



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 12:57 AM UTC

PDB ID : 6LU9 / pdb_00006lu9
EMDB ID : EMD-0979
Title : Rat ionotropic Glutamate Delta-2 receptor in complex with 7-CKA and Calcium
Authors : Kumar, J.; Burada, A.P.
Deposited on : 2020-01-27
Resolution : 8.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

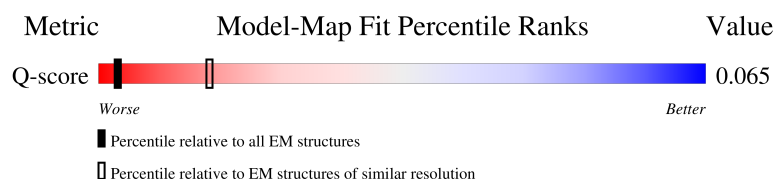
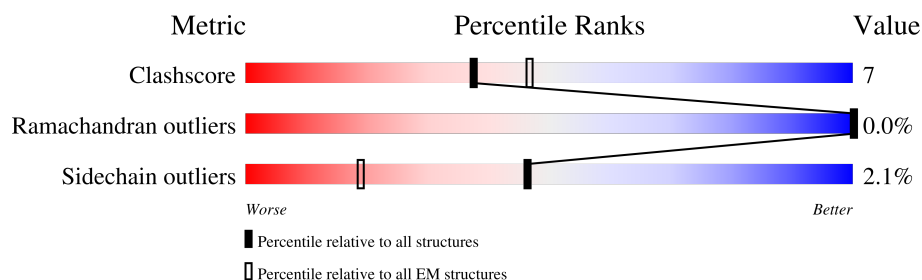
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 8.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	265 (8.30 - 9.30)

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

Mol	Chain	Length	Quality of chain
1	A	877	19% 56% 16% • 25%
1	B	877	22% 58% 15% • 25%
1	C	877	7% 55% 18% • 25%
1	D	877	5% 56% 18% • 25%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20992 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, delta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	660	Total	C	N	O	S	0	0
			5248	3314	910	999	25		
1	B	660	Total	C	N	O	S	0	0
			5248	3314	910	999	25		
1	C	660	Total	C	N	O	S	0	0
			5248	3314	910	999	25		
1	D	660	Total	C	N	O	S	0	0
			5248	3314	910	999	25		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	GLN	GLU	conflict	UNP Q63226
A	871	GLY	-	expression tag	UNP Q63226
A	872	LEU	-	expression tag	UNP Q63226
A	873	VAL	-	expression tag	UNP Q63226
A	874	PRO	-	expression tag	UNP Q63226
A	875	ARG	-	expression tag	UNP Q63226
A	876	GLY	-	expression tag	UNP Q63226
A	877	SER	-	expression tag	UNP Q63226
B	320	GLN	GLU	conflict	UNP Q63226
B	871	GLY	-	expression tag	UNP Q63226
B	872	LEU	-	expression tag	UNP Q63226
B	873	VAL	-	expression tag	UNP Q63226
B	874	PRO	-	expression tag	UNP Q63226
B	875	ARG	-	expression tag	UNP Q63226
B	876	GLY	-	expression tag	UNP Q63226
B	877	SER	-	expression tag	UNP Q63226
C	320	GLN	GLU	conflict	UNP Q63226
C	871	GLY	-	expression tag	UNP Q63226
C	872	LEU	-	expression tag	UNP Q63226
C	873	VAL	-	expression tag	UNP Q63226
C	874	PRO	-	expression tag	UNP Q63226
C	875	ARG	-	expression tag	UNP Q63226

Continued on next page...

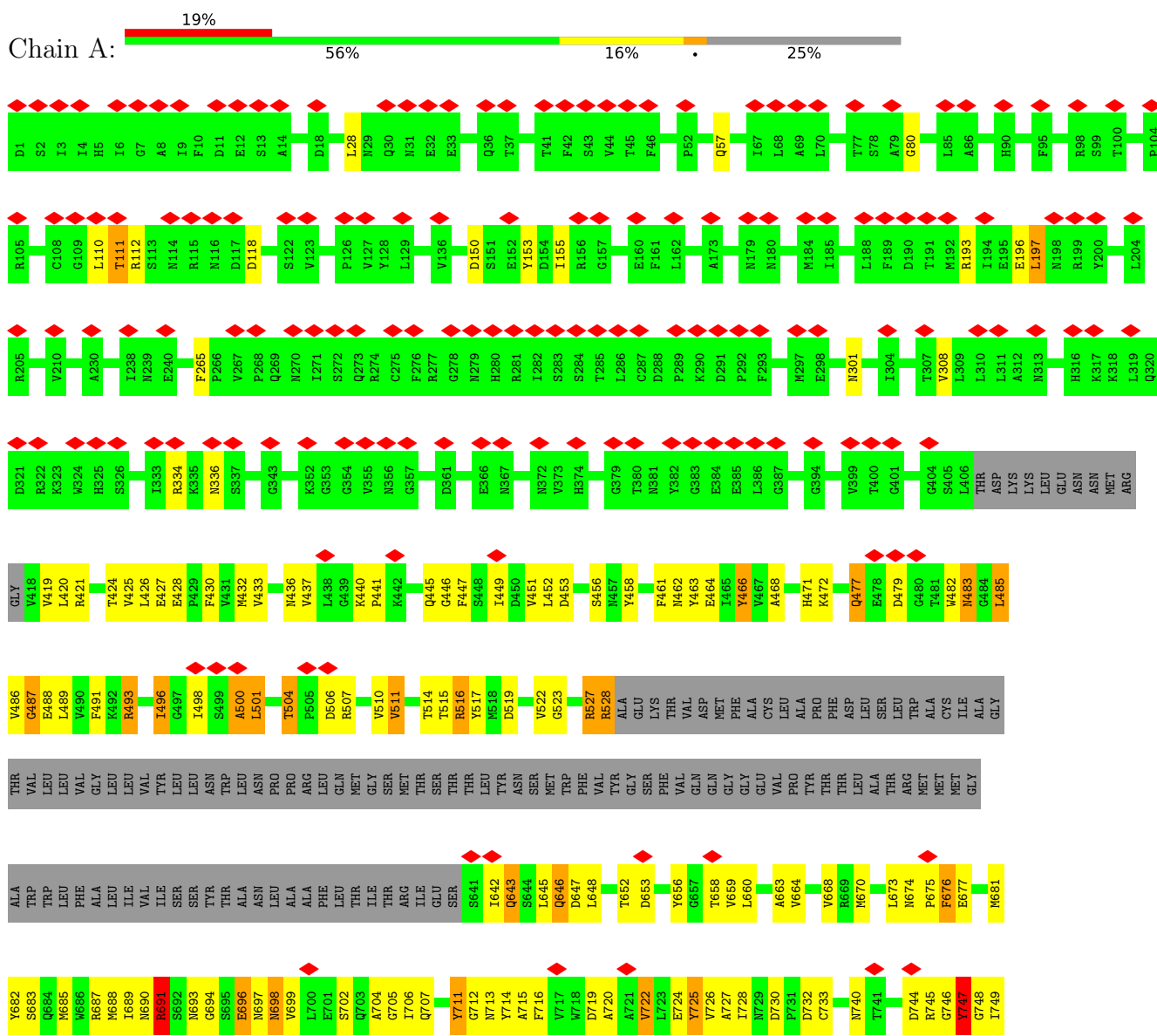
Continued from previous page...

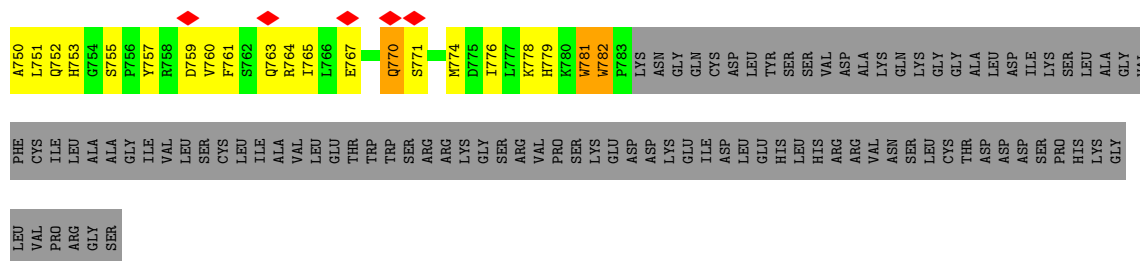
Chain	Residue	Modelled	Actual	Comment	Reference
C	876	GLY	-	expression tag	UNP Q63226
C	877	SER	-	expression tag	UNP Q63226
D	320	GLN	GLU	conflict	UNP Q63226
D	871	GLY	-	expression tag	UNP Q63226
D	872	LEU	-	expression tag	UNP Q63226
D	873	VAL	-	expression tag	UNP Q63226
D	874	PRO	-	expression tag	UNP Q63226
D	875	ARG	-	expression tag	UNP Q63226
D	876	GLY	-	expression tag	UNP Q63226
D	877	SER	-	expression tag	UNP Q63226

3 Residue-property plots

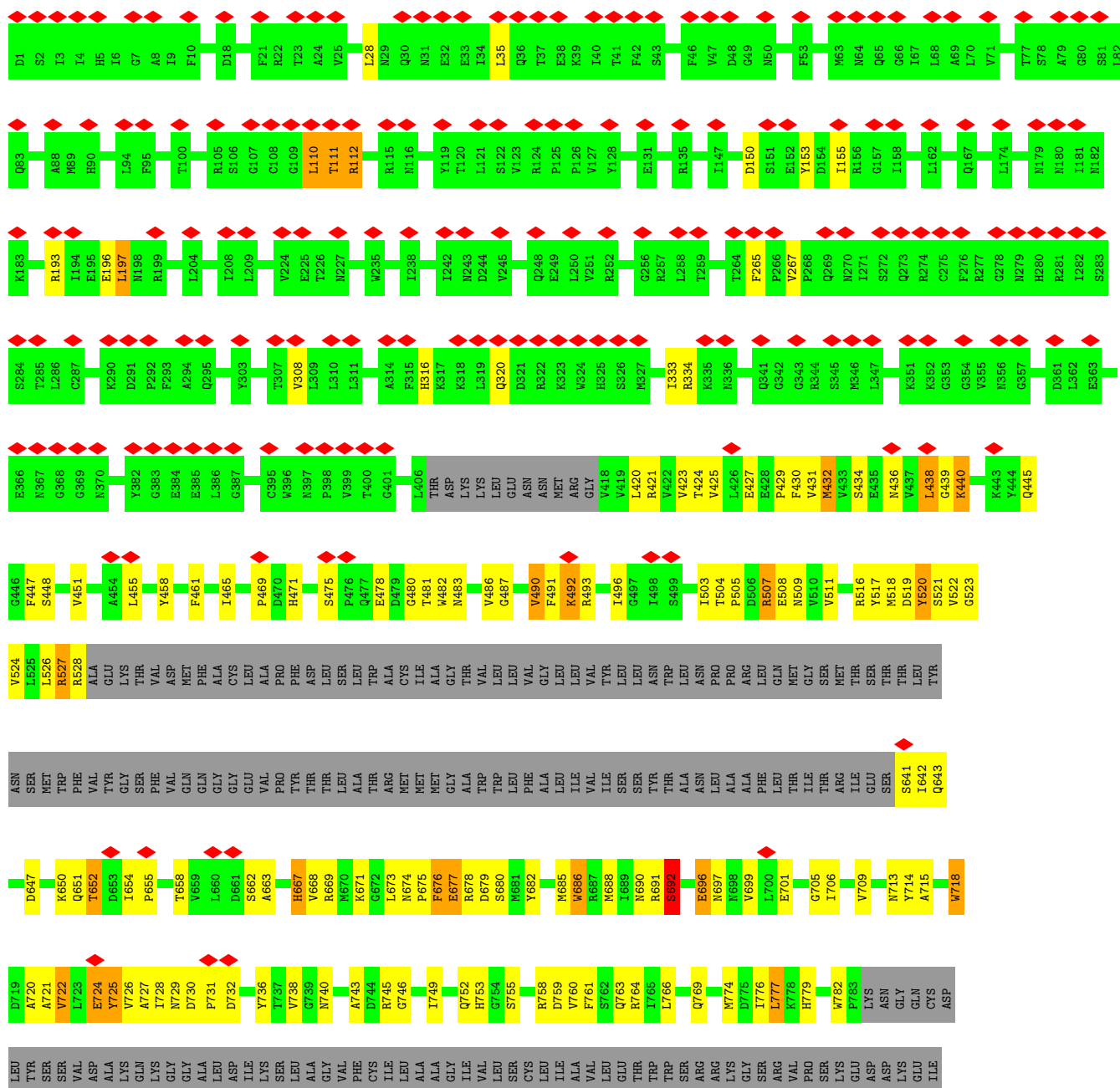
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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, delta-2



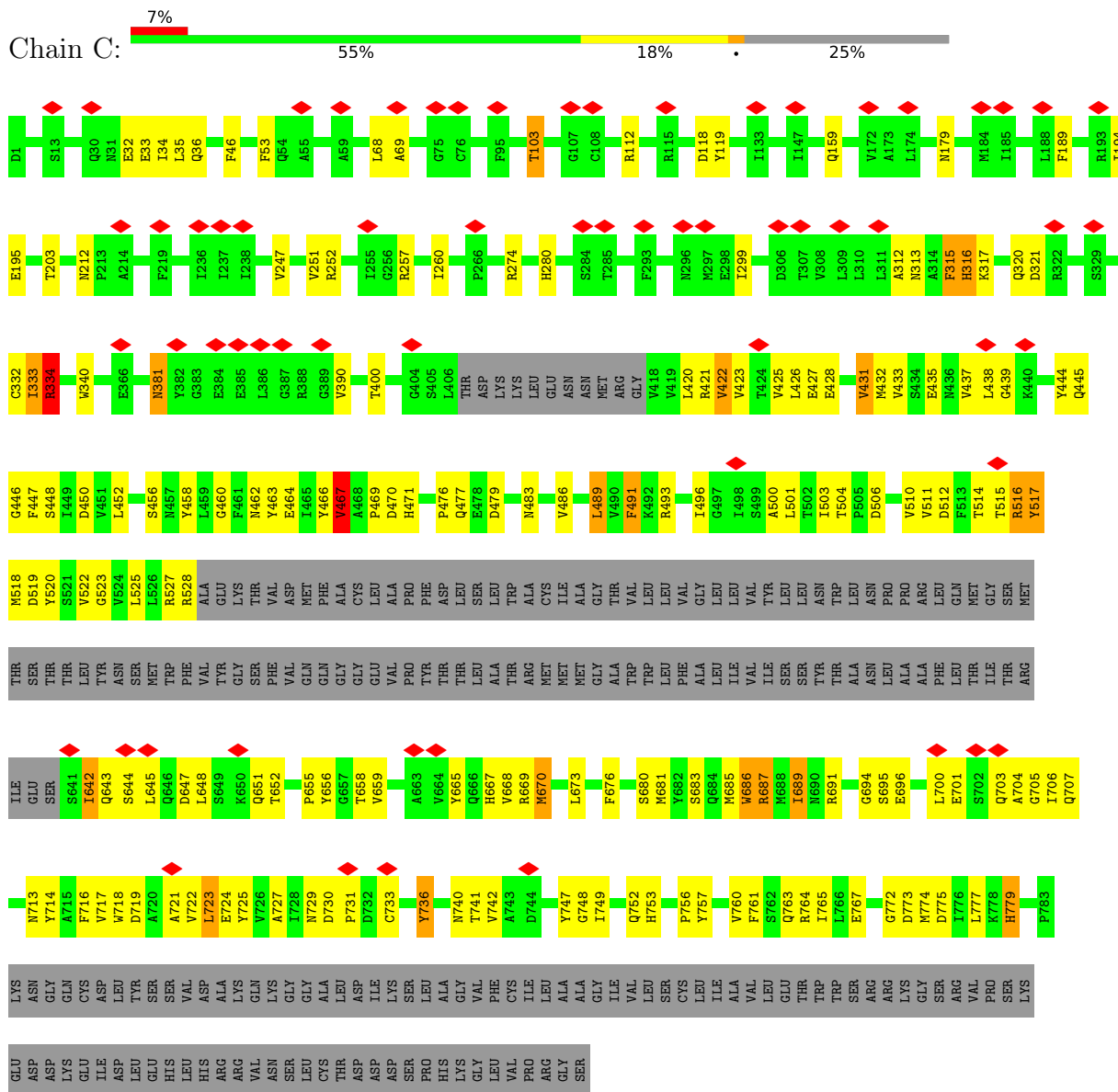


• Molecule 1: Glutamate receptor ionotropic, delta-2

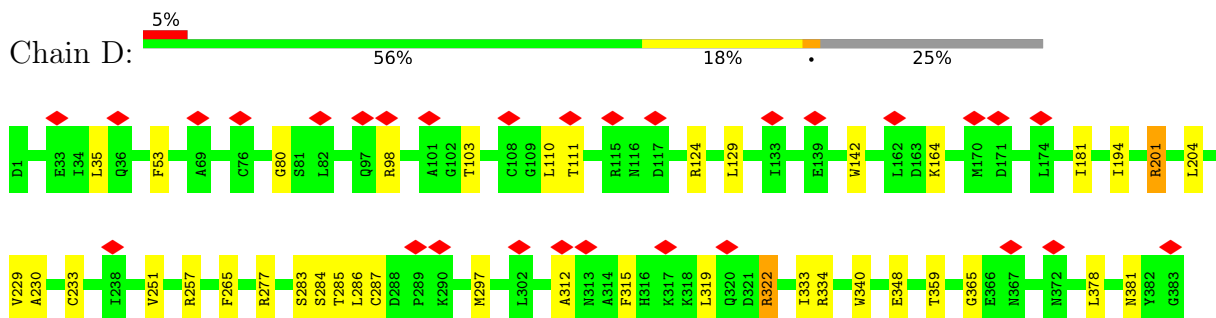


ASP
LEU
GLU
HIS
LEU
HIS
ARG
ARG
VAL
ASN
SER
SER
LEU
CYS
THR
ASP
ASP
SER
PRO
HIS
LYS
GLY
LEU
VAL
PRO
ARG
GLY
SER

• Molecule 1: Glutamate receptor ionotropic, delta-2



• Molecule 1: Glutamate receptor ionotropic, delta-2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	7977	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.38	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.958	Depositor
Minimum map value	-0.463	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.316	Depositor
Map size (Å)	392.0, 392.0, 392.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	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	1.45	61/5352 (1.1%)	1.74	113/7251 (1.6%)
1	B	1.51	60/5352 (1.1%)	1.76	115/7251 (1.6%)
1	C	1.56	78/5352 (1.5%)	1.88	133/7251 (1.8%)
1	D	1.53	68/5352 (1.3%)	1.82	105/7251 (1.4%)
All	All	1.52	267/21408 (1.2%)	1.80	466/29004 (1.6%)

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	7
1	B	0	7
1	C	0	12
1	D	0	17
All	All	0	43

All (267) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	316	HIS	CA-C	-8.59	1.42	1.52
1	A	782	TRP	NE1-CE2	-8.22	1.28	1.37
1	C	652	THR	N-CA	-8.21	1.38	1.46
1	B	642	ILE	CA-CB	-8.07	1.44	1.53
1	D	491	PHE	C-N	8.05	1.44	1.33
1	D	516	ARG	NE-CZ	7.97	1.41	1.33
1	D	423	VAL	CA-CB	7.96	1.64	1.54
1	A	642	ILE	CA-CB	-7.89	1.44	1.54
1	D	475	SER	CA-CB	7.80	1.64	1.53
1	A	485	LEU	C-N	7.65	1.43	1.33
1	A	728	ILE	CA-C	-7.59	1.43	1.52
1	A	496	ILE	C-O	-7.52	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	764	ARG	C-N	7.51	1.43	1.33
1	C	447	PHE	CA-CB	7.45	1.65	1.53
1	B	676	PHE	CA-C	-7.44	1.43	1.53
1	C	439	GLY	CA-C	-7.43	1.42	1.51
1	D	669	ARG	CD-NE	7.40	1.56	1.46
1	D	654	ILE	CA-CB	-7.37	1.47	1.54
1	A	496	ILE	CA-C	7.34	1.61	1.52
1	C	645	LEU	C-N	7.34	1.43	1.33
1	B	521	SER	N-CA	-7.32	1.37	1.46
1	A	702	SER	N-CA	-7.27	1.37	1.46
1	B	641	SER	C-N	7.25	1.43	1.33
1	C	425	VAL	CA-C	-7.15	1.43	1.52
1	D	713	ASN	CA-CB	7.14	1.62	1.53
1	A	733	CYS	C-N	7.06	1.44	1.33
1	C	435	GLU	CA-C	-7.06	1.44	1.52
1	B	724	GLU	N-CA	-7.06	1.37	1.46
1	C	724	GLU	C-N	7.05	1.42	1.33
1	C	470	ASP	C-N	7.04	1.43	1.33
1	D	446	GLY	CA-C	-7.04	1.44	1.52
1	B	421	ARG	CZ-NH2	7.02	1.42	1.33
1	B	654	ILE	N-CA	-7.00	1.41	1.46
1	C	727	ALA	CA-C	-7.00	1.43	1.52
1	D	440	LYS	C-N	6.98	1.42	1.33
1	A	706	ILE	CA-C	-6.95	1.44	1.52
1	B	763	GLN	N-CA	6.92	1.54	1.46
1	D	762	SER	C-N	6.92	1.42	1.33
1	C	740	ASN	CA-C	-6.90	1.44	1.52
1	C	716	PHE	CA-CB	6.90	1.62	1.53
1	C	477	GLN	CA-C	-6.88	1.44	1.52
1	C	706	ILE	CA-CB	6.85	1.63	1.54
1	C	450	ASP	C-N	6.83	1.42	1.33
1	C	511	VAL	N-CA	-6.83	1.38	1.46
1	C	777	LEU	CA-CB	6.82	1.64	1.53
1	A	719	ASP	N-CA	-6.78	1.37	1.46
1	D	425	VAL	CA-CB	-6.72	1.45	1.54
1	C	764	ARG	NE-CZ	6.72	1.40	1.33
1	B	431	VAL	CA-C	-6.71	1.44	1.52
1	C	681	MET	CA-C	-6.70	1.44	1.52
1	C	464	GLU	CA-C	-6.68	1.44	1.52
1	B	701	GLU	CA-C	-6.67	1.44	1.52
1	A	517	TYR	CA-CB	6.64	1.63	1.54
1	B	461	PHE	N-CA	-6.60	1.37	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	705	GLY	C-N	6.58	1.42	1.33
1	D	755	SER	C-N	6.54	1.38	1.33
1	B	490	VAL	CA-CB	6.52	1.62	1.54
1	A	440	LYS	C-N	-6.51	1.25	1.33
1	D	717	VAL	CA-CB	-6.47	1.46	1.54
1	C	528	ARG	NE-CZ	6.44	1.40	1.33
1	D	679	ASP	N-CA	-6.42	1.38	1.46
1	D	781	TRP	CA-CB	6.40	1.63	1.53
1	B	425	VAL	CA-CB	-6.39	1.46	1.54
1	B	686	TRP	CA-CB	6.38	1.63	1.53
1	C	423	VAL	N-CA	-6.38	1.38	1.46
1	B	697	ASN	N-CA	6.37	1.52	1.46
1	A	528	ARG	CD-NE	6.37	1.55	1.46
1	A	496	ILE	N-CA	-6.36	1.38	1.46
1	B	519	ASP	CA-CB	6.36	1.63	1.53
1	C	527	ARG	CA-CB	6.36	1.63	1.53
1	B	423	VAL	CA-CB	-6.35	1.46	1.54
1	C	694	GLY	CA-C	-6.34	1.43	1.51
1	B	523	GLY	CA-C	-6.33	1.45	1.52
1	D	669	ARG	N-CA	-6.25	1.39	1.46
1	A	500	ALA	CA-CB	6.24	1.60	1.52
1	A	725	TYR	CA-CB	6.21	1.62	1.53
1	C	705	GLY	C-N	6.20	1.41	1.33
1	C	500	ALA	CA-C	-6.19	1.46	1.53
1	C	700	LEU	C-N	6.19	1.41	1.33
1	A	468	ALA	C-N	-6.18	1.28	1.33
1	B	745	ARG	NE-CZ	6.17	1.39	1.33
1	A	752	GLN	CA-C	-6.17	1.44	1.53
1	A	419	VAL	N-CA	-6.17	1.38	1.46
1	C	510	VAL	C-N	6.16	1.42	1.33
1	A	763	GLN	N-CA	-6.14	1.39	1.46
1	C	516	ARG	NE-CZ	6.11	1.39	1.33
1	A	747	TYR	CA-C	-6.11	1.45	1.52
1	C	658	THR	N-CA	-6.08	1.39	1.46
1	D	707	GLN	C-N	6.08	1.42	1.34
1	A	493	ARG	NE-CZ	6.08	1.39	1.33
1	A	713	ASN	CA-C	-6.08	1.47	1.53
1	D	673	LEU	N-CA	6.07	1.53	1.46
1	B	749	ILE	CA-CB	-6.05	1.46	1.54
1	B	436	ASN	N-CA	-6.04	1.38	1.46
1	A	504	THR	CA-C	-6.03	1.44	1.52
1	D	486	VAL	C-N	6.01	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	695	SER	C-N	5.98	1.42	1.33
1	A	727	ALA	N-CA	-5.97	1.39	1.46
1	B	753	HIS	ND1-CE1	5.97	1.38	1.32
1	A	767	GLU	N-CA	-5.97	1.39	1.46
1	B	520	TYR	CA-C	-5.96	1.45	1.52
1	B	431	VAL	N-CA	-5.96	1.38	1.46
1	A	522	VAL	CA-C	5.96	1.59	1.52
1	B	504	THR	CA-C	5.95	1.58	1.52
1	C	748	GLY	CA-C	-5.94	1.46	1.52
1	D	521	SER	C-N	5.91	1.41	1.33
1	D	507	ARG	N-CA	-5.90	1.38	1.46
1	A	763	GLN	CA-CB	5.89	1.62	1.53
1	D	454	ALA	N-CA	-5.88	1.39	1.46
1	B	480	GLY	CA-C	-5.88	1.43	1.51
1	C	763	GLN	C-O	-5.87	1.17	1.24
1	C	725	TYR	CA-C	5.86	1.60	1.52
1	B	675	PRO	CA-C	-5.83	1.46	1.52
1	C	516	ARG	CA-C	-5.83	1.45	1.52
1	D	677	GLU	CA-C	5.82	1.60	1.52
1	D	649	SER	CA-C	-5.82	1.44	1.52
1	A	510	VAL	CA-CB	-5.81	1.46	1.54
1	A	458	TYR	N-CA	-5.80	1.39	1.46
1	C	503	ILE	CA-C	5.80	1.60	1.52
1	D	745	ARG	NE-CZ	5.79	1.39	1.33
1	C	448	SER	N-CA	-5.79	1.39	1.46
1	C	452	LEU	CA-C	-5.78	1.45	1.52
1	B	730	ASP	C-N	5.77	1.38	1.33
1	B	725	TYR	C-N	5.77	1.41	1.33
1	C	752	GLN	N-CA	-5.76	1.38	1.46
1	D	458	TYR	CA-C	-5.75	1.45	1.52
1	B	705	GLY	C-N	5.67	1.41	1.33
1	B	763	GLN	CA-CB	5.66	1.62	1.53
1	D	509	ASN	N-CA	-5.65	1.38	1.46
1	C	527	ARG	C-N	5.65	1.41	1.33
1	C	665	TYR	C-N	5.65	1.41	1.34
1	D	454	ALA	CA-CB	5.64	1.62	1.53
1	A	500	ALA	N-CA	-5.63	1.39	1.46
1	A	688	MET	CA-C	-5.62	1.45	1.52
1	C	670	MET	N-CA	-5.62	1.39	1.46
1	D	782	TRP	CA-CB	5.61	1.59	1.53
1	C	466	TYR	CA-C	-5.60	1.45	1.52
1	D	703	GLN	CA-C	5.60	1.60	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	745	ARG	CD-NE	5.60	1.54	1.46
1	A	675	PRO	N-CA	-5.59	1.40	1.47
1	D	758	ARG	NE-CZ	5.59	1.39	1.33
1	D	780	LYS	N-CA	-5.59	1.39	1.46
1	D	461	PHE	CA-C	5.59	1.59	1.52
1	A	646	GLN	C-N	5.58	1.41	1.33
1	D	449	ILE	C-N	5.58	1.41	1.33
1	A	514	THR	CA-C	5.58	1.60	1.53
1	D	421	ARG	C-N	5.56	1.40	1.33
1	C	713	ASN	CA-CB	5.55	1.60	1.53
1	B	769	GLN	N-CA	5.55	1.53	1.46
1	B	526	LEU	N-CA	-5.54	1.39	1.45
1	B	503	ILE	CA-CB	5.53	1.60	1.54
1	D	500	ALA	C-O	-5.52	1.17	1.23
1	A	471	HIS	N-CA	5.51	1.54	1.46
1	B	526	LEU	C-N	5.50	1.40	1.33
1	D	450	ASP	CA-CB	5.50	1.61	1.53
1	B	678	ARG	NE-CZ	5.49	1.39	1.33
1	A	687	ARG	NE-CZ	5.49	1.39	1.33
1	D	500	ALA	N-CA	-5.48	1.39	1.46
1	C	69	ALA	CA-C	-5.47	1.46	1.52
1	C	450	ASP	N-CA	-5.47	1.39	1.46
1	C	696	GLU	N-CA	-5.47	1.39	1.46
1	B	508	GLU	CA-CB	5.46	1.62	1.53
1	C	467	VAL	CA-C	-5.45	1.45	1.52
1	C	471	HIS	ND1-CE1	5.44	1.38	1.32
1	C	512	ASP	CA-C	5.44	1.59	1.52
1	A	712	GLY	C-N	5.43	1.40	1.33
1	A	493	ARG	CD-NE	5.42	1.53	1.46
1	C	456	SER	CA-CB	5.42	1.61	1.53
1	C	714	TYR	C-N	5.41	1.41	1.33
1	A	664	VAL	CA-CB	-5.40	1.48	1.54
1	C	463	TYR	CA-C	-5.40	1.46	1.52
1	A	690	ASN	CA-CB	5.39	1.61	1.53
1	A	464	GLU	CA-C	-5.39	1.46	1.52
1	B	480	GLY	N-CA	-5.39	1.37	1.45
1	C	667	HIS	CA-CB	5.39	1.61	1.53
1	D	523	GLY	CA-C	-5.39	1.45	1.51
1	D	676	PHE	C-N	5.38	1.41	1.33
1	D	645	LEU	CA-C	5.38	1.60	1.52
1	A	487	GLY	CA-C	-5.38	1.45	1.51
1	B	753	HIS	CG-CD2	5.38	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	458	TYR	C-N	5.37	1.42	1.33
1	D	743	ALA	C-N	5.37	1.41	1.33
1	C	460	GLY	C-N	5.36	1.40	1.33
1	D	463	TYR	CA-C	-5.34	1.45	1.52
1	B	740	ASN	CA-C	-5.34	1.46	1.52
1	C	460	GLY	CA-C	5.34	1.59	1.51
1	D	650	LYS	N-CA	-5.33	1.39	1.46
1	A	770	GLN	CA-C	-5.32	1.46	1.52
1	D	340	TRP	CD2-CE2	5.32	1.50	1.41
1	D	493	ARG	CZ-NH2	5.32	1.40	1.33
1	B	650	LYS	N-CA	5.32	1.53	1.46
1	C	772	GLY	C-N	5.31	1.41	1.33
1	D	739	GLY	C-N	5.31	1.40	1.33
1	A	746	GLY	N-CA	-5.30	1.39	1.45
1	D	722	VAL	CA-CB	5.29	1.60	1.54
1	D	365	GLY	C-O	-5.29	1.18	1.23
1	B	518	MET	CA-C	-5.29	1.46	1.52
1	D	738	VAL	N-CA	5.27	1.51	1.46
1	C	420	LEU	CA-C	-5.26	1.45	1.52
1	B	458	TYR	CA-CB	5.26	1.61	1.53
1	D	460	GLY	CA-C	-5.25	1.44	1.51
1	C	438	LEU	CA-CB	5.25	1.61	1.53
1	C	658	THR	C-N	5.25	1.40	1.33
1	C	703	GLN	CA-CB	5.25	1.61	1.53
1	C	317	LYS	N-CA	-5.24	1.40	1.46
1	A	764	ARG	NE-CZ	5.24	1.38	1.33
1	C	334	ARG	CA-C	-5.24	1.48	1.52
1	D	758	ARG	CZ-NH1	5.23	1.40	1.32
1	D	525	LEU	N-CA	-5.22	1.39	1.46
1	B	440	LYS	CA-CB	5.21	1.62	1.53
1	C	489	LEU	CB-CG	5.21	1.63	1.53
1	C	716	PHE	CA-C	-5.20	1.46	1.52
1	D	750	ALA	C-N	5.20	1.40	1.33
1	B	746	GLY	N-CA	-5.20	1.39	1.45
1	C	421	ARG	CZ-NH2	5.20	1.40	1.33
1	C	669	ARG	CD-NE	5.19	1.53	1.46
1	A	516	ARG	CZ-NH2	5.18	1.40	1.33
1	C	680	SER	CA-C	5.18	1.59	1.52
1	C	668	VAL	N-CA	-5.17	1.40	1.46
1	B	692	SER	C-N	5.17	1.40	1.33
1	C	462	ASN	N-CA	-5.17	1.39	1.45
1	A	428	GLU	CA-CB	5.16	1.61	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	523	GLY	CA-C	-5.16	1.44	1.51
1	A	711	TYR	N-CA	-5.16	1.40	1.46
1	C	433	VAL	CA-C	5.16	1.58	1.52
1	C	764	ARG	CD-NE	5.16	1.53	1.46
1	D	654	ILE	CA-C	5.16	1.57	1.52
1	D	658	THR	C-N	5.16	1.40	1.33
1	B	483	ASN	CA-CB	5.15	1.61	1.53
1	B	493	ARG	CD-NE	5.14	1.53	1.46
1	D	768	LEU	C-N	5.13	1.41	1.33
1	A	472	LYS	N-CA	-5.12	1.39	1.45
1	A	719	ASP	CA-CB	5.12	1.61	1.53
1	A	482	TRP	N-CA	-5.12	1.39	1.45
1	D	695	SER	CA-C	-5.12	1.45	1.52
1	D	475	SER	N-CA	5.12	1.50	1.45
1	B	722	VAL	N-CA	5.11	1.52	1.46
1	A	445	GLN	C-N	-5.11	1.26	1.33
1	B	642	ILE	N-CA	-5.11	1.39	1.46
1	C	764	ARG	N-CA	-5.11	1.40	1.46
1	A	683	SER	C-N	5.10	1.40	1.33
1	B	527	ARG	N-CA	-5.10	1.39	1.46
1	D	500	ALA	CA-CB	5.08	1.59	1.52
1	A	698	ASN	CA-C	-5.07	1.46	1.52
1	C	742	VAL	N-CA	-5.07	1.39	1.46
1	B	528	ARG	NE-CZ	5.06	1.38	1.33
1	C	676	PHE	CA-C	-5.06	1.46	1.52
1	D	436	ASN	C-N	5.06	1.39	1.33
1	B	520	TYR	C-N	5.06	1.40	1.33
1	C	670	MET	CA-C	-5.05	1.46	1.52
1	A	753	HIS	C-N	5.05	1.40	1.33
1	D	644	SER	CA-CB	5.04	1.62	1.53
1	D	458	TYR	C-N	5.04	1.41	1.33
1	A	744	ASP	CA-CB	5.04	1.61	1.53
1	D	678	ARG	NE-CZ	5.03	1.38	1.33
1	D	501	LEU	CA-C	-5.03	1.46	1.52
1	D	731	PRO	CA-C	-5.02	1.45	1.52
1	B	430	PHE	C-N	5.02	1.39	1.33
1	B	720	ALA	N-CA	-5.02	1.40	1.46
1	C	517	TYR	CZ-OH	5.02	1.48	1.38
1	D	764	ARG	N-CA	-5.02	1.40	1.46
1	B	424	THR	N-CA	-5.01	1.39	1.45
1	A	764	ARG	CD-NE	5.01	1.53	1.46
1	B	465	ILE	C-N	5.01	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	714	TYR	C-N	5.01	1.40	1.33
1	B	746	GLY	CA-C	-5.00	1.46	1.51
1	D	396	TRP	CD2-CE2	5.00	1.49	1.41

All (466) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	691	ARG	NE-CZ-NH2	9.61	127.85	119.20
1	C	316	HIS	CA-CB-CG	9.21	123.01	113.80
1	B	753	HIS	CB-CG-CD2	-8.93	119.59	131.20
1	D	504	THR	CA-C-N	8.87	128.90	119.05
1	D	504	THR	C-N-CA	8.87	128.90	119.05
1	A	704	ALA	CA-C-N	8.83	131.18	120.14
1	A	704	ALA	C-N-CA	8.83	131.18	120.14
1	D	430	PHE	CA-CB-CG	-8.69	105.11	113.80
1	D	519	ASP	CA-C-N	8.67	133.18	120.87
1	D	519	ASP	C-N-CA	8.67	133.18	120.87
1	B	690	ASN	CA-CB-CG	8.61	121.21	112.60
1	D	749	ILE	N-CA-CB	8.39	119.67	110.53
1	C	691	ARG	NE-CZ-NH1	-8.37	113.13	121.50
1	B	759	ASP	CA-CB-CG	-8.32	104.28	112.60
1	C	471	HIS	CE1-NE2-CD2	-8.29	100.71	109.00
1	D	779	HIS	CA-C-N	8.29	132.90	120.31
1	D	779	HIS	C-N-CA	8.29	132.90	120.31
1	C	658	THR	N-CA-C	-8.27	96.52	108.60
1	A	761	PHE	CA-CB-CG	-8.26	105.55	113.80
1	C	719	ASP	CA-CB-CG	8.24	120.84	112.60
1	C	696	GLU	CA-C-N	8.24	135.14	122.29
1	C	696	GLU	C-N-CA	8.24	135.14	122.29
1	A	445	GLN	N-CA-C	-8.20	96.74	108.96
1	C	527	ARG	NE-CZ-NH2	-8.10	111.91	119.20
1	A	761	PHE	CB-CG-CD1	8.04	134.38	120.70
1	A	447	PHE	CA-CB-CG	-8.01	105.79	113.80
1	D	674	ASN	CA-C-N	8.01	127.72	119.64
1	D	674	ASN	C-N-CA	8.01	127.72	119.64
1	D	663	ALA	CA-C-N	7.90	130.52	120.56
1	D	663	ALA	C-N-CA	7.90	130.52	120.56
1	D	744	ASP	N-CA-C	7.89	122.31	111.90
1	A	730	ASP	CA-CB-CG	7.74	120.34	112.60
1	A	719	ASP	CA-C-O	-7.66	112.01	120.81
1	B	110	LEU	N-CA-C	7.63	121.52	111.75
1	A	445	GLN	OE1-CD-NE2	7.61	130.21	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	483	ASN	CA-CB-CG	7.57	120.17	112.60
1	C	749	ILE	O-C-N	7.56	131.57	122.95
1	C	773	ASP	N-CA-C	-7.50	102.77	112.23
1	D	483	ASN	CA-CB-CG	7.48	120.08	112.60
1	A	782	TRP	CD2-CE2-CZ2	-7.36	115.04	122.40
1	A	437	VAL	N-CA-C	-7.36	96.88	107.77
1	D	674	ASN	CA-C-O	-7.32	112.85	119.59
1	A	781	TRP	N-CA-C	-7.30	103.03	112.23
1	D	667	HIS	CA-C-N	7.29	130.45	120.46
1	D	667	HIS	C-N-CA	7.29	130.45	120.46
1	D	658	THR	N-CA-C	-7.29	97.96	108.60
1	D	758	ARG	CA-C-N	7.27	129.89	120.44
1	D	758	ARG	C-N-CA	7.27	129.89	120.44
1	D	440	LYS	O-C-N	7.27	129.47	122.06
1	D	773	ASP	N-CA-C	-7.25	103.41	111.82
1	B	691	ARG	NH1-CZ-NH2	-7.25	109.87	119.30
1	C	448	SER	CA-C-N	7.25	130.71	120.42
1	C	448	SER	C-N-CA	7.25	130.71	120.42
1	C	316	HIS	CB-CA-C	-7.24	99.46	110.90
1	D	504	THR	O-C-N	-7.21	114.71	121.20
1	C	652	THR	CA-C-O	7.13	126.28	118.65
1	A	760	VAL	CA-C-O	-7.10	112.80	120.47
1	C	655	PRO	N-CA-CB	7.08	109.48	103.25
1	C	760	VAL	CA-C-N	7.06	129.74	120.28
1	C	760	VAL	C-N-CA	7.06	129.74	120.28
1	A	452	LEU	O-C-N	-7.04	114.66	122.12
1	B	696	GLU	N-CA-C	-7.04	104.96	113.97
1	D	498	ILE	N-CA-C	-7.03	96.97	107.37
1	D	777	LEU	CA-C-N	7.02	130.38	120.28
1	D	777	LEU	C-N-CA	7.02	130.38	120.28
1	C	725	TYR	CA-C-N	6.95	129.32	120.56
1	C	725	TYR	C-N-CA	6.95	129.32	120.56
1	C	703	GLN	CA-C-N	6.92	130.83	120.31
1	C	703	GLN	C-N-CA	6.92	130.83	120.31
1	C	779	HIS	CE1-NE2-CD2	-6.91	102.09	109.00
1	B	430	PHE	CA-CB-CG	-6.90	106.90	113.80
1	B	662	SER	O-C-N	-6.90	113.55	122.72
1	A	511	VAL	O-C-N	-6.89	115.76	123.20
1	A	464	GLU	N-CA-C	-6.89	98.55	109.23
1	C	704	ALA	CA-C-N	6.86	127.55	120.00
1	C	704	ALA	C-N-CA	6.86	127.55	120.00
1	A	753	HIS	CG-CD2-NE2	6.84	114.04	107.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	707	GLN	OE1-CD-NE2	-6.83	115.77	122.60
1	C	462	ASN	N-CA-C	-6.82	99.56	110.14
1	B	753	HIS	CB-CG-ND1	6.81	132.92	122.70
1	C	648	LEU	CA-C-O	6.78	127.74	120.55
1	C	767	GLU	O-C-N	6.77	129.04	122.07
1	A	759	ASP	CB-CA-C	-6.75	100.29	110.88
1	A	511	VAL	N-CA-C	-6.70	98.47	108.12
1	B	486	VAL	N-CA-C	6.70	117.45	110.62
1	B	517	TYR	CA-C-O	6.69	126.39	118.69
1	A	668	VAL	N-CA-CB	6.69	119.64	110.54
1	D	670	MET	N-CA-C	6.68	118.22	111.07
1	A	647	ASP	CA-C-N	6.67	129.22	120.28
1	A	647	ASP	C-N-CA	6.67	129.22	120.28
1	A	715	ALA	N-CA-C	-6.66	98.54	109.40
1	A	770	GLN	CA-C-O	-6.65	113.37	120.42
1	A	449	ILE	N-CA-C	6.65	117.40	110.62
1	B	729	ASN	CA-CB-CG	-6.62	105.98	112.60
1	B	731	PRO	N-CA-C	-6.61	105.41	114.80
1	D	722	VAL	N-CA-C	-6.59	104.34	110.53
1	A	451	VAL	CA-C-O	-6.56	114.13	120.95
1	B	669	ARG	CB-CA-C	-6.54	100.61	110.88
1	B	471	HIS	CA-CB-CG	-6.54	107.26	113.80
1	D	773	ASP	CA-C-O	-6.54	112.45	119.97
1	C	668	VAL	N-CA-C	6.54	117.29	110.62
1	B	647	ASP	CA-C-O	-6.51	113.98	120.82
1	A	670	MET	CA-C-N	6.51	129.66	120.28
1	A	670	MET	C-N-CA	6.51	129.66	120.28
1	D	667	HIS	ND1-CE1-NE2	6.49	114.89	108.40
1	A	511	VAL	N-CA-CB	6.49	121.00	111.52
1	B	736	TYR	CA-C-O	-6.48	113.52	121.11
1	A	675	PRO	N-CA-CB	6.48	110.39	103.52
1	B	475	SER	CA-C-O	-6.46	114.12	120.26
1	D	662	SER	CA-C-N	6.45	129.21	120.44
1	D	662	SER	C-N-CA	6.45	129.21	120.44
1	A	724	GLU	CA-C-O	-6.44	113.60	120.42
1	C	515	THR	CA-C-N	6.42	129.99	120.87
1	C	515	THR	C-N-CA	6.42	129.99	120.87
1	C	317	LYS	N-CA-CB	-6.42	100.67	110.16
1	C	730	ASP	CA-C-O	-6.39	113.35	120.25
1	D	461	PHE	CA-CB-CG	-6.39	107.41	113.80
1	D	751	LEU	N-CA-C	-6.36	99.67	109.14
1	C	680	SER	CA-C-N	6.35	129.12	120.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	680	SER	C-N-CA	6.35	129.12	120.54
1	C	723	LEU	N-CA-C	6.33	118.99	111.71
1	B	667	HIS	CG-CD2-NE2	6.32	113.52	107.20
1	A	757	TYR	N-CA-C	-6.31	105.35	114.12
1	B	643	GLN	CA-C-O	6.30	126.33	119.15
1	C	445	GLN	N-CA-C	-6.30	99.76	109.14
1	C	736	TYR	O-C-N	-6.30	115.50	123.24
1	C	686	TRP	CE3-CZ3-CH2	6.29	129.28	121.10
1	D	772	GLY	CA-C-N	6.29	129.87	120.31
1	D	772	GLY	C-N-CA	6.29	129.87	120.31
1	D	681	MET	O-C-N	6.28	128.54	122.07
1	C	446	GLY	N-CA-C	-6.27	105.20	111.85
1	B	658	THR	N-CA-C	-6.27	99.96	108.24
1	C	647	ASP	CA-C-N	6.27	128.68	120.28
1	C	647	ASP	C-N-CA	6.27	128.68	120.28
1	D	447	PHE	N-CA-C	6.27	118.19	111.36
1	C	695	SER	CA-C-N	6.25	129.17	120.29
1	C	695	SER	C-N-CA	6.25	129.17	120.29
1	D	434	SER	N-CA-C	-6.25	104.71	112.90
1	B	671	LYS	CA-C-O	6.24	127.15	119.97
1	C	713	ASN	CA-CB-CG	6.24	118.84	112.60
1	C	486	VAL	O-C-N	6.24	127.92	121.87
1	C	504	THR	CA-C-N	6.23	125.64	118.85
1	C	504	THR	C-N-CA	6.23	125.64	118.85
1	C	515	THR	CB-CA-C	6.22	120.65	109.64
1	C	514	THR	CA-C-N	6.21	129.94	120.82
1	C	514	THR	C-N-CA	6.21	129.94	120.82
1	C	522	VAL	O-C-N	-6.21	116.56	123.26
1	B	691	ARG	NE-CZ-NH2	6.20	124.78	119.20
1	B	713	ASN	OD1-CG-ND2	6.20	128.80	122.60
1	C	658	THR	CA-C-N	6.20	129.74	120.69
1	C	658	THR	C-N-CA	6.20	129.74	120.69
1	B	738	VAL	N-CA-C	-6.19	98.63	108.90
1	D	473	TYR	N-CA-C	-6.18	105.80	113.15
1	C	749	ILE	N-CA-C	-6.18	99.68	108.58
1	C	332	CYS	CA-C-N	6.18	133.09	121.97
1	C	332	CYS	C-N-CA	6.18	133.09	121.97
1	B	758	ARG	CA-C-N	6.15	128.52	120.28
1	B	758	ARG	C-N-CA	6.15	128.52	120.28
1	C	333	ILE	CA-C-N	-6.15	114.16	121.90
1	C	333	ILE	C-N-CA	-6.15	114.16	121.90
1	A	759	ASP	N-CA-C	6.14	117.64	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	424	THR	CA-CB-OG1	6.14	118.80	109.60
1	B	448	SER	CA-C-N	6.12	129.11	120.42
1	B	448	SER	C-N-CA	6.12	129.11	120.42
1	B	782	TRP	CA-C-O	-6.11	114.34	120.64
1	D	739	GLY	CA-C-N	6.10	131.78	122.93
1	D	739	GLY	C-N-CA	6.10	131.78	122.93
1	A	424	THR	N-CA-C	-6.10	100.06	109.14
1	A	436	ASN	N-CA-CB	6.09	120.14	110.57
1	C	779	HIS	ND1-CE1-NE2	6.08	114.48	108.40
1	B	766	LEU	O-C-N	6.08	128.56	122.12
1	B	709	VAL	CA-C-N	6.08	128.92	120.29
1	B	709	VAL	C-N-CA	6.08	128.92	120.29
1	A	719	ASP	O-C-N	6.07	130.40	122.93
1	C	686	TRP	CZ3-CH2-CZ2	-6.06	113.62	121.50
1	D	730	ASP	O-C-N	-6.06	115.55	121.18
1	B	720	ALA	O-C-N	6.04	128.52	122.12
1	A	441	PRO	CB-CA-C	-6.03	103.68	111.46
1	A	673	LEU	N-CA-C	-6.03	105.10	112.88
1	C	760	VAL	N-CA-C	6.03	116.81	110.72
1	C	719	ASP	CA-C-N	6.02	128.35	120.28
1	C	719	ASP	C-N-CA	6.02	128.35	120.28
1	A	456	SER	CA-C-N	6.01	128.82	120.29
1	A	456	SER	C-N-CA	6.01	128.82	120.29
1	C	194	ILE	N-CA-C	5.99	117.45	110.62
1	B	732	ASP	CA-C-N	5.99	130.64	122.19
1	B	732	ASP	C-N-CA	5.99	130.64	122.19
1	D	782	TRP	N-CA-C	-5.99	95.80	108.73
1	D	767	GLU	CA-C-N	5.98	128.90	120.28
1	D	767	GLU	C-N-CA	5.98	128.90	120.28
1	B	745	ARG	N-CA-CB	5.98	121.95	111.13
1	A	458	TYR	CA-CB-CG	5.97	124.66	113.90
1	D	679	ASP	N-CA-C	-5.95	99.70	109.40
1	B	714	TYR	O-C-N	5.94	129.86	123.56
1	C	527	ARG	CD-NE-CZ	-5.94	116.09	124.40
1	A	720	ALA	N-CA-CB	5.93	118.84	110.12
1	B	677	GLU	N-CA-C	-5.93	101.35	109.71
1	A	658	THR	CA-C-N	5.93	128.44	120.50
1	A	658	THR	C-N-CA	5.93	128.44	120.50
1	D	761	PHE	O-C-N	5.92	128.39	122.12
1	B	669	ARG	CA-C-O	-5.92	114.61	120.82
1	D	648	LEU	N-CA-CB	-5.91	101.11	110.22
1	A	523	GLY	O-C-N	-5.88	117.05	123.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	491	PHE	CA-C-N	5.88	131.10	122.63
1	D	491	PHE	C-N-CA	5.88	131.10	122.63
1	C	471	HIS	CG-CD2-NE2	5.87	113.07	107.20
1	D	431	VAL	N-CA-CB	5.87	119.80	111.82
1	D	687	ARG	NE-CZ-NH1	5.86	127.36	121.50
1	A	498	ILE	CA-C-O	-5.86	113.80	120.66
1	C	491	PHE	CA-CB-CG	-5.86	107.94	113.80
1	D	675	PRO	N-CA-CB	5.86	108.91	103.46
1	A	687	ARG	CA-CB-CG	5.86	125.81	114.10
1	B	448	SER	O-C-N	-5.85	115.48	122.15
1	D	516	ARG	CA-C-O	5.85	127.94	121.56
1	D	432	MET	CA-C-O	5.84	127.38	120.66
1	A	663	ALA	CA-C-N	5.84	128.13	120.60
1	A	663	ALA	C-N-CA	5.84	128.13	120.60
1	B	680	SER	N-CA-C	5.83	119.86	112.87
1	B	492	LYS	N-CA-C	5.83	117.72	110.91
1	C	685	MET	CA-C-N	5.82	128.08	120.28
1	C	685	MET	C-N-CA	5.82	128.08	120.28
1	A	486	VAL	CA-C-N	5.81	127.60	120.22
1	A	486	VAL	C-N-CA	5.81	127.60	120.22
1	B	455	LEU	CA-C-N	5.81	128.53	120.29
1	B	455	LEU	C-N-CA	5.81	128.53	120.29
1	D	749	ILE	N-CA-C	-5.80	101.24	108.89
1	A	719	ASP	CA-C-N	5.77	128.01	120.28
1	A	719	ASP	C-N-CA	5.77	128.01	120.28
1	C	761	PHE	N-CA-C	-5.76	105.00	111.28
1	D	391	ARG	NE-CZ-NH2	5.76	124.38	119.20
1	C	479	ASP	N-CA-CB	5.75	119.24	110.44
1	C	316	HIS	N-CA-C	5.75	117.35	111.14
1	C	431	VAL	N-CA-C	5.74	117.10	107.18
1	B	755	SER	O-C-N	-5.72	115.36	121.42
1	B	777	LEU	N-CA-CB	5.72	118.53	110.12
1	B	763	GLN	CA-C-O	-5.71	114.50	120.55
1	B	777	LEU	CA-C-N	5.71	127.93	120.28
1	B	777	LEU	C-N-CA	5.71	127.93	120.28
1	A	265	PHE	CA-CB-CG	-5.70	108.10	113.80
1	A	767	GLU	N-CA-CB	5.69	118.49	110.12
1	C	464	GLU	N-CA-C	-5.69	99.39	109.06
1	A	501	LEU	N-CA-C	-5.68	99.93	108.96
1	A	642	ILE	CA-C-N	5.67	127.82	120.44
1	A	642	ILE	C-N-CA	5.67	127.82	120.44
1	A	699	VAL	N-CA-C	-5.67	100.25	108.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	501	LEU	CA-C-O	-5.67	114.51	120.58
1	C	471	HIS	ND1-CE1-NE2	5.67	114.07	108.40
1	C	722	VAL	O-C-N	-5.66	116.37	121.91
1	D	515	THR	CA-C-N	5.65	129.81	120.94
1	D	515	THR	C-N-CA	5.65	129.81	120.94
1	C	489	LEU	CA-C-N	5.64	128.19	120.46
1	C	489	LEU	C-N-CA	5.64	128.19	120.46
1	C	643	GLN	CB-CG-CD	5.64	122.18	112.60
1	B	483	ASN	N-CA-C	-5.63	102.12	110.46
1	B	668	VAL	N-CA-CB	5.62	118.18	110.54
1	A	426	LEU	N-CA-CB	5.61	119.02	109.87
1	B	662	SER	CA-C-N	5.58	128.02	120.44
1	B	662	SER	C-N-CA	5.58	128.02	120.44
1	C	644	SER	CA-C-N	5.58	128.79	120.31
1	C	644	SER	C-N-CA	5.58	128.79	120.31
1	B	669	ARG	N-CA-C	5.57	117.03	111.07
1	C	506	ASP	CA-CB-CG	5.57	118.17	112.60
1	C	721	ALA	N-CA-CB	5.57	118.31	110.12
1	C	722	VAL	CB-CA-C	-5.57	104.84	111.97
1	D	475	SER	CA-C-N	5.57	126.80	119.84
1	D	475	SER	C-N-CA	5.57	126.80	119.84
1	C	668	VAL	N-CA-CB	5.56	118.11	110.54
1	A	757	TYR	CA-C-N	5.56	127.67	120.44
1	A	757	TYR	C-N-CA	5.56	127.67	120.44
1	D	436	ASN	N-CA-C	-5.56	100.12	109.07
1	C	422	VAL	N-CA-CB	5.56	117.71	111.21
1	C	686	TRP	CG-CD2-CE3	-5.54	128.36	133.90
1	C	321	ASP	CA-CB-CG	5.54	118.14	112.60
1	B	522	VAL	N-CA-C	-5.53	100.51	108.48
1	D	425	VAL	CA-CB-CG1	5.53	119.81	110.40
1	B	423	VAL	N-CA-C	-5.53	100.47	108.71
1	C	433	VAL	N-CA-CB	5.53	117.14	110.95
1	D	662	SER	N-CA-C	-5.53	101.03	109.65
1	A	767	GLU	CB-CA-C	-5.52	101.63	110.79
1	C	686	TRP	CA-CB-CG	5.52	124.08	113.60
1	C	729	ASN	CA-C-O	5.51	125.80	119.35
1	A	682	TYR	CA-C-O	-5.51	112.60	119.38
1	B	655	PRO	N-CD-CG	5.51	111.47	103.20
1	B	706	ILE	O-C-N	5.51	127.50	121.83
1	B	727	ALA	CB-CA-C	-5.51	100.10	110.67
1	D	722	VAL	CA-C-O	-5.49	114.95	121.05
1	A	751	LEU	N-CA-C	-5.49	100.95	109.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	697	ASN	N-CA-C	-5.49	105.73	113.20
1	B	685	MET	N-CA-C	5.49	117.34	111.36
1	D	497	GLY	N-CA-C	-5.49	100.18	113.18
1	A	483	ASN	CB-CG-ND2	-5.48	108.18	116.40
1	C	779	HIS	CA-C-O	-5.48	113.67	119.97
1	D	742	VAL	N-CA-C	-5.48	98.04	107.24
1	C	527	ARG	NE-CZ-NH1	5.47	126.97	121.50
1	B	761	PHE	N-CA-CB	5.47	117.94	110.01
1	B	265	PHE	CA-CB-CG	-5.47	108.33	113.80
1	B	669	ARG	CA-CB-CG	5.46	125.03	114.10
1	A	646	GLN	CA-C-N	5.46	127.53	120.44
1	A	646	GLN	C-N-CA	5.46	127.53	120.44
1	D	512	ASP	CA-C-N	5.46	130.78	122.65
1	D	512	ASP	C-N-CA	5.46	130.78	122.65
1	A	732	ASP	CA-C-N	5.44	130.09	122.36
1	A	732	ASP	C-N-CA	5.44	130.09	122.36
1	D	432	MET	O-C-N	-5.44	116.63	123.27
1	B	690	ASN	CA-C-O	-5.44	113.31	119.78
1	A	471	HIS	CE1-NE2-CD2	-5.44	103.56	109.00
1	A	519	ASP	CA-C-O	-5.43	114.86	121.05
1	C	676	PHE	CA-CB-CG	-5.43	108.37	113.80
1	A	451	VAL	CB-CA-C	-5.43	104.81	112.14
1	C	469	PRO	N-CA-CB	5.43	109.28	103.52
1	C	703	GLN	CG-CD-NE2	5.43	124.54	116.40
1	D	475	SER	CA-C-O	-5.42	115.35	120.34
1	C	689	ILE	CB-CA-C	5.42	119.46	112.14
1	B	776	ILE	CA-C-N	5.42	127.54	120.28
1	B	776	ILE	C-N-CA	5.42	127.54	120.28
1	A	504	THR	CA-CB-OG1	5.42	117.73	109.60
1	D	142	TRP	CG-CD2-CE3	-5.41	128.49	133.90
1	B	667	HIS	CE1-NE2-CD2	-5.41	103.59	109.00
1	B	458	TYR	CB-CG-CD1	5.40	128.90	120.80
1	D	422	VAL	N-CA-CB	5.39	118.26	111.46
1	B	491	PHE	CB-CG-CD1	-5.38	111.55	120.70
1	A	763	GLN	OE1-CD-NE2	-5.38	117.22	122.60
1	B	267	VAL	CA-C-N	5.38	125.38	119.89
1	B	267	VAL	C-N-CA	5.38	125.38	119.89
1	B	519	ASP	O-C-N	-5.38	116.67	123.01
1	C	724	GLU	N-CA-C	5.37	117.21	111.36
1	A	716	PHE	CA-CB-CG	5.37	119.17	113.80
1	A	452	LEU	CA-C-N	5.36	128.46	120.31
1	A	452	LEU	C-N-CA	5.36	128.46	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	501	LEU	N-CA-CB	5.36	118.73	110.21
1	D	652	THR	O-C-N	5.36	128.62	122.25
1	B	763	GLN	N-CA-C	5.36	117.12	111.28
1	A	691	ARG	NE-CZ-NH2	-5.35	114.38	119.20
1	C	669	ARG	CA-C-N	5.35	127.39	120.44
1	C	669	ARG	C-N-CA	5.35	127.39	120.44
1	C	753	HIS	ND1-CE1-NE2	5.35	113.75	108.40
1	C	765	ILE	CA-C-N	5.35	127.39	120.44
1	C	765	ILE	C-N-CA	5.35	127.39	120.44
1	C	462	ASN	CA-CB-CG	-5.34	107.26	112.60
1	C	670	MET	CG-SD-CE	-5.34	89.16	100.90
1	B	729	ASN	N-CA-C	-5.33	105.42	112.94
1	D	740	ASN	CA-CB-CG	5.33	117.93	112.60
1	C	466	TYR	N-CA-C	-5.33	101.08	109.50
1	D	648	LEU	N-CA-C	5.32	117.83	111.71
1	B	760	VAL	CA-C-N	5.32	127.35	120.44
1	B	760	VAL	C-N-CA	5.32	127.35	120.44
1	A	647	ASP	N-CA-C	5.31	116.76	111.07
1	B	505	PRO	CA-C-N	5.31	127.34	120.44
1	B	505	PRO	C-N-CA	5.31	127.34	120.44
1	A	453	ASP	CA-C-O	-5.30	113.87	119.97
1	B	738	VAL	CA-C-O	-5.30	116.38	121.63
1	D	667	HIS	CE1-NE2-CD2	-5.30	103.70	109.00
1	B	755	SER	CA-C-N	5.29	126.46	119.84
1	B	755	SER	C-N-CA	5.29	126.46	119.84
1	D	651	GLN	OE1-CD-NE2	5.29	127.89	122.60
1	B	481	THR	CA-CB-OG1	5.28	117.52	109.60
1	B	699	VAL	CB-CA-C	5.28	118.78	111.49
1	B	761	PHE	CA-C-N	5.28	127.78	120.29
1	B	761	PHE	C-N-CA	5.28	127.78	120.29
1	A	647	ASP	CB-CA-C	-5.27	102.60	110.88
1	B	475	SER	N-CA-C	-5.27	103.47	108.22
1	C	447	PHE	N-CA-C	5.27	116.71	111.07
1	C	707	GLN	N-CA-C	5.27	117.94	111.82
1	C	701	GLU	O-C-N	5.27	129.38	123.48
1	B	724	GLU	N-CA-C	-5.26	105.62	111.36
1	C	431	VAL	CA-C-O	-5.26	115.53	120.22
1	A	516	ARG	N-CA-CB	5.26	117.74	109.69
1	B	650	LYS	CA-C-O	5.26	125.84	119.11
1	A	515	THR	CA-C-N	5.25	128.23	120.82
1	A	515	THR	C-N-CA	5.25	128.23	120.82
1	A	755	SER	O-C-N	5.25	125.94	121.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	ASN	CA-CB-CG	5.25	117.85	112.60
1	A	782	TRP	CH2-CZ2-CE2	5.25	124.32	117.50
1	C	103	THR	CA-C-O	-5.24	115.01	120.88
1	C	512	ASP	N-CA-CB	5.24	118.96	110.42
1	D	696	GLU	CB-CG-CD	-5.24	103.69	112.60
1	B	475	SER	CA-C-N	5.23	126.38	119.84
1	B	475	SER	C-N-CA	5.23	126.38	119.84
1	B	763	GLN	O-C-N	5.23	127.67	122.12
1	B	451	VAL	CA-C-O	5.23	126.39	120.95
1	B	718	TRP	CA-CB-CG	5.23	123.53	113.60
1	A	462	ASN	CA-CB-CG	-5.23	107.37	112.60
1	B	764	ARG	O-C-N	-5.22	116.20	122.15
1	C	518	MET	CG-SD-CE	-5.22	89.41	100.90
1	C	652	THR	CA-CB-OG1	5.22	117.43	109.60
1	D	686	TRP	CB-CG-CD2	-5.22	119.50	126.80
1	C	444	TYR	N-CA-C	-5.21	101.38	109.72
1	D	431	VAL	N-CA-C	-5.21	100.06	107.77
1	A	501	LEU	CB-CA-C	5.21	118.91	110.22
1	A	656	TYR	CA-C-O	-5.21	115.88	121.45
1	D	694	GLY	O-C-N	5.20	128.28	122.50
1	D	708	LYS	O-C-N	5.20	128.67	122.27
1	A	707	GLN	CA-C-N	5.20	128.21	120.31
1	A	707	GLN	C-N-CA	5.20	128.21	120.31
1	C	437	VAL	CA-CB-CG2	-5.19	101.57	110.40
1	B	652	THR	N-CA-C	-5.19	105.28	113.02
1	A	761	PHE	CB-CG-CD2	-5.19	111.88	120.70
1	A	463	TYR	CB-CG-CD2	5.19	128.58	120.80
1	C	519	ASP	CB-CA-C	-5.18	101.40	109.84
1	A	722	VAL	O-C-N	5.18	126.99	121.91
1	B	743	ALA	CA-C-N	5.18	129.91	122.40
1	B	743	ALA	C-N-CA	5.18	129.91	122.40
1	D	738	VAL	N-CA-C	-5.18	100.41	108.95
1	D	778	LYS	O-C-N	-5.18	116.16	122.22
1	C	316	HIS	CB-CG-ND1	-5.17	114.94	122.70
1	B	520	TYR	CB-CA-C	5.17	118.49	109.65
1	C	476	PRO	CB-CA-C	-5.17	105.00	111.56
1	C	642	ILE	O-C-N	5.17	128.62	122.83
1	A	765	ILE	CA-C-O	-5.17	115.58	120.95
1	C	46	PHE	CA-CB-CG	-5.16	108.64	113.80
1	D	742	VAL	CA-C-O	5.16	125.37	120.31
1	A	749	ILE	N-CA-C	-5.16	101.03	108.87
1	B	679	ASP	N-CA-C	-5.15	99.70	108.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	704	ALA	O-C-N	-5.15	116.28	122.15
1	D	507	ARG	NE-CZ-NH2	5.15	123.83	119.20
1	B	726	VAL	CB-CA-C	-5.14	105.39	111.97
1	C	717	VAL	CB-CA-C	-5.14	104.54	110.91
1	A	668	VAL	CB-CA-C	-5.13	105.22	112.14
1	C	733	CYS	N-CA-C	-5.13	104.34	111.52
1	D	691	ARG	N-CA-C	-5.13	102.69	110.28
1	D	764	ARG	CD-NE-CZ	-5.12	117.23	124.40
1	B	478	GLU	N-CA-C	-5.12	107.06	113.72
1	B	667	HIS	CA-C-N	5.11	127.47	120.46
1	B	667	HIS	C-N-CA	5.11	127.47	120.46
1	A	676	PHE	CB-CG-CD2	-5.11	112.02	120.70
1	A	653	ASP	N-CA-C	-5.11	106.56	112.89
1	C	159	GLN	N-CA-C	5.11	116.53	111.07
1	D	651	GLN	CA-C-N	5.11	130.56	122.60
1	D	651	GLN	C-N-CA	5.11	130.56	122.60
1	B	732	ASP	N-CA-CB	5.10	118.16	110.30
1	A	643	GLN	N-CA-C	5.10	116.53	111.07
1	A	690	ASN	CB-CG-ND2	-5.10	108.75	116.40
1	B	526	LEU	O-C-N	5.09	129.80	123.19
1	C	724	GLU	CB-CG-CD	-5.09	103.95	112.60
1	A	748	GLY	N-CA-C	-5.08	103.68	111.10
1	A	730	ASP	CA-C-O	-5.08	115.24	119.76
1	B	471	HIS	CG-CD2-NE2	5.08	112.28	107.20
1	A	506	ASP	CA-CB-CG	-5.08	107.52	112.60
1	D	124	ARG	CA-C-N	5.07	123.36	119.66
1	D	124	ARG	C-N-CA	5.07	123.36	119.66
1	D	513	PHE	N-CA-CB	5.07	118.89	110.52
1	B	663	ALA	CA-C-N	5.07	127.68	120.53
1	B	663	ALA	C-N-CA	5.07	127.68	120.53
1	B	692	SER	CA-C-N	5.07	131.01	123.05
1	B	692	SER	C-N-CA	5.07	131.01	123.05
1	A	336	ASN	CA-CB-CG	-5.07	107.53	112.60
1	D	733	CYS	CA-C-N	5.06	130.88	122.73
1	D	733	CYS	C-N-CA	5.06	130.88	122.73
1	C	447	PHE	O-C-N	5.06	127.28	122.07
1	D	493	ARG	O-C-N	5.06	128.14	122.27
1	D	522	VAL	N-CA-C	-5.06	101.19	108.48
1	B	481	THR	CA-C-N	5.06	127.95	120.82
1	B	481	THR	C-N-CA	5.06	127.95	120.82
1	A	468	ALA	O-C-N	-5.05	116.25	121.60
1	C	299	ILE	CA-C-N	5.04	127.03	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	299	ILE	C-N-CA	5.04	127.03	120.28
1	D	194	ILE	N-CA-C	5.04	115.65	110.36
1	A	527	ARG	CA-C-O	-5.03	116.21	121.55
1	B	436	ASN	CA-CB-CG	5.03	117.63	112.60
1	A	488	GLU	CA-C-O	-5.02	114.20	119.97
1	C	683	SER	O-C-N	5.02	127.87	122.15
1	C	716	PHE	CA-CB-CG	5.02	118.82	113.80
1	D	438	LEU	CA-C-N	5.01	129.03	120.91
1	D	438	LEU	C-N-CA	5.01	129.03	120.91
1	A	764	ARG	O-C-N	5.01	127.43	122.12
1	B	721	ALA	CA-C-O	-5.01	115.11	120.42

There are no chirality outliers.

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	516	ARG	Sidechain
1	A	527	ARG	Sidechain
1	A	528	ARG	Sidechain
1	A	691	ARG	Sidechain
1	A	711	TYR	Sidechain
1	A	725	TYR	Sidechain
1	A	747	TYR	Sidechain
1	B	507	ARG	Sidechain
1	B	516	ARG	Sidechain
1	B	520	TYR	Sidechain
1	B	527	ARG	Sidechain
1	B	682	TYR	Sidechain
1	B	725	TYR	Sidechain
1	B	779	HIS	Sidechain
1	C	119	TYR	Sidechain
1	C	252	ARG	Sidechain
1	C	257	ARG	Sidechain
1	C	274	ARG	Sidechain
1	C	315	PHE	Sidechain
1	C	458	TYR	Sidechain
1	C	516	ARG	Sidechain
1	C	520	TYR	Sidechain
1	C	656	TYR	Sidechain
1	C	687	ARG	Sidechain
1	C	736	TYR	Sidechain
1	C	747	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	D	201	ARG	Sidechain
1	D	257	ARG	Sidechain
1	D	277	ARG	Sidechain
1	D	458	TYR	Sidechain
1	D	491	PHE	Sidechain
1	D	493	ARG	Sidechain
1	D	507	ARG	Sidechain
1	D	665	TYR	Sidechain
1	D	682	TYR	Sidechain
1	D	687	ARG	Sidechain
1	D	691	ARG	Sidechain
1	D	711	TYR	Sidechain
1	D	714	TYR	Sidechain
1	D	747	TYR	Sidechain
1	D	757	TYR	Sidechain
1	D	758	ARG	Sidechain
1	D	98	ARG	Sidechain

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	5248	0	5160	112	0
1	B	5248	0	5160	78	0
1	C	5248	0	5158	112	0
1	D	5248	0	5160	94	0
All	All	20992	0	20638	310	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 7.

All (310) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:LEU:HD22	1:D:297:MET:SD	1.16	1.71
1:C:334:ARG:CG	1:D:334:ARG:NH2	1.81	1.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLY:HA2	1:A:110:LEU:CD2	1.50	1.41
1:D:286:LEU:CD2	1:D:297:MET:SD	2.13	1.36
1:C:333:ILE:CD1	1:D:53:PHE:HE1	1.37	1.35
1:B:316:HIS:NE2	1:B:320:GLN:NE2	1.76	1.33
1:C:35:LEU:HD11	1:C:316:HIS:CA	1.60	1.27
1:C:334:ARG:HG3	1:D:334:ARG:NH2	0.92	1.24
1:A:643:GLN:NE2	1:B:696:GLU:OE1	1.71	1.23
1:A:80:GLY:CA	1:A:110:LEU:HD21	1.68	1.22
1:C:35:LEU:CD1	1:C:316:HIS:HA	1.68	1.22
1:A:80:GLY:CA	1:A:110:LEU:CD2	2.17	1.22
1:A:112:ARG:NH2	1:A:118:ASP:CB	2.02	1.21
1:A:643:GLN:HB3	1:B:696:GLU:CG	1.73	1.18
1:C:35:LEU:HD11	1:C:316:HIS:N	1.60	1.17
1:A:771:SER:O	1:B:440:LYS:HD2	1.44	1.16
1:A:112:ARG:NH2	1:A:118:ASP:CA	2.09	1.16
1:C:333:ILE:CD1	1:D:53:PHE:CE1	2.27	1.16
1:A:112:ARG:HH22	1:A:118:ASP:HB2	1.03	1.14
1:A:646:GLN:OE1	1:B:692:SER:HB3	1.49	1.12
1:A:643:GLN:CB	1:B:696:GLU:HG3	1.79	1.12
1:C:35:LEU:CD2	1:C:316:HIS:HD1	1.63	1.12
1:C:53:PHE:HE1	1:D:333:ILE:HD11	1.15	1.11
1:D:286:LEU:HD13	1:D:297:MET:HE1	1.21	1.11
1:C:333:ILE:HD11	1:D:53:PHE:HE1	1.09	1.11
1:C:334:ARG:HG3	1:D:334:ARG:CZ	1.79	1.10
1:C:35:LEU:HD23	1:C:316:HIS:HD1	1.11	1.07
1:C:779:HIS:CE1	1:D:675:PRO:HG2	1.90	1.06
1:A:643:GLN:CD	1:B:696:GLU:CD	2.24	1.05
1:C:35:LEU:HD23	1:C:316:HIS:ND1	1.71	1.04
1:C:333:ILE:HD13	1:D:53:PHE:CE1	1.92	1.04
1:A:112:ARG:NH2	1:A:118:ASP:HB2	1.66	1.03
1:C:53:PHE:CZ	1:D:333:ILE:HG12	1.93	1.03
1:D:694:GLY:O	1:D:698:ASN:OD1	1.73	1.03
1:C:316:HIS:CD2	1:C:320:GLN:OE1	2.03	1.02
1:A:80:GLY:HA2	1:A:110:LEU:HD21	1.08	1.02
1:A:643:GLN:NE2	1:B:696:GLU:CD	2.18	1.00
1:C:333:ILE:HD13	1:D:53:PHE:HE1	1.25	1.00
1:C:333:ILE:HD11	1:D:53:PHE:CE1	1.96	0.99
1:A:80:GLY:CA	1:A:110:LEU:HD22	1.91	0.99
1:A:643:GLN:CD	1:B:696:GLU:OE1	2.04	0.99
1:C:35:LEU:HG	1:C:316:HIS:HB2	1.44	0.98
1:A:112:ARG:NH2	1:A:118:ASP:HA	1.76	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:LEU:HD11	1:C:316:HIS:HA	0.98	0.98
1:C:334:ARG:CG	1:D:334:ARG:CZ	2.39	0.97
1:C:35:LEU:CD2	1:C:316:HIS:ND1	2.25	0.96
1:A:112:ARG:CZ	1:A:118:ASP:CG	2.39	0.96
1:A:112:ARG:HH22	1:A:118:ASP:CB	1.69	0.95
1:A:112:ARG:NH1	1:A:118:ASP:OD2	1.98	0.95
1:A:691:ARG:HB3	1:A:696:GLU:OE1	1.68	0.93
1:C:491:PHE:HD2	1:C:493:ARG:HH11	1.16	0.92
1:B:652:THR:HB	1:B:688:MET:CE	2.01	0.91
1:A:771:SER:O	1:B:440:LYS:CD	2.19	0.89
1:A:155:ILE:HD12	1:B:155:ILE:CD1	2.02	0.89
1:C:35:LEU:HG	1:C:316:HIS:CB	2.01	0.89
1:C:53:PHE:CE1	1:D:333:ILE:HD11	2.07	0.89
1:C:334:ARG:HG3	1:D:334:ARG:HH21	1.28	0.89
1:C:35:LEU:CD1	1:C:316:HIS:N	2.36	0.89
1:D:230:ALA:HA	1:D:233:CYS:SG	2.13	0.89
1:A:112:ARG:HH21	1:A:118:ASP:HA	1.36	0.89
1:C:53:PHE:HE1	1:D:333:ILE:CD1	1.86	0.88
1:C:334:ARG:CG	1:D:334:ARG:HH22	1.61	0.88
1:C:53:PHE:HZ	1:D:333:ILE:HG12	1.33	0.87
1:D:286:LEU:HD13	1:D:297:MET:CE	2.02	0.87
1:C:779:HIS:CE1	1:D:675:PRO:CG	2.58	0.87
1:D:204:LEU:HB3	1:D:229:VAL:HG21	1.56	0.86
1:C:35:LEU:CG	1:C:316:HIS:HA	2.06	0.86
1:C:35:LEU:CD1	1:C:316:HIS:CA	2.38	0.85
1:D:286:LEU:CD1	1:D:297:MET:HE1	2.06	0.85
1:D:467:VAL:HG11	1:D:471:HIS:CD2	2.11	0.85
1:B:652:THR:HB	1:B:688:MET:HE3	1.58	0.85
1:C:334:ARG:HG3	1:D:334:ARG:HH22	1.08	0.85
1:A:155:ILE:CD1	1:B:155:ILE:CD1	2.56	0.84
1:C:35:LEU:HD11	1:C:315:PHE:C	2.01	0.84
1:B:676:PHE:CE1	1:C:189:PHE:CD2	2.66	0.84
1:A:771:SER:C	1:B:440:LYS:HD2	2.04	0.83
1:A:776:ILE:HD11	1:B:439:GLY:HA3	1.61	0.82
1:D:467:VAL:HG11	1:D:471:HIS:HD2	1.43	0.82
1:A:432:MET:HE1	1:A:781:TRP:CZ3	2.14	0.82
1:A:643:GLN:HB3	1:B:696:GLU:HG3	0.87	0.82
1:A:80:GLY:HA2	1:A:110:LEU:HD22	1.47	0.80
1:A:80:GLY:HA3	1:A:110:LEU:CD2	2.11	0.80
1:D:527:ARG:HD3	1:D:709:VAL:O	1.83	0.79
1:A:112:ARG:HH21	1:A:118:ASP:CA	1.92	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:779:HIS:CE1	1:D:676:PHE:CE1	2.71	0.79
1:C:35:LEU:CG	1:C:316:HIS:HD1	1.96	0.78
1:A:155:ILE:HD12	1:B:155:ILE:HD12	1.62	0.78
1:B:35:LEU:H	1:B:316:HIS:HD1	1.30	0.78
1:D:204:LEU:HB3	1:D:229:VAL:CG2	2.13	0.78
1:C:53:PHE:CZ	1:D:333:ILE:CG1	2.67	0.78
1:C:779:HIS:NE2	1:D:675:PRO:HB2	2.01	0.76
1:C:34:ILE:HD13	1:C:313:ASN:HA	1.66	0.76
1:A:112:ARG:CZ	1:A:118:ASP:CB	2.64	0.76
1:A:150:ASP:OD1	1:A:153:TYR:HB2	1.86	0.76
1:A:112:ARG:NH1	1:A:118:ASP:CG	2.43	0.75
1:C:32:GLU:HB3	1:C:36:GLN:NE2	2.02	0.75
1:B:150:ASP:OD1	1:B:153:TYR:HB2	1.87	0.74
1:D:286:LEU:HD22	1:D:297:MET:CE	2.17	0.74
1:B:193:ARG:O	1:B:197:LEU:HB2	1.88	0.74
1:C:775:ASP:HB2	1:D:676:PHE:HE2	1.53	0.73
1:A:155:ILE:CD1	1:B:155:ILE:HD12	2.17	0.72
1:C:35:LEU:CG	1:C:316:HIS:CA	2.67	0.72
1:B:447:PHE:CE1	1:B:777:LEU:HB2	2.24	0.72
1:A:193:ARG:O	1:A:197:LEU:HB2	1.88	0.72
1:C:779:HIS:HE1	1:D:676:PHE:CE1	2.08	0.71
1:C:34:ILE:HG23	1:C:316:HIS:HB2	1.72	0.71
1:A:155:ILE:HD12	1:B:155:ILE:HD11	1.73	0.71
1:A:80:GLY:HA3	1:A:110:LEU:HD21	1.66	0.71
1:C:35:LEU:CD2	1:C:316:HIS:HA	2.20	0.70
1:C:428:GLU:HG2	1:C:432:MET:HG2	1.74	0.69
1:C:35:LEU:HD21	1:C:316:HIS:HA	1.72	0.69
1:A:646:GLN:OE1	1:B:692:SER:CB	2.36	0.69
1:D:283:SER:HB3	1:D:285:THR:HG22	1.75	0.69
1:A:432:MET:HE1	1:A:781:TRP:CE3	2.28	0.68
1:A:776:ILE:CD1	1:B:439:GLY:HA3	2.22	0.68
1:B:724:GLU:O	1:B:728:ILE:HG13	1.94	0.68
1:A:643:GLN:CB	1:B:696:GLU:CG	2.53	0.67
1:C:779:HIS:HE1	1:D:675:PRO:HG2	1.53	0.67
1:C:53:PHE:HZ	1:D:333:ILE:CG1	2.04	0.67
1:A:489:LEU:HB2	1:A:511:VAL:HG11	1.77	0.66
1:B:316:HIS:CD2	1:B:320:GLN:NE2	2.62	0.66
1:B:674:ASN:ND2	1:B:677:GLU:HB3	2.10	0.66
1:C:32:GLU:HB3	1:C:36:GLN:CD	2.21	0.66
1:C:53:PHE:CE1	1:D:333:ILE:CD1	2.71	0.66
1:C:426:LEU:HG	1:C:467:VAL:HG11	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:643:GLN:CB	1:B:696:GLU:CD	2.69	0.65
1:A:501:LEU:CD1	1:A:507:ARG:NH1	2.60	0.65
1:D:286:LEU:CD1	1:D:297:MET:CE	2.69	0.65
1:C:316:HIS:HD2	1:C:320:GLN:OE1	1.75	0.65
1:C:53:PHE:CE1	1:D:333:ILE:CG1	2.80	0.65
1:C:35:LEU:CG	1:C:316:HIS:CB	2.74	0.65
1:A:477:GLN:H	1:A:477:GLN:NE2	1.94	0.65
1:B:447:PHE:HE1	1:B:777:LEU:HB2	1.61	0.64
1:D:204:LEU:O	1:D:229:VAL:HG21	1.97	0.64
1:C:491:PHE:CD2	1:C:493:ARG:NH1	2.67	0.64
1:C:251:VAL:HG11	1:C:381:ASN:HB3	1.80	0.63
1:B:193:ARG:HG2	1:B:196:GLU:HG3	1.81	0.62
1:A:774:MET:HG3	1:A:778:LYS:NZ	2.14	0.62
1:C:53:PHE:CE1	1:D:333:ILE:HG12	2.32	0.62
1:C:334:ARG:HG2	1:D:334:ARG:NH2	2.07	0.62
1:A:487:GLY:O	1:A:491:PHE:HD2	1.81	0.62
1:A:696:GLU:C	1:A:698:ASN:H	2.07	0.62
1:A:779:HIS:HA	1:A:782:TRP:O	2.00	0.61
1:A:501:LEU:HD11	1:A:507:ARG:NH1	2.16	0.61
1:B:316:HIS:CD2	1:B:320:GLN:CD	2.79	0.61
1:C:35:LEU:HD21	1:C:316:HIS:CA	2.31	0.61
1:B:111:THR:HG23	1:B:111:THR:O	2.00	0.61
1:A:420:LEU:HD12	1:A:461:PHE:CE1	2.36	0.60
1:B:728:ILE:HG22	1:B:728:ILE:O	2.01	0.60
1:B:316:HIS:CE1	1:B:320:GLN:NE2	2.65	0.60
1:D:696:GLU:HG2	1:D:697:ASN:OD1	2.00	0.60
1:A:193:ARG:HG2	1:A:196:GLU:HG3	1.84	0.60
1:B:429:PRO:HA	1:B:432:MET:HG2	1.83	0.59
1:C:381:ASN:N	1:C:381:ASN:HD22	1.99	0.59
1:A:430:PHE:CG	1:A:500:ALA:HB2	2.38	0.59
1:C:775:ASP:HB2	1:D:676:PHE:CE2	2.37	0.59
1:D:230:ALA:O	1:D:233:CYS:SG	2.58	0.59
1:A:111:THR:HG23	1:A:111:THR:O	2.01	0.59
1:D:322:ARG:HD2	1:D:322:ARG:N	2.14	0.59
1:C:333:ILE:HG12	1:D:53:PHE:CZ	2.39	0.58
1:A:677:GLU:HG3	1:A:677:GLU:O	2.03	0.58
1:C:34:ILE:CG2	1:C:316:HIS:HB2	2.33	0.58
1:C:334:ARG:CD	1:D:334:ARG:CZ	2.82	0.57
1:D:319:LEU:HG	1:D:319:LEU:O	2.03	0.57
1:A:643:GLN:CD	1:B:696:GLU:CG	2.77	0.57
1:B:316:HIS:NE2	1:B:320:GLN:CD	2.56	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:ARG:O	1:D:229:VAL:HG11	2.04	0.57
1:A:334:ARG:CZ	1:B:334:ARG:CZ	2.83	0.57
1:C:426:LEU:HD23	1:C:431:VAL:HG12	1.86	0.57
1:C:422:VAL:HG22	1:C:496:ILE:HD11	1.86	0.57
1:D:201:ARG:O	1:D:229:VAL:CG1	2.54	0.56
1:D:477:GLN:O	1:D:481:THR:O	2.24	0.56
1:D:286:LEU:CD2	1:D:297:MET:CE	2.80	0.56
1:A:491:PHE:HB2	1:A:493:ARG:NE	2.21	0.56
1:D:527:ARG:CD	1:D:709:VAL:O	2.53	0.56
1:B:673:LEU:HD21	1:B:686:TRP:NE1	2.20	0.56
1:A:776:ILE:HD11	1:B:439:GLY:CA	2.34	0.55
1:B:492:LYS:HG2	1:B:752:GLN:OE1	2.06	0.55
1:C:334:ARG:HD3	1:D:334:ARG:CZ	2.36	0.55
1:A:150:ASP:OD1	1:A:153:TYR:CB	2.54	0.55
1:C:334:ARG:HG2	1:D:334:ARG:HH22	1.65	0.55
1:D:35:LEU:HD21	1:D:315:PHE:HB2	1.88	0.55
1:D:204:LEU:CB	1:D:229:VAL:HG21	2.34	0.55
1:A:421:ARG:NE	1:A:466:TYR:CE2	2.75	0.55
1:B:507:ARG:O	1:B:511:VAL:HG22	2.06	0.55
1:A:112:ARG:NH2	1:A:118:ASP:N	2.55	0.55
1:A:155:ILE:CD1	1:B:155:ILE:HD11	2.31	0.55
1:B:434:SER:HB2	1:B:445:GLN:CD	2.32	0.55
1:A:430:PHE:CZ	1:A:747:TYR:CE2	2.94	0.54
1:A:674:ASN:HB3	1:A:677:GLU:HB3	1.89	0.54
1:D:229:VAL:HG23	1:D:229:VAL:O	2.08	0.54
1:A:489:LEU:HB2	1:A:511:VAL:CG1	2.38	0.54
1:A:501:LEU:HD12	1:A:507:ARG:NH1	2.23	0.53
1:B:673:LEU:HD21	1:B:686:TRP:HE1	1.72	0.53
1:C:35:LEU:CD1	1:C:315:PHE:C	2.75	0.53
1:D:204:LEU:C	1:D:229:VAL:HG21	2.33	0.53
1:A:80:GLY:N	1:A:110:LEU:HD22	2.24	0.53
1:A:689:ILE:HA	1:A:698:ASN:HD21	1.74	0.53
1:C:35:LEU:CG	1:C:316:HIS:ND1	2.67	0.53
1:C:35:LEU:HG	1:C:316:HIS:ND1	2.23	0.53
1:C:333:ILE:HG12	1:D:53:PHE:HZ	1.73	0.53
1:A:477:GLN:H	1:A:477:GLN:HE21	1.55	0.53
1:B:110:LEU:HG	1:B:112:ARG:HB2	1.91	0.53
1:A:430:PHE:CD2	1:A:500:ALA:HB2	2.44	0.52
1:A:722:VAL:O	1:A:726:VAL:HG23	2.10	0.52
1:A:155:ILE:HD11	1:B:155:ILE:CD1	2.38	0.52
1:B:110:LEU:CD2	1:B:112:ARG:HB2	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:MET:HG3	1:A:685:MET:HE3	1.91	0.52
1:B:150:ASP:OD1	1:B:153:TYR:CB	2.55	0.52
1:D:181:ILE:HD12	1:D:181:ILE:H	1.75	0.51
1:D:265:PHE:CD1	1:D:359:THR:HA	2.46	0.51
1:A:643:GLN:OE1	1:B:696:GLU:OE1	2.28	0.51
1:C:779:HIS:HE1	1:D:676:PHE:CD1	2.29	0.51
1:D:80:GLY:HA3	1:D:110:LEU:HD13	1.91	0.51
1:A:489:LEU:HD13	1:A:750:ALA:HB1	1.93	0.51
1:B:447:PHE:HZ	1:B:774:MET:SD	2.34	0.50
1:A:477:GLN:OE1	1:A:483:ASN:ND2	2.44	0.50
1:C:316:HIS:O	1:C:320:GLN:HG3	2.12	0.50
1:A:432:MET:CE	1:A:781:TRP:CZ3	2.92	0.50
1:A:112:ARG:CZ	1:A:118:ASP:HB2	2.33	0.50
1:A:155:ILE:HD11	1:B:155:ILE:HG13	1.93	0.50
1:B:674:ASN:HD22	1:B:677:GLU:HB3	1.75	0.49
1:A:477:GLN:NE2	1:A:477:GLN:N	2.60	0.49
1:C:334:ARG:HG2	1:D:334:ARG:NH1	2.27	0.49
1:D:428:GLU:HG3	1:D:722:VAL:HG13	1.94	0.49
1:A:643:GLN:HB2	1:B:696:GLU:OE2	2.13	0.49
1:A:770:GLN:HG2	1:B:469:PRO:HB3	1.93	0.49
1:C:112:ARG:HH21	1:C:118:ASP:CG	2.20	0.49
1:C:334:ARG:CG	1:D:334:ARG:NH1	2.76	0.49
1:C:334:ARG:HG2	1:D:334:ARG:CZ	2.39	0.49
1:C:68:LEU:HD22	1:C:340:TRP:CH2	2.48	0.49
1:D:230:ALA:CA	1:D:233:CYS:SG	2.96	0.49
1:A:420:LEU:HD13	1:A:496:ILE:HD13	1.93	0.49
1:A:776:ILE:CG1	1:B:439:GLY:HA3	2.43	0.48
1:C:756:PRO:HG2	1:C:757:TYR:CD2	2.47	0.48
1:D:322:ARG:HD2	1:D:322:ARG:H	1.78	0.48
1:C:33:GLU:OE2	1:C:280:HIS:HB2	2.13	0.48
1:D:688:MET:HG3	1:D:697:ASN:HD22	1.78	0.48
1:A:433:VAL:O	1:A:433:VAL:HG13	2.14	0.48
1:A:774:MET:HG3	1:A:778:LYS:HZ1	1.79	0.48
1:D:204:LEU:HB3	1:D:229:VAL:HG22	1.96	0.47
1:C:381:ASN:HD22	1:C:381:ASN:H	1.60	0.47
1:A:660:LEU:HD13	1:A:694:GLY:HA3	1.96	0.47
1:C:333:ILE:O	1:C:333:ILE:HG22	2.13	0.47
1:C:381:ASN:H	1:C:381:ASN:ND2	2.13	0.47
1:C:642:ILE:HD11	1:C:651:GLN:HG2	1.97	0.47
1:D:429:PRO:O	1:D:432:MET:HE2	2.15	0.47
1:A:430:PHE:CE2	1:A:747:TYR:CD2	3.02	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:428:GLU:OE2	1:D:722:VAL:CG1	2.63	0.47
1:A:432:MET:HE2	1:A:446:GLY:HA2	1.97	0.46
1:C:779:HIS:CE1	1:D:676:PHE:CZ	3.03	0.46
1:C:525:LEU:N	1:C:723:LEU:HD13	2.30	0.46
1:A:57:GLN:HG3	1:B:333:ILE:HG23	1.98	0.46
1:A:334:ARG:NE	1:B:334:ARG:NE	2.63	0.46
1:B:420:LEU:HD13	1:B:496:ILE:HD13	1.96	0.46
1:C:32:GLU:HB3	1:C:36:GLN:CG	2.46	0.46
1:C:34:ILE:HG23	1:C:316:HIS:CB	2.45	0.46
1:A:645:LEU:HD12	1:A:740:ASN:OD1	2.16	0.46
1:C:35:LEU:HG	1:C:316:HIS:CG	2.51	0.46
1:A:643:GLN:HB2	1:B:696:GLU:CD	2.40	0.46
1:C:32:GLU:HB3	1:C:36:GLN:HG2	1.98	0.46
1:C:35:LEU:CD2	1:C:316:HIS:CA	2.91	0.46
1:B:427:GLU:HA	1:B:427:GLU:OE1	2.16	0.45
1:C:427:GLU:HA	1:C:427:GLU:OE2	2.17	0.45
1:C:689:ILE:HD12	1:C:689:ILE:HA	1.78	0.45
1:D:283:SER:C	1:D:285:THR:H	2.25	0.45
1:D:164:LYS:HE2	1:D:164:LYS:HA	1.99	0.45
1:D:467:VAL:CG1	1:D:471:HIS:CD2	2.92	0.44
1:C:775:ASP:CB	1:D:676:PHE:CE2	2.99	0.44
1:A:501:LEU:HD12	1:A:507:ARG:HH12	1.81	0.44
1:B:524:VAL:CG2	1:B:715:ALA:HB1	2.46	0.44
1:A:778:LYS:O	1:A:782:TRP:HB2	2.18	0.44
1:B:507:ARG:O	1:B:511:VAL:CG2	2.65	0.44
1:D:378:LEU:HB3	1:D:390:VAL:HG11	2.00	0.44
1:A:112:ARG:NH2	1:A:118:ASP:CG	2.56	0.43
1:C:333:ILE:CG1	1:D:53:PHE:CE1	2.97	0.43
1:A:696:GLU:C	1:A:698:ASN:N	2.74	0.43
1:C:33:GLU:OE2	1:C:280:HIS:CG	2.71	0.43
1:C:35:LEU:CD2	1:C:316:HIS:CG	3.00	0.43
1:D:284:SER:HA	1:D:287:CYS:SG	2.59	0.43
1:B:509:ASN:ND2	1:C:179:ASN:OD1	2.52	0.43
1:A:155:ILE:HD11	1:B:155:ILE:CG1	2.49	0.43
1:A:776:ILE:HD11	1:B:438:LEU:O	2.19	0.43
1:C:673:LEU:HD21	1:C:686:TRP:CZ2	2.53	0.43
1:A:659:VAL:HG12	1:A:660:LEU:O	2.19	0.43
1:A:504:THR:OG1	1:A:507:ARG:HG3	2.18	0.42
1:C:779:HIS:CE1	1:D:675:PRO:CB	3.01	0.42
1:C:34:ILE:HG21	1:C:312:ALA:O	2.20	0.42
1:D:251:VAL:HG13	1:D:381:ASN:HB3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:378:LEU:HB3	1:D:390:VAL:CG1	2.50	0.42
1:B:482:TRP:HB2	1:B:487:GLY:HA2	2.02	0.42
1:B:676:PHE:CE1	1:C:189:PHE:CE2	3.07	0.41
1:A:28:LEU:HD12	1:A:308:VAL:HG12	2.02	0.41
1:B:316:HIS:O	1:B:320:GLN:HG3	2.20	0.41
1:A:693:ASN:N	1:A:693:ASN:HD22	2.18	0.41
1:C:381:ASN:N	1:C:381:ASN:ND2	2.64	0.41
1:D:283:SER:C	1:D:285:THR:N	2.79	0.41
1:B:427:GLU:OE2	1:B:722:VAL:HG11	2.20	0.41
1:A:776:ILE:HD11	1:B:438:LEU:C	2.45	0.41
1:B:28:LEU:HD12	1:B:308:VAL:HG12	2.02	0.41
1:C:251:VAL:CG1	1:C:381:ASN:HB3	2.46	0.41
1:C:247:VAL:HG11	1:C:390:VAL:HG21	2.02	0.41
1:C:517:TYR:HB2	1:C:774:MET:HE3	2.03	0.41
1:A:420:LEU:HD13	1:A:496:ILE:CD1	2.50	0.41
1:C:68:LEU:HD22	1:C:340:TRP:CZ2	2.55	0.41
1:A:80:GLY:HA3	1:A:110:LEU:CD1	2.50	0.41
1:D:35:LEU:HD11	1:D:312:ALA:HA	2.04	0.40
1:A:776:ILE:HG12	1:B:439:GLY:HA3	2.03	0.40
1:B:434:SER:HB2	1:B:445:GLN:CG	2.51	0.40
1:D:656:TYR:HB3	1:D:715:ALA:HB3	2.03	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	654/877 (75%)	636 (97%)	17 (3%)	1 (0%)	43	78
1	B	654/877 (75%)	639 (98%)	15 (2%)	0	100	100
1	C	654/877 (75%)	629 (96%)	25 (4%)	0	100	100
1	D	654/877 (75%)	621 (95%)	33 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2616/3508 (75%)	2525 (96%)	90 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	696	GLU

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	580/764 (76%)	569 (98%)	11 (2%)	50	67
1	B	580/764 (76%)	570 (98%)	10 (2%)	53	69
1	C	580/764 (76%)	564 (97%)	16 (3%)	38	60
1	D	580/764 (76%)	569 (98%)	11 (2%)	50	67
All	All	2320/3056 (76%)	2272 (98%)	48 (2%)	46	65

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	THR
1	A	197	LEU
1	A	425	VAL
1	A	427	GLU
1	A	466	TYR
1	A	477	GLN
1	A	479	ASP
1	A	485	LEU
1	A	648	LEU
1	A	652	THR
1	A	676	PHE
1	B	111	THR
1	B	112	ARG
1	B	197	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	432	MET
1	B	438	LEU
1	B	490	VAL
1	B	651	GLN
1	B	667	HIS
1	B	692	SER
1	B	718	TRP
1	C	103	THR
1	C	195	GLU
1	C	203	THR
1	C	212	ASN
1	C	260	ILE
1	C	334	ARG
1	C	381	ASN
1	C	400	THR
1	C	467	VAL
1	C	489	LEU
1	C	659	VAL
1	C	670	MET
1	C	687	ARG
1	C	718	TRP
1	C	731	PRO
1	C	741	THR
1	D	103	THR
1	D	111	THR
1	D	129	LEU
1	D	322	ARG
1	D	348	GLU
1	D	433	VAL
1	D	479	ASP
1	D	481	THR
1	D	483	ASN
1	D	502	THR
1	D	710	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	GLN
1	A	462	ASN
1	A	477	GLN
1	A	483	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	684	GLN
1	A	690	ASN
1	A	693	ASN
1	A	697	ASN
1	A	698	ASN
1	A	753	HIS
1	B	263	GLN
1	B	320	GLN
1	B	477	GLN
1	B	684	GLN
1	C	29	ASN
1	C	31	ASN
1	C	64	ASN
1	C	90	HIS
1	C	143	GLN
1	C	159	GLN
1	C	175	GLN
1	C	212	ASN
1	C	270	ASN
1	C	313	ASN
1	C	381	ASN
1	C	471	HIS
1	C	477	GLN
1	C	698	ASN
1	C	703	GLN
1	C	707	GLN
1	C	753	HIS
1	C	779	HIS
1	D	30	GLN
1	D	57	GLN
1	D	175	GLN
1	D	336	ASN
1	D	374	HIS
1	D	471	HIS
1	D	483	ASN
1	D	698	ASN
1	D	713	ASN
1	D	729	ASN
1	D	779	HIS

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.

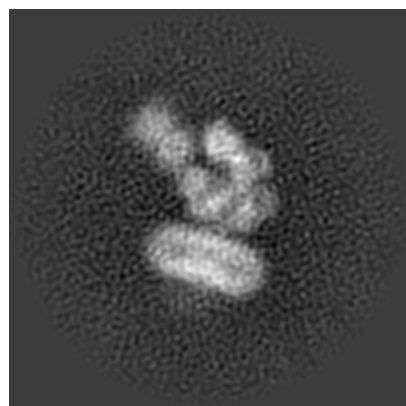
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0979. These allow visual inspection of the internal detail of the map and identification of artifacts.

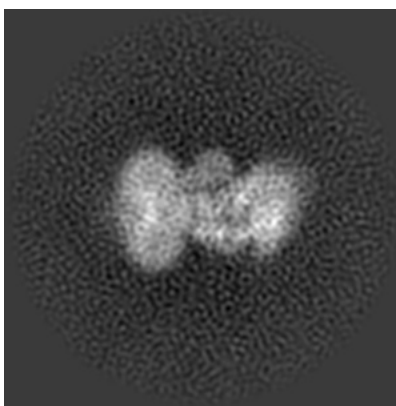
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

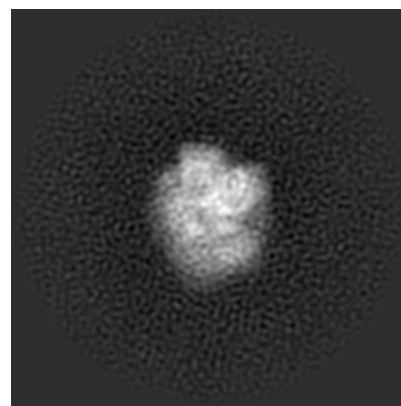
6.1.1 Primary map



X

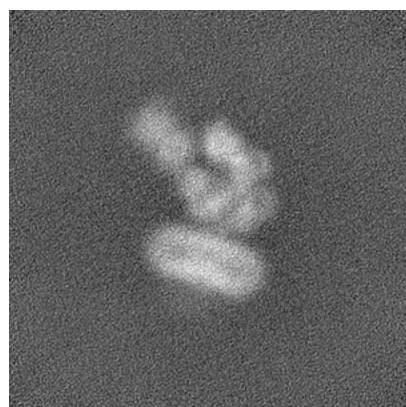


Y

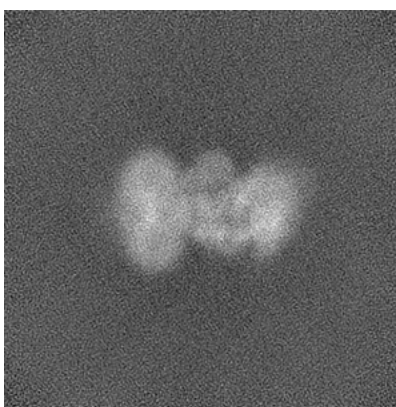


Z

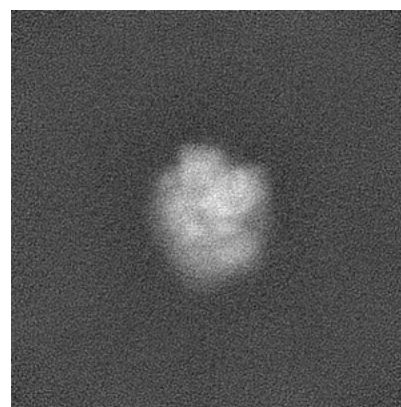
6.1.2 Raw map



X



Y

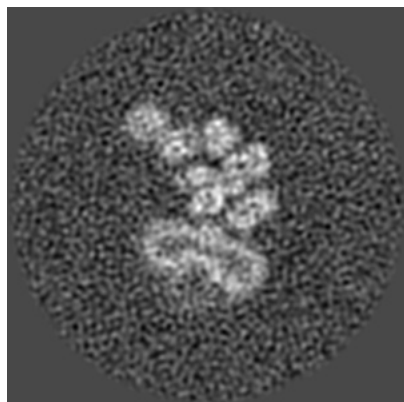


Z

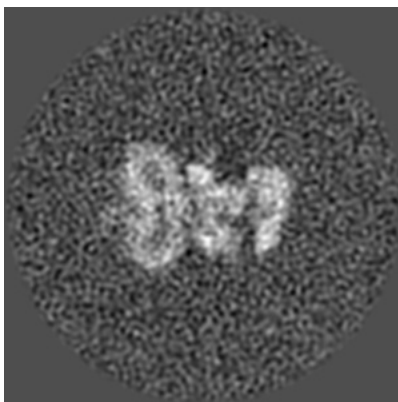
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

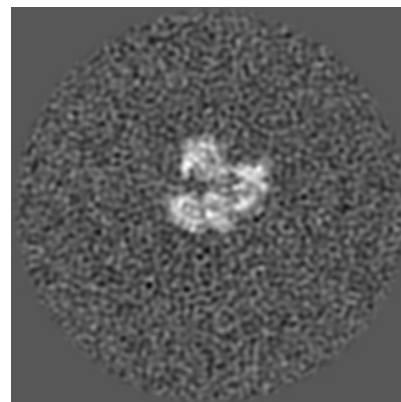
6.2.1 Primary map



X Index: 140

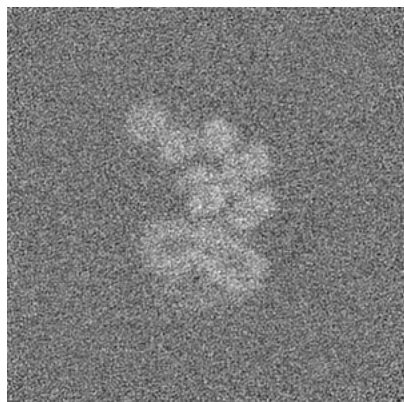


Y Index: 140

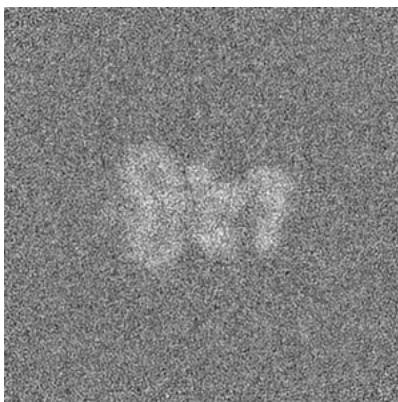


Z Index: 140

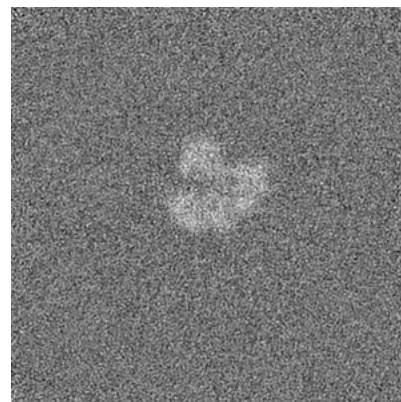
6.2.2 Raw map



X Index: 140



Y Index: 140

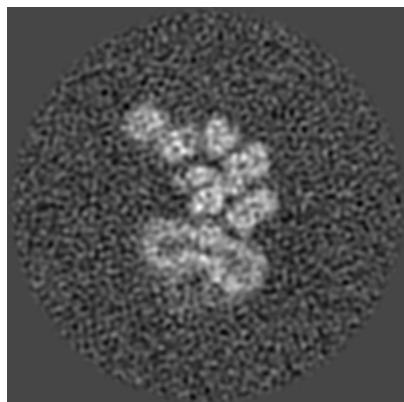


Z Index: 140

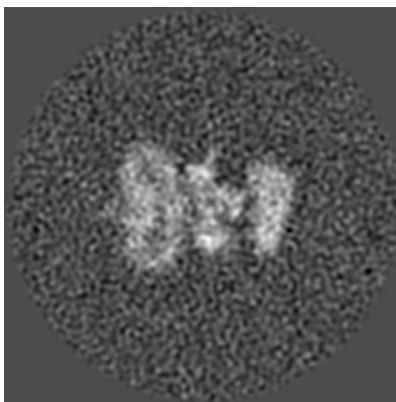
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

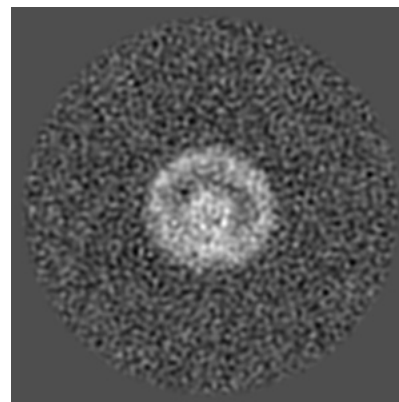
6.3.1 Primary map



X Index: 139

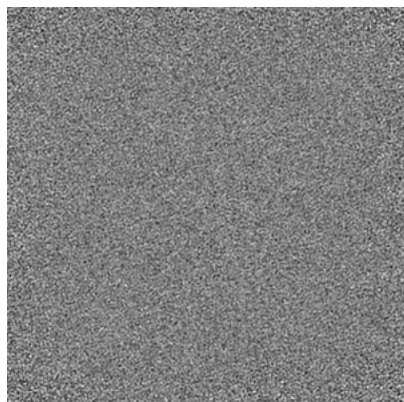


Y Index: 142

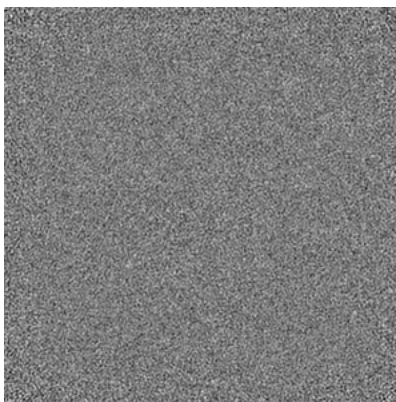


Z Index: 101

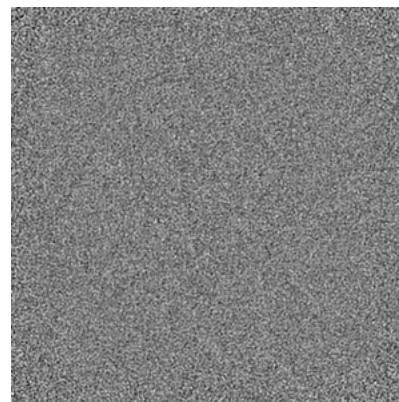
6.3.2 Raw map



X Index: 0



Y Index: 0

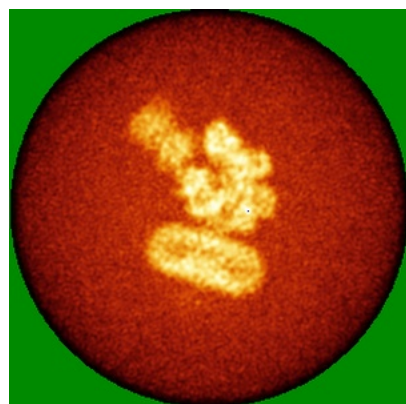


Z Index: 0

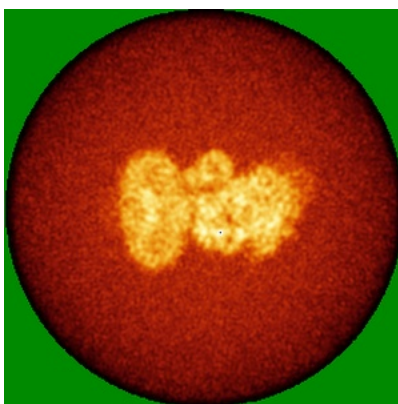
The images above show the largest variance slices of the map in three orthogonal directions.

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

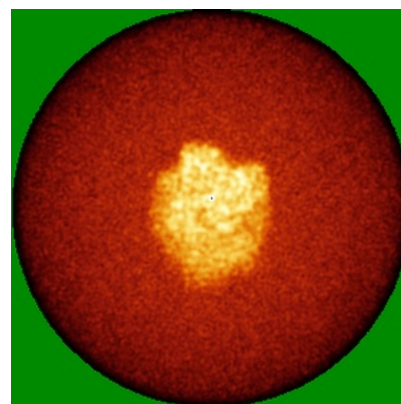
6.4.1 Primary map



X

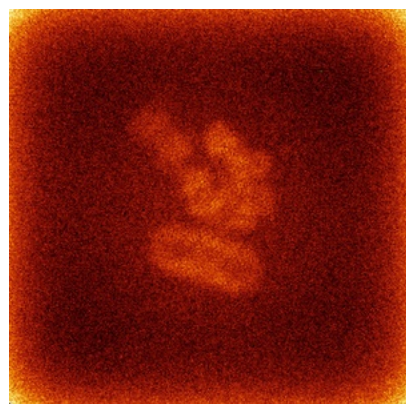


Y

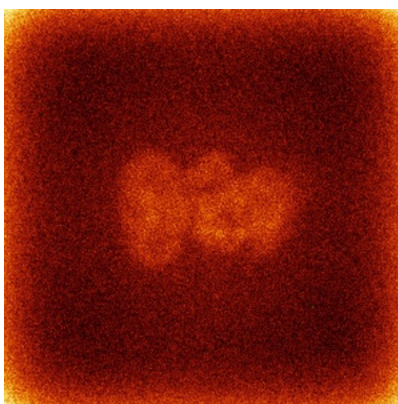


Z

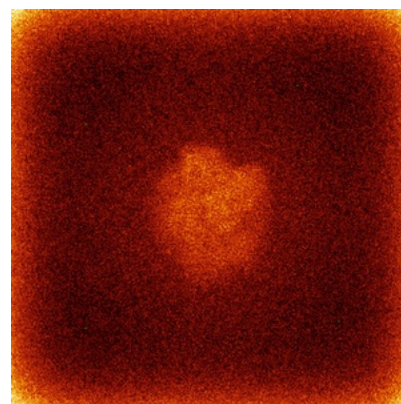
6.4.2 Raw map



X



Y

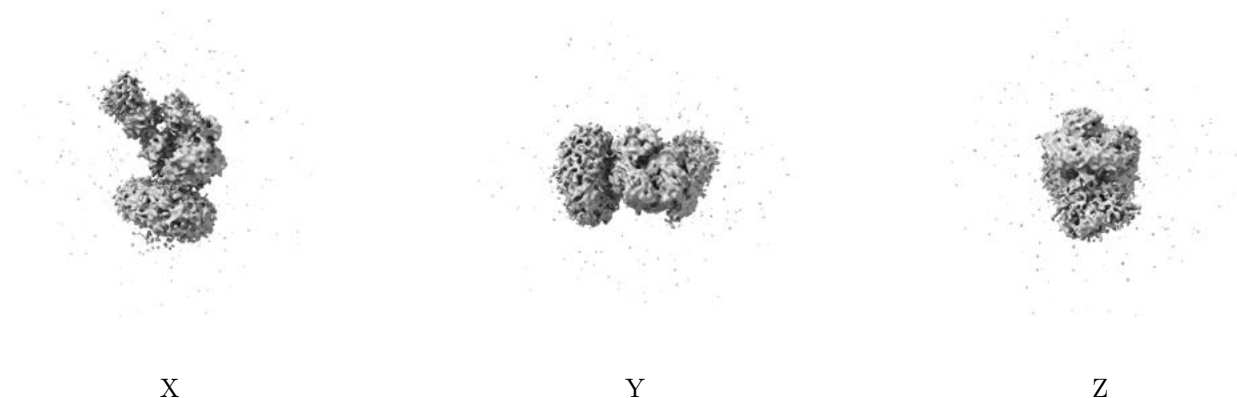


Z

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.

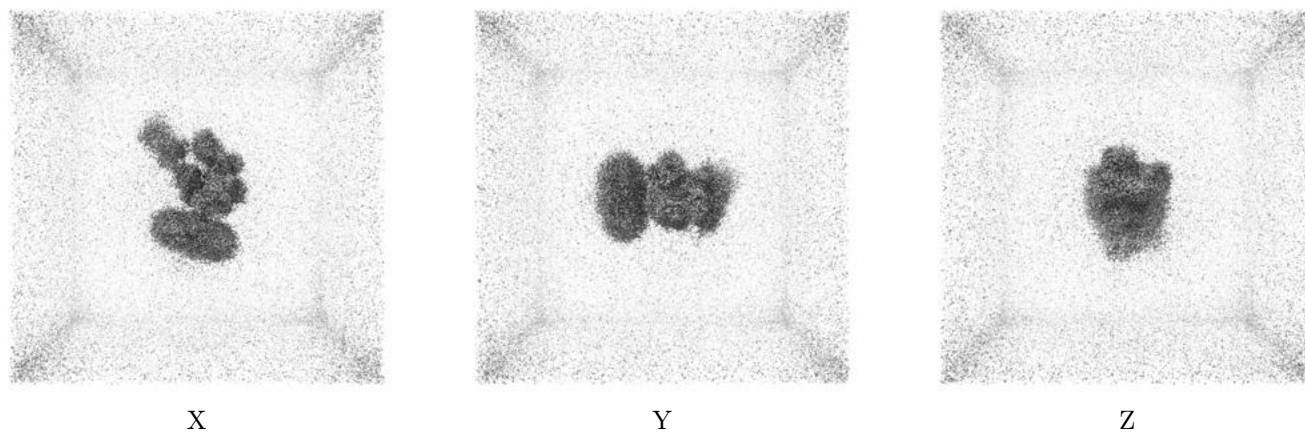
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.316. 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.

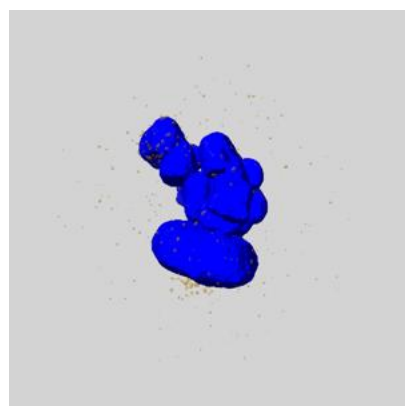
6.6 Mask visualisation [i](#)

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

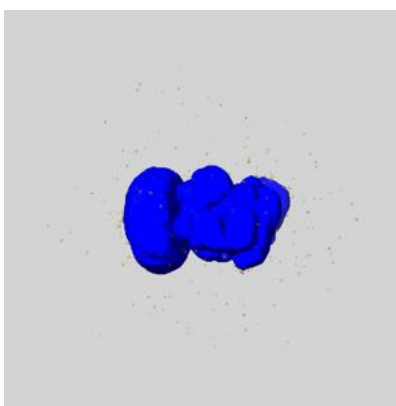
A mask typically either:

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

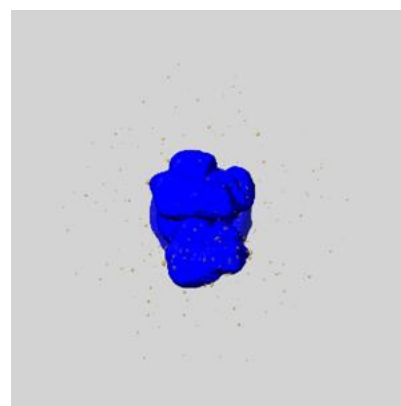
6.6.1 emd_0979_msk_1.map [i](#)



X



Y

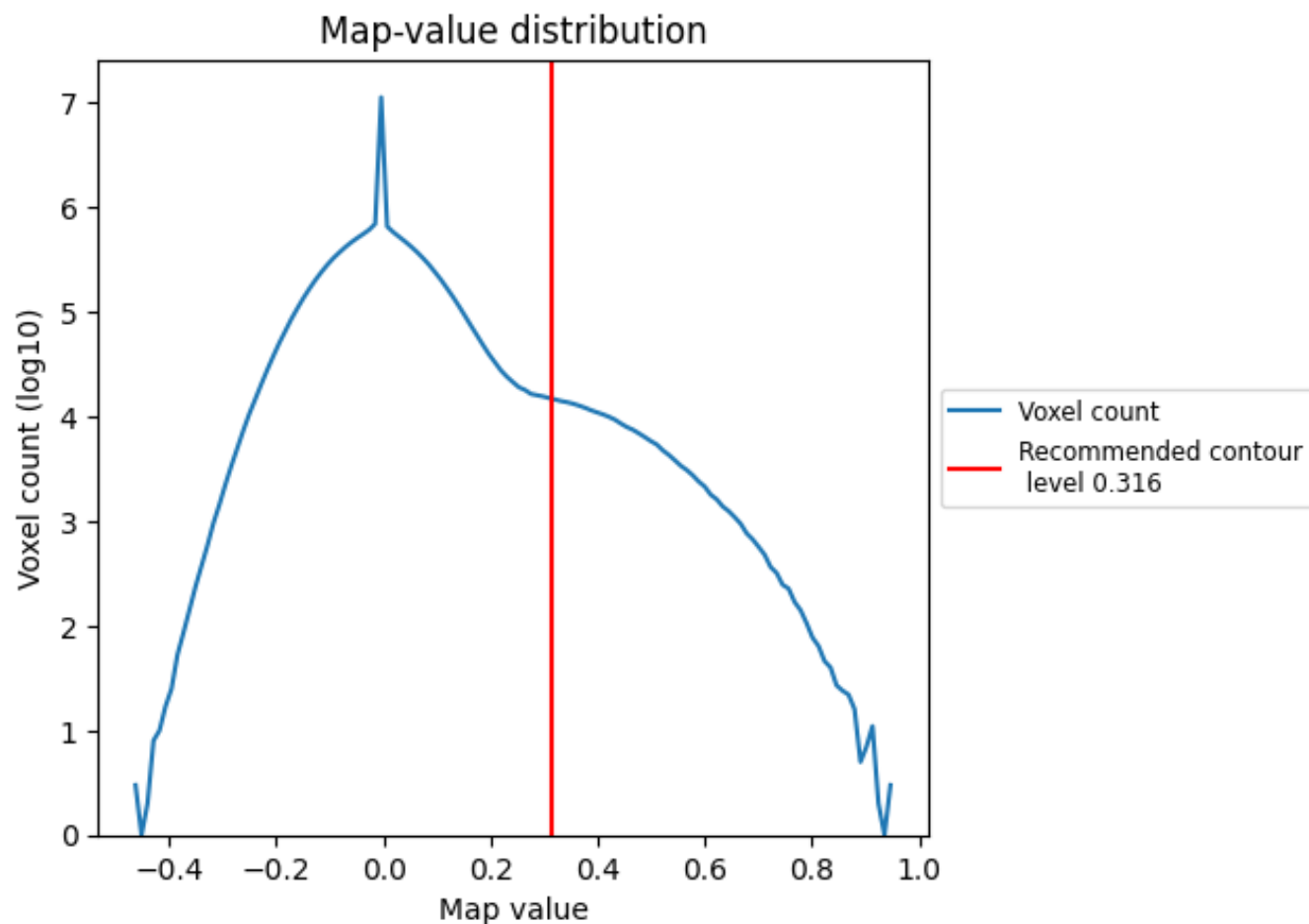


Z

7 Map analysis [i](#)

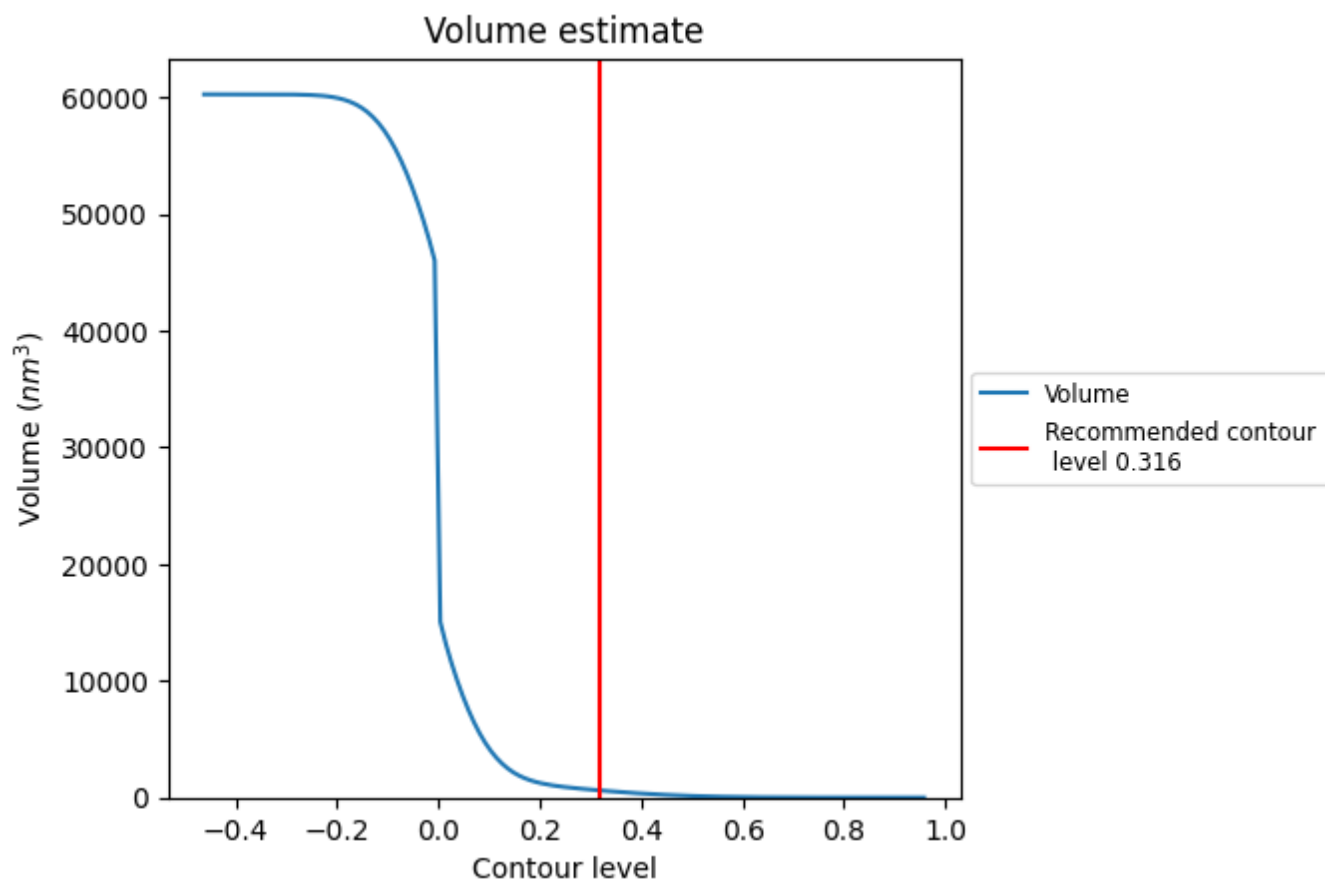
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

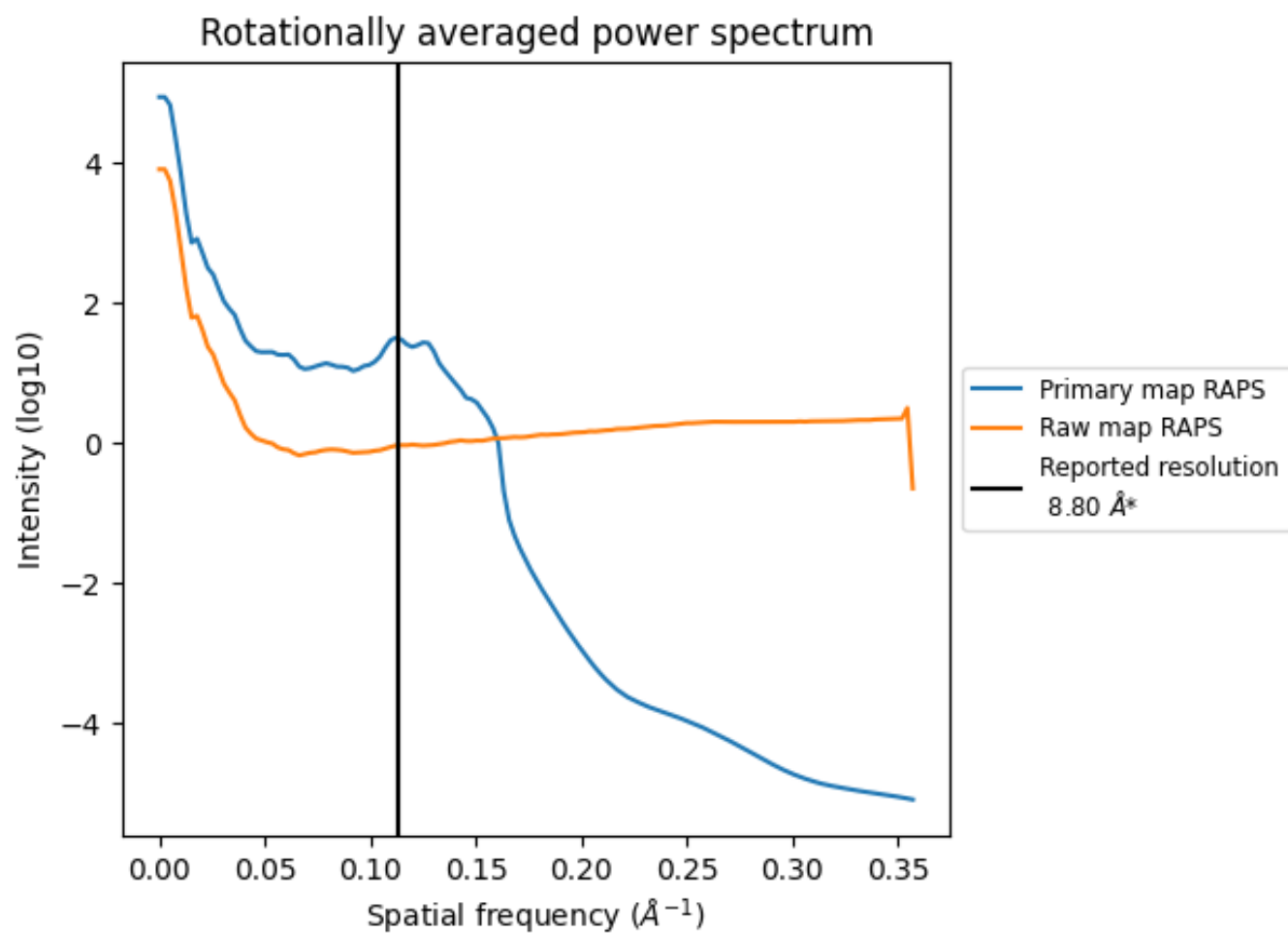
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 621 nm³; this corresponds to an approximate mass of 561 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

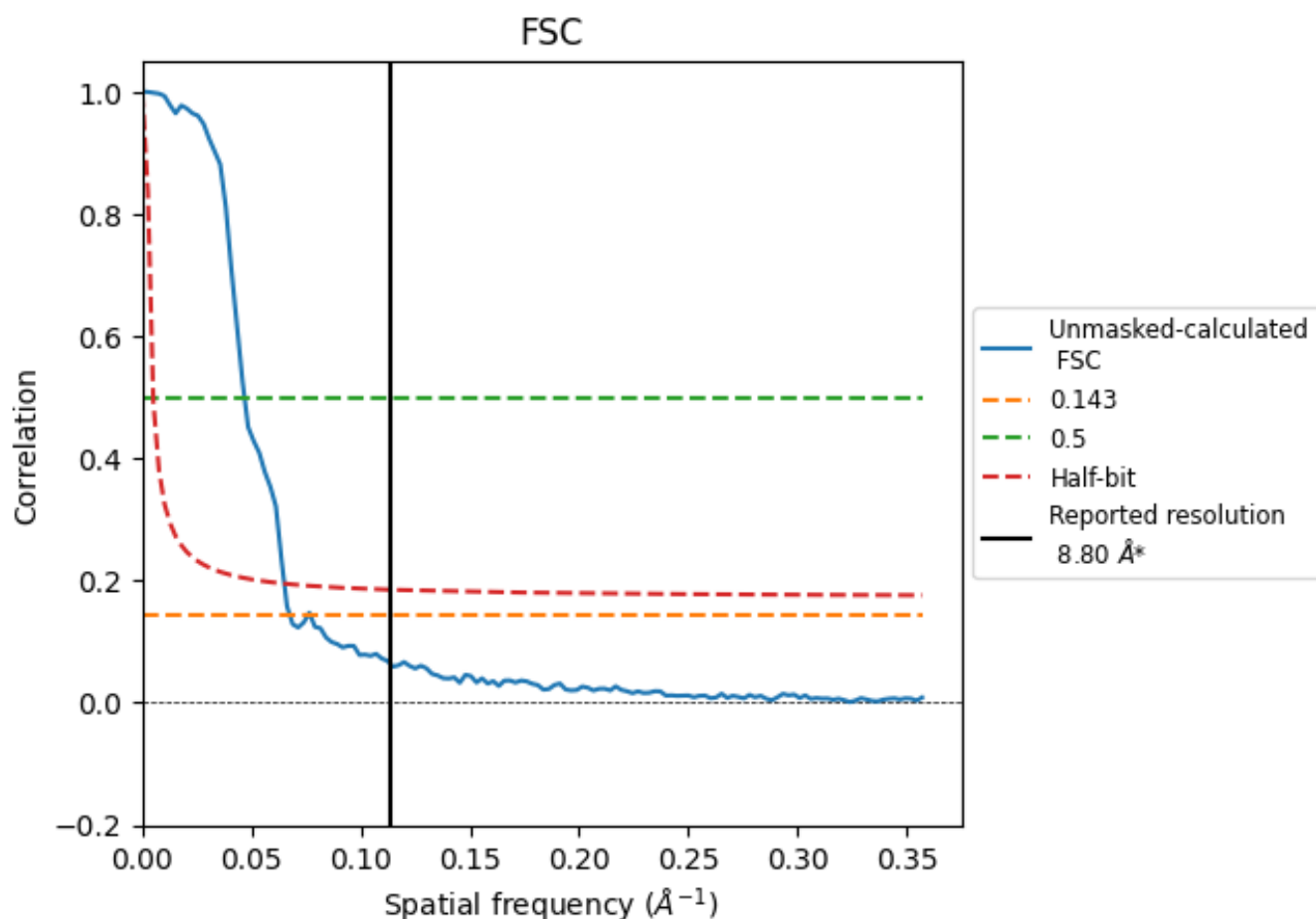


*Reported resolution corresponds to spatial frequency of 0.114 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.114 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

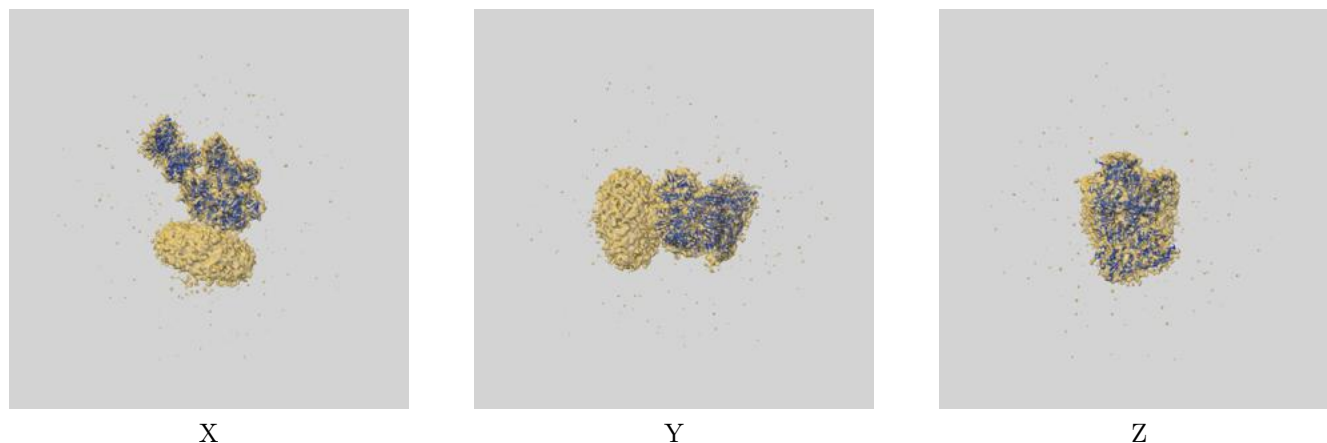
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	14.79	21.37	15.36

*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 14.79 differs from the reported value 8.8 by more than 10 %

9 Map-model fit [i](#)

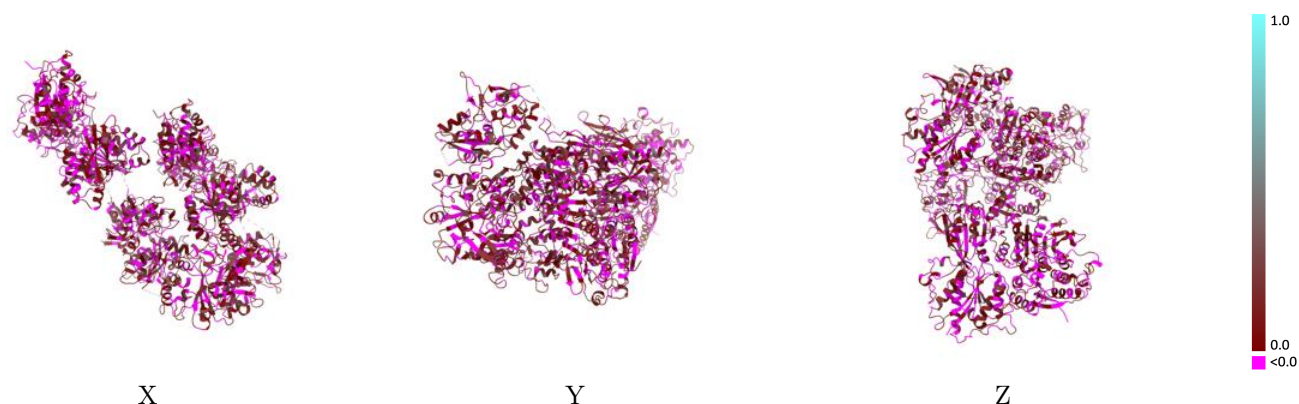
This section contains information regarding the fit between EMDB map EMD-0979 and PDB model 6LU9. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



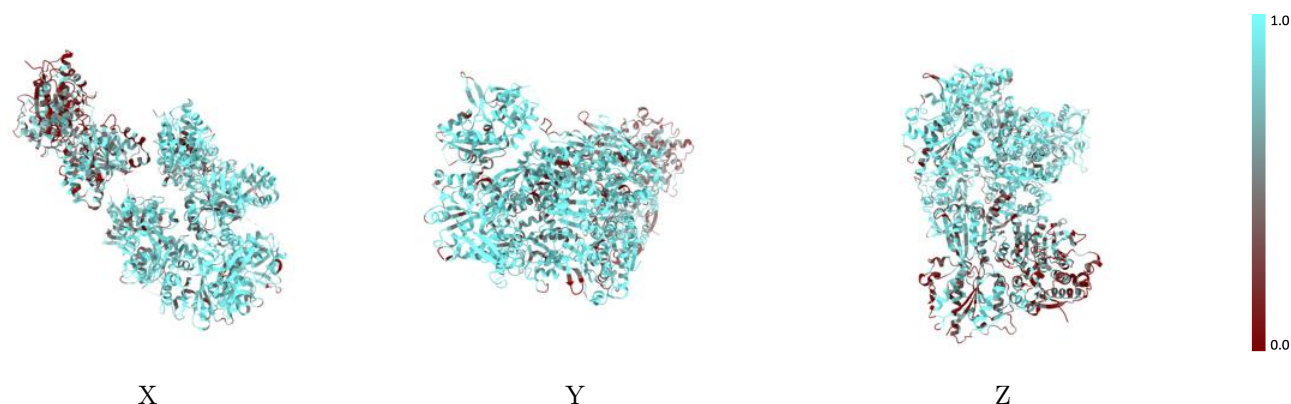
The images above show the 3D surface view of the map at the recommended contour level 0.316 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



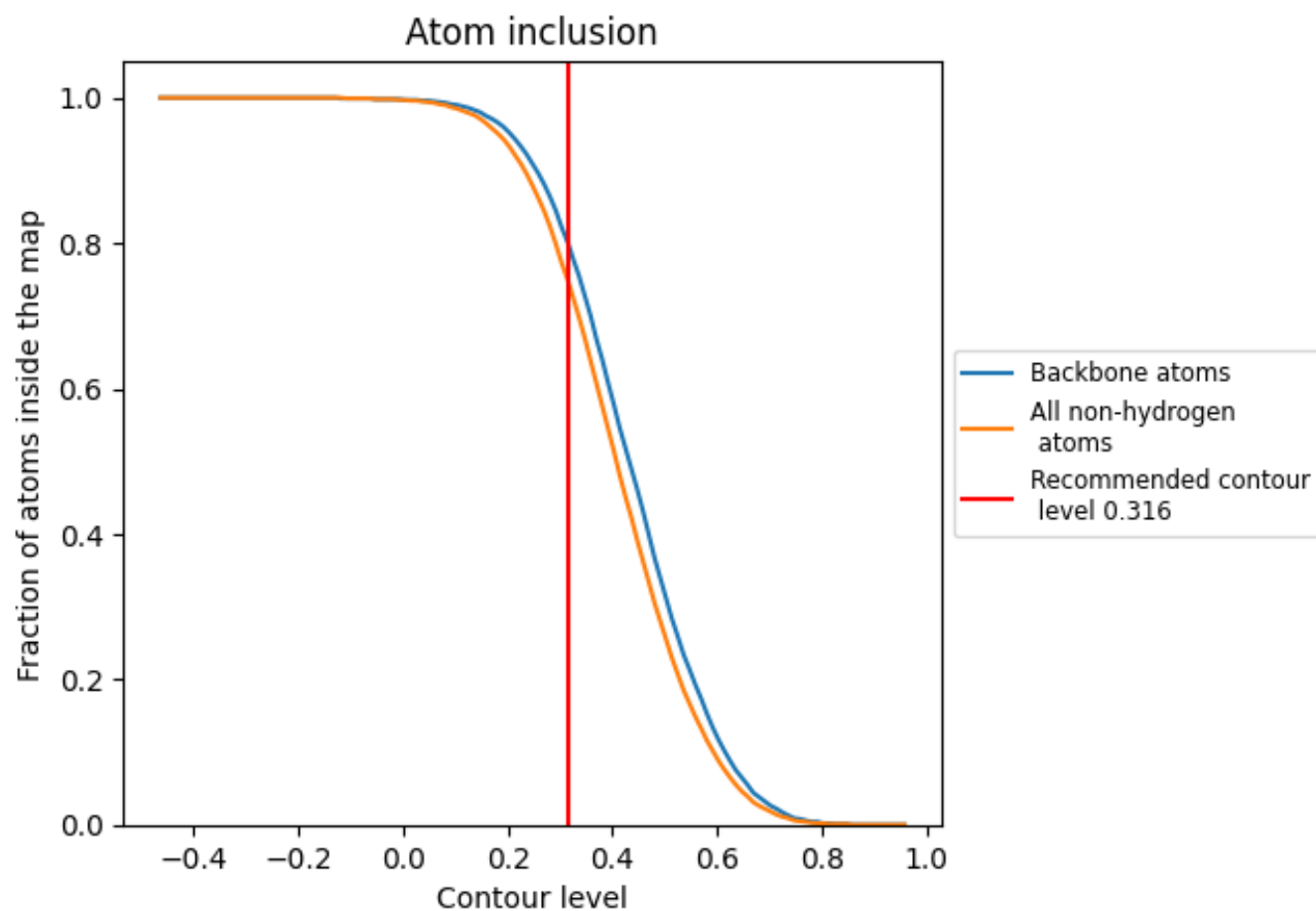
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.316).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 75% 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 (0.316) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7470	0.0650
A	0.6760	0.0450
B	0.6330	0.0550
C	0.8370	0.0860
D	0.8420	0.0730

