



Full wwPDB EM Validation Report ⓘ

May 4, 2026 – 12:58 PM EDT

PDB ID : 9OSG / pdb_00009osg
EMDB ID : EMD-70806
Title : The partially ruptured LBD state of GluK2/K5 with 5-iodowillardine and kynurenic acid sodium salt
Authors : Khanra, N.K.; Meyerson, J.R.
Deposited on : 2025-05-24
Resolution : 3.83 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

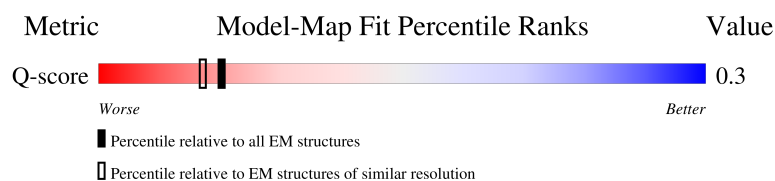
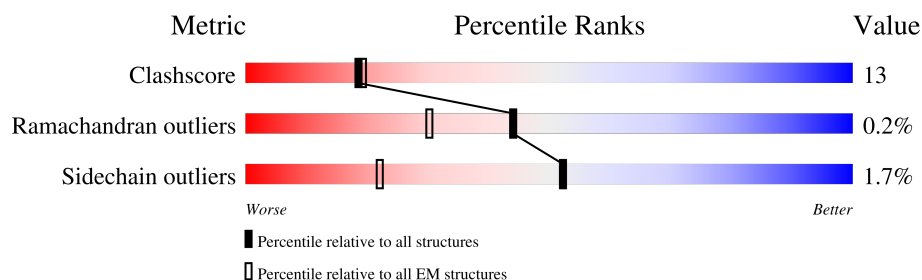
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.83 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9087 (3.33 - 4.33)

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	1101	
1	C	1101	
2	B	942	
2	D	942	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21712 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 Glutamate receptor ionotropic, kainate 5, Green fluorescent protein chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	747	Total	C	N	O	S	0	0
			5462	3490	925	1020	27		
1	C	747	Total	C	N	O	S	0	0
			5170	3279	893	977	21		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	559	VAL	CYS	conflict	UNP Q63273
A	578	SER	CYS	conflict	UNP Q63273
A	619	ILE	CYS	conflict	UNP Q63273
A	813	ALA	CYS	conflict	UNP Q63273
A	828	TYR	-	linker	UNP Q63273
A	829	LYS	-	linker	UNP Q63273
A	830	SER	-	linker	UNP Q63273
A	831	ARG	-	linker	UNP Q63273
A	832	ALA	-	linker	UNP Q63273
A	833	GLU	-	linker	UNP Q63273
A	834	ALA	-	linker	UNP Q63273
A	835	LYS	-	linker	UNP Q63273
A	836	ARG	-	linker	UNP Q63273
A	837	MET	-	linker	UNP Q63273
A	838	LYS	-	linker	UNP Q63273
A	839	GLY	-	linker	UNP Q63273
A	840	LEU	-	linker	UNP Q63273
A	841	VAL	-	linker	UNP Q63273
A	842	PRO	-	linker	UNP Q63273
A	843	ARG	-	linker	UNP Q63273
A	844	GLY	-	linker	UNP Q63273
A	845	SER	-	linker	UNP Q63273
A	846	ALA	-	linker	UNP Q63273
A	847	ALA	-	linker	UNP Q63273
A	848	ALA	-	linker	UNP Q63273

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Chain	Residue	Modelled	Actual	Comment	Reference
A	849	ALA	-	linker	UNP Q63273
A	850	MET	-	linker	UNP Q63273
A	851	VAL	-	linker	UNP Q63273
C	559	VAL	CYS	conflict	UNP Q63273
C	578	SER	CYS	conflict	UNP Q63273
C	619	ILE	CYS	conflict	UNP Q63273
C	813	ALA	CYS	conflict	UNP Q63273
C	828	TYR	-	linker	UNP Q63273
C	829	LYS	-	linker	UNP Q63273
C	830	SER	-	linker	UNP Q63273
C	831	ARG	-	linker	UNP Q63273
C	832	ALA	-	linker	UNP Q63273
C	833	GLU	-	linker	UNP Q63273
C	834	ALA	-	linker	UNP Q63273
C	835	LYS	-	linker	UNP Q63273
C	836	ARG	-	linker	UNP Q63273
C	837	MET	-	linker	UNP Q63273
C	838	LYS	-	linker	UNP Q63273
C	839	GLY	-	linker	UNP Q63273
C	840	LEU	-	linker	UNP Q63273
C	841	VAL	-	linker	UNP Q63273
C	842	PRO	-	linker	UNP Q63273
C	843	ARG	-	linker	UNP Q63273
C	844	GLY	-	linker	UNP Q63273
C	845	SER	-	linker	UNP Q63273
C	846	ALA	-	linker	UNP Q63273
C	847	ALA	-	linker	UNP Q63273
C	848	ALA	-	linker	UNP Q63273
C	849	ALA	-	linker	UNP Q63273
C	850	MET	-	linker	UNP Q63273
C	851	VAL	-	linker	UNP Q63273

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	755	Total	C	N	O	S	0	0
			5398	3456	913	1007	22		
2	D	755	Total	C	N	O	S	0	0
			5682	3667	947	1044	24		

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	567	VAL	ILE	conflict	UNP P42260
B	576	VAL	CYS	conflict	UNP P42260
B	595	SER	CYS	conflict	UNP P42260
B	909	SER	-	expression tag	UNP P42260
B	910	GLY	-	expression tag	UNP P42260
B	911	LEU	-	expression tag	UNP P42260
B	912	ARG	-	expression tag	UNP P42260
B	913	SER	-	expression tag	UNP P42260
B	914	ALA	-	expression tag	UNP P42260
B	915	TRP	-	expression tag	UNP P42260
B	916	SER	-	expression tag	UNP P42260
B	917	HIS	-	expression tag	UNP P42260
B	918	PRO	-	expression tag	UNP P42260
B	919	GLN	-	expression tag	UNP P42260
B	920	PHE	-	expression tag	UNP P42260
B	921	GLU	-	expression tag	UNP P42260
B	922	LYS	-	expression tag	UNP P42260
B	923	GLY	-	expression tag	UNP P42260
B	924	GLY	-	expression tag	UNP P42260
B	925	GLY	-	expression tag	UNP P42260
B	926	SER	-	expression tag	UNP P42260
B	927	GLY	-	expression tag	UNP P42260
B	928	GLY	-	expression tag	UNP P42260
B	929	GLY	-	expression tag	UNP P42260
B	930	SER	-	expression tag	UNP P42260
B	931	GLY	-	expression tag	UNP P42260
B	932	GLY	-	expression tag	UNP P42260
B	933	GLY	-	expression tag	UNP P42260
B	934	SER	-	expression tag	UNP P42260
B	935	TRP	-	expression tag	UNP P42260
B	936	SER	-	expression tag	UNP P42260
B	937	HIS	-	expression tag	UNP P42260
B	938	PRO	-	expression tag	UNP P42260
B	939	GLN	-	expression tag	UNP P42260
B	940	PHE	-	expression tag	UNP P42260
B	941	GLU	-	expression tag	UNP P42260
B	942	LYS	-	expression tag	UNP P42260
D	567	VAL	ILE	conflict	UNP P42260
D	576	VAL	CYS	conflict	UNP P42260
D	595	SER	CYS	conflict	UNP P42260
D	909	SER	-	expression tag	UNP P42260
D	910	GLY	-	expression tag	UNP P42260
D	911	LEU	-	expression tag	UNP P42260

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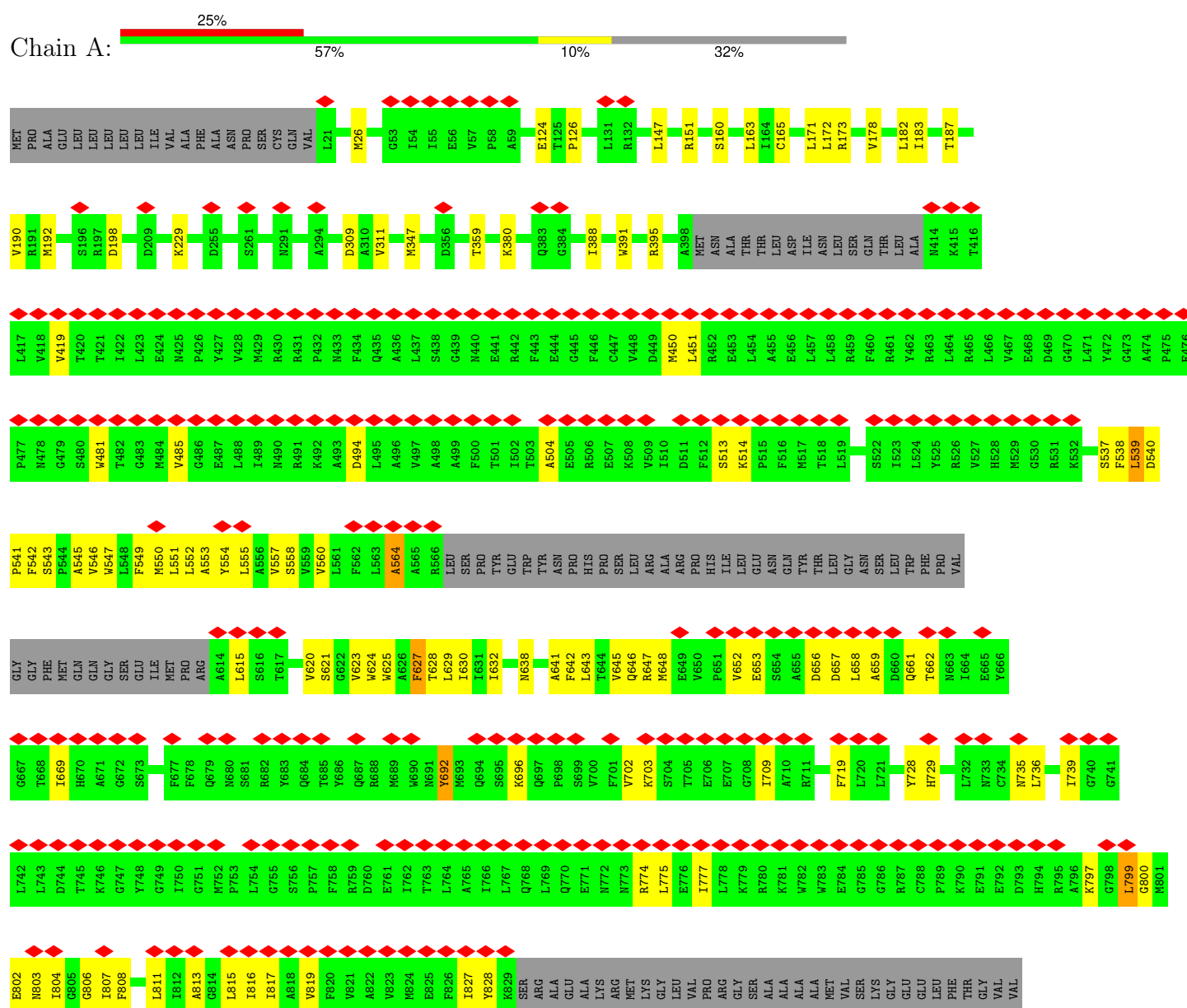
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Chain	Residue	Modelled	Actual	Comment	Reference
D	912	ARG	-	expression tag	UNP P42260
D	913	SER	-	expression tag	UNP P42260
D	914	ALA	-	expression tag	UNP P42260
D	915	TRP	-	expression tag	UNP P42260
D	916	SER	-	expression tag	UNP P42260
D	917	HIS	-	expression tag	UNP P42260
D	918	PRO	-	expression tag	UNP P42260
D	919	GLN	-	expression tag	UNP P42260
D	920	PHE	-	expression tag	UNP P42260
D	921	GLU	-	expression tag	UNP P42260
D	922	LYS	-	expression tag	UNP P42260
D	923	GLY	-	expression tag	UNP P42260
D	924	GLY	-	expression tag	UNP P42260
D	925	GLY	-	expression tag	UNP P42260
D	926	SER	-	expression tag	UNP P42260
D	927	GLY	-	expression tag	UNP P42260
D	928	GLY	-	expression tag	UNP P42260
D	929	GLY	-	expression tag	UNP P42260
D	930	SER	-	expression tag	UNP P42260
D	931	GLY	-	expression tag	UNP P42260
D	932	GLY	-	expression tag	UNP P42260
D	933	GLY	-	expression tag	UNP P42260
D	934	SER	-	expression tag	UNP P42260
D	935	TRP	-	expression tag	UNP P42260
D	936	SER	-	expression tag	UNP P42260
D	937	HIS	-	expression tag	UNP P42260
D	938	PRO	-	expression tag	UNP P42260
D	939	GLN	-	expression tag	UNP P42260
D	940	PHE	-	expression tag	UNP P42260
D	941	GLU	-	expression tag	UNP P42260
D	942	LYS	-	expression tag	UNP P42260

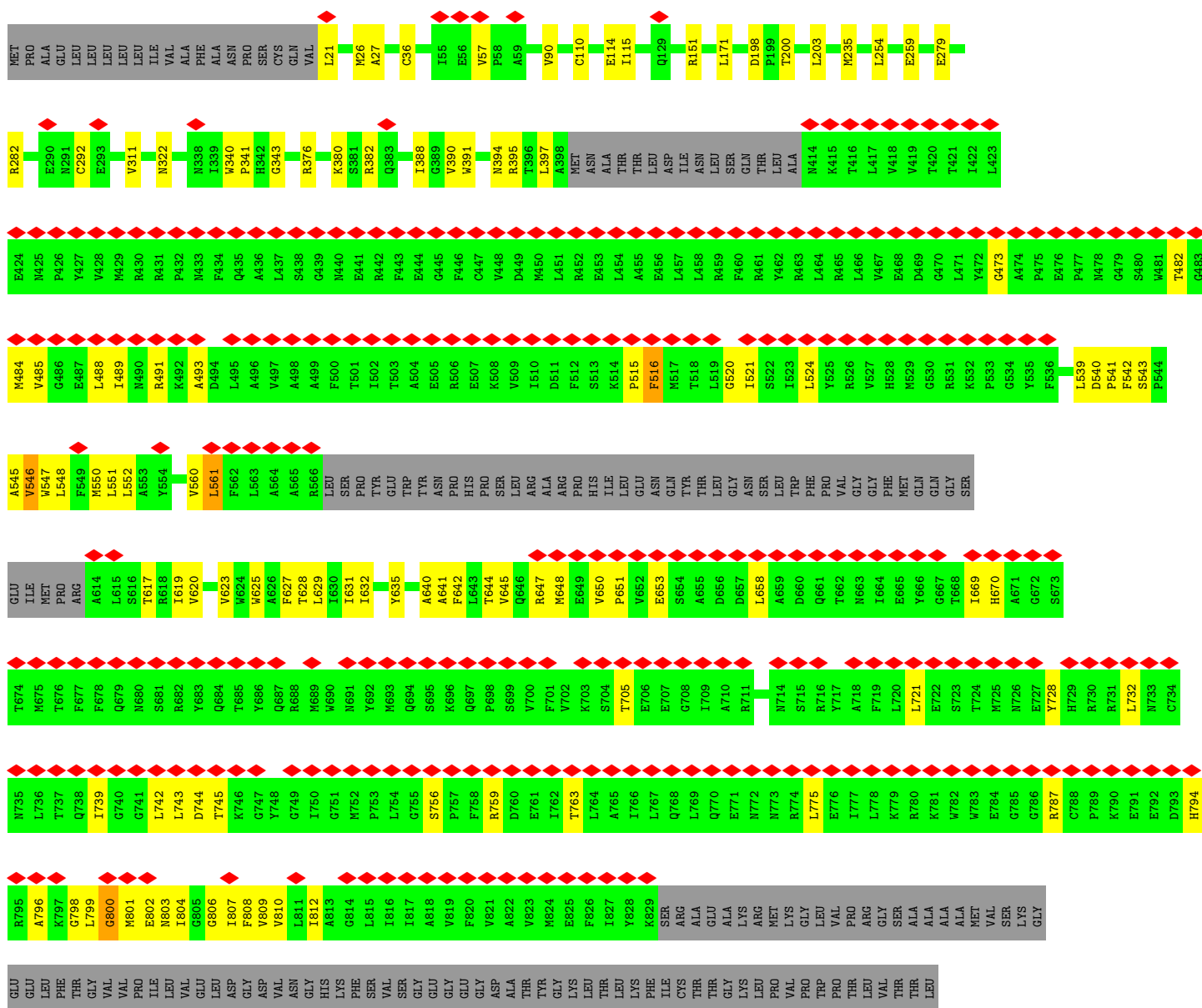
3 Residue-property plots

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: Glutamate receptor ionotropic, kainate 5, Green fluorescent protein chimera

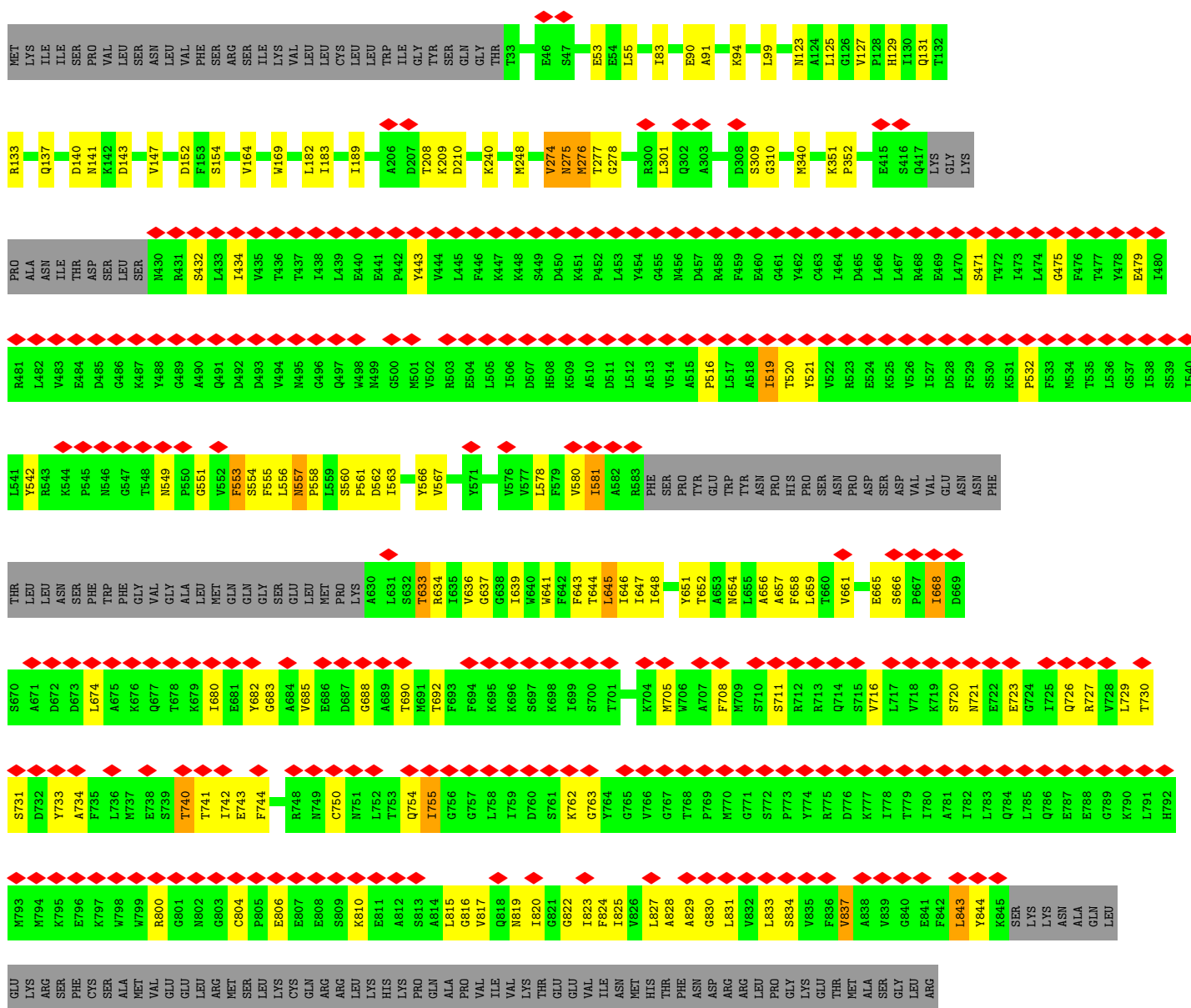


- Molecule 1: Glutamate receptor ionotropic, kainate 5, Green fluorescent protein chimera



THR	SER	GLN	VAL	ALA	PRO	ALA	THR	ASN	LEU	THR	GLY	THR	THR
								ASN	GLY	LEU	GLY	GLY	THR
								PRO	ILE	GLY	ILE	GLY	GLY
								GLY	ASP	ASP	ASP	ASP	GLN
								ASP	PHE	PHE	PHE	CYS	VAL
								GLY	LYS	LYS	LYS	PHE	THR
								PRO	GLU	GLU	GLU	SER	SER
								LEU	ASP	ASP	ASP	ARG	THR
								PRO	ASN	ASN	ASN	PRO	THR
								ASP	ILE	ILE	ASP	HIS	ASP
								ASN	LEU	LEU	GLY	MET	LYS
								THR	HIS	HIS	GLN	LYS	GLN
								LEU	LEU	LEU	LEU	HIS	ASP
								SER	SER	GLU	THR	ASP	THR
								THR	THR	THR	THR	PHE	THR
								GLN	ASN	ASN	ASN	PHE	THR
								SER	LYS	LYS	LYS	SER	THR
								LEU	ASN	ASN	ASN	SER	THR
								SER	HIS	HIS	ALA	MET	THR
								LYS	ASN	ASN	PRO	MET	THR
								ASP	VAL	VAL	GLY	GLU	GLY
								PRO	THR	THR	THR	TYR	TYR
								ASN	ILE	ILE	VAL	VAL	VAL
								GLU	MET	ALA	GLN	GLU	GLN
								LYS	ALA	ASP	GLU	GLU	GLU
								ARG	LYS	LYS	ARG	ARG	ARG
								ASP	GLN	THR	THR	ALA	ALA
								HIS	LYS	ILE	ILE	ALA	GLU
								MET	ASN	ASN	ASN	ALA	GLU
								VAL	ASN	ASN	GLY	ASN	THR
								LEU	GLY	ILE	LYS	LYS	THR
								LEU	ILE	LYS	ASP	ASP	THR
								GLU	LYS	VAL	VAL	ASP	VAL
								VAL	ASN	ASN	GLY	GLY	GLY
								THR	PHE	LYS	TYR	TYR	THR
								ALA	LYS	ILE	LYS	THR	THR
								GLY	ARG	ARG	ALA	ALA	LEU
								LEU	ILE	ILE	GLU	GLU	VAL
								GLY	GLU	GLU	VAL	GLY	VAL
								MET	ASP	ASP	LYS	LYS	LEU
								ASP	GLY	PHE	PHE	PHE	VAL
								GLU	SER	SER	GLY	GLY	VAL
								LEU	VAL	GLN	ASP	ASP	ASN
								THR	LEU	THR	THR	THR	ASN
								ARG	THR	THR	THR	THR	ARG
								THR	GLN	GLN	ILE	ILE	THR
								GLN	GLN	GLN	GLN	GLN	GLN

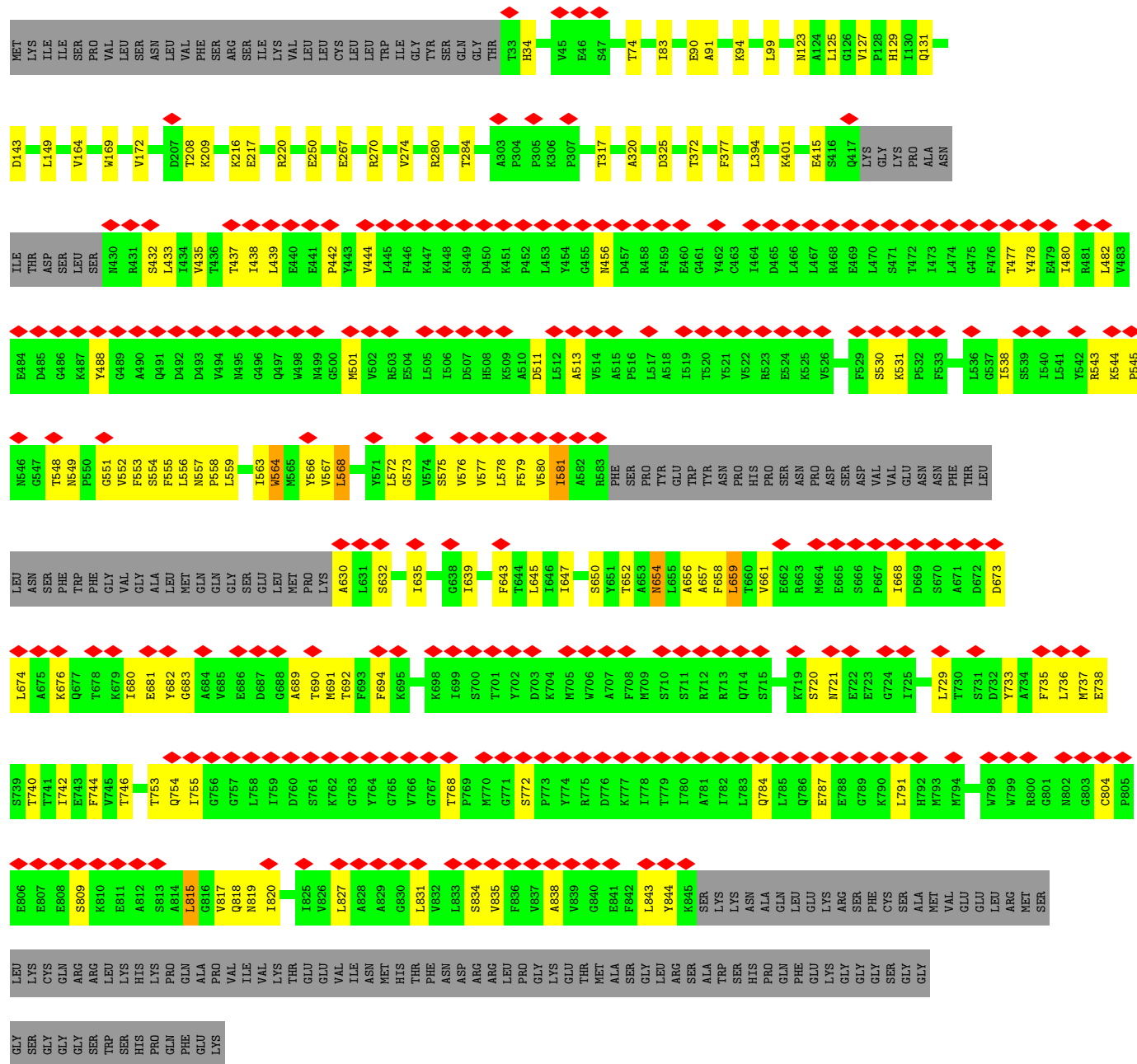
- Molecule 2: Glutamate receptor ionotropic, kainate 2



SER
ALA
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS
GLY
GLY
GLY
SER
GLY
GLY
GLY
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS

● Molecule 2: Glutamate receptor ionotropic, kainate 2

Chain D: 26% 65% 15% 20%



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Property	Value	Source
Map value standard deviation	0.020	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	408.96, 408.96, 408.96	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.852, 0.852, 0.852	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	0.57	0/5563	0.82	8/7582 (0.1%)
1	C	0.61	4/5248 (0.1%)	0.83	4/7170 (0.1%)
2	B	0.68	6/5505 (0.1%)	0.86	21/7512 (0.3%)
2	D	0.58	1/5807 (0.0%)	0.80	6/7905 (0.1%)
All	All	0.61	11/22123 (0.0%)	0.83	39/30169 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	515	PRO	C-O	-8.07	1.13	1.24
2	B	532	PRO	C-O	-6.71	1.14	1.23
2	B	519	ILE	CA-C	-6.64	1.46	1.53
2	B	276	MET	C-O	-6.59	1.16	1.23
1	C	516	PHE	C-O	-6.35	1.15	1.23
2	B	519	ILE	C-O	-5.99	1.15	1.23
1	C	516	PHE	CA-C	-5.69	1.44	1.52
2	B	532	PRO	CA-C	-5.66	1.45	1.52
2	D	654	ASN	CA-C	-5.64	1.45	1.52
2	B	275	ASN	C-O	-5.30	1.17	1.24
1	C	515	PRO	CA-CB	-5.26	1.46	1.53

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	564	ALA	N-CA-C	11.27	123.56	111.28
1	A	802	GLU	N-CA-C	10.00	123.22	111.02
1	A	615	LEU	N-CA-C	8.91	120.99	111.28
1	A	799	LEU	N-CA-C	-8.72	102.19	112.92
2	B	666	SER	CA-C-N	8.71	129.87	120.11
2	B	666	SER	C-N-CA	8.71	129.87	120.11
1	C	803	ASN	N-CA-C	8.33	120.36	111.28
1	C	388	ILE	N-CA-C	-7.85	105.49	113.10
2	B	763	GLY	N-CA-C	7.19	121.64	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	734	ALA	N-CA-C	-7.10	98.39	109.25
2	D	804	CYS	CA-C-N	7.06	128.67	119.84
2	D	804	CYS	C-N-CA	7.06	128.67	119.84
1	A	388	ILE	N-CA-C	-6.51	106.79	113.10
2	B	633	THR	N-CA-C	-6.43	104.28	111.28
2	D	564	TRP	CA-C-N	6.15	133.29	121.54
2	D	564	TRP	C-N-CA	6.15	133.29	121.54
2	B	810	LYS	N-CA-C	6.10	117.39	107.32
2	B	580	VAL	CA-C-N	5.85	128.44	120.77
2	B	580	VAL	C-N-CA	5.85	128.44	120.77
2	B	634	ARG	N-CA-C	5.83	118.11	111.11
2	D	630	ALA	CA-C-N	5.82	128.40	120.54
2	D	630	ALA	C-N-CA	5.82	128.40	120.54
2	B	549	ASN	CA-C-N	-5.73	112.67	119.84
2	B	549	ASN	C-N-CA	-5.73	112.67	119.84
2	B	274	VAL	CB-CA-C	-5.72	103.73	111.63
1	C	787	ARG	N-CA-C	5.62	117.41	111.28
2	B	762	LYS	O-C-N	-5.56	116.44	123.17
1	A	696	LYS	CA-C-N	5.50	127.84	120.58
1	A	696	LYS	C-N-CA	5.50	127.84	120.58
1	C	802	GLU	N-CA-C	-5.49	99.11	110.80
2	B	519	ILE	N-CA-CB	-5.26	106.22	111.90
2	B	532	PRO	N-CA-CB	-5.21	98.50	103.19
1	A	627	PHE	N-CA-C	-5.12	106.98	113.43
2	B	557	ASN	CA-C-N	5.10	126.22	119.84
2	B	557	ASN	C-N-CA	5.10	126.22	119.84
2	B	479	GLU	N-CA-C	-5.08	98.99	107.99
2	B	553	PHE	N-CA-C	-5.05	104.42	111.39
2	B	532	PRO	CB-CA-C	-5.04	105.24	111.64
2	B	581	ILE	CA-C-O	-5.01	116.20	121.41

There are no chirality outliers.

There are no planarity outliers.

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	5462	0	5161	161	0
1	C	5170	0	4697	131	0
2	B	5398	0	4896	181	0
2	D	5682	0	5461	181	0
All	All	21712	0	20215	543	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 13.

All (543) 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:727:ARG:HB3	2:B:733:TYR:CD2	1.58	1.39
1:C:550:MET:SD	1:C:631:ILE:HD11	1.72	1.28
2:D:735:PHE:CE2	2:D:737:MET:HB2	1.70	1.25
2:D:581:ILE:CD1	2:D:632:SER:HB3	1.70	1.20
2:D:581:ILE:HD13	2:D:632:SER:CB	1.71	1.19
1:A:538:PHE:CE2	1:A:806:GLY:HA3	1.79	1.17
1:A:632:ILE:HD12	2:D:645:LEU:HD21	1.24	1.16
2:B:711:SER:CB	1:C:743:LEU:O	1.94	1.15
1:C:625:TRP:CZ2	1:C:629:LEU:HD11	1.84	1.11
1:A:560:VAL:O	1:A:564:ALA:HB3	1.50	1.10
2:B:711:SER:HB2	1:C:743:LEU:C	1.77	1.09
2:B:643:PHE:HA	1:C:807:ILE:HD11	1.28	1.09
2:D:721:ASN:HD21	2:D:737:MET:HE2	1.04	1.09
2:B:563:ILE:HD13	1:C:804:ILE:HD11	1.34	1.08
2:B:711:SER:HB2	1:C:743:LEU:O	1.53	1.08
1:C:623:VAL:HG12	2:D:827:LEU:HD12	1.33	1.08
2:D:581:ILE:HD13	2:D:632:SER:HB3	1.08	1.07
1:C:541:PRO:HG2	1:C:635:TYR:CE1	1.90	1.06
2:D:721:ASN:HD21	2:D:737:MET:CE	1.69	1.05
2:B:668:ILE:HD11	2:B:680:ILE:HD12	1.33	1.05
1:C:625:TRP:CE2	1:C:629:LEU:HD11	1.90	1.05
1:C:541:PRO:HG2	1:C:635:TYR:HE1	1.22	1.05
1:A:627:PHE:HD1	2:B:823:ILE:HG12	1.22	1.04
2:B:551:GLY:HA3	2:B:819:ASN:HA	1.35	1.04
2:D:721:ASN:ND2	2:D:737:MET:HE2	1.72	1.04
1:C:623:VAL:HG12	2:D:827:LEU:CD1	1.88	1.03
1:A:538:PHE:HE2	1:A:806:GLY:HA3	0.91	1.02
1:A:774:ARG:O	1:A:777:ILE:HG22	1.59	1.02
2:D:581:ILE:CD1	2:D:632:SER:CB	2.35	1.01
1:A:538:PHE:HE2	1:A:806:GLY:CA	1.73	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:560:VAL:HG21	2:D:831:LEU:HD21	1.44	1.00
1:A:813:ALA:O	1:A:816:ILE:HG12	1.60	1.00
1:C:550:MET:SD	1:C:631:ILE:CD1	2.49	0.99
1:A:560:VAL:O	1:A:564:ALA:CB	2.08	0.99
1:C:623:VAL:CG1	2:D:827:LEU:HD12	1.93	0.98
1:A:662:THR:HG23	1:A:692:TYR:OH	1.60	0.98
2:D:576:VAL:HA	2:D:579:PHE:CD2	1.98	0.97
2:B:443:TYR:OH	2:B:740:THR:HG21	1.66	0.96
2:B:556:LEU:HD23	2:B:556:LEU:O	1.66	0.95
2:B:727:ARG:HB3	2:B:733:TYR:HD2	1.21	0.95
2:B:682:TYR:CZ	2:B:708:PHE:CB	2.50	0.94
2:B:643:PHE:HD1	1:C:807:ILE:CD1	1.81	0.93
2:B:711:SER:HB3	1:C:743:LEU:O	1.66	0.93
1:A:542:PHE:HD2	1:A:547:TRP:HZ3	1.14	0.91
2:B:553:PHE:CB	2:B:557:ASN:HB2	2.00	0.91
2:D:735:PHE:HE2	2:D:737:MET:HB2	1.18	0.89
1:A:630:ILE:HB	2:B:823:ILE:HD12	1.53	0.88
1:A:538:PHE:CE2	1:A:806:GLY:CA	2.53	0.88
1:A:627:PHE:CD1	2:B:823:ILE:HG12	2.09	0.87
1:A:632:ILE:CD1	2:D:645:LEU:HD21	2.04	0.87
2:B:682:TYR:CZ	2:B:705:MET:HA	2.09	0.87
2:B:727:ARG:CB	2:B:733:TYR:CD2	2.54	0.87
2:B:557:ASN:N	2:B:558:PRO:HD2	1.90	0.86
2:B:682:TYR:HE1	2:B:705:MET:O	1.59	0.86
1:A:813:ALA:O	1:A:816:ILE:CG1	2.23	0.85
1:A:629:LEU:HD11	2:B:648:ILE:HG21	1.58	0.85
2:B:682:TYR:OH	2:B:705:MET:HA	1.77	0.85
1:C:560:VAL:CG2	2:D:831:LEU:HD21	2.05	0.84
2:B:555:PHE:CD1	2:B:555:PHE:O	2.30	0.84
1:C:524:LEU:HD11	1:C:721:LEU:HD12	1.59	0.84
1:C:524:LEU:CD1	1:C:721:LEU:HD12	2.08	0.84
2:D:735:PHE:HE2	2:D:737:MET:CB	1.90	0.84
1:C:548:LEU:O	1:C:552:LEU:HD13	1.77	0.84
2:D:577:VAL:O	2:D:580:VAL:HG22	1.75	0.84
2:B:843:LEU:C	2:B:843:LEU:HD13	2.03	0.83
2:B:646:ILE:HB	1:C:807:ILE:HD12	1.61	0.83
2:B:727:ARG:HD2	2:B:733:TYR:CE2	2.12	0.83
1:A:542:PHE:HD2	1:A:547:TRP:CZ3	1.96	0.82
2:B:668:ILE:HD11	2:B:680:ILE:CD1	2.10	0.82
2:D:737:MET:HG3	2:D:738:GLU:H	1.42	0.82
1:C:625:TRP:CZ2	1:C:629:LEU:CD1	2.63	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:799:LEU:HD22	2:D:654:ASN:HD22	1.45	0.82
2:B:563:ILE:HD13	1:C:804:ILE:CD1	2.11	0.81
2:D:815:LEU:HG	2:D:820:ILE:CG2	2.11	0.81
2:B:645:LEU:HD21	1:C:632:ILE:HD11	1.61	0.81
2:D:737:MET:HG3	2:D:738:GLU:N	1.95	0.81
2:B:682:TYR:O	2:B:682:TYR:CD1	2.35	0.80
2:D:551:GLY:HA2	2:D:819:ASN:HA	1.61	0.79
2:D:735:PHE:CE2	2:D:737:MET:CB	2.60	0.79
2:B:682:TYR:CE1	2:B:705:MET:O	2.36	0.79
1:A:630:ILE:HB	2:B:823:ILE:CD1	2.12	0.78
1:C:560:VAL:HG21	2:D:831:LEU:CD2	2.12	0.78
2:D:815:LEU:HG	2:D:820:ILE:HG23	1.63	0.78
1:C:651:PRO:O	1:C:653:GLU:HG3	1.84	0.77
1:A:816:ILE:HG13	1:A:817:ILE:N	1.98	0.77
1:A:816:ILE:HG13	1:A:817:ILE:H	1.51	0.76
2:D:581:ILE:CD1	2:D:632:SER:OG	2.33	0.75
2:D:581:ILE:HD11	2:D:632:SER:OG	1.85	0.75
1:A:538:PHE:CE2	1:A:806:GLY:C	2.65	0.75
1:A:799:LEU:O	2:D:563:ILE:HD11	1.86	0.75
1:A:647:ARG:HG2	2:D:661:VAL:HG21	1.69	0.74
2:D:149:LEU:HD23	2:D:377:PHE:HE1	1.50	0.74
2:B:560:SER:HB3	1:C:798:GLY:O	1.87	0.74
2:B:682:TYR:OH	2:B:708:PHE:CB	2.36	0.74
2:B:682:TYR:CE1	2:B:705:MET:HB3	2.24	0.73
2:B:645:LEU:HD21	1:C:632:ILE:CD1	2.17	0.73
1:A:647:ARG:CG	2:D:661:VAL:HG21	2.19	0.73
1:A:638:ASN:ND2	2:B:815:LEU:HB2	2.03	0.72
2:B:658:PHE:HE1	1:C:647:ARG:CZ	2.03	0.72
2:B:551:GLY:CA	2:B:819:ASN:HA	2.16	0.72
2:D:433:LEU:HD22	2:D:511:ASP:OD2	1.89	0.72
2:B:820:ILE:O	2:B:823:ILE:HG22	1.90	0.71
1:C:759:ARG:O	1:C:763:THR:HG23	1.89	0.71
2:B:562:ASP:HB3	2:B:566:TYR:CZ	2.25	0.71
2:B:558:PRO:CG	2:B:651:TYR:CE1	2.74	0.71
2:B:558:PRO:HG3	2:B:651:TYR:CE1	2.26	0.71
1:A:627:PHE:HD1	2:B:823:ILE:CG1	2.02	0.71
1:A:632:ILE:HD12	2:D:645:LEU:CD2	2.15	0.71
2:B:727:ARG:HB3	2:B:733:TYR:CG	2.23	0.70
2:D:820:ILE:HD12	2:D:820:ILE:O	1.92	0.70
1:A:542:PHE:CD2	1:A:547:TRP:HZ3	2.04	0.70
1:A:629:LEU:HD21	2:B:648:ILE:HD12	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:MET:HE3	2:B:274:VAL:HG21	1.74	0.70
2:B:682:TYR:CE2	2:B:708:PHE:CB	2.75	0.69
1:A:774:ARG:O	1:A:777:ILE:CG2	2.40	0.69
2:B:711:SER:O	1:C:745:THR:HG23	1.93	0.69
1:A:658:LEU:O	1:A:661:GLN:N	2.25	0.69
1:A:638:ASN:HD21	2:B:815:LEU:HB2	1.58	0.69
2:B:643:PHE:CD1	1:C:807:ILE:CD1	2.73	0.68
2:D:576:VAL:O	2:D:580:VAL:HG13	1.93	0.67
1:A:538:PHE:CZ	1:A:806:GLY:C	2.73	0.67
1:A:630:ILE:CB	2:B:823:ILE:HD12	2.24	0.67
1:C:653:GLU:OE1	1:C:658:LEU:HD21	1.94	0.67
1:A:800:GLY:O	2:D:563:ILE:CG1	2.43	0.67
1:A:804:ILE:O	1:A:808:PHE:CG	2.48	0.67
1:A:800:GLY:HA2	2:D:563:ILE:CD1	2.25	0.67
1:A:543:SER:OG	2:B:816:GLY:HA2	1.93	0.66
2:B:726:GLN:O	2:B:730:THR:HG23	1.96	0.66
1:A:804:ILE:HA	1:A:807:ILE:HG22	1.77	0.66
1:A:807:ILE:HG21	2:D:647:ILE:HD11	1.78	0.66
1:C:669:ILE:CD1	1:C:705:THR:HG22	2.27	0.65
1:A:799:LEU:O	2:D:563:ILE:CD1	2.45	0.65
1:A:669:ILE:HG22	1:A:719:PHE:HZ	1.62	0.65
1:A:652:VAL:O	1:A:653:GLU:HG3	1.97	0.64
2:B:668:ILE:CD1	2:B:680:ILE:HD12	2.20	0.64
1:A:647:ARG:CD	2:D:661:VAL:HG21	2.28	0.64
2:B:643:PHE:CA	1:C:807:ILE:HD11	2.17	0.64
2:D:554:SER:O	2:D:557:ASN:HB2	1.98	0.64
2:B:843:LEU:C	2:B:843:LEU:CD1	2.71	0.64
2:D:149:LEU:HD23	2:D:377:PHE:CE1	2.32	0.64
2:B:643:PHE:HD1	1:C:807:ILE:HD11	1.63	0.63
2:B:551:GLY:O	2:B:554:SER:O	2.16	0.63
1:C:561:LEU:HD21	1:C:617:THR:HG22	1.78	0.63
1:C:560:VAL:HG21	2:D:831:LEU:CG	2.28	0.63
1:A:800:GLY:O	2:D:563:ILE:HG13	1.98	0.63
1:C:653:GLU:HB2	1:C:739:ILE:HG21	1.81	0.63
2:B:641:TRP:O	2:B:644:THR:HG22	1.98	0.62
1:A:813:ALA:C	1:A:816:ILE:HG12	2.25	0.62
2:D:564:TRP:O	2:D:567:VAL:N	2.32	0.62
1:A:165:CYS:HB2	1:A:192:MET:HG2	1.82	0.62
1:C:548:LEU:O	1:C:552:LEU:CD1	2.47	0.62
1:A:647:ARG:HD2	2:D:661:VAL:CG2	2.29	0.62
1:C:520:GLY:HA3	1:C:742:LEU:HD22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:VAL:HG12	1:A:703:LYS:N	2.16	0.61
1:A:728:TYR:HD2	1:A:729:HIS:CD2	2.19	0.61
1:C:473:GLY:HA2	1:C:482:THR:O	2.00	0.61
2:D:557:ASN:HB3	2:D:558:PRO:HD3	1.82	0.61
1:C:669:ILE:CD1	1:C:705:THR:CG2	2.78	0.61
1:C:627:PHE:CD2	2:D:827:LEU:HD22	2.35	0.60
2:D:815:LEU:CD2	2:D:820:ILE:HG21	2.30	0.60
2:B:560:SER:CB	1:C:798:GLY:O	2.50	0.60
1:C:547:TRP:O	1:C:551:LEU:HG	2.02	0.60
2:B:674:LEU:O	2:B:674:LEU:HG	2.00	0.60
2:B:682:TYR:OH	2:B:705:MET:CA	2.50	0.59
1:A:799:LEU:HD22	2:D:654:ASN:ND2	2.17	0.59
1:A:542:PHE:CD2	1:A:547:TRP:CZ3	2.84	0.59
2:D:568:LEU:O	2:D:572:LEU:HG	2.02	0.59
2:D:149:LEU:HD21	2:D:377:PHE:CZ	2.37	0.59
1:A:804:ILE:O	1:A:808:PHE:CD2	2.56	0.59
2:B:665:GLU:O	2:B:665:GLU:HG3	2.03	0.59
1:C:560:VAL:HG21	2:D:831:LEU:HD11	1.85	0.58
1:A:151:ARG:HD2	1:A:391:TRP:HE1	1.67	0.58
1:A:151:ARG:NH1	1:A:395:ARG:O	2.36	0.58
1:A:629:LEU:HD21	2:B:648:ILE:CD1	2.32	0.58
1:A:540:ASP:HB3	1:A:642:PHE:HE2	1.67	0.58
2:B:578:LEU:HD21	2:B:636:VAL:HG21	1.85	0.58
1:C:617:THR:O	1:C:620:VAL:HG12	2.04	0.58
2:D:123:ASN:ND2	2:D:143:ASP:OD1	2.37	0.58
1:C:650:VAL:HG23	1:C:650:VAL:O	2.02	0.58
1:A:629:LEU:HD11	2:B:648:ILE:CG2	2.31	0.58
2:B:646:ILE:CB	1:C:807:ILE:HD12	2.34	0.58
2:B:820:ILE:CG2	2:B:823:ILE:CG2	2.82	0.58
1:C:669:ILE:HD11	1:C:705:THR:HG22	1.84	0.58
2:B:643:PHE:HD1	1:C:807:ILE:CG1	2.17	0.58
2:B:646:ILE:HB	1:C:807:ILE:CD1	2.32	0.58
1:C:625:TRP:CE2	1:C:629:LEU:CD1	2.77	0.58
2:D:149:LEU:HD21	2:D:377:PHE:HZ	1.68	0.57
2:B:750:CYS:HB3	2:B:806:GLU:CB	2.34	0.57
1:C:669:ILE:HD11	1:C:705:THR:CG2	2.34	0.57
2:B:668:ILE:CD1	2:B:680:ILE:CD1	2.82	0.57
1:A:774:ARG:C	1:A:777:ILE:HG22	2.29	0.57
2:B:643:PHE:CD1	1:C:807:ILE:HG12	2.39	0.57
1:A:811:LEU:HD12	2:D:639:ILE:HG22	1.87	0.57
2:B:682:TYR:CZ	2:B:705:MET:CA	2.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:543:SER:O	1:C:546:VAL:HG13	2.05	0.57
1:C:521:ILE:HG22	1:C:743:LEU:HD12	1.86	0.57
1:A:641:ALA:O	1:A:645:VAL:HG22	2.04	0.56
1:A:647:ARG:HD2	2:D:661:VAL:HG21	1.88	0.56
1:A:647:ARG:CD	2:D:661:VAL:CG2	2.83	0.56
2:B:674:LEU:HD21	2:B:682:TYR:HB3	1.86	0.56
1:C:545:ALA:HB3	2:D:817:VAL:HG22	1.87	0.56
2:D:433:LEU:CD2	2:D:511:ASP:OD2	2.53	0.56
2:B:658:PHE:HE1	1:C:647:ARG:NH1	2.03	0.56
1:C:524:LEU:HD13	1:C:721:LEU:HD12	1.85	0.56
2:D:566:TYR:HD1	2:D:566:TYR:H	1.53	0.56
2:D:737:MET:CG	2:D:738:GLU:H	2.15	0.56
2:B:560:SER:HB2	2:B:561:PRO:HD2	1.87	0.56
1:A:800:GLY:HA2	2:D:563:ILE:HD11	1.88	0.56
2:B:558:PRO:HG2	2:B:651:TYR:CE1	2.40	0.55
1:C:623:VAL:HG11	2:D:827:LEU:HD12	1.85	0.55
2:B:562:ASP:HB3	2:B:566:TYR:CE2	2.42	0.55
2:B:820:ILE:CG2	2:B:823:ILE:HG22	2.36	0.55
2:B:820:ILE:O	2:B:820:ILE:HG22	2.06	0.55
1:C:539:LEU:HD12	1:C:539:LEU:O	2.07	0.55
2:B:682:TYR:CE1	2:B:705:MET:CA	2.89	0.55
1:C:539:LEU:HD12	1:C:539:LEU:C	2.32	0.55
1:A:560:VAL:O	1:A:564:ALA:HB2	2.05	0.55
1:C:259:GLU:O	1:C:382:ARG:NH2	2.39	0.55
1:C:647:ARG:O	1:C:647:ARG:HG2	2.07	0.55
2:D:99:LEU:HD13	2:D:125:LEU:HD12	1.89	0.55
1:A:819:VAL:HG22	2:D:577:VAL:HG13	1.89	0.54
1:A:811:LEU:HD12	2:D:639:ILE:CG2	2.38	0.54
2:B:277:THR:OG1	2:B:278:GLY:N	2.41	0.54
2:B:828:ALA:O	2:B:829:ALA:C	2.50	0.54
2:D:438:ILE:HD13	2:D:488:TYR:HB3	1.89	0.54
2:B:123:ASN:ND2	2:B:143:ASP:OD1	2.40	0.54
2:B:633:THR:HA	2:B:636:VAL:HG12	1.88	0.54
1:A:504:ALA:CB	2:D:787:GLU:OE1	2.56	0.54
2:B:53:GLU:OE2	2:B:133:ARG:NH2	2.40	0.54
1:C:516:PHE:O	1:C:775:LEU:HD21	2.08	0.54
1:A:813:ALA:O	1:A:816:ILE:HG13	2.08	0.54
2:B:556:LEU:O	2:B:556:LEU:CD2	2.47	0.54
1:C:110:CYS:HB2	1:C:115:ILE:HB	1.89	0.53
2:D:538:ILE:HD13	2:D:690:THR:HA	1.90	0.53
2:D:543:ARG:NH2	2:D:729:LEU:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:815:LEU:HD23	2:D:820:ILE:HG21	1.88	0.53
2:D:433:LEU:HD13	2:D:511:ASP:OD2	2.08	0.53
2:D:557:ASN:H	2:D:558:PRO:HD2	1.73	0.53
2:D:149:LEU:CD2	2:D:377:PHE:CE1	2.92	0.53
1:A:542:PHE:HE1	2:B:820:ILE:CD1	2.21	0.53
2:D:530:SER:OG	2:D:531:LYS:N	2.39	0.53
2:B:711:SER:HB2	1:C:744:ASP:N	2.22	0.53
1:C:541:PRO:HG2	1:C:635:TYR:CD1	2.38	0.53
1:A:632:ILE:HG23	2:D:645:LEU:HD11	1.89	0.53
1:C:545:ALA:HB3	2:D:817:VAL:CG2	2.38	0.53
1:A:646:GLN:C	1:A:648:MET:H	2.15	0.53
1:A:658:LEU:O	1:A:661:GLN:HB2	2.09	0.53
2:D:437:THR:HG22	2:D:438:ILE:N	2.23	0.53
1:A:656:ASP:O	1:A:657:ASP:C	2.52	0.52
1:A:799:LEU:HD12	1:A:803:ASN:CB	2.39	0.52
2:B:563:ILE:HD13	1:C:804:ILE:CG1	2.39	0.52
2:B:643:PHE:HD1	1:C:807:ILE:HD13	1.71	0.52
1:C:151:ARG:NH1	1:C:395:ARG:O	2.43	0.52
2:B:820:ILE:HG22	2:B:823:ILE:HG22	1.91	0.52
2:D:668:ILE:HG12	2:D:674:LEU:HD21	1.91	0.52
2:B:443:TYR:CD2	2:B:516:PRO:HG3	2.44	0.52
2:D:720:SER:OG	2:D:721:ASN:N	2.42	0.52
2:D:553:PHE:HB2	2:D:555:PHE:CE1	2.43	0.52
1:A:546:VAL:HG13	2:B:824:PHE:CZ	2.44	0.52
2:D:576:VAL:HA	2:D:579:PHE:CE2	2.42	0.52
1:A:799:LEU:HD21	2:D:650:SER:HB3	1.91	0.52
2:D:544:LYS:HG3	2:D:545:PRO:HD2	1.92	0.52
2:D:768:THR:HB	2:D:772:SER:OG	2.09	0.52
1:A:163:LEU:HD12	1:A:190:VAL:HG22	1.92	0.51
1:A:419:VAL:HG21	1:A:451:LEU:HD21	1.92	0.51
1:A:827:ILE:O	1:A:828:TYR:C	2.53	0.51
2:D:557:ASN:N	2:D:558:PRO:HD2	2.25	0.51
2:B:661:VAL:HG11	1:C:647:ARG:HG2	1.93	0.51
2:B:741:THR:O	2:B:744:PHE:HB3	2.10	0.51
1:A:555:LEU:O	1:A:558:SER:HB3	2.11	0.51
2:B:843:LEU:HD13	2:B:843:LEU:O	2.09	0.51
1:A:653:GLU:HB2	1:A:739:ILE:HG12	1.93	0.51
2:B:557:ASN:H	2:B:558:PRO:HD2	1.69	0.51
2:B:274:VAL:HG12	2:B:275:ASN:N	2.25	0.51
2:B:558:PRO:CG	2:B:651:TYR:HE1	2.22	0.51
2:D:682:TYR:CZ	2:D:736:LEU:HD21	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:800:ARG:O	2:B:804:CYS:N	2.44	0.50
2:B:560:SER:N	1:C:798:GLY:O	2.44	0.50
2:B:720:SER:OG	2:B:721:ASN:N	2.44	0.50
2:D:90:GLU:OE2	2:D:94:LYS:NZ	2.44	0.50
2:D:544:LYS:HB2	2:D:753:THR:HG23	1.93	0.50
2:B:551:GLY:HA2	2:B:819:ASN:HD22	1.76	0.50
1:C:628:THR:O	1:C:631:ILE:HG22	2.11	0.50
2:D:456:ASN:ND2	2:D:478:TYR:O	2.45	0.50
1:A:632:ILE:CG2	2:D:645:LEU:HD11	2.42	0.50
2:B:90:GLU:OE2	2:B:94:LYS:NZ	2.43	0.50
2:B:137:GLN:OE1	2:B:141:ASN:ND2	2.40	0.50
2:B:643:PHE:HD1	1:C:807:ILE:HG12	1.76	0.50
2:D:575:SER:O	2:D:579:PHE:CD1	2.65	0.50
1:A:702:VAL:CG1	1:A:703:LYS:N	2.74	0.50
2:B:643:PHE:CD1	1:C:807:ILE:HD13	2.46	0.50
1:C:21:LEU:HD11	1:C:322:ASN:HD21	1.76	0.50
1:A:543:SER:C	1:A:545:ALA:H	2.20	0.50
1:A:669:ILE:CG2	1:A:719:PHE:HZ	2.25	0.50
2:B:182:LEU:HD22	2:B:189:ILE:HD11	1.94	0.50
1:C:542:PHE:CG	1:C:546:VAL:HG21	2.47	0.50
1:A:513:SER:OG	1:A:514:LYS:N	2.41	0.49
1:A:549:PHE:O	1:A:552:LEU:HB2	2.13	0.49
1:A:641:ALA:O	1:A:642:PHE:C	2.55	0.49
1:A:652:VAL:HG12	1:A:653:GLU:N	2.27	0.49
2:B:555:PHE:O	2:B:555:PHE:HD1	1.88	0.49
2:D:581:ILE:O	2:D:581:ILE:HG22	2.11	0.49
1:A:549:PHE:HA	1:A:552:LEU:HD12	1.94	0.49
1:A:652:VAL:C	1:A:653:GLU:HG3	2.36	0.49
1:A:813:ALA:HA	1:A:816:ILE:CD1	2.41	0.49
2:B:558:PRO:HG2	2:B:651:TYR:HE1	1.76	0.49
2:B:833:LEU:O	2:B:837:VAL:HG13	2.12	0.49
1:C:560:VAL:HG21	2:D:831:LEU:CD1	2.43	0.49
1:A:481:TRP:HB3	1:A:485:VAL:HG13	1.95	0.49
1:A:807:ILE:HG12	2:D:643:PHE:HD1	1.78	0.49
2:B:682:TYR:O	2:B:682:TYR:CG	2.64	0.49
1:C:547:TRP:HA	1:C:550:MET:HE2	1.94	0.49
1:C:645:VAL:O	1:C:648:MET:HB2	2.12	0.49
2:B:682:TYR:CE1	2:B:705:MET:CB	2.95	0.49
2:B:843:LEU:O	2:B:844:TYR:C	2.55	0.49
1:C:26:MET:HE1	1:C:311:VAL:HA	1.94	0.49
1:A:550:MET:O	1:A:551:LEU:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:688:GLY:O	2:B:692:THR:HG23	2.12	0.49
1:A:124:GLU:HG2	1:A:173:ARG:HH21	1.77	0.48
1:C:36:CYS:HB3	1:C:292:CYS:HB3	1.58	0.48
1:C:489:ILE:C	1:C:491:ARG:H	2.21	0.48
2:D:553:PHE:HB2	2:D:555:PHE:HE1	1.78	0.48
1:A:504:ALA:HB1	2:D:784:GLN:HG3	1.95	0.48
1:C:198:ASP:OD2	1:C:200:THR:OG1	2.31	0.48
2:D:437:THR:HG21	2:D:444:VAL:HG21	1.93	0.48
2:B:683:GLY:HA3	2:B:716:VAL:O	2.14	0.48
2:D:581:ILE:HD12	2:D:632:SER:HB3	1.83	0.48
1:A:799:LEU:HD11	2:D:650:SER:HB3	1.96	0.48
2:B:140:ASP:OD1	2:B:140:ASP:N	2.41	0.48
2:B:542:TYR:HB3	2:B:755:ILE:HD13	1.94	0.48
2:D:721:ASN:ND2	2:D:737:MET:CE	2.50	0.48
2:D:432:SER:HB2	2:D:477:THR:HG23	1.96	0.48
2:D:129:HIS:CD2	2:D:131:GLN:HE21	2.32	0.47
2:B:555:PHE:O	2:B:555:PHE:CG	2.64	0.47
1:C:653:GLU:CD	1:C:658:LEU:HD21	2.39	0.47
2:D:280:ARG:NH1	2:D:284:THR:OG1	2.47	0.47
1:A:800:GLY:CA	2:D:563:ILE:HD11	2.43	0.47
2:B:742:ILE:HG21	2:B:754:GLN:HG3	1.96	0.47
2:D:564:TRP:O	2:D:567:VAL:HB	2.13	0.47
1:A:537:SER:C	1:A:539:LEU:H	2.21	0.47
2:B:643:PHE:CD1	1:C:807:ILE:HD11	2.45	0.47
1:C:808:PHE:O	1:C:812:ILE:HG12	2.15	0.47
1:A:557:VAL:HG21	1:A:624:TRP:CE3	2.49	0.47
1:A:799:LEU:HD23	2:D:559:LEU:HD23	1.96	0.47
1:A:816:ILE:CG1	1:A:817:ILE:N	2.75	0.47
2:B:820:ILE:HG23	2:B:823:ILE:CG2	2.45	0.47
2:D:267:GLU:OE2	2:D:270:ARG:NH2	2.45	0.47
2:D:572:LEU:O	2:D:576:VAL:HG13	2.15	0.47
1:A:172:LEU:HD12	2:B:183:ILE:HD11	1.96	0.47
1:A:646:GLN:C	1:A:648:MET:N	2.72	0.47
2:B:820:ILE:HG22	2:B:823:ILE:CG2	2.44	0.47
1:C:623:VAL:HG12	2:D:827:LEU:HD13	1.86	0.47
1:A:545:ALA:O	1:A:546:VAL:C	2.57	0.47
1:A:643:LEU:O	1:A:646:GLN:N	2.48	0.47
2:B:639:ILE:HD11	1:C:810:VAL:HG12	1.97	0.47
2:B:682:TYR:CE1	2:B:705:MET:HA	2.49	0.47
1:C:625:TRP:CH2	1:C:629:LEU:CD1	2.98	0.46
1:C:799:LEU:HA	1:C:800:GLY:HA3	1.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:208:THR:OG1	2:D:209:LYS:N	2.48	0.46
1:A:540:ASP:N	1:A:541:PRO:CD	2.78	0.46
1:A:546:VAL:HG13	2:B:824:PHE:HZ	1.81	0.46
2:B:99:LEU:HD13	2:B:125:LEU:HD12	1.97	0.46
1:C:114:GLU:HB3	1:C:343:GLY:HA3	1.97	0.46
1:A:494:ASP:OD1	1:A:494:ASP:N	2.45	0.46
2:B:210:ASP:OD1	2:B:210:ASP:N	2.49	0.46
2:D:737:MET:CG	2:D:738:GLU:N	2.68	0.46
2:B:731:SER:OG	2:B:733:TYR:CE2	2.67	0.46
1:C:806:GLY:O	1:C:809:VAL:HG12	2.16	0.46
2:D:216:LYS:HB2	2:D:216:LYS:HE3	1.79	0.46
2:D:566:TYR:CD1	2:D:566:TYR:N	2.84	0.46
2:D:573:GLY:O	2:D:576:VAL:HG22	2.16	0.46
1:A:652:VAL:O	1:A:653:GLU:CG	2.63	0.46
1:A:657:ASP:O	1:A:658:LEU:C	2.58	0.46
2:B:563:ILE:HG21	1:C:804:ILE:HD11	1.98	0.46
2:B:659:LEU:HD23	2:B:659:LEU:HA	1.55	0.46
1:C:484:MET:O	1:C:485:VAL:C	2.59	0.46
2:D:83:ILE:HD13	2:D:91:ALA:HB2	1.98	0.46
2:D:683:GLY:HA3	2:D:733:TYR:HE1	1.80	0.46
2:B:208:THR:OG1	2:B:209:LYS:N	2.48	0.46
2:B:658:PHE:CE1	1:C:647:ARG:CZ	2.91	0.46
2:B:820:ILE:O	2:B:820:ILE:CG2	2.64	0.46
2:B:340:MET:HE2	2:B:340:MET:HB3	1.84	0.46
2:D:742:ILE:HG21	2:D:754:GLN:HG3	1.97	0.46
2:D:831:LEU:O	2:D:834:SER:HB3	2.16	0.46
1:A:450:MET:HB3	1:A:450:MET:HE2	1.83	0.46
1:A:538:PHE:O	1:A:538:PHE:CD1	2.69	0.46
2:B:55:LEU:HD22	2:B:301:LEU:HD13	1.97	0.45
2:B:563:ILE:HD11	1:C:801:MET:H	1.80	0.45
1:C:524:LEU:HD13	1:C:721:LEU:CD1	2.46	0.45
2:D:501:MET:HE2	2:D:513:ALA:HB1	1.96	0.45
1:A:630:ILE:CG2	2:B:823:ILE:HD12	2.47	0.45
2:B:685:VAL:HG12	2:B:690:THR:CG2	2.46	0.45
1:C:644:THR:O	1:C:645:VAL:C	2.58	0.45
2:B:578:LEU:HD21	2:B:636:VAL:HG11	1.99	0.45
2:D:682:TYR:CE2	2:D:736:LEU:HD11	2.51	0.45
1:A:658:LEU:O	1:A:659:ALA:C	2.59	0.45
2:B:551:GLY:HA2	2:B:819:ASN:ND2	2.31	0.45
2:D:682:TYR:OH	2:D:736:LEU:HD21	2.17	0.45
1:A:538:PHE:CE2	1:A:807:ILE:N	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:819:VAL:CG2	2:D:577:VAL:HG13	2.46	0.45
1:C:151:ARG:HD2	1:C:391:TRP:HE1	1.82	0.45
2:D:557:ASN:N	2:D:558:PRO:CD	2.80	0.45
2:D:643:PHE:HE1	2:D:647:ILE:HD11	1.81	0.45
2:D:689:ALA:O	2:D:690:THR:C	2.60	0.45
2:D:691:MET:O	2:D:692:THR:C	2.60	0.45
2:D:815:LEU:CG	2:D:820:ILE:CG2	2.91	0.45
2:B:558:PRO:O	2:B:654:ASN:ND2	2.41	0.45
1:C:560:VAL:CG2	2:D:831:LEU:HD11	2.47	0.45
1:A:182:LEU:O	1:A:187:THR:OG1	2.26	0.45
2:D:99:LEU:HD21	2:D:127:VAL:HG21	1.99	0.44
2:B:743:GLU:O	2:B:743:GLU:HG2	2.16	0.44
2:D:548:THR:O	2:D:549:ASN:C	2.61	0.44
1:A:552:LEU:O	1:A:553:ALA:C	2.60	0.44
1:A:804:ILE:HA	1:A:807:ILE:CG2	2.47	0.44
1:A:804:ILE:CB	1:A:808:PHE:CZ	3.00	0.44
1:A:811:LEU:CD1	2:D:639:ILE:HG22	2.46	0.44
2:B:309:SER:OG	2:B:310:GLY:N	2.51	0.44
2:B:682:TYR:OH	2:B:705:MET:C	2.60	0.44
1:C:391:TRP:HD1	1:C:397:LEU:HB3	1.82	0.44
1:A:620:VAL:O	1:A:621:SER:C	2.60	0.44
2:B:99:LEU:HD21	2:B:127:VAL:HG21	1.97	0.44
2:B:829:ALA:O	2:B:830:GLY:C	2.61	0.44
1:A:662:THR:CG2	1:A:692:TYR:OH	2.49	0.44
1:C:151:ARG:HB3	1:C:397:LEU:HD22	1.98	0.44
1:C:376:ARG:HD3	1:C:390:VAL:HG12	2.00	0.44
1:C:547:TRP:CE3	1:C:550:MET:HE1	2.53	0.44
1:A:347:MET:HE2	1:A:347:MET:HB2	1.89	0.44
1:A:648:MET:HE3	1:A:648:MET:HB2	1.78	0.44
2:B:432:SER:C	2:B:434:ILE:N	2.73	0.44
2:B:636:VAL:HG13	2:B:637:GLY:N	2.33	0.44
1:C:641:ALA:O	1:C:642:PHE:C	2.61	0.44
1:C:489:ILE:C	1:C:491:ARG:N	2.75	0.44
2:D:659:LEU:HD23	2:D:659:LEU:N	2.31	0.44
1:A:543:SER:HB3	2:B:815:LEU:O	2.18	0.43
1:C:759:ARG:O	1:C:763:THR:CG2	2.64	0.43
2:D:681:GLU:O	2:D:733:TYR:HD1	2.01	0.43
2:D:815:LEU:HG	2:D:820:ILE:HG21	1.98	0.43
1:A:160:SER:O	1:A:160:SER:OG	2.34	0.43
2:B:432:SER:C	2:B:434:ILE:H	2.26	0.43
2:B:656:ALA:O	2:B:657:ALA:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:691:MET:O	2:D:694:PHE:N	2.50	0.43
1:A:647:ARG:HH12	1:A:797:LYS:N	2.16	0.43
1:C:27:ALA:HB2	1:C:90:VAL:HG11	2.01	0.43
2:D:791:LEU:HD23	2:D:791:LEU:HA	1.83	0.43
1:A:627:PHE:HA	2:B:823:ILE:HD11	2.01	0.43
2:B:578:LEU:O	2:B:581:ILE:CB	2.67	0.43
2:D:835:VAL:O	2:D:838:ALA:HB3	2.19	0.43
2:B:685:VAL:HG12	2:B:690:THR:HG22	2.00	0.43
2:D:217:GLU:OE2	2:D:220:ARG:NH2	2.51	0.43
1:A:504:ALA:HB3	2:D:787:GLU:OE1	2.19	0.43
1:C:279:GLU:OE1	1:C:282:ARG:NH2	2.40	0.43
1:A:669:ILE:CG2	1:A:719:PHE:CZ	3.01	0.43
2:B:723:GLU:O	2:B:727:ARG:HG2	2.19	0.43
1:A:807:ILE:CG1	2:D:643:PHE:HD1	2.32	0.43
2:D:317:THR:HG23	2:D:320:ALA:H	1.83	0.43
1:A:504:ALA:N	2:D:787:GLU:OE1	2.44	0.43
1:A:807:ILE:CG1	2:D:643:PHE:CD1	3.02	0.43
2:D:552:VAL:HA	2:D:553:PHE:HA	1.57	0.43
1:A:709:ILE:HD12	1:A:729:HIS:HB3	2.00	0.42
2:B:83:ILE:HD13	2:B:91:ALA:HB2	2.01	0.42
2:B:520:THR:OG1	2:B:521:TYR:N	2.51	0.42
2:D:34:HIS:HB2	2:D:74:THR:HG22	2.00	0.42
1:A:775:LEU:HD12	1:A:775:LEU:HA	1.90	0.42
2:D:815:LEU:HD12	2:D:815:LEU:HA	1.60	0.42
1:A:26:MET:HE1	1:A:311:VAL:HA	2.00	0.42
2:B:152:ASP:OD2	2:B:154:SER:OG	2.32	0.42
2:B:164:VAL:HG13	2:B:169:TRP:HB2	2.00	0.42
1:A:309:ASP:OD2	1:A:359:THR:OG1	2.33	0.42
1:A:647:ARG:HH12	1:A:797:LYS:H	1.67	0.42
2:B:443:TYR:OH	2:B:740:THR:CG2	2.53	0.42
1:C:488:LEU:HA	1:C:493:ALA:O	2.19	0.42
2:B:240:LYS:HE3	2:B:240:LYS:HB2	1.85	0.42
1:C:641:ALA:O	1:C:645:VAL:HG22	2.19	0.42
2:D:572:LEU:O	2:D:575:SER:OG	2.32	0.42
2:D:575:SER:O	2:D:578:LEU:HB2	2.19	0.42
1:A:171:LEU:HD23	1:A:171:LEU:HA	1.86	0.42
1:A:632:ILE:CD1	2:D:645:LEU:CD2	2.88	0.42
1:C:203:LEU:HB3	1:C:235:MET:HE1	2.00	0.42
2:D:439:LEU:HG	2:D:482:LEU:HD11	2.00	0.42
2:D:555:PHE:CG	2:D:556:LEU:N	2.87	0.42
2:B:729:LEU:HD23	2:B:729:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:164:VAL:HG13	2:D:169:TRP:HB2	2.01	0.42
2:D:433:LEU:CD1	2:D:511:ASP:OD2	2.67	0.42
1:A:728:TYR:HD2	1:A:729:HIS:HD2	1.64	0.42
2:B:351:LYS:HE2	2:B:352:PRO:HD2	2.02	0.42
1:C:254:LEU:HD12	1:C:380:LYS:HG3	2.02	0.42
2:D:657:ALA:O	2:D:661:VAL:HG22	2.19	0.42
2:B:471:SER:O	2:B:475:GLY:N	2.51	0.42
1:C:171:LEU:HD23	1:C:171:LEU:HA	1.91	0.42
1:C:394:ASN:OD1	1:C:395:ARG:N	2.52	0.42
2:D:442:PRO:HG3	2:D:744:PHE:CE1	2.55	0.42
1:A:178:VAL:HG13	1:A:183:ILE:HD11	2.02	0.41
1:C:340:TRP:HA	1:C:341:PRO:HD3	1.96	0.41
1:C:756:SER:OG	1:C:759:ARG:CB	2.67	0.41
2:D:401:LYS:HB2	2:D:401:LYS:HE3	1.86	0.41
2:D:656:ALA:O	2:D:657:ALA:C	2.62	0.41
2:D:721:ASN:HD21	2:D:737:MET:HE1	1.73	0.41
1:A:147:LEU:HD23	1:A:147:LEU:HA	1.92	0.41
2:B:683:GLY:CA	2:B:716:VAL:HG12	2.49	0.41
1:C:539:LEU:HA	1:C:547:TRP:CZ2	2.55	0.41
2:D:673:ASP:HA	2:D:676:LYS:HD2	2.02	0.41
2:D:843:LEU:O	2:D:844:TYR:C	2.63	0.41
2:D:576:VAL:HA	2:D:579:PHE:CG	2.52	0.41
2:D:668:ILE:HG12	2:D:674:LEU:HD11	2.03	0.41
1:A:553:ALA:O	1:A:554:TYR:C	2.63	0.41
1:C:548:LEU:C	1:C:552:LEU:HD13	2.45	0.41
1:C:640:ALA:O	1:C:641:ALA:C	2.63	0.41
1:C:728:TYR:O	1:C:732:LEU:HG	2.20	0.41
2:D:668:ILE:HG23	2:D:674:LEU:CD1	2.50	0.41
1:A:625:TRP:HA	1:A:628:THR:HG22	2.02	0.41
1:C:669:ILE:HG22	1:C:670:HIS:N	2.36	0.41
2:D:554:SER:O	2:D:555:PHE:C	2.64	0.41
2:D:573:GLY:HA2	2:D:576:VAL:HG22	2.02	0.41
2:B:822:GLY:O	2:B:825:ILE:HB	2.21	0.41
2:D:437:THR:CG2	2:D:438:ILE:N	2.83	0.41
1:A:807:ILE:HG13	2:D:643:PHE:CD1	2.55	0.41
2:D:325:ASP:OD2	2:D:372:THR:OG1	2.34	0.41
1:A:537:SER:C	1:A:539:LEU:N	2.79	0.41
1:A:543:SER:C	1:A:545:ALA:N	2.79	0.40
2:B:641:TRP:HA	2:B:644:THR:HG22	2.03	0.40
2:B:682:TYR:CE1	2:B:705:MET:C	2.98	0.40
1:C:669:ILE:HD13	1:C:705:THR:CG2	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:689:ALA:C	2:D:691:MET:N	2.78	0.40
1:A:553:ALA:HB1	2:B:827:LEU:HD21	2.02	0.40
1:A:709:ILE:CD1	1:A:729:HIS:HB3	2.52	0.40
2:B:55:LEU:HD13	2:B:301:LEU:HB3	2.03	0.40
2:B:831:LEU:O	2:B:834:SER:HB3	2.21	0.40
1:C:619:ILE:O	1:C:623:VAL:HG23	2.21	0.40
2:D:683:GLY:HA3	2:D:733:TYR:CE1	2.55	0.40
1:A:198:ASP:OD1	1:A:229:LYS:NZ	2.48	0.40
1:A:380:LYS:HD3	1:A:380:LYS:HA	1.94	0.40
1:A:627:PHE:O	2:B:823:ILE:HD11	2.21	0.40
1:C:540:ASP:N	1:C:541:PRO:CD	2.84	0.40
2:D:643:PHE:CE1	2:D:647:ILE:CG1	3.04	0.40
1:A:647:ARG:CZ	2:D:658:PHE:HE1	2.35	0.40
2:B:555:PHE:HE2	2:B:822:GLY:C	2.29	0.40
2:D:581:ILE:HD13	2:D:632:SER:OG	2.03	0.40
2:D:668:ILE:HG21	2:D:755:ILE:HG21	2.03	0.40
1:A:126:PRO:HD3	1:A:172:LEU:HD11	2.03	0.40
2:B:129:HIS:CD2	2:B:131:GLN:HE21	2.40	0.40
2:D:274:VAL:HG23	2:D:394:LEU:HD23	2.03	0.40
2:D:432:SER:CA	2:D:477:THR:HG23	2.52	0.40
2:D:551:GLY:HA3	2:D:818:GLN:O	2.21	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	741/1101 (67%)	662 (89%)	78 (10%)	1 (0%)	48	80
1	C	741/1101 (67%)	672 (91%)	66 (9%)	3 (0%)	30	64
2	B	749/942 (80%)	673 (90%)	76 (10%)	0	100	100
2	D	749/942 (80%)	686 (92%)	62 (8%)	1 (0%)	48	80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2980/4086 (73%)	2693 (90%)	282 (10%)	5 (0%)	44	74

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	809	SER
1	A	735	ASN
1	C	794	HIS
1	C	796	ALA
1	C	800	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	533/950 (56%)	528 (99%)	5 (1%)	70	75
1	C	462/950 (49%)	459 (99%)	3 (1%)	78	80
2	B	491/817 (60%)	478 (97%)	13 (3%)	40	61
2	D	572/817 (70%)	558 (98%)	14 (2%)	43	63
All	All	2058/3534 (58%)	2023 (98%)	35 (2%)	52	68

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	539	LEU
1	A	623	VAL
1	A	692	TYR
1	A	736	LEU
1	A	815	LEU
2	B	147	VAL
2	B	276	MET
2	B	519	ILE
2	B	567	VAL
2	B	645	LEU

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Mol	Chain	Res	Type
2	B	647	ILE
2	B	652	THR
2	B	668	ILE
2	B	740	THR
2	B	755	ILE
2	B	817	VAL
2	B	837	VAL
2	B	843	LEU
1	C	57	VAL
1	C	546	VAL
1	C	561	LEU
2	D	172	VAL
2	D	250	GLU
2	D	415	GLU
2	D	435	VAL
2	D	480	ILE
2	D	568	LEU
2	D	581	ILE
2	D	635	ILE
2	D	652	THR
2	D	659	LEU
2	D	680	ILE
2	D	740	THR
2	D	746	THR
2	D	815	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	HIS
1	A	312	HIS
1	A	342	HIS
1	A	348	ASN
1	A	638	ASN
1	A	729	HIS
2	B	81	GLN
2	B	123	ASN
2	B	129	HIS
2	B	203	GLN
2	B	253	HIS
2	B	328	HIS
2	B	412	ASN

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Mol	Chain	Res	Type
2	B	819	ASN
1	C	322	ASN
2	D	116	ASN
2	D	123	ASN
2	D	129	HIS
2	D	203	GLN
2	D	328	HIS
2	D	412	ASN
2	D	654	ASN
2	D	721	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

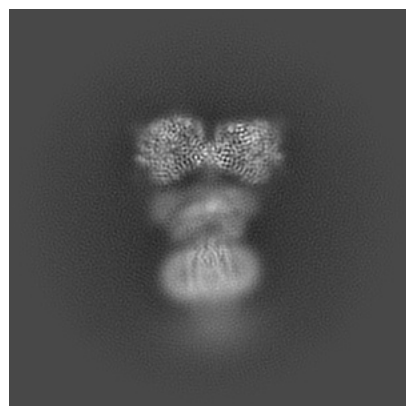
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70806. These allow visual inspection of the internal detail of the map and identification of artifacts.

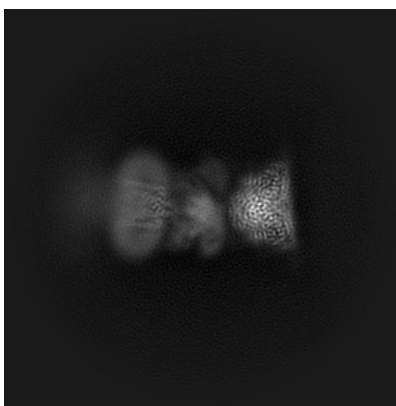
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

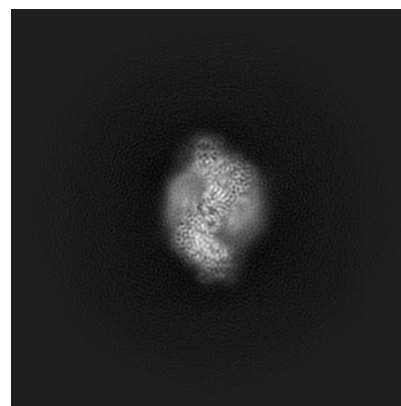
6.1.1 Primary map



X

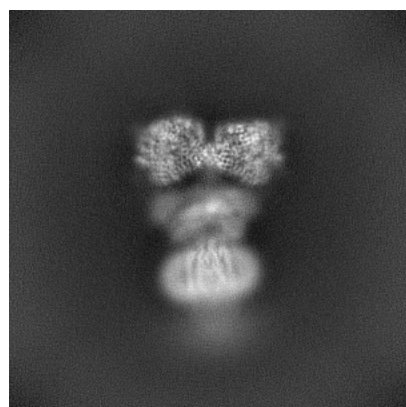


Y

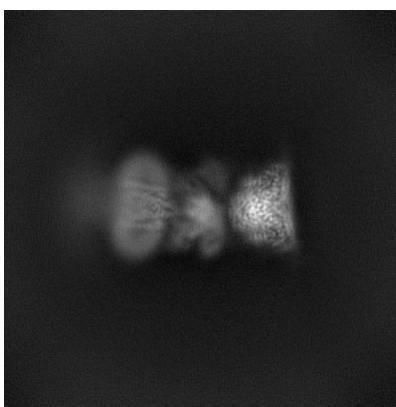


Z

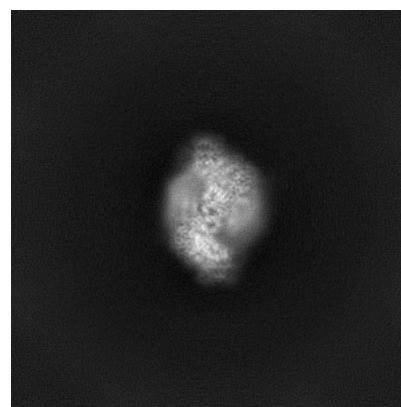
6.1.2 Raw map



X



Y

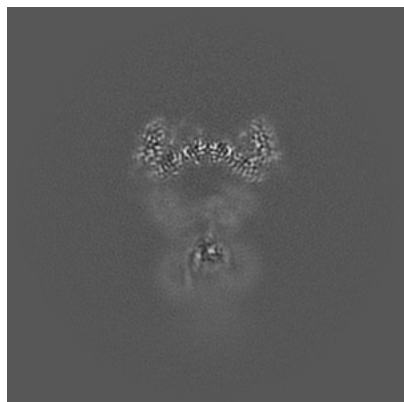


Z

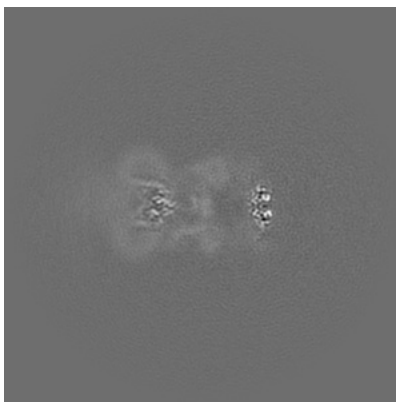
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

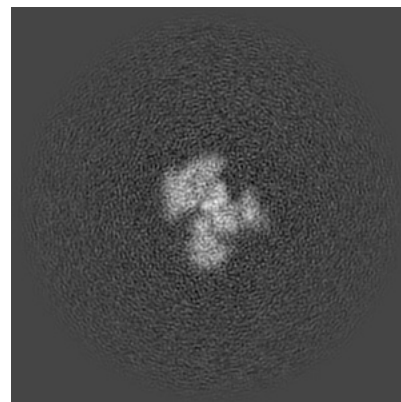
6.2.1 Primary map



X Index: 240

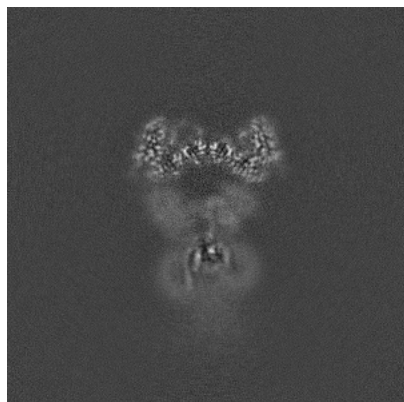


Y Index: 240

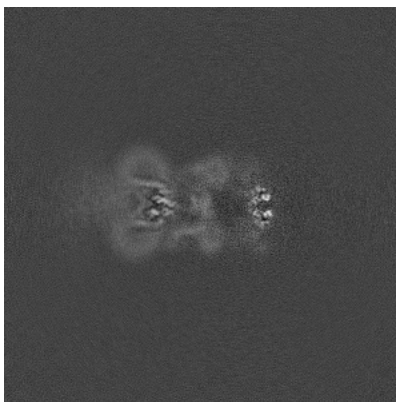


Z Index: 240

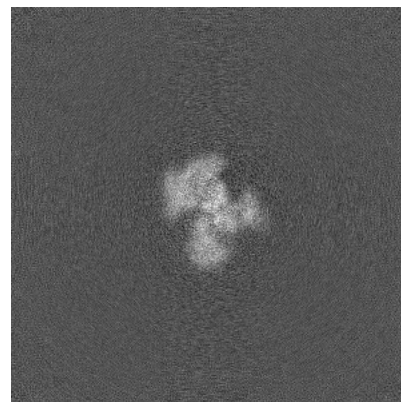
6.2.2 Raw map



X Index: 240



Y Index: 240

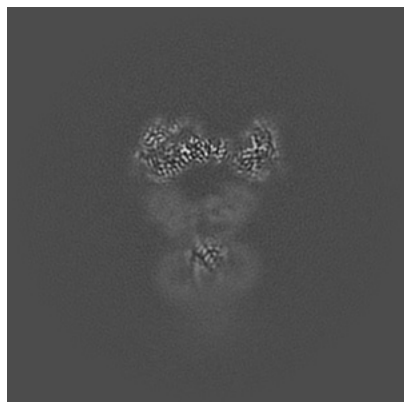


Z Index: 240

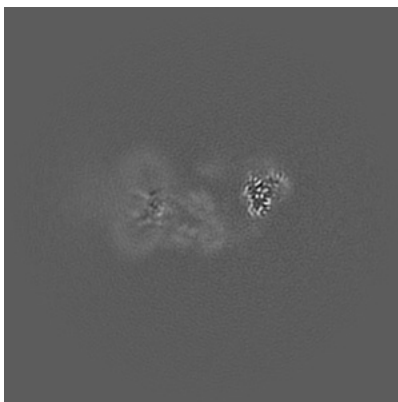
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

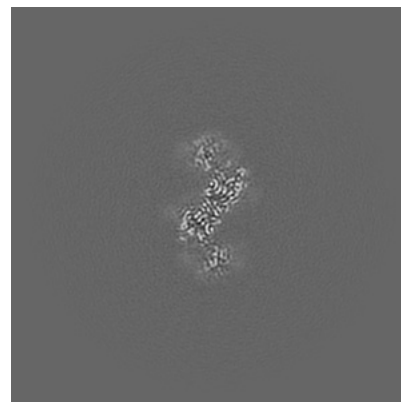
6.3.1 Primary map



X Index: 235



Y Index: 254

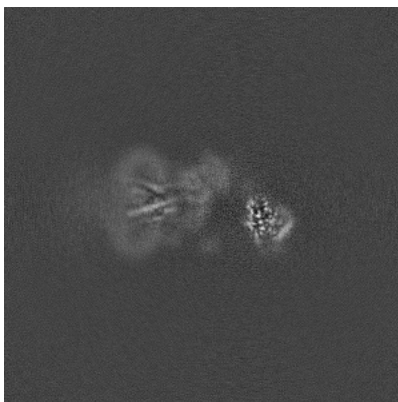


Z Index: 307

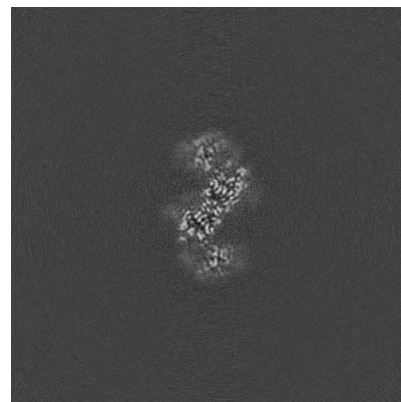
6.3.2 Raw map



X Index: 235



Y Index: 228

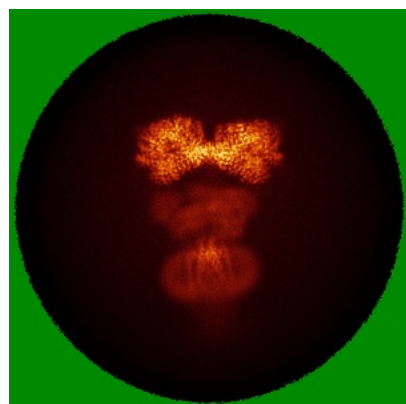


Z Index: 307

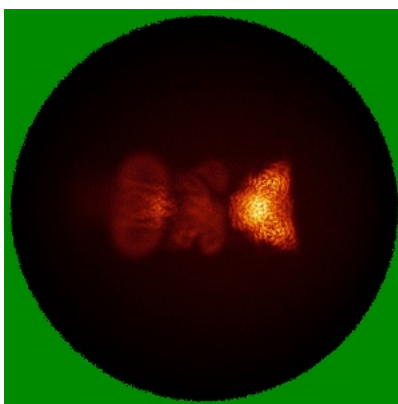
The images above show the largest variance slices of the map in three orthogonal directions.

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

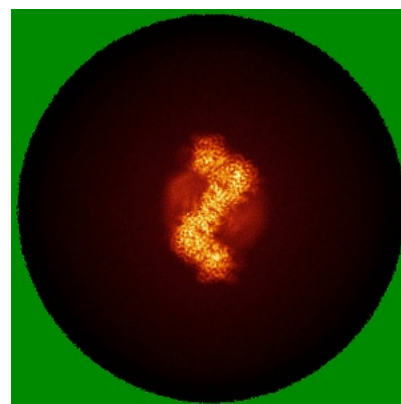
6.4.1 Primary map



X

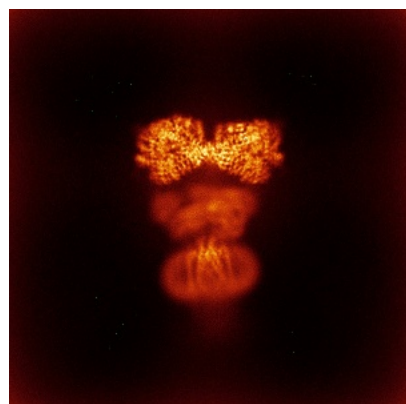


Y

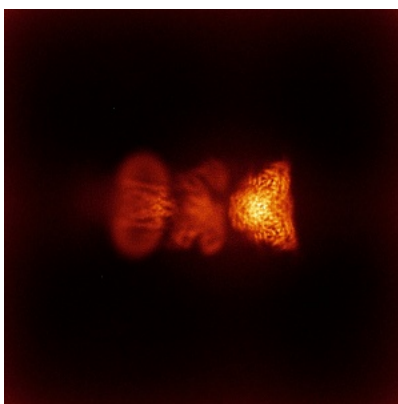


Z

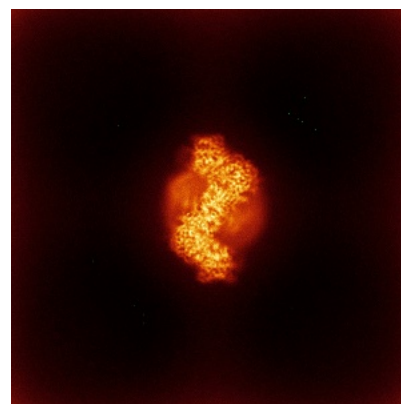
6.4.2 Raw map



X



Y

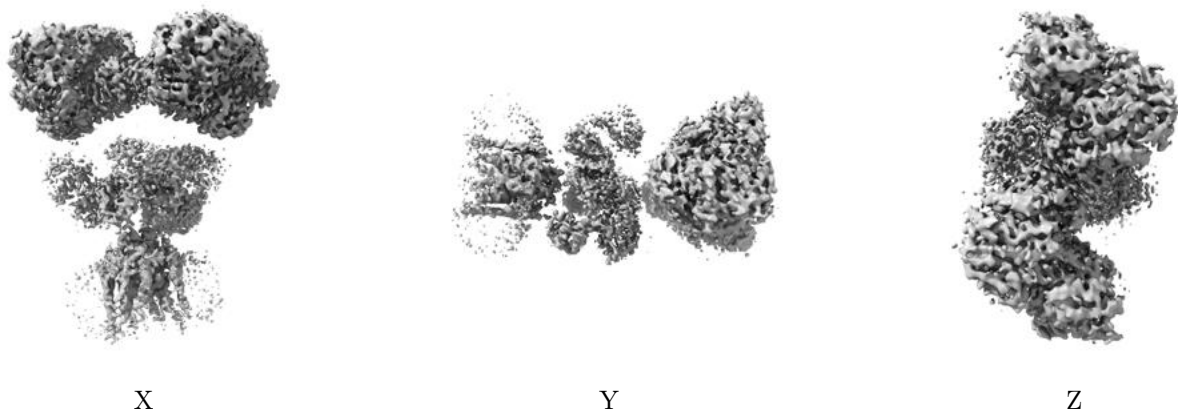


Z

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

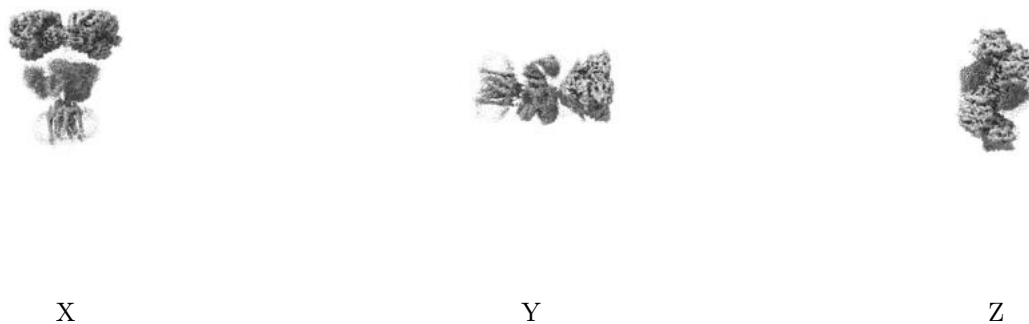
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

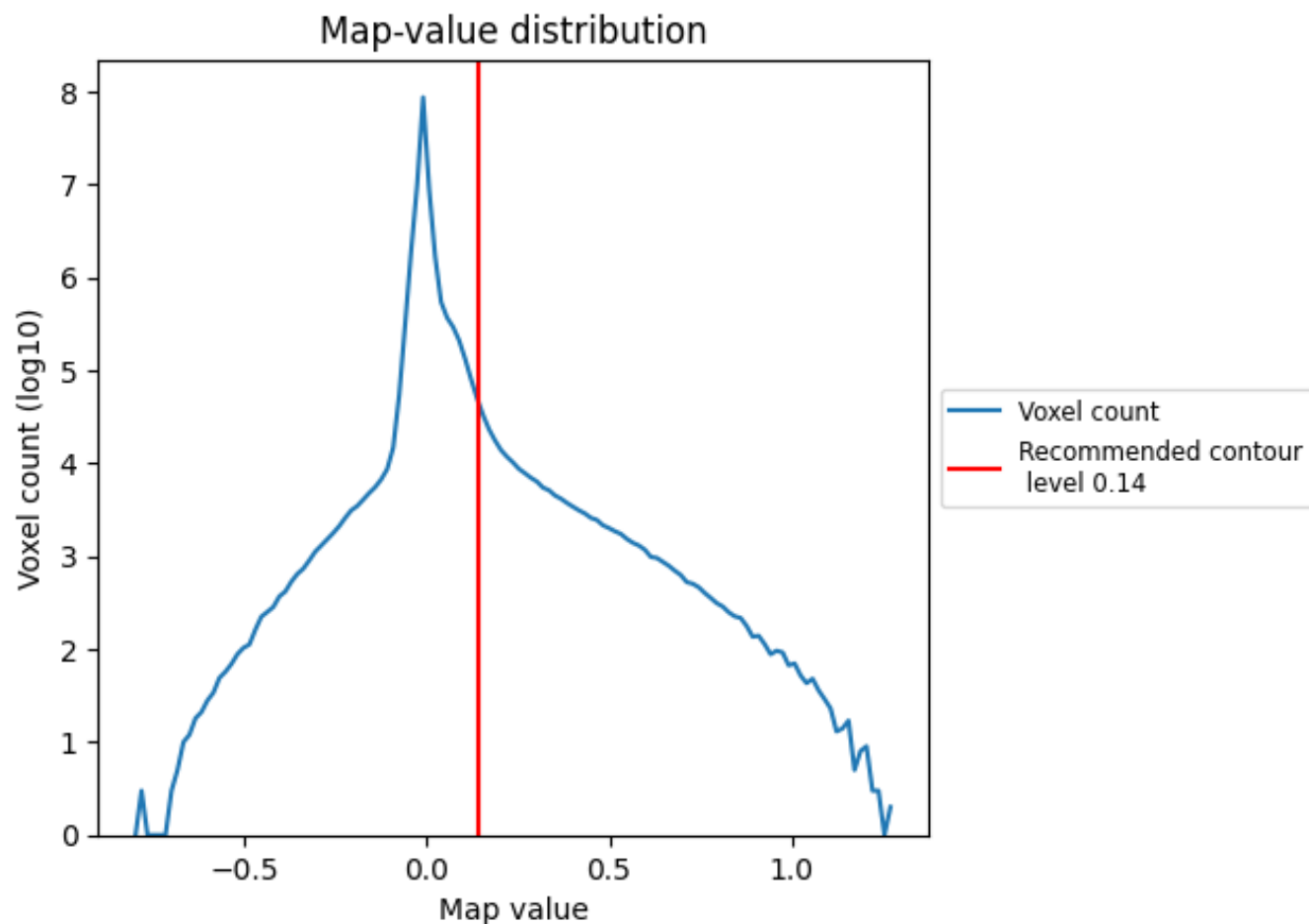
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

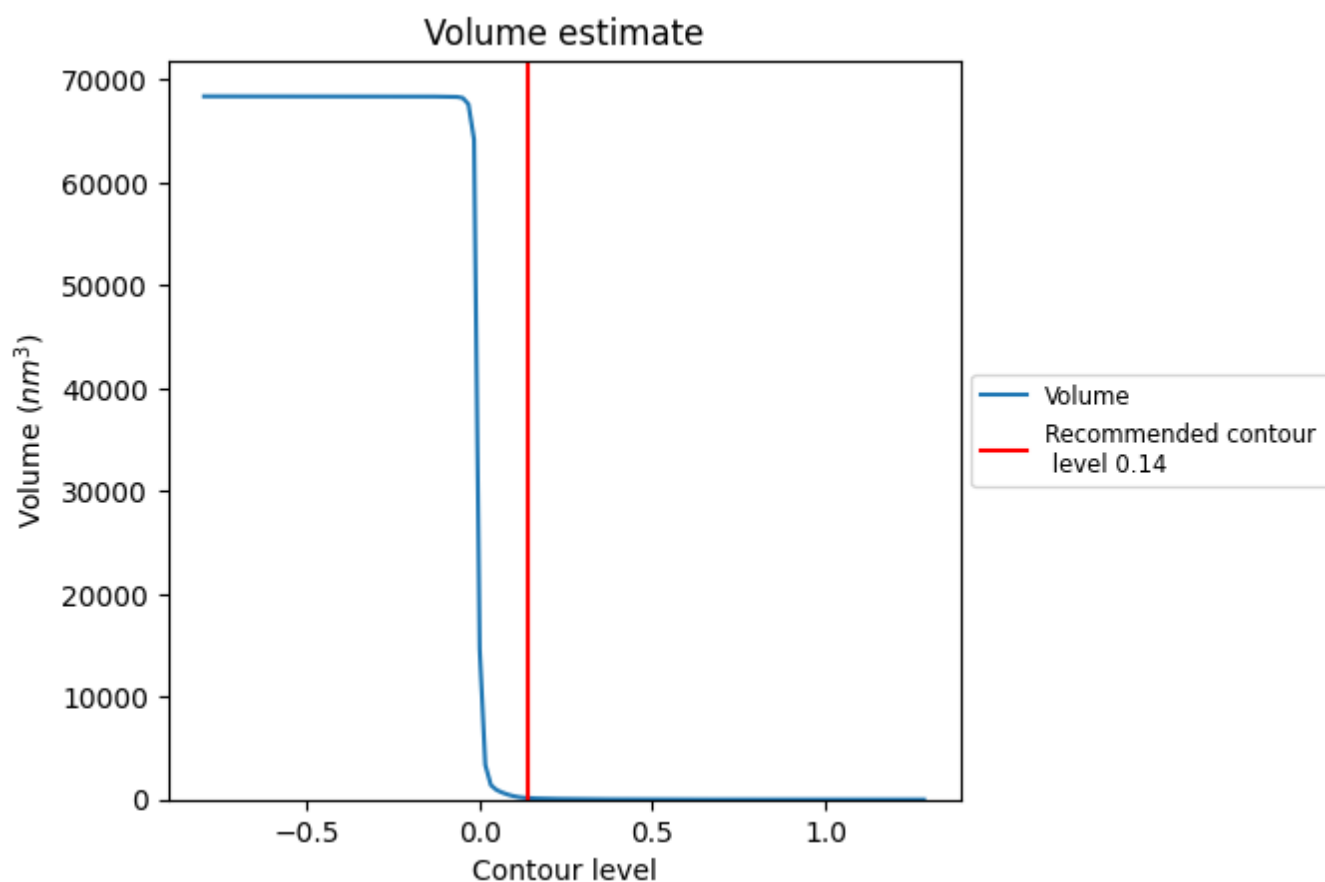
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

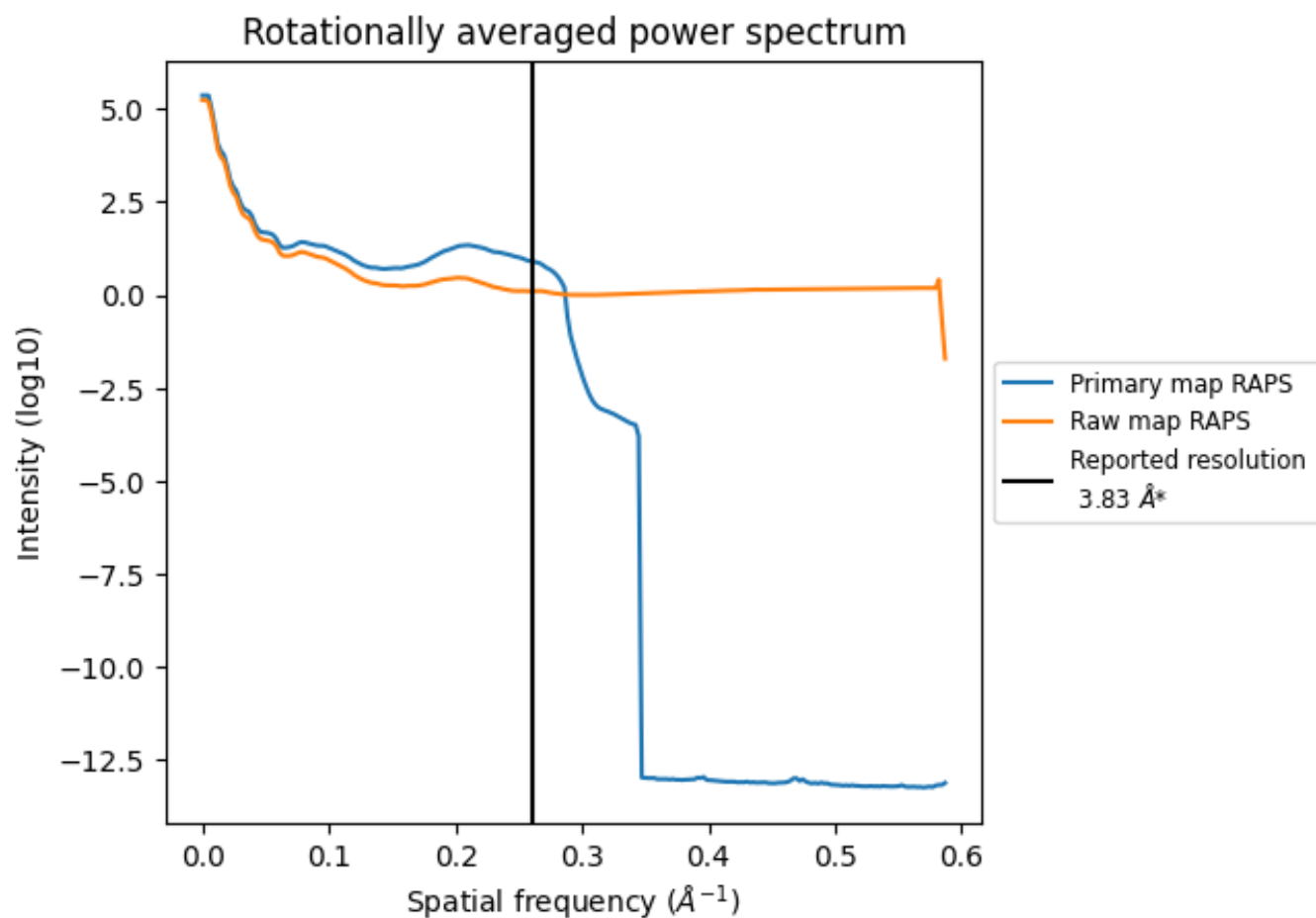
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 152 nm³; this corresponds to an approximate mass of 137 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 ⓘ

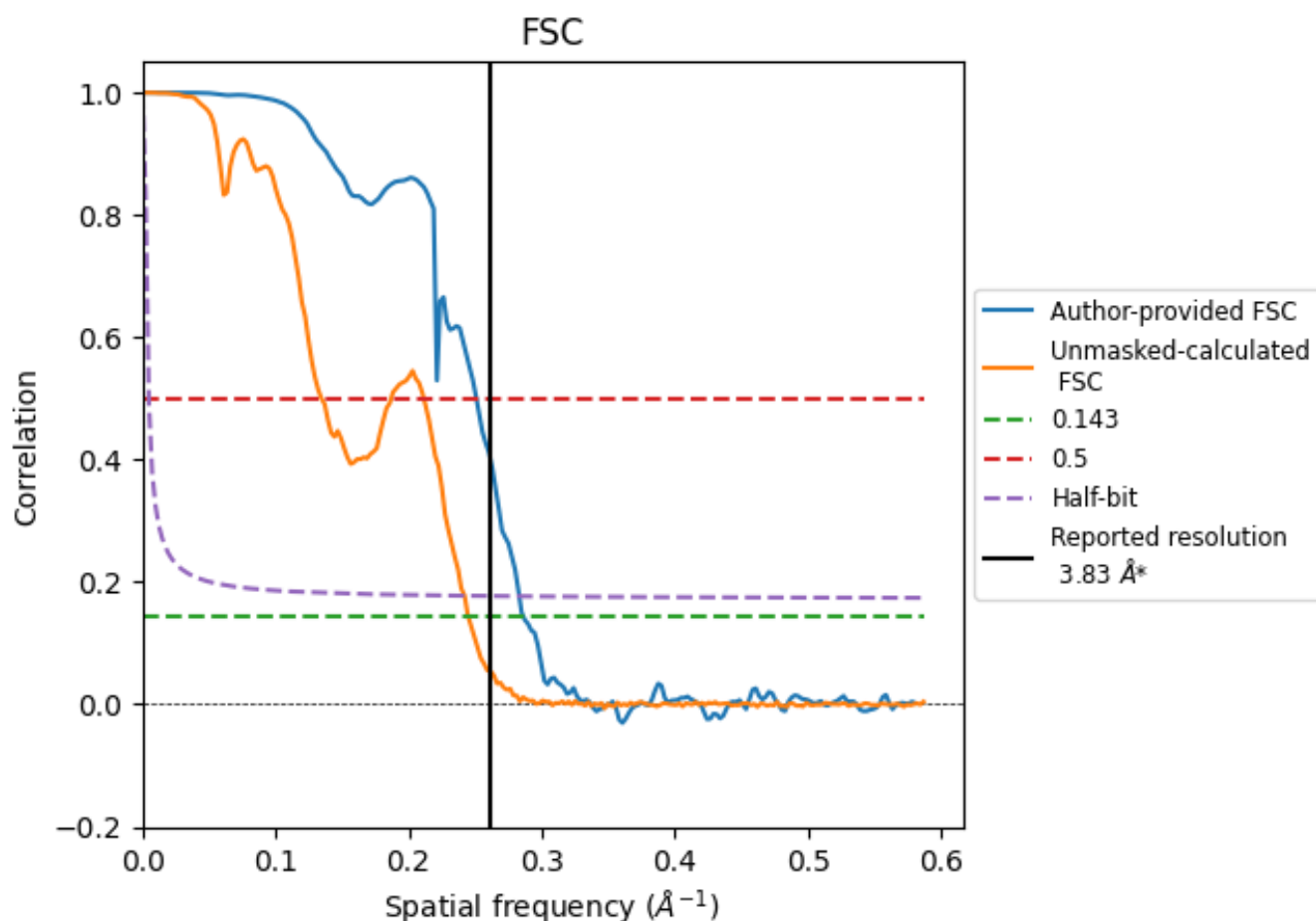


*Reported resolution corresponds to spatial frequency of 0.261 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.261 \AA^{-1}

8.2 Resolution estimates [i](#)

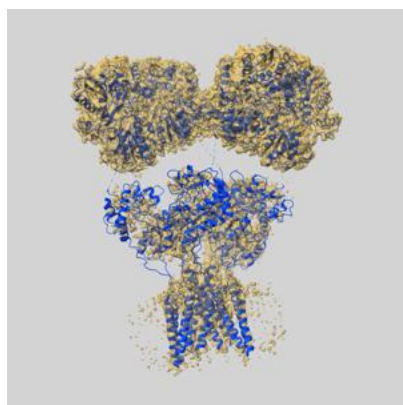
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	3.49	3.99	3.53
Unmasked-calculated*	4.08	7.44	4.13

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

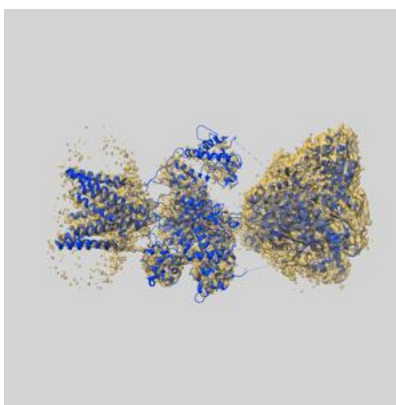
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70806 and PDB model 9OSG. Per-residue inclusion information can be found in section 3 on page 7.

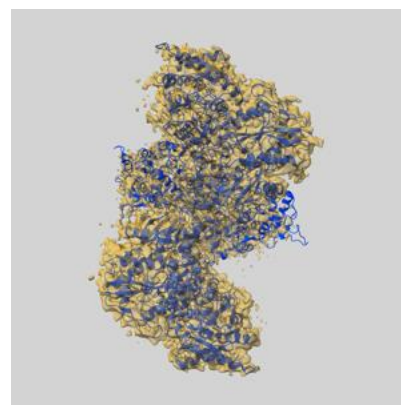
9.1 Map-model overlay [i](#)



X



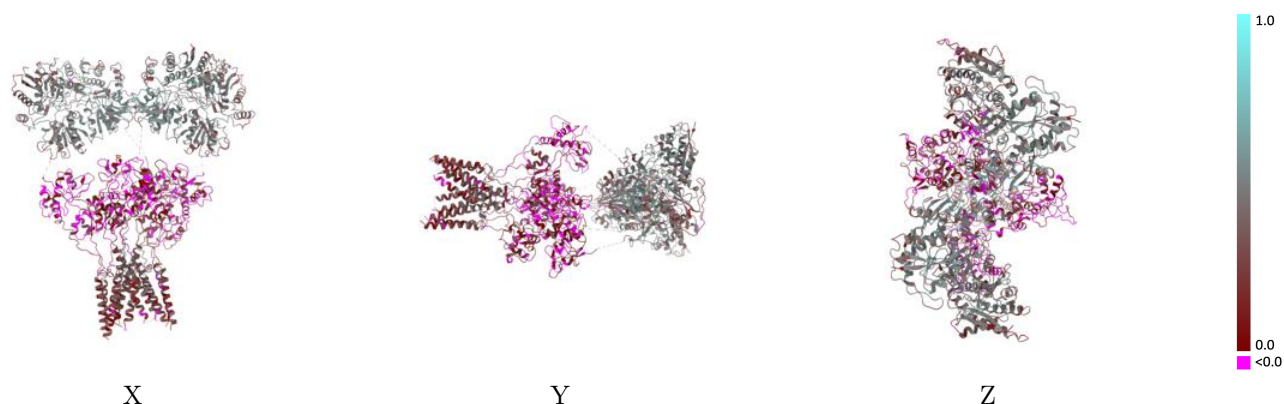
Y



Z

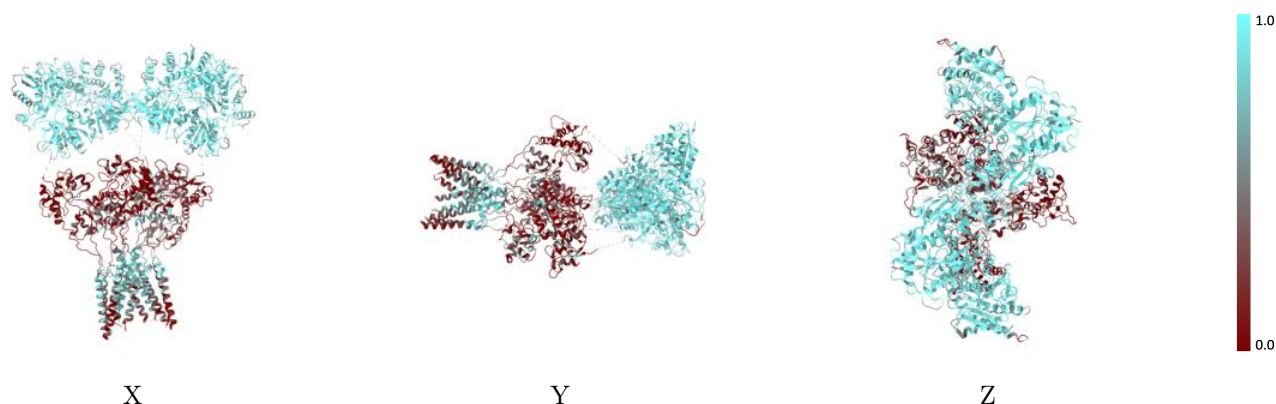
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



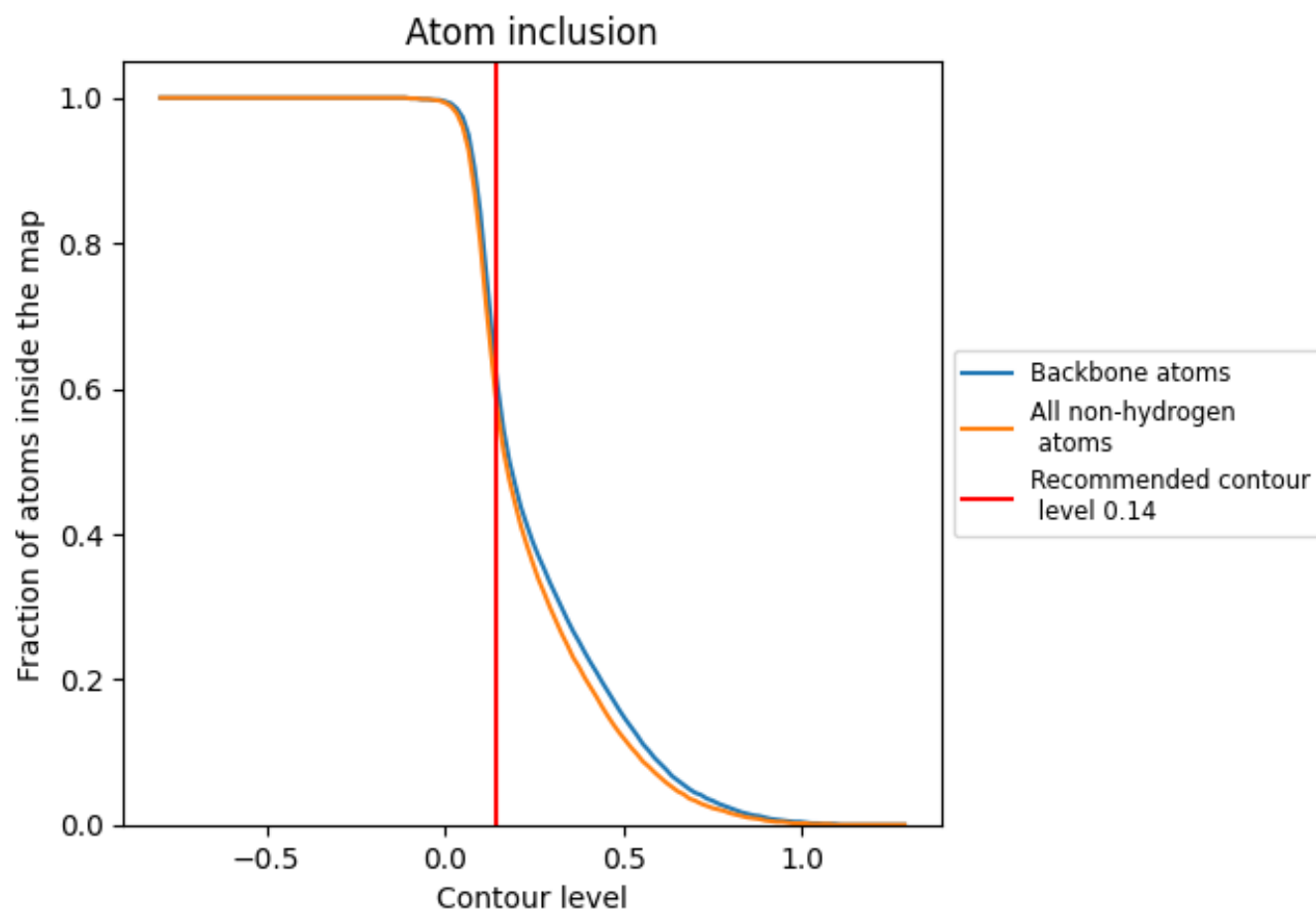
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.14).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 60% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5960	<div></div> 0.3000
A	<div></div> 0.5700	<div></div> 0.2730
B	<div></div> 0.6130	<div></div> 0.3270
C	<div></div> 0.5750	<div></div> 0.2810
D	<div></div> 0.6230	<div></div> 0.3200

