
1:A:598:LEU:CG	1:A:653:LEU:HD23	2.12	0.78
2:D:513:LEU:O	2:D:514:THR:HG23	1.81	0.78
1:C:795:LEU:HD12	1:C:795:LEU:O	1.84	0.78
2:B:517:GLU:HG3	1:C:795:LEU:CD1	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:LEU:HD23	2:D:649:ASN:OD1	1.85	0.77
2:B:513:LEU:O	2:B:514:THR:HG23	1.81	0.76
1:C:554:PHE:HB3	1:C:797:ILE:HD12	1.67	0.76
2:B:406:LEU:HD22	2:B:507:TYR:CD2	2.21	0.76
2:D:406:LEU:HD22	2:D:507:TYR:CD2	2.21	0.76
1:A:431:TYR:HB2	1:A:477:TYR:O	1.85	0.76
1:C:431:TYR:HB2	1:C:477:TYR:O	1.85	0.76
1:A:670:ALA:HB1	2:B:651:ALA:HA	1.67	0.75
1:C:419:LEU:CD1	1:C:493:PHE:CE1	2.69	0.75
2:B:648:ALA:HB1	1:C:673:ALA:CB	2.17	0.75
1:A:572:LEU:CD1	1:A:675:PHE:CE2	2.70	0.75
1:A:577:GLN:O	2:B:812:GLN:NE2	2.20	0.75
1:A:419:LEU:CD1	1:A:493:PHE:CE1	2.69	0.74
1:C:830:THR:C	1:C:832:GLU:H	1.91	0.74
1:A:554:PHE:HB3	1:A:797:ILE:HD12	1.67	0.74
2:B:429:CYS:SG	2:B:430:MET:N	2.61	0.73
1:C:572:LEU:CD1	1:C:675:PHE:CE2	2.70	0.73
1:A:676:LEU:HD21	2:D:649:ASN:OD1	1.89	0.73
2:D:429:CYS:SG	2:D:430:MET:N	2.61	0.72
1:A:456:ILE:H	1:A:456:ILE:CD1	1.99	0.72
1:C:424:ILE:O	1:C:430:VAL:HG11	1.90	0.72
1:A:429:PHE:CE1	1:A:479:PHE:HD2	2.06	0.72
1:C:672:LEU:HD23	1:C:672:LEU:C	2.11	0.71
1:A:424:ILE:O	1:A:430:VAL:HG11	1.90	0.71
1:A:672:LEU:HD23	1:A:672:LEU:C	2.11	0.71
1:A:830:THR:C	1:A:832:GLU:H	1.91	0.70
2:B:648:ALA:HA	1:C:673:ALA:HB2	1.72	0.70
1:C:572:LEU:HD13	1:C:675:PHE:CE2	2.26	0.70
1:A:572:LEU:HD13	1:A:675:PHE:CE2	2.26	0.70
1:A:429:PHE:HE1	1:A:479:PHE:CE2	2.10	0.70
1:C:598:LEU:HG	1:C:653:LEU:CD2	2.22	0.70
1:A:598:LEU:HG	1:A:653:LEU:CD2	2.22	0.69
1:C:429:PHE:HE1	1:C:479:PHE:CE2	2.10	0.69
1:C:456:ILE:HG12	1:C:456:ILE:O	1.93	0.69
1:C:601:LEU:HB3	1:C:649:SER:HG	1.55	0.69
2:D:834:ILE:HD12	2:D:834:ILE:C	2.13	0.69
1:C:795:LEU:HD12	1:C:795:LEU:C	2.14	0.68
1:A:456:ILE:HG12	1:A:456:ILE:O	1.93	0.68
1:C:456:ILE:HD13	1:C:456:ILE:N	2.04	0.68
1:A:795:LEU:CD1	2:D:517:GLU:HG3	2.23	0.68
2:B:834:ILE:HD12	2:B:834:ILE:C	2.13	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:GLY:O	1:A:655:MET:C	2.33	0.67
1:C:598:LEU:CD2	1:C:653:LEU:CD2	2.71	0.66
1:A:795:LEU:HD12	1:A:795:LEU:C	2.14	0.65
1:A:92:VAL:HG11	1:A:104:PRO:HB3	1.78	0.65
1:A:78:VAL:HG21	1:A:107:VAL:HG12	1.79	0.65
1:A:598:LEU:CD2	1:A:653:LEU:CD2	2.71	0.65
1:A:602:ASP:HA	1:A:647:SER:OG	1.97	0.65
1:C:92:VAL:HG11	1:C:104:PRO:HB3	1.78	0.65
1:C:602:ASP:HA	1:C:647:SER:OG	1.97	0.65
1:A:635:LEU:O	1:A:635:LEU:HG	1.93	0.65
1:A:669:THR:HG22	2:D:644:ALA:HB1	1.79	0.65
1:A:829:LEU:HD23	2:D:649:ASN:CG	2.16	0.64
1:C:654:GLY:O	1:C:655:MET:C	2.33	0.64
1:C:675:PHE:C	1:C:675:PHE:HD2	2.01	0.64
1:C:78:VAL:HG21	1:C:107:VAL:HG12	1.79	0.64
1:A:675:PHE:HD2	1:A:675:PHE:C	2.01	0.63
1:A:598:LEU:HG	1:A:653:LEU:HD23	1.80	0.63
2:B:685:THR:HG22	2:B:730:ILE:HB	1.80	0.63
2:B:644:ALA:CB	1:C:669:THR:CG2	2.70	0.63
1:C:598:LEU:HG	1:C:653:LEU:HD23	1.79	0.63
1:A:552:LYS:HG2	1:A:794:SER:OG	1.99	0.63
1:A:456:ILE:HD13	1:A:456:ILE:N	2.04	0.62
1:C:632:TRP:HA	1:C:632:TRP:CE3	2.35	0.62
1:C:552:LYS:HG2	1:C:794:SER:OG	1.99	0.62
1:A:638:SER:HG	1:A:639:GLY:H	1.45	0.62
1:A:795:LEU:HD13	2:D:517:GLU:HG3	1.82	0.62
2:D:406:LEU:HD22	2:D:507:TYR:CE2	2.35	0.62
2:D:685:THR:HG22	2:D:730:ILE:HB	1.80	0.61
1:C:456:ILE:H	1:C:456:ILE:CD1	1.99	0.61
1:C:638:SER:HG	1:C:639:GLY:H	1.45	0.61
2:B:824:MET:O	2:B:824:MET:HG2	1.99	0.61
2:B:406:LEU:HD22	2:B:507:TYR:CE2	2.35	0.61
1:A:632:TRP:HA	1:A:632:TRP:CE3	2.35	0.61
1:C:455:VAL:HG23	1:C:455:VAL:O	1.99	0.60
1:C:645:PRO:HG2	1:C:645:PRO:O	2.01	0.60
1:A:455:VAL:O	1:A:455:VAL:HG23	1.99	0.60
1:C:632:TRP:HA	1:C:632:TRP:HE3	1.66	0.60
1:A:632:TRP:HA	1:A:632:TRP:HE3	1.66	0.60
1:C:677:VAL:HG22	1:C:677:VAL:O	2.01	0.60
1:A:792:GLN:NE2	1:A:792:GLN:HA	2.17	0.60
1:C:675:PHE:C	1:C:675:PHE:CD2	2.75	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:PHE:C	1:A:675:PHE:CD2	2.75	0.60
1:A:429:PHE:CE1	1:A:479:PHE:CE2	2.89	0.60
1:A:677:VAL:HG22	1:A:677:VAL:O	2.01	0.60
1:C:792:GLN:HA	1:C:792:GLN:NE2	2.17	0.60
2:D:824:MET:HG2	2:D:824:MET:O	1.99	0.59
2:D:731:TYR:HB3	2:D:736:LEU:HG	1.85	0.59
1:C:417:THR:O	1:C:494:THR:OG1	2.19	0.59
1:A:645:PRO:O	1:A:645:PRO:HG2	2.01	0.58
2:D:741:GLY:O	2:D:800:ILE:N	2.31	0.58
1:A:431:TYR:O	1:A:476:CYS:HB2	2.03	0.58
1:A:571:THR:O	1:A:571:THR:HG22	2.03	0.58
1:C:431:TYR:O	1:C:476:CYS:HB2	2.03	0.58
2:D:241:PHE:O	2:D:245:ASN:ND2	2.37	0.58
1:C:526:LEU:HA	1:C:531:ALA:HB3	1.86	0.58
2:B:618:VAL:HG12	2:B:618:VAL:O	2.04	0.57
2:B:731:TYR:HB3	2:B:736:LEU:HG	1.85	0.57
1:C:458:THR:O	1:C:458:THR:OG1	2.18	0.57
1:C:491:MET:CE	1:C:792:GLN:HG3	2.34	0.57
1:C:677:VAL:O	1:C:677:VAL:HG13	2.04	0.57
1:A:491:MET:CE	1:A:792:GLN:HG3	2.34	0.57
1:A:526:LEU:HA	1:A:531:ALA:HB3	1.86	0.57
1:C:429:PHE:CE1	1:C:479:PHE:CE2	2.88	0.57
1:A:458:THR:O	1:A:458:THR:OG1	2.18	0.57
1:A:677:VAL:O	1:A:677:VAL:HG13	2.04	0.57
2:B:515:ILE:HG22	2:B:515:ILE:O	2.05	0.57
2:D:679:PRO:O	2:D:705:TYR:OH	2.23	0.57
2:B:241:PHE:O	2:B:245:ASN:ND2	2.37	0.57
1:C:571:THR:O	1:C:571:THR:HG22	2.03	0.57
2:D:618:VAL:HG12	2:D:618:VAL:O	2.04	0.56
1:A:417:THR:O	1:A:494:THR:OG1	2.19	0.56
1:A:672:LEU:HD22	2:D:648:ALA:CB	2.35	0.56
2:B:679:PRO:O	2:B:705:TYR:OH	2.23	0.56
1:C:670:ALA:HB1	2:D:651:ALA:HA	1.87	0.56
2:D:515:ILE:O	2:D:515:ILE:HG22	2.05	0.55
1:A:672:LEU:CD2	2:D:648:ALA:CB	2.85	0.55
1:A:566:GLU:O	1:A:566:GLU:HG2	2.07	0.55
1:C:830:THR:O	1:C:830:THR:HG23	2.06	0.55
2:D:34:SER:HA	2:D:65:VAL:H	1.73	0.54
1:A:554:PHE:HB3	1:A:797:ILE:CD1	2.38	0.54
1:A:634:VAL:HG23	2:B:617:SER:HA	1.90	0.54
2:B:34:SER:HA	2:B:65:VAL:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:663:VAL:HG21	2:B:668:ASP:HB2	1.89	0.54
1:C:312:ALA:HB1	1:C:342:PHE:HE1	1.72	0.54
1:C:300:ALA:HB1	1:C:355:VAL:HG21	1.89	0.54
1:C:652:ILE:O	1:C:652:ILE:HD12	2.08	0.54
1:A:830:THR:O	1:A:830:THR:HG23	2.06	0.53
1:A:426:GLN:H	1:A:430:VAL:HG12	1.74	0.53
1:A:652:ILE:HD12	1:A:652:ILE:O	2.08	0.53
2:B:653:PHE:CZ	1:C:826:PRO:HG2	2.43	0.53
2:D:663:VAL:HG21	2:D:668:ASP:HB2	1.89	0.53
2:D:664:SER:HB2	2:D:667:SER:OG	2.08	0.53
1:A:300:ALA:HB1	1:A:355:VAL:HG21	1.89	0.53
1:A:312:ALA:HB1	1:A:342:PHE:HE1	1.72	0.53
1:C:426:GLN:HG3	1:C:428:PRO:HD2	1.89	0.53
1:A:83:ILE:HG22	1:A:329:CYS:H	1.74	0.53
2:B:509:ALA:HB3	2:B:765:ALA:HB3	1.91	0.53
2:B:664:SER:HB2	2:B:667:SER:OG	2.08	0.53
1:A:426:GLN:HG3	1:A:428:PRO:HD2	1.89	0.53
2:B:663:VAL:HG13	2:B:664:SER:H	1.74	0.53
2:D:663:VAL:HG13	2:D:664:SER:H	1.74	0.53
1:C:426:GLN:H	1:C:430:VAL:HG12	1.74	0.53
1:C:463:THR:OG1	1:C:467:SER:O	2.27	0.53
1:A:579:PHE:CE1	2:B:813:LEU:HD22	2.44	0.53
1:A:601:LEU:HB3	1:A:649:SER:HG	1.71	0.53
2:B:116:SER:HB3	2:B:141:SER:HB3	1.90	0.53
1:C:591:VAL:HG11	1:C:632:TRP:CE3	2.44	0.53
2:B:644:ALA:HA	1:C:669:THR:HG21	1.91	0.52
2:D:116:SER:HB3	2:D:141:SER:HB3	1.90	0.52
1:A:591:VAL:HG11	1:A:632:TRP:CE3	2.45	0.52
1:A:672:LEU:CD2	2:D:648:ALA:HB1	2.40	0.52
2:B:524:ASP:OD1	2:B:525:PHE:N	2.42	0.52
1:C:457:CYS:HB3	1:C:497:VAL:CG2	2.40	0.52
2:D:524:ASP:OD1	2:D:525:PHE:N	2.42	0.52
1:C:83:ILE:HG22	1:C:329:CYS:H	1.74	0.52
1:A:457:CYS:HB3	1:A:497:VAL:CG2	2.40	0.52
1:C:552:LYS:H	1:C:794:SER:HG	1.58	0.52
1:C:572:LEU:HD11	1:C:675:PHE:CZ	2.44	0.52
1:A:457:CYS:HB3	1:A:497:VAL:HG23	1.91	0.52
1:A:463:THR:OG1	1:A:467:SER:O	2.27	0.52
1:C:602:ASP:HA	1:C:647:SER:CB	2.40	0.52
2:D:64:VAL:HG21	2:D:301:THR:HG23	1.91	0.52
2:D:509:ALA:HB3	2:D:765:ALA:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:555:SER:OG	1:C:828:THR:HG21	2.10	0.52
2:B:834:ILE:HD12	2:B:835:THR:N	2.25	0.52
2:D:794:ALA:HA	2:D:798:THR:HG23	1.92	0.52
2:D:834:ILE:HD12	2:D:835:THR:N	2.25	0.52
1:C:457:CYS:HB3	1:C:497:VAL:HG23	1.91	0.52
1:A:552:LYS:H	1:A:794:SER:HG	1.58	0.51
2:B:64:VAL:HG21	2:B:301:THR:HG23	1.91	0.51
1:C:566:GLU:O	1:C:566:GLU:HG2	2.07	0.51
1:A:32:VAL:HG12	1:A:90:ILE:HD11	1.92	0.51
2:B:613:VAL:HA	2:B:639:ALA:HB1	1.92	0.51
1:C:32:VAL:HG12	1:C:90:ILE:HD11	1.92	0.51
1:C:634:VAL:O	1:C:634:VAL:HG13	2.09	0.51
2:B:794:ALA:HA	2:B:798:THR:HG23	1.92	0.51
1:A:602:ASP:HA	1:A:647:SER:CB	2.40	0.51
1:A:648:PHE:C	1:A:648:PHE:CD1	2.84	0.51
2:B:406:LEU:HD13	2:B:508:MET:CE	2.41	0.51
2:D:406:LEU:HD13	2:D:508:MET:CE	2.41	0.51
1:A:594:VAL:HG22	1:A:653:LEU:HD21	1.92	0.51
1:C:591:VAL:HG22	1:C:657:TRP:HZ2	1.76	0.50
1:C:648:PHE:CD1	1:C:648:PHE:C	2.84	0.50
1:C:594:VAL:HG22	1:C:653:LEU:HD21	1.92	0.50
2:D:669:LYS:O	2:D:673:ARG:N	2.45	0.50
2:D:361:LYS:HA	2:D:380:LYS:HA	1.94	0.50
2:D:613:VAL:HA	2:D:639:ALA:HB1	1.92	0.50
1:A:591:VAL:HG22	1:A:657:TRP:CZ2	2.47	0.50
2:B:669:LYS:O	2:B:673:ARG:N	2.45	0.50
2:D:498:ILE:HD11	2:D:513:LEU:CD1	2.42	0.50
1:A:792:GLN:NE2	1:A:792:GLN:CA	2.71	0.50
2:B:654:MET:HE1	2:B:813:LEU:HD21	1.94	0.50
1:C:554:PHE:HB3	1:C:797:ILE:CD1	2.38	0.50
1:C:591:VAL:HG22	1:C:657:TRP:CZ2	2.47	0.50
1:C:594:VAL:CG2	1:C:653:LEU:HD21	2.42	0.50
1:A:491:MET:HE2	1:A:792:GLN:HG3	1.93	0.50
1:A:759:PHE:HB2	1:A:814:VAL:HG23	1.94	0.50
1:A:552:LYS:HG3	1:A:798:LEU:HD11	1.94	0.49
1:A:591:VAL:HG22	1:A:657:TRP:HZ2	1.76	0.49
2:B:498:ILE:HD11	2:B:513:LEU:CD1	2.42	0.49
1:C:552:LYS:HG3	1:C:798:LEU:HD11	1.94	0.49
1:A:594:VAL:CG2	1:A:653:LEU:HD21	2.42	0.49
1:A:803:ASN:N	1:A:803:ASN:ND2	2.60	0.49
2:D:242:GLU:HA	2:D:245:ASN:HD21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:LEU:H	1:A:165:LEU:HD23	1.78	0.49
2:D:343:THR:OG1	2:D:347:ARG:O	2.29	0.49
1:A:579:PHE:HE1	2:B:813:LEU:HD22	1.77	0.49
2:B:361:LYS:HA	2:B:380:LYS:HA	1.94	0.49
2:B:436:CYS:HB3	2:B:478:LEU:HD22	1.94	0.49
1:C:165:LEU:H	1:C:165:LEU:HD23	1.78	0.49
2:B:343:THR:OG1	2:B:347:ARG:O	2.29	0.49
1:A:829:LEU:HD22	2:D:649:ASN:OD1	2.11	0.49
2:B:741:GLY:O	2:B:800:ILE:N	2.31	0.49
2:B:242:GLU:HA	2:B:245:ASN:HD21	1.77	0.49
1:C:792:GLN:NE2	1:C:792:GLN:CA	2.71	0.49
1:A:676:LEU:CD2	2:D:649:ASN:OD1	2.60	0.48
1:C:759:PHE:HB2	1:C:814:VAL:HG23	1.94	0.48
2:D:436:CYS:HB3	2:D:478:LEU:HD22	1.94	0.48
2:B:648:ALA:HA	1:C:673:ALA:CB	2.43	0.48
2:D:515:ILE:HG12	2:D:525:PHE:CD1	2.49	0.48
1:A:545:ALA:O	2:D:774:ARG:NH2	2.46	0.48
1:A:634:VAL:HG22	1:A:634:VAL:O	2.14	0.48
1:A:673:ALA:HB2	2:D:648:ALA:HB1	1.95	0.48
1:C:421:ILE:HB	1:C:497:VAL:HG12	1.96	0.48
1:C:458:THR:HA	1:C:473:PRO:HA	1.96	0.48
2:D:732:ASP:OD2	2:D:762:TYR:OH	2.32	0.48
1:C:634:VAL:O	1:C:634:VAL:HG22	2.14	0.48
1:A:458:THR:HA	1:A:473:PRO:HA	1.96	0.48
2:B:515:ILE:HG12	2:B:525:PHE:CD1	2.49	0.48
2:B:644:ALA:HB1	1:C:669:THR:CG2	2.15	0.48
1:C:651:ARG:HE	1:C:651:ARG:HB2	1.51	0.48
1:A:421:ILE:HB	1:A:497:VAL:HG12	1.96	0.47
1:A:656:VAL:HG11	2:B:828:ALA:HB2	1.96	0.47
2:D:38:ALA:HB3	2:D:97:VAL:HG22	1.96	0.47
1:C:628:MET:O	1:C:632:TRP:HB2	2.15	0.47
1:A:628:MET:O	1:A:632:TRP:HB2	2.15	0.47
2:B:38:ALA:HB3	2:B:97:VAL:HG22	1.96	0.47
2:B:553:PRO:HG3	2:B:650:LEU:HD13	1.97	0.47
1:C:644:ALA:HB1	1:C:645:PRO:HD2	1.97	0.47
1:A:572:LEU:HD11	1:A:675:PHE:CZ	2.44	0.47
1:C:429:PHE:HE1	1:C:479:PHE:HE2	1.58	0.47
1:C:598:LEU:CG	1:C:653:LEU:CD2	2.84	0.46
1:C:803:ASN:N	1:C:803:ASN:ND2	2.60	0.46
2:D:608:LEU:HA	2:D:619:PRO:HB3	1.97	0.46
1:C:577:GLN:O	2:D:812:GLN:NE2	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ASN:HA	1:A:210:PRO:HG3	1.98	0.46
1:A:673:ALA:HB2	2:D:648:ALA:CB	2.45	0.46
1:C:598:LEU:HD21	1:C:653:LEU:CD2	2.26	0.46
2:D:795:LEU:HB3	2:D:796:TRP:CD1	2.50	0.46
1:A:644:ALA:HB1	1:A:645:PRO:HD2	1.97	0.46
1:A:648:PHE:CD1	1:A:648:PHE:O	2.69	0.46
2:D:205:LEU:HD22	2:D:216:ILE:HG12	1.97	0.46
2:D:417:VAL:HG23	2:D:457:CYS:HB3	1.96	0.46
2:B:417:VAL:HG23	2:B:457:CYS:HB3	1.96	0.46
1:C:161:ASN:HA	1:C:210:PRO:HG3	1.98	0.46
2:D:654:MET:HE1	2:D:813:LEU:HD21	1.98	0.46
1:A:587:VAL:O	1:A:591:VAL:HG23	2.16	0.46
2:B:406:LEU:CD2	2:B:507:TYR:CE2	2.99	0.46
2:D:406:LEU:HD13	2:D:508:MET:HE1	1.97	0.46
2:D:498:ILE:HD11	2:D:513:LEU:HD12	1.98	0.46
1:A:429:PHE:HE1	1:A:479:PHE:HE2	1.58	0.46
2:B:608:LEU:HA	2:B:619:PRO:HB3	1.97	0.46
2:B:795:LEU:HB3	2:B:796:TRP:CD1	2.50	0.46
1:C:675:PHE:CD2	1:C:675:PHE:O	2.69	0.46
1:A:459:GLY:C	1:A:461:ASN:N	2.67	0.46
1:A:634:VAL:O	1:A:634:VAL:HG13	2.16	0.46
2:B:653:PHE:CE2	1:C:826:PRO:HG2	2.51	0.46
1:C:648:PHE:CD1	1:C:648:PHE:O	2.69	0.46
1:C:459:GLY:C	1:C:461:ASN:N	2.67	0.46
1:C:587:VAL:O	1:C:591:VAL:HG23	2.16	0.46
2:B:498:ILE:HD11	2:B:513:LEU:HD12	1.98	0.45
2:D:409:VAL:H	2:D:509:ALA:HA	1.81	0.45
2:D:553:PRO:HG3	2:D:650:LEU:HD13	1.97	0.45
1:A:256:ALA:O	1:A:260:ASP:N	2.49	0.45
2:B:406:LEU:HD22	2:B:507:TYR:HD2	1.77	0.45
2:B:732:ASP:OD2	2:B:762:TYR:OH	2.32	0.45
1:C:256:ALA:O	1:C:260:ASP:N	2.49	0.45
1:C:654:GLY:O	1:C:656:VAL:N	2.49	0.45
2:D:406:LEU:CD2	2:D:507:TYR:CE2	2.99	0.45
1:A:651:ARG:HE	1:A:651:ARG:HB2	1.51	0.45
2:B:205:LEU:HD22	2:B:216:ILE:HG12	1.97	0.45
2:D:498:ILE:HA	2:D:501:VAL:HG12	1.98	0.45
1:A:654:GLY:O	1:A:656:VAL:N	2.49	0.45
1:A:675:PHE:CD2	1:A:675:PHE:O	2.69	0.45
2:B:409:VAL:H	2:B:509:ALA:HA	1.81	0.45
2:B:498:ILE:HA	2:B:501:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:ILE:CD1	1:A:456:ILE:N	2.72	0.45
2:D:834:ILE:HD12	2:D:834:ILE:O	2.17	0.45
1:A:338:THR:O	1:A:342:PHE:HB3	2.16	0.45
2:B:513:LEU:HD22	2:B:513:LEU:HA	1.63	0.45
2:B:655:ILE:HG23	2:B:656:GLN:HG3	1.99	0.45
1:C:338:THR:O	1:C:342:PHE:HB3	2.16	0.45
2:B:534:ILE:HG12	2:B:691:THR:HG22	1.99	0.45
2:D:406:LEU:O	2:D:476:TYR:HA	2.17	0.45
2:D:513:LEU:HD22	2:D:513:LEU:HA	1.63	0.45
1:C:431:TYR:HD1	1:C:431:TYR:HA	1.65	0.45
2:B:532:THR:HA	2:B:733:ALA:HB3	1.99	0.45
1:C:562:LEU:HD11	1:C:767:LEU:HD13	1.99	0.45
2:D:532:THR:HA	2:D:733:ALA:HB3	1.98	0.45
1:A:562:LEU:HD11	1:A:767:LEU:HD13	1.99	0.44
1:A:673:ALA:HB2	2:D:648:ALA:HA	1.99	0.44
1:C:431:TYR:N	1:C:477:TYR:O	2.50	0.44
1:A:385:VAL:HG21	1:A:400:ILE:HD13	2.00	0.44
2:B:148:PRO:HG3	2:B:362:LEU:HD21	1.99	0.44
1:C:491:MET:HE2	1:C:792:GLN:HG3	1.98	0.44
1:A:46:VAL:HG11	1:A:62:ALA:HB2	2.00	0.44
1:A:671:ASN:ND2	1:A:671:ASN:O	2.51	0.44
2:B:406:LEU:O	2:B:476:TYR:HA	2.17	0.44
2:B:834:ILE:HD12	2:B:834:ILE:O	2.17	0.44
1:C:602:ASP:CA	1:C:647:SER:OG	2.66	0.44
1:C:672:LEU:HD23	1:C:672:LEU:O	2.17	0.44
1:C:484:LEU:HD12	1:C:535:VAL:HG21	1.98	0.44
1:C:565:LYS:HD2	1:C:565:LYS:O	2.17	0.44
2:D:534:ILE:HG12	2:D:691:THR:HG22	1.99	0.44
1:A:431:TYR:N	1:A:477:TYR:O	2.50	0.44
1:A:562:LEU:HD21	1:A:767:LEU:HD22	2.00	0.44
2:B:240:ILE:HA	2:B:243:VAL:HG22	1.99	0.44
1:C:385:VAL:HG21	1:C:400:ILE:HD13	2.00	0.44
1:C:562:LEU:HD21	1:C:767:LEU:HD22	2.00	0.44
1:C:671:ASN:O	1:C:671:ASN:ND2	2.51	0.44
1:A:457:CYS:HB2	1:A:498:HIS:HA	2.00	0.44
1:A:484:LEU:HD12	1:A:535:VAL:HG21	1.98	0.44
2:B:100:ALA:HA	2:B:128:GLY:HA2	2.00	0.44
2:B:648:ALA:HB1	1:C:673:ALA:CA	2.47	0.44
1:C:457:CYS:HB2	1:C:498:HIS:HA	2.00	0.44
1:A:306:VAL:HA	1:A:309:VAL:HG22	1.99	0.44
1:C:456:ILE:N	1:C:456:ILE:CD1	2.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:517:GLU:O	2:D:521:GLU:HG3	2.18	0.44
2:D:655:ILE:HG23	2:D:656:GLN:HG3	1.99	0.44
1:A:565:LYS:HD2	1:A:565:LYS:O	2.17	0.44
1:C:419:LEU:HD12	1:C:493:PHE:CE2	2.52	0.44
2:D:406:LEU:HD22	2:D:507:TYR:HD2	1.77	0.43
1:A:90:ILE:HG23	1:A:118:VAL:HG23	2.00	0.43
2:B:649:ASN:OD1	1:C:676:LEU:HD23	2.16	0.43
1:C:306:VAL:HA	1:C:309:VAL:HG22	1.98	0.43
2:D:240:ILE:HA	2:D:243:VAL:HG22	1.99	0.43
1:A:105:THR:HB	2:B:114:PHE:CE1	2.53	0.43
2:D:148:PRO:HG3	2:D:362:LEU:HD21	1.99	0.43
1:A:672:LEU:HD23	1:A:672:LEU:O	2.18	0.43
2:B:774:ARG:NH2	1:C:546:GLN:O	2.51	0.43
1:C:46:VAL:HG11	1:C:62:ALA:HB2	2.00	0.43
1:C:90:ILE:HG23	1:C:118:VAL:HG23	2.00	0.43
1:C:564:LYS:HA	1:C:767:LEU:HB3	2.00	0.43
1:C:567:ILE:H	1:C:567:ILE:HG13	1.51	0.43
2:D:100:ALA:HA	2:D:128:GLY:HA2	2.00	0.43
1:A:91:LEU:HD23	1:A:91:LEU:H	1.84	0.43
1:A:564:LYS:HA	1:A:767:LEU:HB3	2.00	0.43
2:B:517:GLU:O	2:B:521:GLU:HG3	2.18	0.43
2:B:516:ASN:OD1	2:B:517:GLU:N	2.51	0.43
2:B:440:ILE:HD11	2:B:480:LEU:HD23	2.01	0.42
2:B:97:VAL:HB	2:B:123:ILE:HG22	2.02	0.42
2:B:834:ILE:C	2:B:834:ILE:CD1	2.83	0.42
2:B:128:GLY:HA3	2:B:131:SER:OG	2.20	0.42
2:D:440:ILE:HD11	2:D:480:LEU:HD23	2.01	0.42
1:A:551:SER:OG	1:A:552:LYS:N	2.52	0.42
2:B:614:PHE:O	2:B:615:ASN:C	2.56	0.42
1:C:91:LEU:HD23	1:C:91:LEU:H	1.84	0.42
1:C:551:SER:OG	1:C:552:LYS:N	2.52	0.42
1:C:652:ILE:O	1:C:652:ILE:CG1	2.67	0.42
1:A:30:GLY:HA2	1:A:63:THR:HB	2.02	0.42
1:A:117:PRO:HG2	1:A:342:PHE:HD2	1.85	0.42
2:B:303:ALA:HB2	2:B:342:VAL:HG21	2.01	0.42
2:D:128:GLY:HA3	2:D:131:SER:OG	2.20	0.42
2:D:303:ALA:HB2	2:D:342:VAL:HG21	2.01	0.42
2:B:663:VAL:O	2:B:664:SER:OG	2.31	0.42
1:A:704:THR:OG1	1:A:705:VAL:N	2.53	0.42
2:B:683:PHE:HB3	2:B:728:ALA:HB3	2.02	0.42
1:C:117:PRO:HG2	1:C:342:PHE:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:428:THR:HG22	2:D:429:CYS:H	1.85	0.42
1:A:852:ILE:HB	2:D:627:THR:HG21	2.01	0.41
1:C:491:MET:HE1	1:C:792:GLN:HG3	2.00	0.41
2:D:464:ILE:HD12	2:D:464:ILE:HA	1.96	0.41
2:B:299:ILE:HD13	2:B:299:ILE:HA	1.94	0.41
2:B:428:THR:HG22	2:B:429:CYS:H	1.85	0.41
1:A:652:ILE:O	1:A:652:ILE:CG1	2.67	0.41
1:A:671:ASN:ND2	1:A:671:ASN:C	2.72	0.41
2:B:515:ILE:HD13	2:B:515:ILE:HG21	1.85	0.41
1:A:105:THR:HB	2:B:114:PHE:CZ	2.54	0.41
2:B:660:VAL:HG23	2:B:661:ASP:H	1.86	0.41
1:A:602:ASP:CA	1:A:647:SER:OG	2.66	0.41
2:D:97:VAL:HB	2:D:123:ILE:HG22	2.02	0.41
2:D:660:VAL:HG23	2:D:661:ASP:H	1.86	0.41
1:C:704:THR:OG1	1:C:705:VAL:N	2.53	0.41
2:D:380:LYS:O	2:D:383:SER:OG	2.31	0.41
1:A:419:LEU:HD12	1:A:493:PHE:CE2	2.52	0.41
1:C:457:CYS:CB	1:C:497:VAL:HG23	2.51	0.41
1:C:636:LEU:HD23	1:C:636:LEU:H	1.86	0.41
1:A:673:ALA:HB2	2:D:648:ALA:CA	2.51	0.41
1:C:117:PRO:HG2	1:C:342:PHE:CD2	2.56	0.41
1:C:423:THR:HG22	1:C:424:ILE:H	1.86	0.41
2:D:516:ASN:OD1	2:D:517:GLU:N	2.51	0.41
1:A:117:PRO:HG2	1:A:342:PHE:CD2	2.56	0.41
1:A:670:ALA:HB1	2:B:651:ALA:CA	2.44	0.41
1:A:841:VAL:HG23	2:D:634:VAL:HG12	2.03	0.41
1:A:422:VAL:HA	1:A:498:HIS:O	2.21	0.40
2:B:517:GLU:HG3	1:C:795:LEU:HD11	2.01	0.40
1:A:829:LEU:HD23	2:D:649:ASN:CB	2.51	0.40
1:C:118:VAL:HG13	1:C:137:PHE:HD1	1.87	0.40
1:C:430:VAL:O	1:C:430:VAL:CG1	2.69	0.40
1:A:567:ILE:H	1:A:567:ILE:HG13	1.51	0.40
2:B:429:CYS:HB3	2:B:435:PRO:HG3	2.03	0.40
1:C:652:ILE:O	1:C:652:ILE:CD1	2.70	0.40
2:D:429:CYS:HB3	2:D:435:PRO:HG3	2.03	0.40
1:A:660:PHE:CD1	2:B:821:VAL:HG12	2.57	0.40
2:D:683:PHE:HB3	2:D:728:ALA:HB3	2.02	0.40
2:B:172:VAL:HG22	2:B:203:LEU:HD13	2.03	0.40
1:C:30:GLY:HA2	1:C:63:THR:HB	2.02	0.40
1:C:184:LEU:HD13	1:C:211:LYS:O	2.22	0.40
1:C:422:VAL:HA	1:C:498:HIS:O	2.21	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	793/959 (83%)	743 (94%)	49 (6%)	1 (0%)	51	84
1	C	793/959 (83%)	742 (94%)	50 (6%)	1 (0%)	51	84
2	B	781/883 (88%)	719 (92%)	59 (8%)	3 (0%)	34	71
2	D	781/883 (88%)	720 (92%)	58 (7%)	3 (0%)	34	71
All	All	3148/3684 (86%)	2924 (93%)	216 (7%)	8 (0%)	44	75

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	831	CYS
2	B	616	ASN
1	C	831	CYS
2	D	616	ASN
2	B	669	LYS
2	D	669	LYS
2	B	128	GLY
2	D	128	GLY

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	439/826 (53%)	398 (91%)	41 (9%)	9	34
1	C	439/826 (53%)	398 (91%)	41 (9%)	9	34
2	B	412/762 (54%)	385 (93%)	27 (7%)	16	46
2	D	412/762 (54%)	385 (93%)	27 (7%)	16	46
All	All	1702/3176 (54%)	1566 (92%)	136 (8%)	16	41

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	A	87	VAL
1	A	103	THR
1	A	105	THR
1	A	180	LEU
1	A	329	CYS
1	A	391	THR
1	A	393	VAL
1	A	423	THR
1	A	431	TYR
1	A	455	VAL
1	A	456	ILE
1	A	473	PRO
1	A	475	CYS
1	A	479	PHE
1	A	493	PHE
1	A	505	PHE
1	A	539	THR
1	A	559	LEU
1	A	565	LYS
1	A	567	ILE
1	A	569	ARG
1	A	571	THR
1	A	583	LEU
1	A	623	THR
1	A	632	TRP
1	A	675	PHE
1	A	677	VAL
1	A	714	PHE
1	A	718	VAL
1	A	767	LEU
1	A	773	LEU
1	A	786	ASP

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Mol	Chain	Res	Type
1	A	793	VAL
1	A	794	SER
1	A	795	LEU
1	A	797	ILE
1	A	801	HIS
1	A	803	ASN
1	A	813	TRP
1	A	831	CYS
2	B	131	SER
2	B	268	THR
2	B	275	THR
2	B	308	LEU
2	B	349	LEU
2	B	410	THR
2	B	411	LEU
2	B	417	VAL
2	B	419	VAL
2	B	428	THR
2	B	433	THR
2	B	456	CYS
2	B	465	LEU
2	B	486	HIS
2	B	513	LEU
2	B	536	VAL
2	B	554	PHE
2	B	566	LEU
2	B	627	THR
2	B	641	ILE
2	B	653	PHE
2	B	660	VAL
2	B	749	VAL
2	B	784	PHE
2	B	795	LEU
2	B	824	MET
2	B	834	ILE
1	C	27	VAL
1	C	87	VAL
1	C	103	THR
1	C	105	THR
1	C	180	LEU
1	C	329	CYS
1	C	391	THR

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Mol	Chain	Res	Type
1	C	393	VAL
1	C	423	THR
1	C	431	TYR
1	C	455	VAL
1	C	456	ILE
1	C	473	PRO
1	C	475	CYS
1	C	479	PHE
1	C	493	PHE
1	C	505	PHE
1	C	539	THR
1	C	559	LEU
1	C	565	LYS
1	C	567	ILE
1	C	569	ARG
1	C	571	THR
1	C	583	LEU
1	C	623	THR
1	C	632	TRP
1	C	675	PHE
1	C	677	VAL
1	C	714	PHE
1	C	718	VAL
1	C	767	LEU
1	C	773	LEU
1	C	786	ASP
1	C	793	VAL
1	C	794	SER
1	C	795	LEU
1	C	797	ILE
1	C	801	HIS
1	C	803	ASN
1	C	813	TRP
1	C	831	CYS
2	D	131	SER
2	D	268	THR
2	D	275	THR
2	D	308	LEU
2	D	349	LEU
2	D	410	THR
2	D	411	LEU
2	D	417	VAL

Continued on next page...

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Mol	Chain	Res	Type
2	D	419	VAL
2	D	428	THR
2	D	433	THR
2	D	456	CYS
2	D	465	LEU
2	D	486	HIS
2	D	513	LEU
2	D	536	VAL
2	D	554	PHE
2	D	566	LEU
2	D	627	THR
2	D	641	ILE
2	D	653	PHE
2	D	660	VAL
2	D	749	VAL
2	D	784	PHE
2	D	795	LEU
2	D	824	MET
2	D	834	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	498	HIS
1	A	577	GLN
1	A	792	GLN
1	A	803	ASN
2	B	245	ASN
2	B	357	GLN
2	B	615	ASN
2	B	697	ASN
2	B	710	ASN
2	B	775	GLN
1	C	498	HIS
1	C	577	GLN
1	C	792	GLN
1	C	803	ASN
2	D	245	ASN
2	D	357	GLN
2	D	615	ASN
2	D	697	ASN
2	D	710	ASN

Continued from previous page...

Mol	Chain	Res	Type
2	D	775	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)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\| > 2$	Counts	RMSZ	#$\|Z\| > 2$
3	GLU	D	901	-	8,9,9	1.06	1 (12%)	10,11,11	1.26	2 (20%)
3	GLU	B	901	-	8,9,9	1.06	1 (12%)	10,11,11	1.26	2 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLU	D	901	-	-	0/9/9/9	-
3	GLU	B	901	-	-	0/9/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	901	GLU	OXT-C	-2.14	1.23	1.30
3	B	901	GLU	OXT-C	-2.13	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	901	GLU	OXT-C-O	-2.65	118.07	124.09
3	D	901	GLU	OXT-C-O	-2.64	118.09	124.09
3	B	901	GLU	OXT-C-CA	2.22	120.94	113.38
3	D	901	GLU	OXT-C-CA	2.21	120.92	113.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GLU D 901

Bond lengths

Bond angles

Torsions

Rings

Ligand GLU B 901

Bond lengths

Bond angles

Torsions

Rings
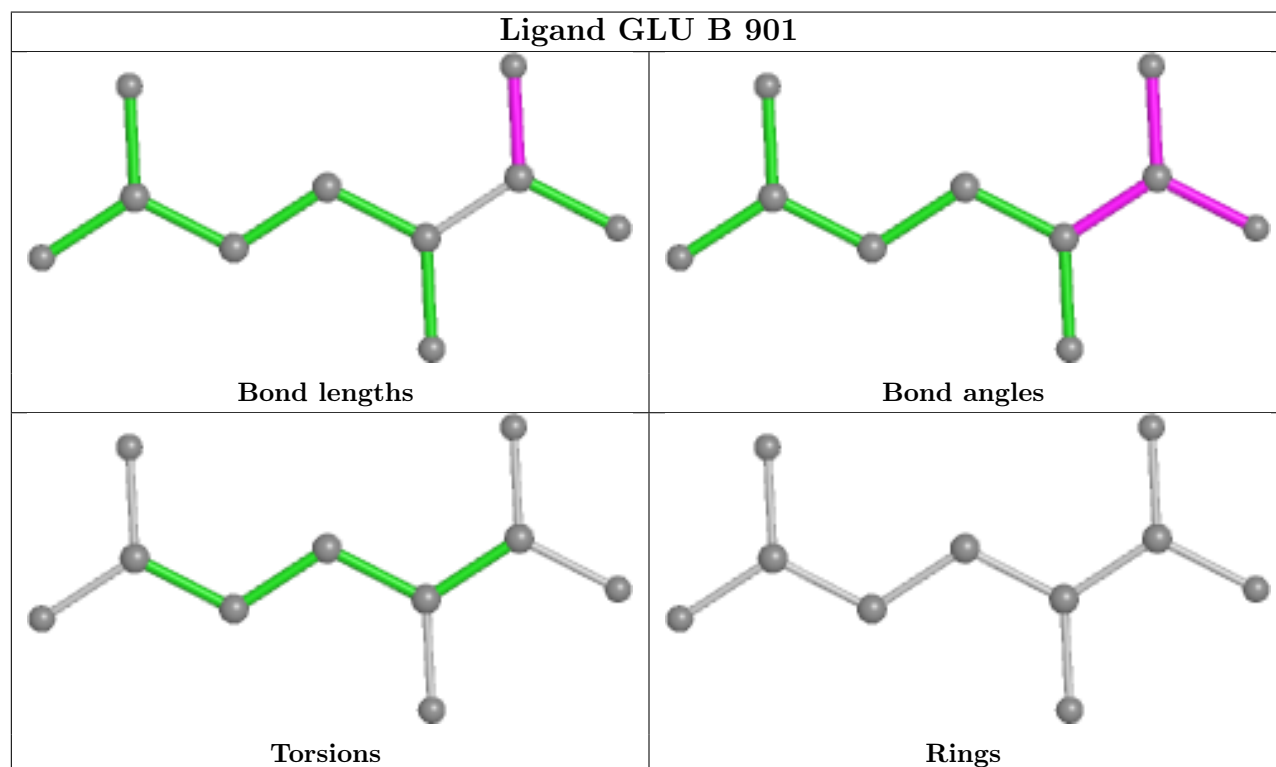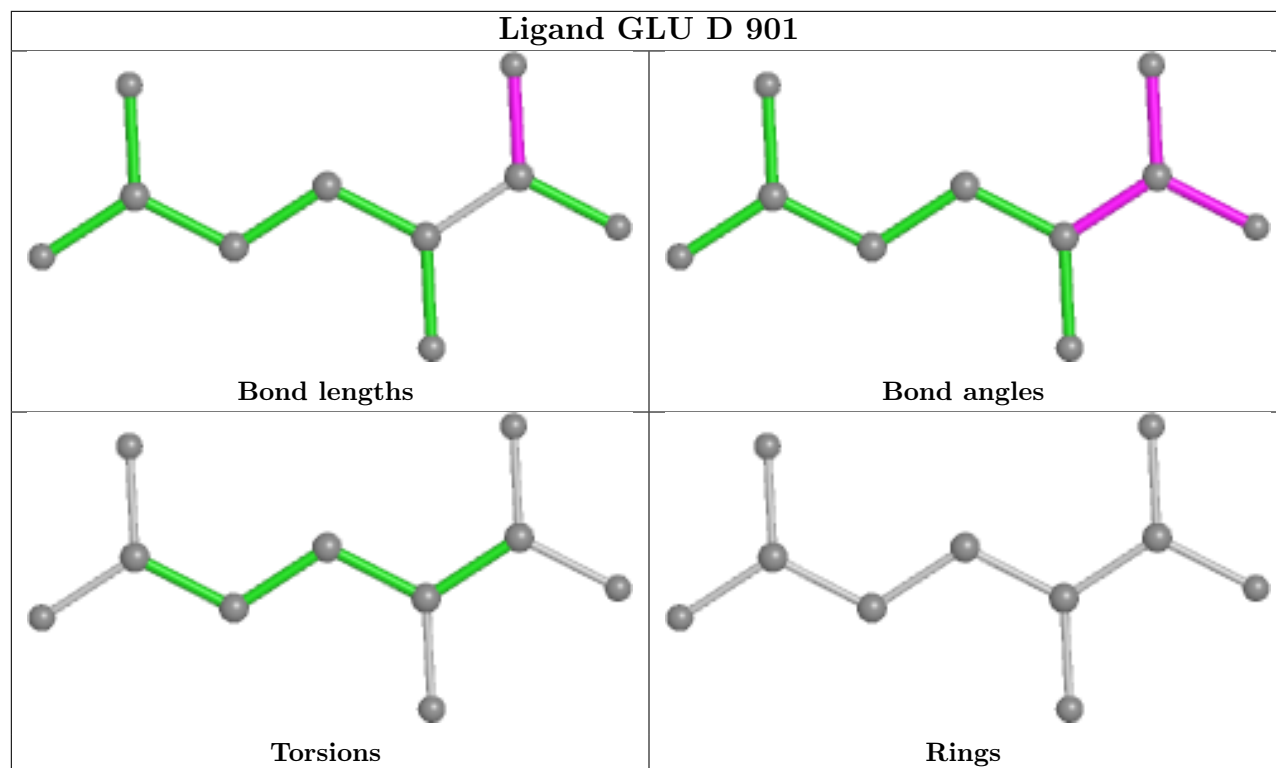
5.7　Other polymers ⓘ

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-43783. 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
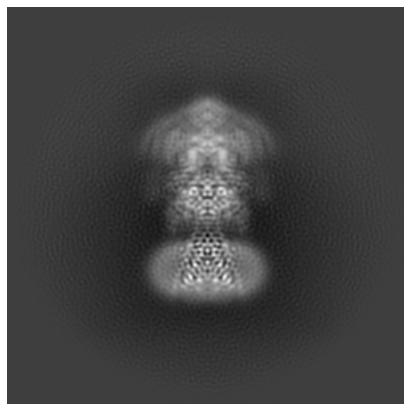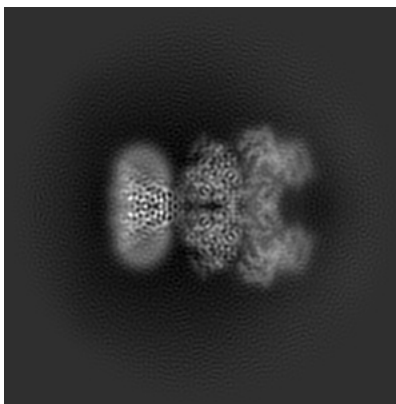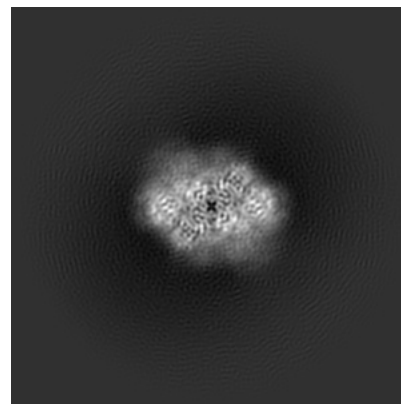
X	Y	Z

6.1.2 Raw map

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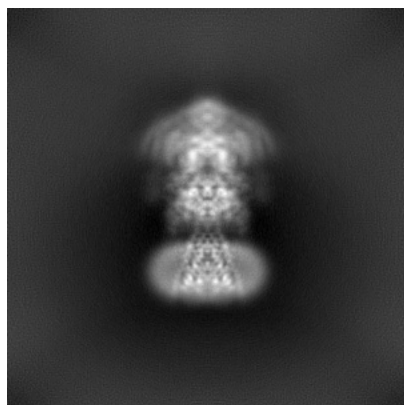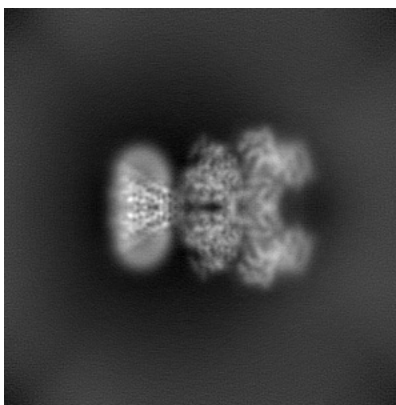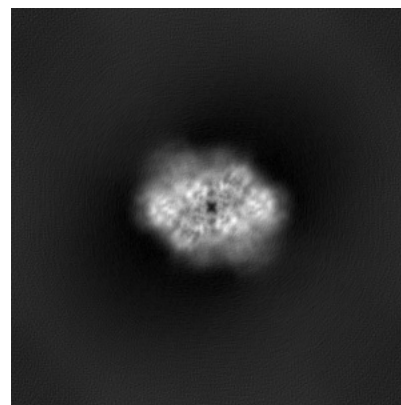
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
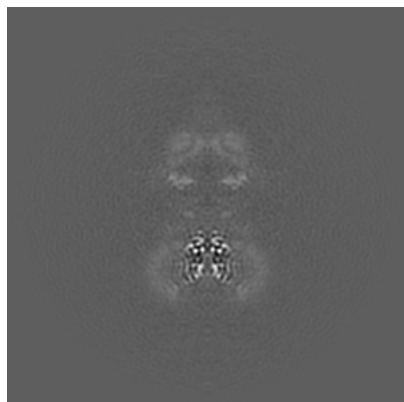
6.2.1 Primary map
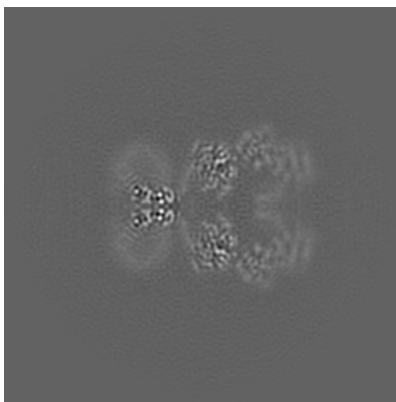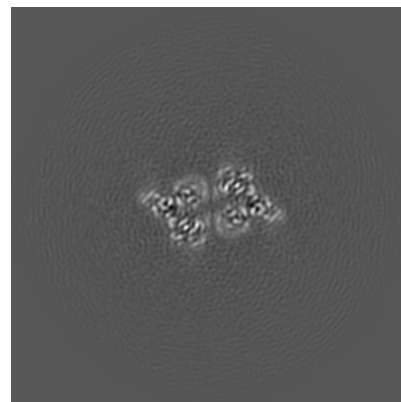
| X Index: 160 | Y Index: 160 | Z Index: 160 |

6.2.2 Raw map
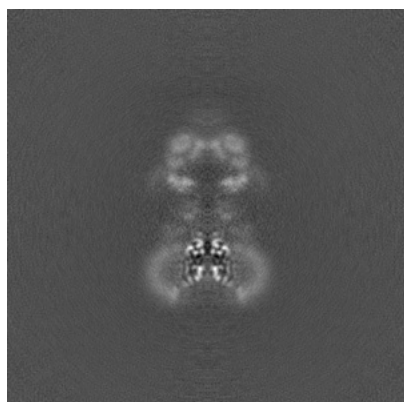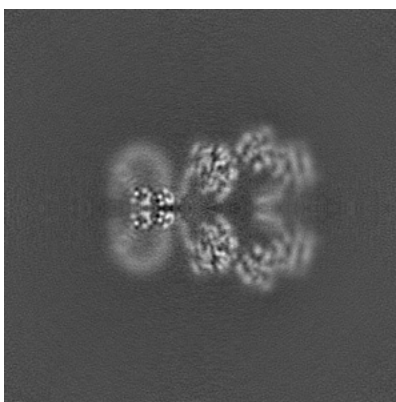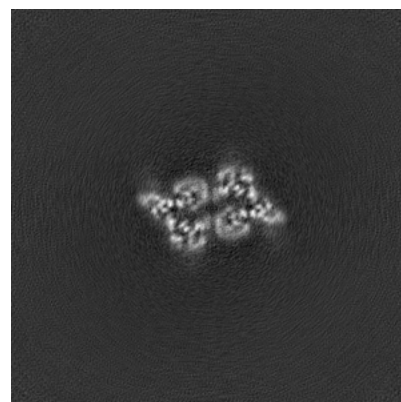
| X Index: 160 | Y Index: 160 | Z Index: 160 |

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

6.3 Largest variance slices (i)

6.3.1 Primary map
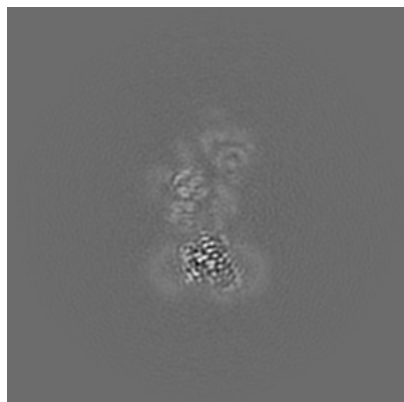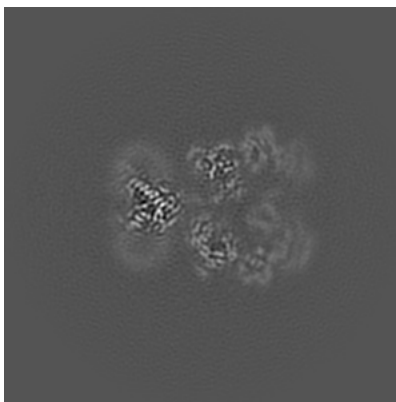
| X Index: 152 | Y Index: 165 | Z Index: 125 |
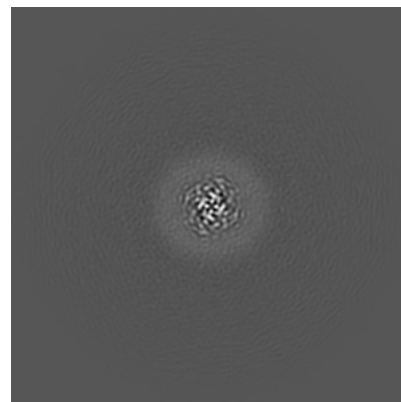
6.3.2 Raw map
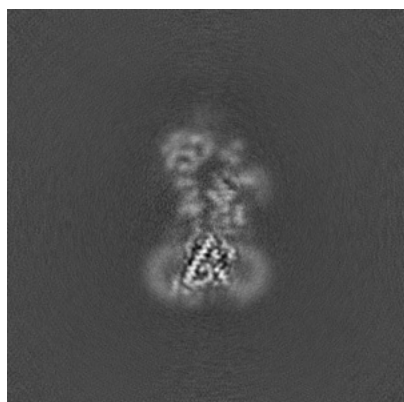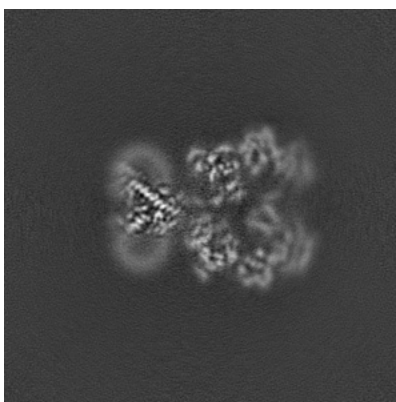
| X Index: 166 | Y Index: 165 | Z Index: 173 |
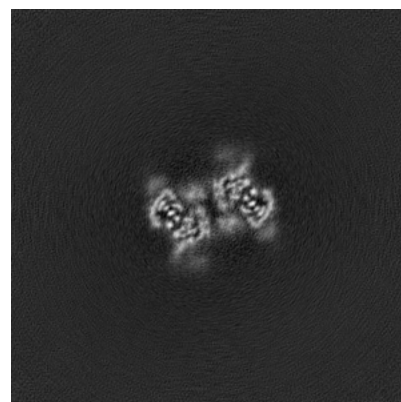
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map
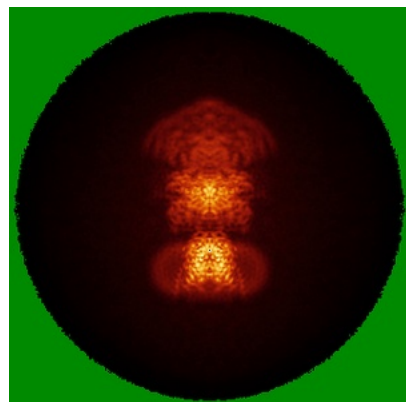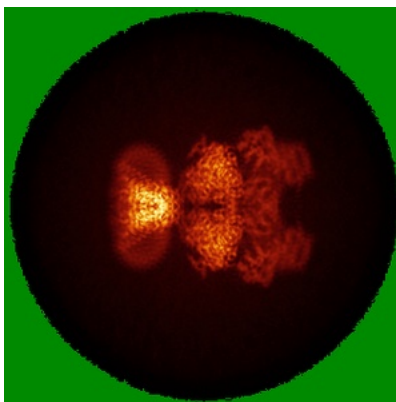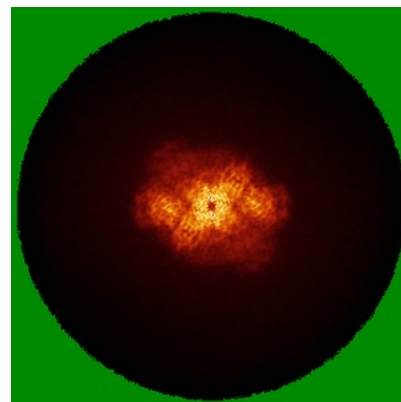
X   Y   Z

6.4.2 Raw map

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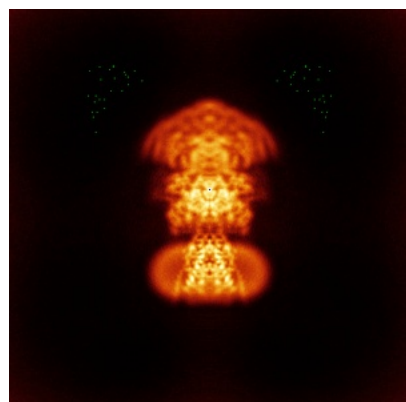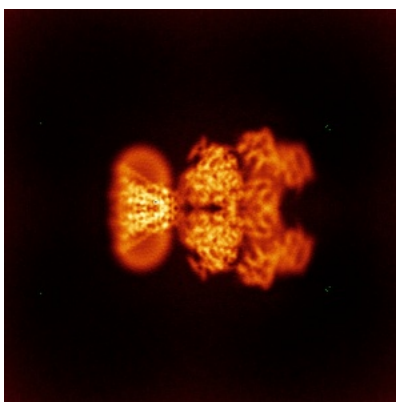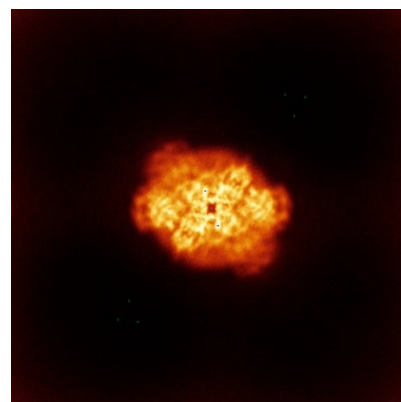
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X   Y   Z

The images above show the 3D surface view of the map at the recommended contour level 0.0915. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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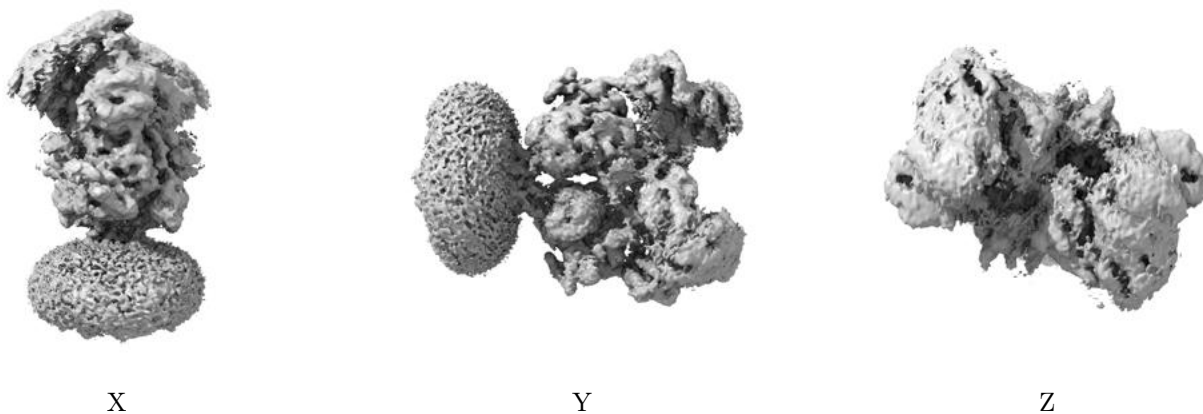
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation ⓘ

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

7   Map analysis ⓘ

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

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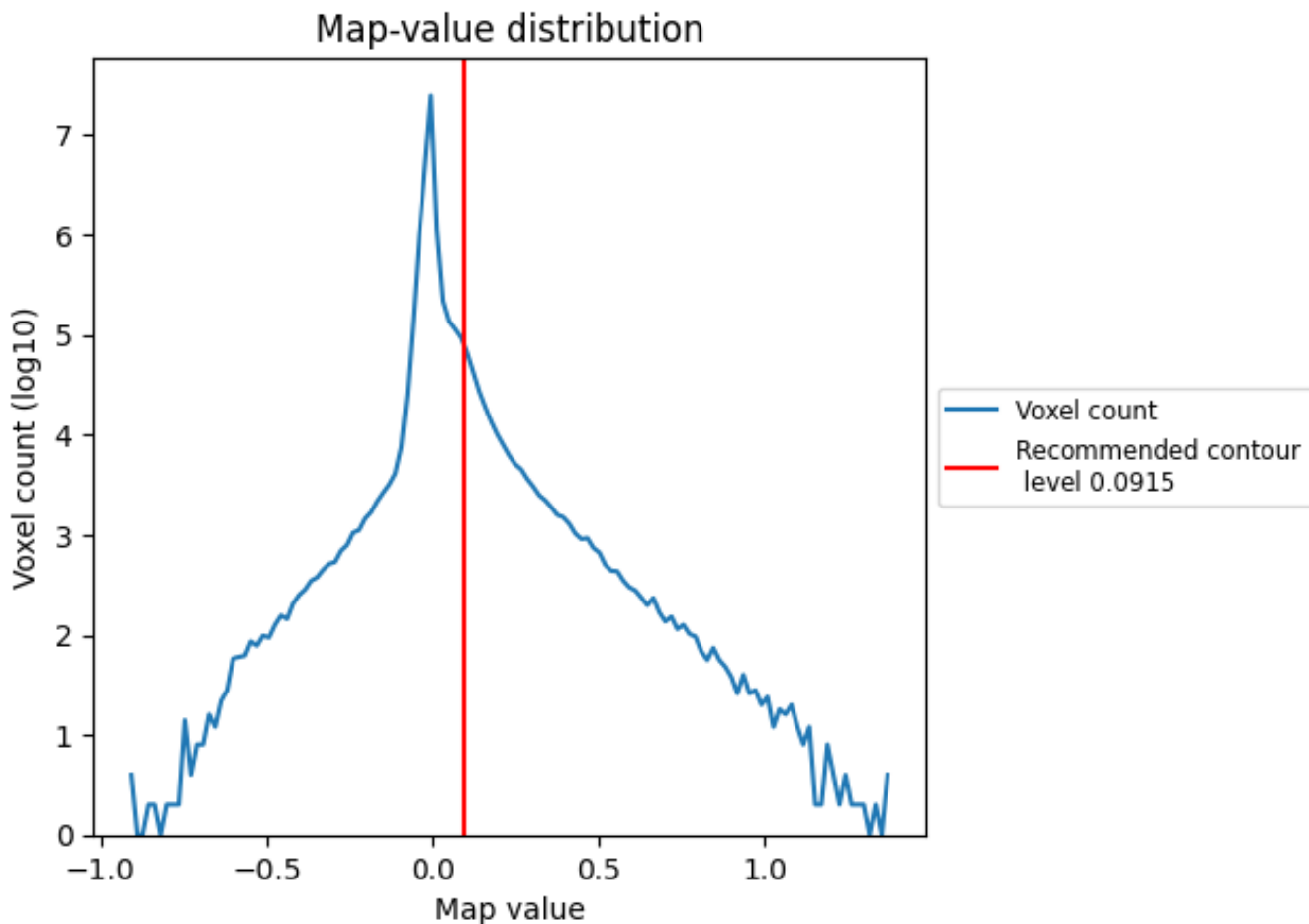
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
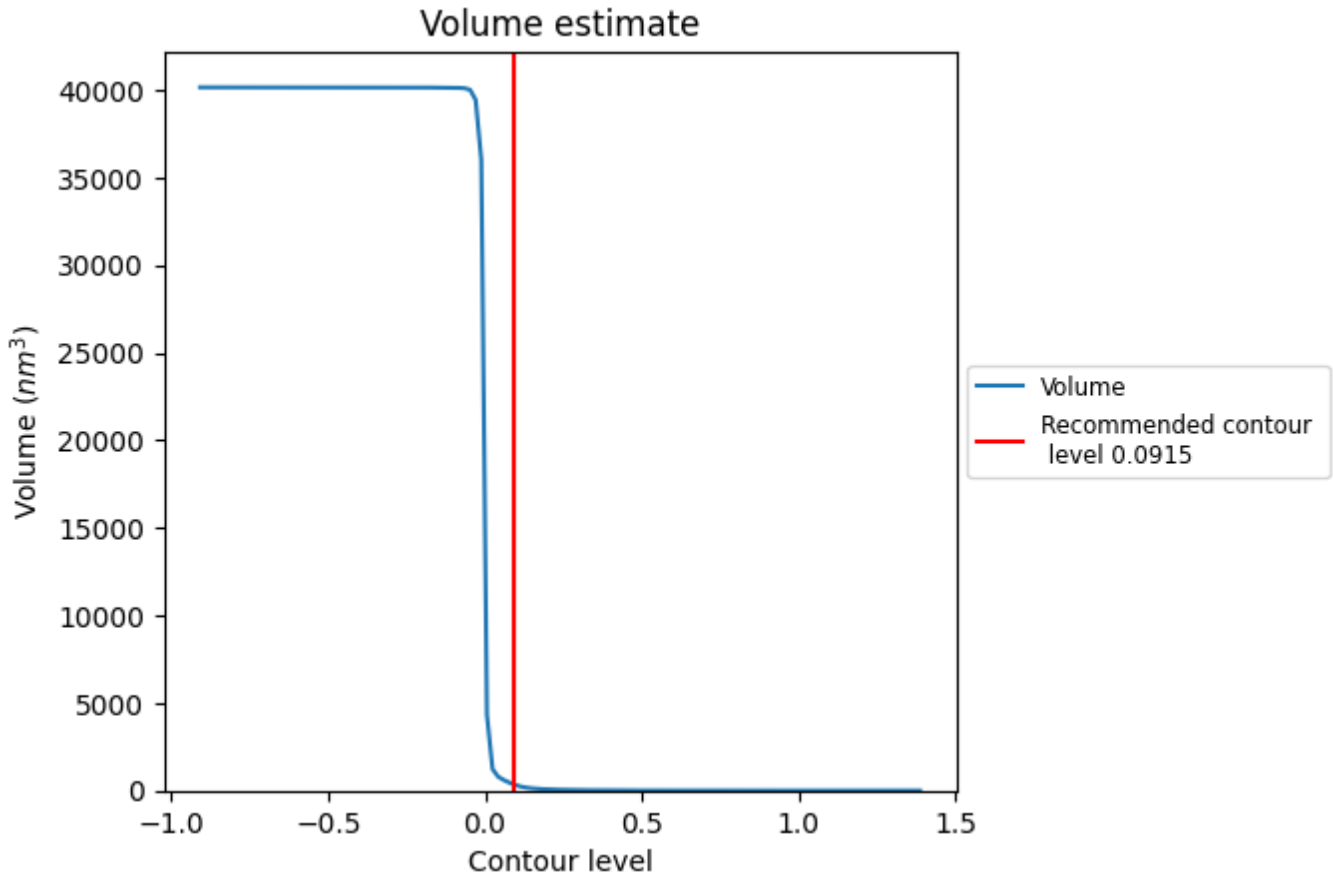
The volume at the recommended contour level is 356 nm^3; this corresponds to an approximate mass of 321 kDa.

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 ⓘ
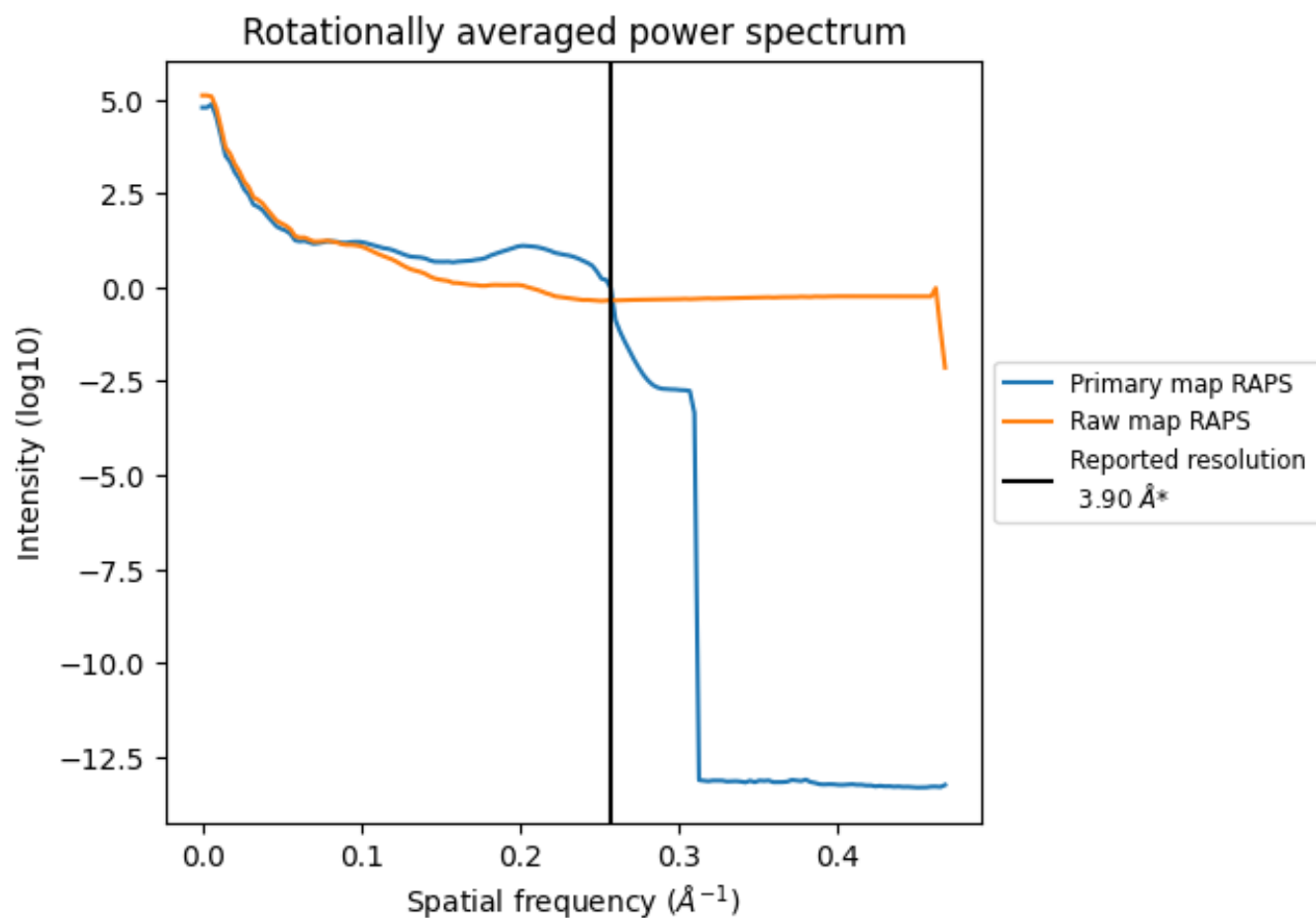
*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8   Fourier-Shell correlation ⓘ

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 ⓘ
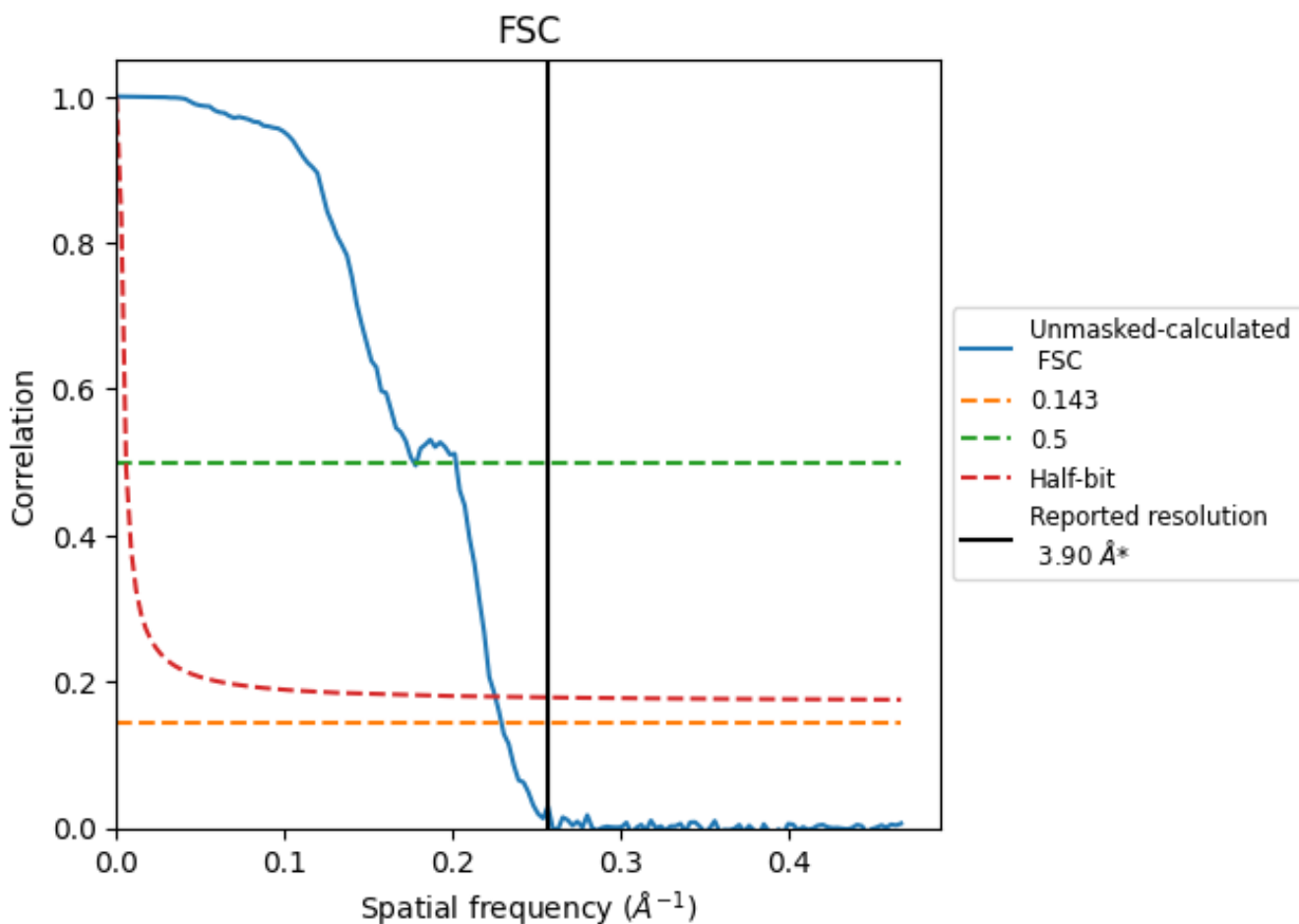
*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.36	5.65	4.43

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.36 differs from the reported value 3.9 by more than 10 %

9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-43783 and PDB model 9ARI. Per-residue inclusion information can be found in section 3 on page 8.

9.1   Map-model overlay ⓘ
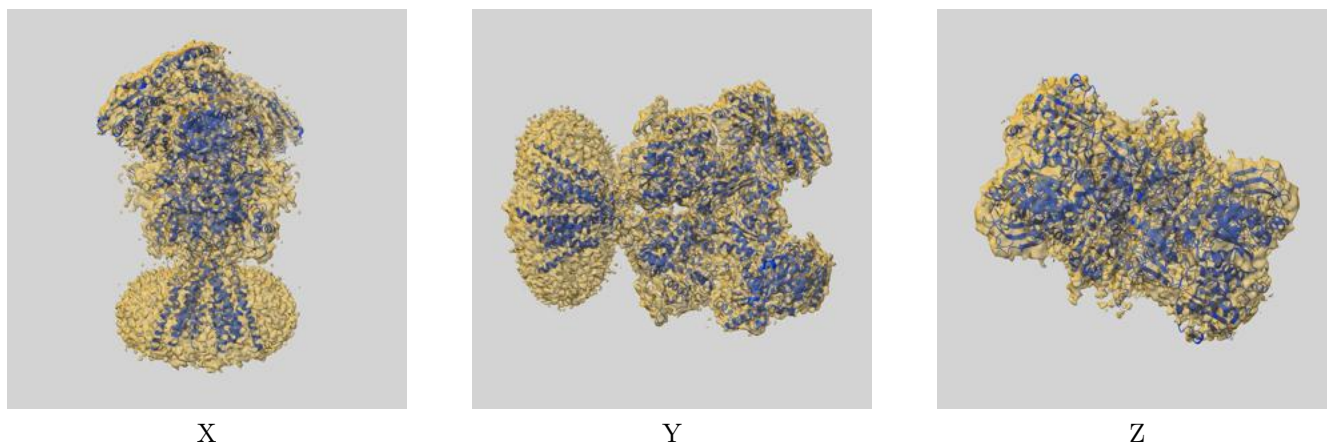
X	Y	Z

The images above show the 3D surface view of the map at the recommended contour level 0.0915 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.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

9.2 Q-score mapped to coordinate model ⓘ

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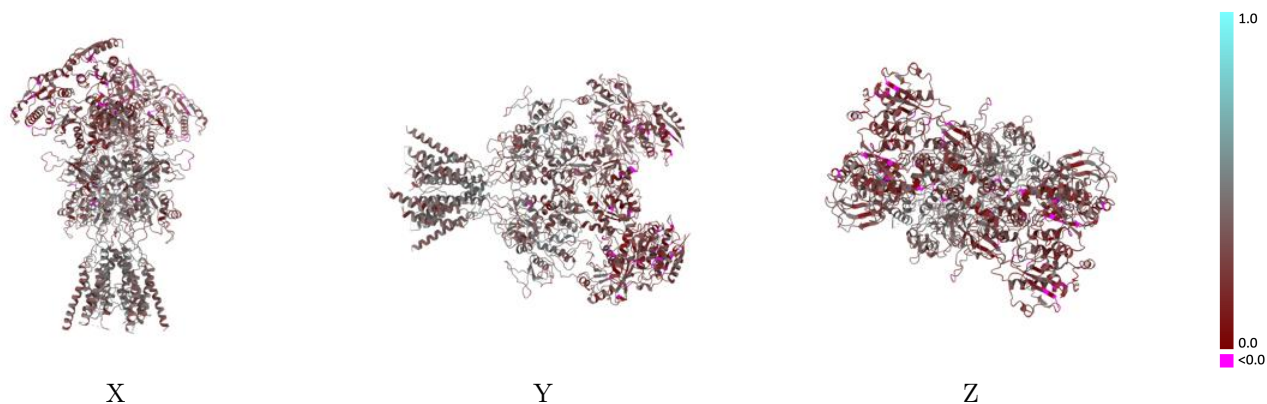
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model ⓘ

X   Y   Z
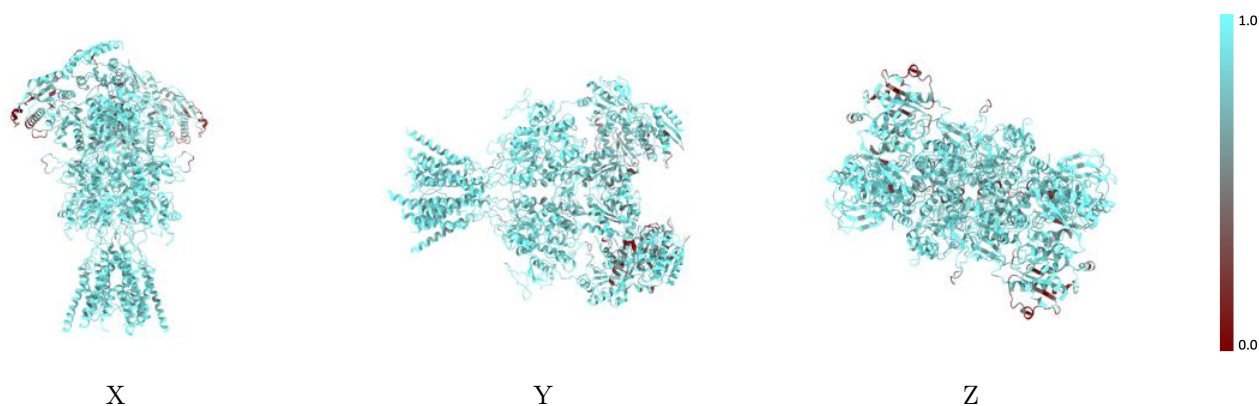
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0915).

9.4 Atom inclusion ⓘ
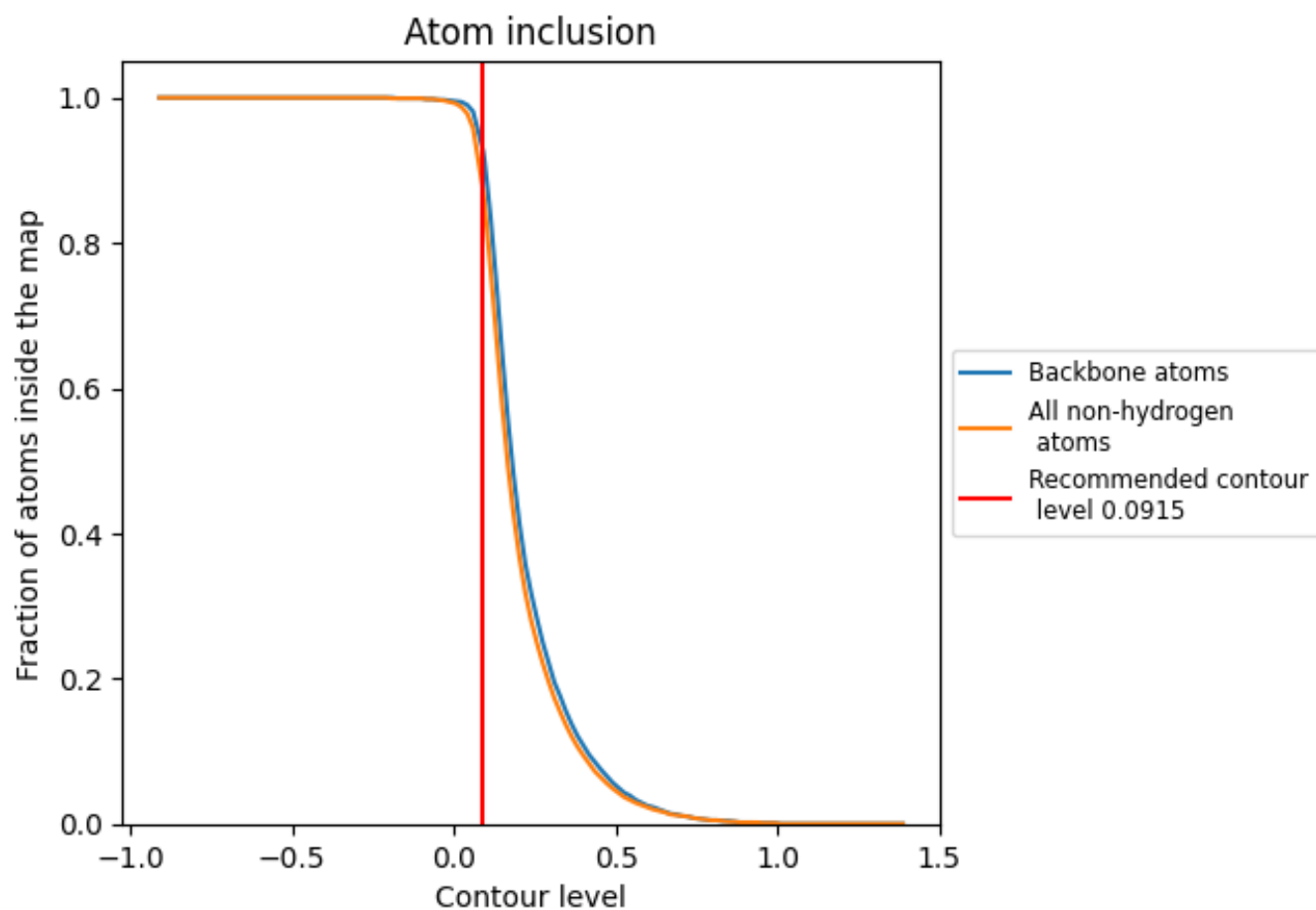
At the recommended contour level, 93% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0915) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8710	0.3420
A	0.8960	0.3550
B	0.8450	0.3290
C	0.8950	0.3520
D	0.8450	0.3310

1.0

0.0

<0.0