



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 01:41 AM UTC

PDB ID : 6L6F / pdb_00006l6f
EMDB ID : EMD-0839
Title : GluK3 receptor complex with UBP301
Authors : Kumar, J.; Kumari, J.; Burada, A.P.
Deposited on : 2019-10-28
Resolution : 10.60 Å(reported)
Based on initial model : 6JFY

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

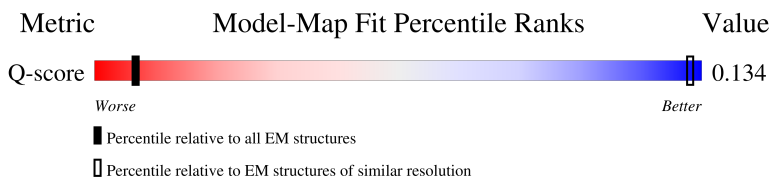
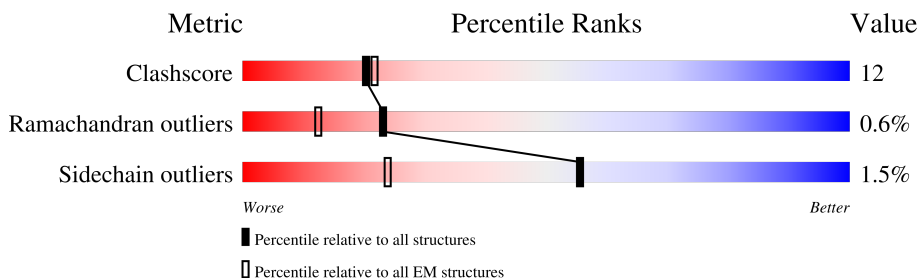
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.60 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	97 (10.10 - 11.10)

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	832	 65% 20% 14%
1	B	832	 63% 22% 14%
1	C	832	 61% 24% 14%
1	D	832	 65% 20% 14%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22836 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 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	715	Total	C	N	O	S	0	0
			5710	3672	970	1038	30		
1	B	715	Total	C	N	O	S	0	0
			5710	3672	970	1038	30		
1	C	715	Total	C	N	O	S	0	0
			5706	3670	970	1036	30		
1	D	715	Total	C	N	O	S	0	0
			5710	3672	970	1038	30		

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	THR	CYS	engineered mutation	UNP G3V9I2
A	305	THR	CYS	engineered mutation	UNP G3V9I2
A	547	VAL	CYS	engineered mutation	UNP G3V9I2
A	825	ARG	-	expression tag	UNP G3V9I2
A	826	SER	-	expression tag	UNP G3V9I2
A	827	GLY	-	expression tag	UNP G3V9I2
A	828	LEU	-	expression tag	UNP G3V9I2
A	829	VAL	-	expression tag	UNP G3V9I2
A	830	PRO	-	expression tag	UNP G3V9I2
A	831	ARG	-	expression tag	UNP G3V9I2
A	832	GLY	-	expression tag	UNP G3V9I2
B	86	THR	CYS	engineered mutation	UNP G3V9I2
B	305	THR	CYS	engineered mutation	UNP G3V9I2
B	547	VAL	CYS	engineered mutation	UNP G3V9I2
B	825	ARG	-	expression tag	UNP G3V9I2
B	826	SER	-	expression tag	UNP G3V9I2
B	827	GLY	-	expression tag	UNP G3V9I2
B	828	LEU	-	expression tag	UNP G3V9I2
B	829	VAL	-	expression tag	UNP G3V9I2
B	830	PRO	-	expression tag	UNP G3V9I2
B	831	ARG	-	expression tag	UNP G3V9I2
B	832	GLY	-	expression tag	UNP G3V9I2

Continued on next page...

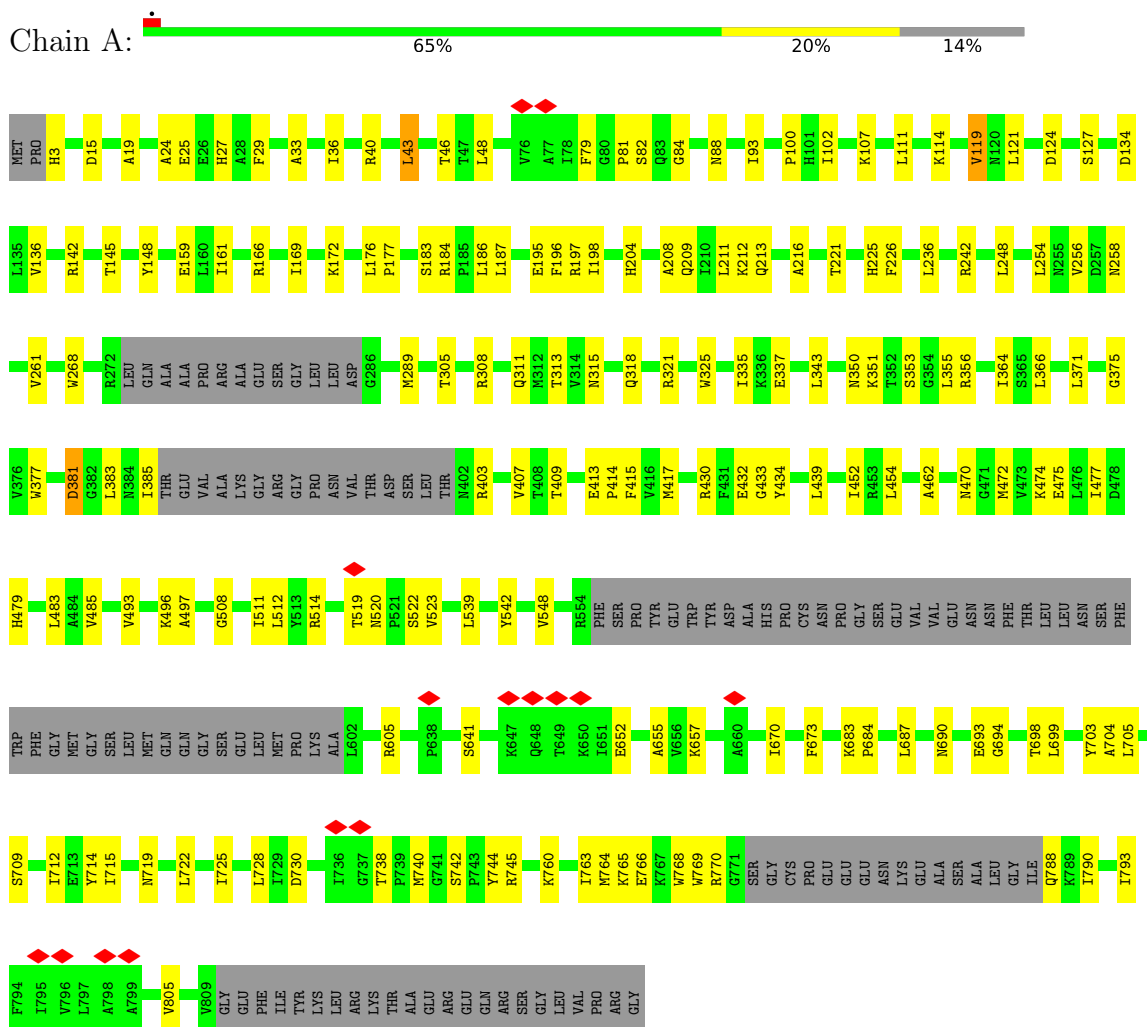
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	86	THR	CYS	engineered mutation	UNP G3V9I2
C	305	THR	CYS	engineered mutation	UNP G3V9I2
C	547	VAL	CYS	engineered mutation	UNP G3V9I2
C	825	ARG	-	expression tag	UNP G3V9I2
C	826	SER	-	expression tag	UNP G3V9I2
C	827	GLY	-	expression tag	UNP G3V9I2
C	828	LEU	-	expression tag	UNP G3V9I2
C	829	VAL	-	expression tag	UNP G3V9I2
C	830	PRO	-	expression tag	UNP G3V9I2
C	831	ARG	-	expression tag	UNP G3V9I2
C	832	GLY	-	expression tag	UNP G3V9I2
D	86	THR	CYS	engineered mutation	UNP G3V9I2
D	305	THR	CYS	engineered mutation	UNP G3V9I2
D	547	VAL	CYS	engineered mutation	UNP G3V9I2
D	825	ARG	-	expression tag	UNP G3V9I2
D	826	SER	-	expression tag	UNP G3V9I2
D	827	GLY	-	expression tag	UNP G3V9I2
D	828	LEU	-	expression tag	UNP G3V9I2
D	829	VAL	-	expression tag	UNP G3V9I2
D	830	PRO	-	expression tag	UNP G3V9I2
D	831	ARG	-	expression tag	UNP G3V9I2
D	832	GLY	-	expression tag	UNP G3V9I2

3 Residue-property plots

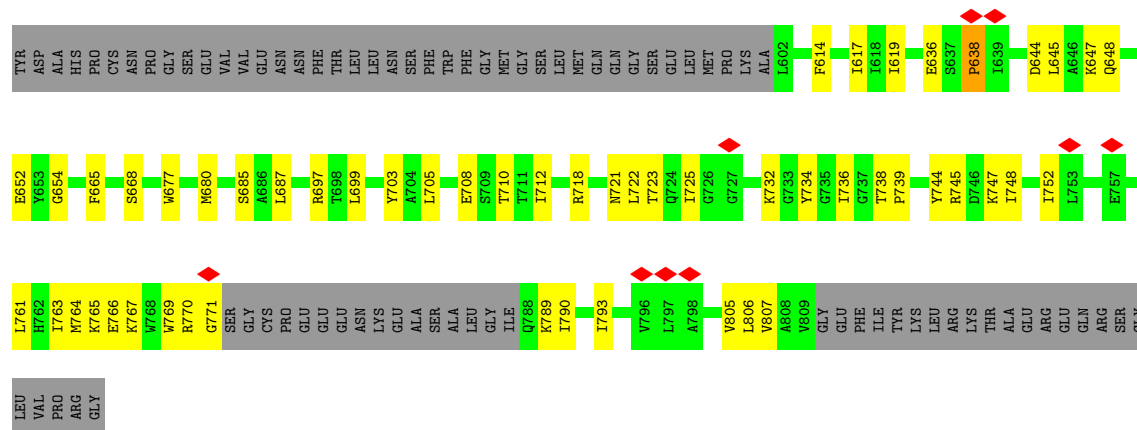
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 3

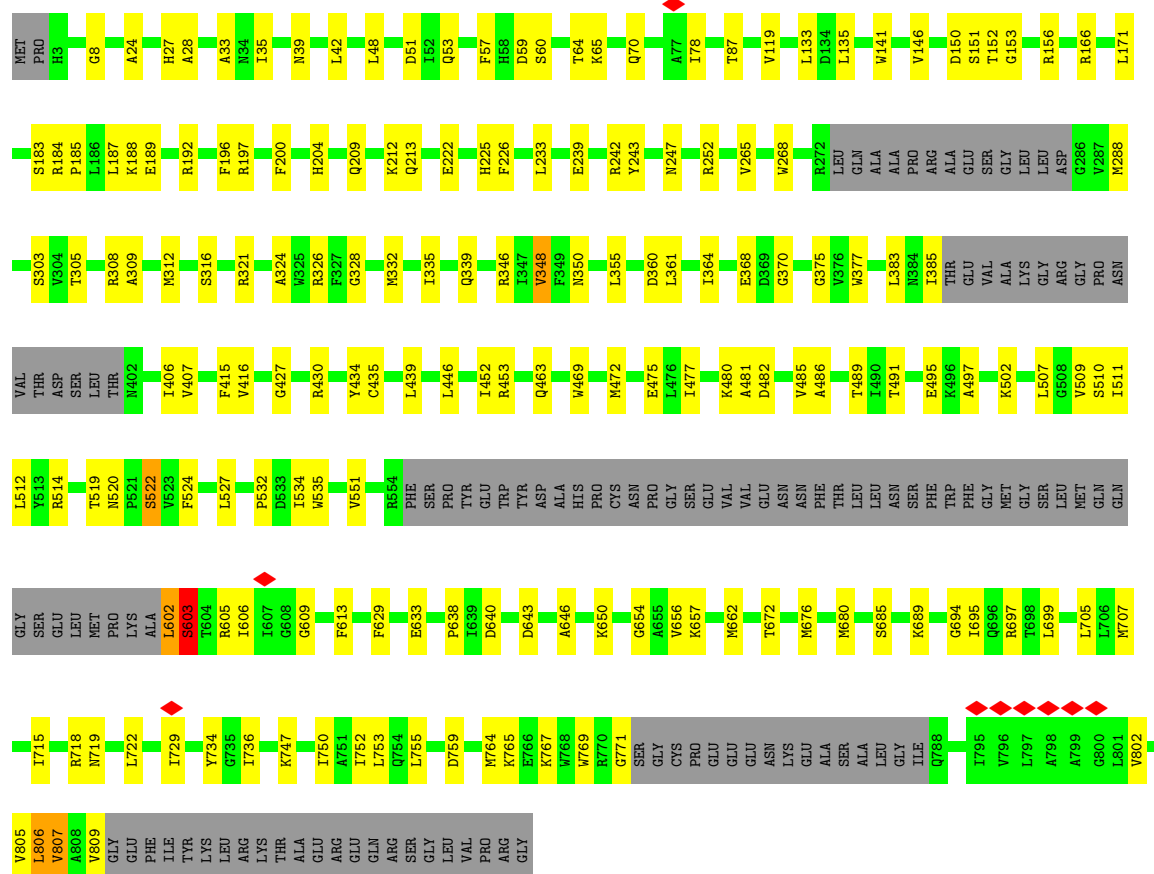


- Molecule 1: Glutamate receptor ionotropic, kainate 3





• Molecule 1: Glutamate receptor ionotropic, kainate 3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27997	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	16.73	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	3.246	Depositor
Minimum map value	-1.230	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.196	Depositor
Recommended contour level	0.936	Depositor
Map size ($\text{\AA}$)	419.1, 419.1, 419.1	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.27, 1.27, 1.27	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	0.28	0/5834	0.70	0/7896
1	B	0.29	0/5834	0.76	4/7896 (0.1%)
1	C	0.27	0/5830	0.72	6/7891 (0.1%)
1	D	0.25	0/5834	0.70	1/7896 (0.0%)
All	All	0.27	0/23332	0.72	11/31579 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	637	SER	CA-C-N	10.92	133.49	119.84
1	B	637	SER	C-N-CA	10.92	133.49	119.84
1	C	530	LEU	CA-C-N	6.04	129.27	120.51
1	C	530	LEU	C-N-CA	6.04	129.27	120.51
1	D	522	SER	CB-CA-C	-5.96	108.69	115.79
1	C	520	ASN	CA-C-N	5.52	126.74	119.84
1	C	520	ASN	C-N-CA	5.52	126.74	119.84
1	B	516	PRO	CA-C-N	5.26	131.59	121.54
1	B	516	PRO	C-N-CA	5.26	131.59	121.54
1	C	222	GLU	CA-CB-CG	5.26	124.62	114.10
1	C	516	PRO	N-CA-C	-5.03	106.54	113.53

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	5710	0	5741	142	0
1	B	5710	0	5741	162	0
1	C	5706	0	5736	149	0
1	D	5710	0	5741	126	0
All	All	22836	0	22959	560	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (560) 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:C:548:VAL:CG1	1:C:552:ILE:HD11	1.35	1.54
1:C:548:VAL:HG12	1:C:552:ILE:CD1	1.46	1.45
1:C:268:TRP:CZ2	1:C:272:ARG:C	1.96	1.44
1:B:803:LEU:O	1:B:807:VAL:CG1	1.67	1.42
1:C:718:ARG:HG2	1:C:771:GLY:C	1.44	1.42
1:B:637:SER:CB	1:B:638:PRO:HD2	1.49	1.34
1:B:637:SER:CB	1:B:638:PRO:CD	2.06	1.33
1:B:717:GLN:HG3	1:B:771:GLY:O	1.30	1.25
1:B:803:LEU:O	1:B:807:VAL:HG12	1.40	1.17
1:A:433:GLY:HA2	1:A:768:TRP:CZ3	1.81	1.15
1:A:605:ARG:NH1	1:B:549:LEU:HD13	1.60	1.15
1:D:377:TRP:HD1	1:D:383:LEU:HB2	1.09	1.15
1:B:548:VAL:HG13	1:B:552:ILE:HD11	1.21	1.14
1:B:629:PHE:CZ	1:B:633:GLU:OE2	2.00	1.14
1:B:803:LEU:O	1:B:807:VAL:HG11	1.34	1.14
1:B:548:VAL:O	1:B:552:ILE:HG13	1.40	1.14
1:B:548:VAL:CG1	1:B:552:ILE:HD11	1.80	1.12
1:B:637:SER:HB2	1:B:638:PRO:CD	1.74	1.09
1:B:714:TYR:HB2	1:B:769:TRP:CD1	1.89	1.07
1:B:637:SER:HB3	1:B:638:PRO:CD	1.79	1.06
1:C:718:ARG:CG	1:C:771:GLY:C	2.29	1.05
1:D:718:ARG:NH2	1:D:771:GLY:H	1.55	1.03
1:C:267:LYS:O	1:C:271:GLU:HG3	1.58	1.02
1:A:433:GLY:CA	1:A:768:TRP:CH2	2.44	1.01
1:A:433:GLY:C	1:A:768:TRP:CZ2	2.39	1.01
1:A:605:ARG:HH11	1:B:549:LEU:HD13	1.12	1.00
1:B:629:PHE:CE2	1:B:633:GLU:OE2	2.14	1.00
1:B:511:ILE:HD12	1:B:642:ALA:HB1	1.41	1.00
1:B:548:VAL:CG1	1:B:552:ILE:CD1	2.40	0.99
1:A:134:ASP:HB3	1:A:383:LEU:HD22	1.44	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:717:GLN:HG3	1:B:771:GLY:C	1.88	0.97
1:B:637:SER:HB3	1:B:638:PRO:HD3	1.42	0.97
1:D:377:TRP:CD1	1:D:383:LEU:HB2	2.01	0.95
1:A:433:GLY:O	1:A:768:TRP:CZ2	2.19	0.95
1:A:433:GLY:HA2	1:A:768:TRP:CH2	2.03	0.94
1:A:522:SER:HB2	1:A:523:VAL:HA	1.49	0.93
1:D:629:PHE:CE2	1:D:633:GLU:OE2	2.21	0.93
1:B:717:GLN:CG	1:B:771:GLY:O	2.17	0.90
1:B:548:VAL:HG13	1:B:552:ILE:CD1	2.00	0.90
1:B:24:ALA:HA	1:B:268:TRP:HH2	1.36	0.90
1:B:714:TYR:HB2	1:B:769:TRP:HD1	1.35	0.90
1:C:268:TRP:CH2	1:C:272:ARG:C	2.49	0.89
1:D:802:VAL:O	1:D:806:LEU:HB3	1.71	0.89
1:B:548:VAL:HG12	1:B:552:ILE:HD12	1.54	0.89
1:C:268:TRP:CE2	1:C:272:ARG:C	2.50	0.89
1:D:718:ARG:NH2	1:D:771:GLY:N	2.21	0.89
1:D:522:SER:OG	1:D:524:PHE:CD2	2.25	0.89
1:D:718:ARG:NE	1:D:771:GLY:C	2.32	0.88
1:B:548:VAL:O	1:B:552:ILE:CG1	2.22	0.87
1:A:605:ARG:NH1	1:B:549:LEU:CD1	2.37	0.86
1:B:511:ILE:CD1	1:B:642:ALA:HB1	2.06	0.86
1:B:548:VAL:HG12	1:B:552:ILE:CD1	2.06	0.85
1:D:522:SER:OG	1:D:524:PHE:HD2	1.59	0.85
1:B:637:SER:HB2	1:B:638:PRO:HD2	0.85	0.85
1:A:434:TYR:HA	1:A:768:TRP:NE1	1.93	0.84
1:D:375:GLY:HA2	1:D:385:ILE:HG22	1.59	0.84
1:C:515:LYS:HG3	1:C:723:THR:HB	1.59	0.82
1:A:433:GLY:N	1:A:768:TRP:CH2	2.48	0.82
1:A:765:LYS:HD2	1:A:769:TRP:CE3	2.16	0.80
1:C:548:VAL:HA	1:C:551:VAL:HG12	1.63	0.80
1:D:602:LEU:HD23	1:D:606:ILE:HG23	1.62	0.79
1:D:718:ARG:CZ	1:D:771:GLY:H	1.96	0.79
1:D:718:ARG:CZ	1:D:771:GLY:C	2.57	0.78
1:A:134:ASP:CB	1:A:383:LEU:HD22	2.14	0.78
1:D:602:LEU:CD2	1:D:606:ILE:HG23	2.13	0.77
1:A:766:GLU:HA	1:A:770:ARG:HB2	1.67	0.76
1:C:268:TRP:CZ2	1:C:272:ARG:O	2.40	0.74
1:A:377:TRP:HD1	1:A:383:LEU:CD1	2.02	0.73
1:B:714:TYR:CB	1:B:769:TRP:HD1	2.02	0.73
1:D:806:LEU:C	1:D:806:LEU:HD13	2.14	0.72
1:C:515:LYS:CG	1:C:723:THR:HB	2.19	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:640:ASP:O	1:B:725:ILE:HG21	1.91	0.70
1:D:629:PHE:O	1:D:633:GLU:HG3	1.92	0.70
1:D:629:PHE:CZ	1:D:633:GLU:OE2	2.46	0.69
1:C:548:VAL:CG1	1:C:552:ILE:CD1	2.31	0.69
1:A:134:ASP:HB3	1:A:383:LEU:CD2	2.21	0.69
1:C:520:ASN:HB3	1:C:789:LYS:HD3	1.73	0.69
1:A:377:TRP:CD1	1:A:383:LEU:HD13	2.27	0.69
1:A:766:GLU:HG2	1:A:770:ARG:HD2	1.74	0.69
1:A:433:GLY:C	1:A:768:TRP:CE2	2.70	0.69
1:B:803:LEU:C	1:B:807:VAL:HG12	2.18	0.68
1:C:765:LYS:O	1:C:769:TRP:HB2	1.94	0.68
1:B:515:LYS:HE2	1:B:723:THR:HB	1.74	0.67
1:A:377:TRP:HD1	1:A:383:LEU:HD13	1.59	0.67
1:C:515:LYS:HB2	1:C:721:ASN:C	2.19	0.67
1:A:493:VAL:HA	1:A:496:LYS:HD3	1.76	0.67
1:C:548:VAL:HG12	1:C:552:ILE:CG1	2.23	0.67
1:A:184:ARG:HE	1:A:213:GLN:HA	1.57	0.67
1:C:267:LYS:O	1:C:271:GLU:CG	2.40	0.66
1:A:605:ARG:HH12	1:B:549:LEU:HD22	1.60	0.66
1:C:101:HIS:H	1:C:117:PHE:HB3	1.60	0.66
1:B:802:VAL:O	1:B:806:LEU:HB3	1.95	0.66
1:A:407:VAL:HG22	1:A:483:LEU:HB2	1.78	0.65
1:A:433:GLY:HA2	1:A:768:TRP:CE3	2.30	0.65
1:C:507:LEU:HB3	1:C:710:THR:HG23	1.78	0.65
1:C:525:SER:HA	1:C:528:ASN:OD1	1.97	0.65
1:A:209:GLN:HG3	1:A:213:GLN:HE21	1.63	0.64
1:D:407:VAL:HB	1:D:452:ILE:HA	1.79	0.64
1:B:143:SER:HB3	1:B:170:ARG:HH11	1.63	0.64
1:B:512:LEU:HB3	1:B:705:LEU:HB3	1.80	0.62
1:A:208:ALA:HB2	1:A:236:LEU:HD22	1.80	0.62
1:A:407:VAL:HB	1:A:452:ILE:HA	1.80	0.62
1:D:718:ARG:HE	1:D:771:GLY:C	2.05	0.62
1:C:744:TYR:HA	1:C:747:LYS:HB2	1.82	0.62
1:C:268:TRP:CE2	1:C:272:ARG:O	2.52	0.62
1:A:714:TYR:HD1	1:A:769:TRP:HA	1.65	0.62
1:D:718:ARG:NH2	1:D:771:GLY:CA	2.63	0.61
1:A:433:GLY:C	1:A:768:TRP:CH2	2.77	0.61
1:D:383:LEU:O	1:D:383:LEU:HG	2.01	0.61
1:D:718:ARG:NH2	1:D:771:GLY:C	2.59	0.60
1:D:602:LEU:HG	1:D:605:ARG:HB2	1.82	0.60
1:D:446:LEU:HD22	1:D:747:LYS:HB3	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:522:SER:HA	1:C:790:ILE:HD13	1.82	0.60
1:B:147:VAL:HG12	1:B:176:LEU:HD12	1.81	0.60
1:B:148:TYR:HA	1:B:201:ASP:HB3	1.84	0.60
1:A:134:ASP:C	1:A:383:LEU:HD22	2.27	0.60
1:C:53:GLN:HE21	1:C:66:LYS:HD2	1.66	0.60
1:A:539:LEU:O	1:A:542:TYR:HB3	2.02	0.59
1:B:473:VAL:HG13	1:B:498:ILE:HD11	1.83	0.59
1:C:514:ARG:HA	1:C:722:LEU:HA	1.84	0.59
1:B:101:HIS:O	1:B:118:TYR:HA	2.02	0.59
1:C:381:ASP:OD2	1:C:384:ASN:ND2	2.35	0.59
1:C:507:LEU:HD12	1:C:732:LYS:HB2	1.85	0.59
1:C:415:PHE:HA	1:C:434:TYR:HB3	1.84	0.59
1:C:269:SER:HB3	1:C:287:VAL:H	1.68	0.59
1:D:200:PHE:HE2	1:D:226:PHE:HB3	1.66	0.59
1:A:124:ASP:HB3	1:A:127:SER:HB3	1.84	0.59
1:C:614:PHE:HA	1:C:617:ILE:HD12	1.85	0.59
1:D:222:GLU:O	1:D:247:ASN:ND2	2.35	0.58
1:C:317:LEU:HA	1:C:323:LYS:HE3	1.84	0.58
1:C:261:VAL:HG13	1:C:343:LEU:HB3	1.84	0.58
1:A:605:ARG:HH12	1:B:549:LEU:HD13	1.65	0.58
1:B:268:TRP:CE3	1:B:288:MET:HE2	2.38	0.58
1:B:714:TYR:CB	1:B:769:TRP:CD1	2.75	0.58
1:B:159:GLU:O	1:B:166:ARG:NH2	2.36	0.58
1:B:332:MET:HE2	1:B:336:LYS:HE3	1.83	0.58
1:B:714:TYR:CA	1:B:769:TRP:HD1	2.17	0.58
1:C:27:HIS:HB3	1:C:268:TRP:HH2	1.69	0.58
1:C:718:ARG:CD	1:C:771:GLY:C	2.76	0.57
1:B:512:LEU:HD11	1:B:722:LEU:HB3	1.85	0.57
1:B:767:LYS:HA	1:B:770:ARG:HE	1.68	0.57
1:A:605:ARG:HH12	1:B:549:LEU:CD2	2.16	0.57
1:A:46:THR:OG1	1:A:311:GLN:NE2	2.38	0.57
1:A:715:ILE:O	1:A:719:ASN:N	2.36	0.57
1:D:427:GLY:HA2	1:D:430:ARG:HH11	1.68	0.57
1:C:527:LEU:HD22	1:C:532:PRO:HB3	1.86	0.57
1:A:25:GLU:O	1:A:29:PHE:N	2.38	0.57
1:B:348:VAL:HG13	1:B:358:ASP:HB3	1.87	0.57
1:C:552:ILE:HG22	1:C:552:ILE:O	2.04	0.57
1:C:416:VAL:HG13	1:C:436:ILE:HD11	1.86	0.57
1:B:154:LEU:HA	1:B:157:LEU:HB2	1.87	0.56
1:C:552:ILE:C	1:C:554:ARG:H	2.12	0.56
1:C:512:LEU:HD23	1:C:705:LEU:HD23	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:TRP:HB2	1:D:383:LEU:HD13	1.86	0.56
1:C:513:TYR:HB3	1:C:725:ILE:HG13	1.88	0.56
1:A:121:LEU:HD12	1:A:356:ARG:HB2	1.87	0.56
1:A:315:ASN:HD22	1:A:325:TRP:HA	1.71	0.56
1:D:239:GLU:HA	1:D:242:ARG:HE	1.71	0.56
1:D:350:ASN:N	1:D:355:LEU:O	2.37	0.56
1:A:548:VAL:HG21	1:B:801:LEU:HD22	1.87	0.56
1:B:15:ASP:HB3	1:B:18:ASN:HB2	1.87	0.56
1:D:806:LEU:HD13	1:D:806:LEU:O	2.06	0.56
1:B:106:TRP:HD1	1:B:122:TYR:HD2	1.54	0.56
1:B:707:MET:SD	1:B:711:THR:OG1	2.60	0.56
1:B:350:ASN:HB2	1:B:357:THR:HG22	1.88	0.55
1:C:162:MET:HB2	1:C:166:ARG:HH21	1.70	0.55
1:B:26:GLU:HG2	1:B:30:ARG:HE	1.70	0.55
1:C:301:ILE:HD11	1:C:347:ILE:HG21	1.87	0.55
1:D:509:VAL:HG12	1:D:729:ILE:HD12	1.87	0.55
1:B:532:PRO:HA	1:B:535:TRP:HD1	1.71	0.55
1:C:515:LYS:HE3	1:C:723:THR:HB	1.87	0.55
1:D:718:ARG:HH22	1:D:771:GLY:H	1.46	0.55
1:B:265:VAL:HG13	1:B:287:VAL:HA	1.88	0.55
1:A:714:TYR:CD1	1:A:769:TRP:HA	2.41	0.55
1:C:512:LEU:HB3	1:C:705:LEU:HB3	1.87	0.55
1:B:24:ALA:CA	1:B:268:TRP:HH2	2.15	0.55
1:A:377:TRP:CD1	1:A:383:LEU:CD1	2.87	0.55
1:C:3:HIS:HB3	1:C:46:THR:HG22	1.89	0.55
1:C:736:ILE:HD11	1:C:752:ILE:HD11	1.89	0.54
1:A:84:GLY:O	1:A:88:ASN:HB2	2.06	0.54
1:C:346:ARG:O	1:C:356:ARG:NH2	2.40	0.54
1:B:243:TYR:HA	1:B:368:GLU:HG3	1.88	0.54
1:D:346:ARG:NH2	1:D:360:ASP:OD2	2.40	0.54
1:D:489:THR:HA	1:D:734:TYR:HA	1.89	0.54
1:D:685:SER:O	1:D:697:ARG:NH2	2.40	0.54
1:B:163:ALA:O	1:B:167:TYR:N	2.39	0.54
1:A:511:ILE:HB	1:A:725:ILE:HB	1.88	0.54
1:C:117:PHE:HD1	1:C:332:MET:HG3	1.72	0.54
1:A:159:GLU:OE1	1:A:166:ARG:NH2	2.41	0.54
1:B:349:PHE:HA	1:B:356:ARG:HA	1.90	0.54
1:C:435:CYS:HA	1:C:438:LEU:HB3	1.88	0.54
1:C:654:GLY:HA2	1:C:680:MET:HE2	1.89	0.54
1:D:809:VAL:O	1:D:809:VAL:HG23	2.08	0.54
1:A:605:ARG:HH11	1:B:549:LEU:CD1	2.01	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:VAL:HG22	1:B:174:ARG:HB2	1.89	0.54
1:A:690:ASN:HD22	1:A:693:GLU:HB2	1.72	0.53
1:B:24:ALA:HA	1:B:268:TRP:CH2	2.29	0.53
1:A:364:ILE:HD12	1:A:371:LEU:HD21	1.91	0.53
1:A:605:ARG:HH12	1:B:549:LEU:CD1	2.19	0.53
1:B:268:TRP:HE3	1:B:288:MET:HE2	1.73	0.53
1:B:603:SER:O	1:B:606:ILE:HG12	2.08	0.53
1:D:406:ILE:HB	1:D:481:ALA:HA	1.89	0.53
1:A:3:HIS:HB3	1:A:46:THR:HA	1.91	0.53
1:C:308:ARG:HH12	1:C:338:ALA:HA	1.72	0.53
1:A:208:ALA:HA	1:A:211:LEU:HD12	1.90	0.53
1:A:522:SER:CB	1:A:523:VAL:HA	2.29	0.53
1:B:714:TYR:HB2	1:B:769:TRP:NE1	2.23	0.53
1:D:477:ILE:HD11	1:D:497:ALA:HB1	1.90	0.53
1:A:430:ARG:HH12	1:A:454:LEU:HD11	1.74	0.53
1:A:439:LEU:HD22	1:A:485:VAL:HG21	1.90	0.53
1:D:209:GLN:HE21	1:D:213:GLN:HE21	1.57	0.53
1:A:375:GLY:HA3	1:A:385:ILE:HA	1.91	0.53
1:B:71:LEU:HD22	1:B:317:LEU:HB2	1.90	0.53
1:B:376:VAL:HG22	1:B:384:ASN:HD22	1.73	0.53
1:C:551:VAL:HG11	1:D:805:VAL:HG13	1.90	0.53
1:A:709:SER:HA	1:A:712:ILE:HD12	1.90	0.53
1:C:100:PRO:HG3	1:C:332:MET:HG2	1.91	0.53
1:A:111:LEU:HD11	1:A:353:SER:HB2	1.91	0.53
1:D:415:PHE:HA	1:D:434:TYR:HB3	1.91	0.53
1:A:350:ASN:H	1:A:355:LEU:H	1.57	0.52
1:D:602:LEU:HD23	1:D:606:ILE:CG2	2.34	0.52
1:D:715:ILE:O	1:D:719:ASN:N	2.42	0.52
1:D:430:ARG:HH12	1:D:453:ARG:HA	1.72	0.52
1:D:609:GLY:O	1:D:613:PHE:HB2	2.09	0.52
1:B:56:HIS:ND1	1:B:62:GLU:OE1	2.39	0.52
1:B:249:THR:HA	1:B:365:SER:HA	1.91	0.52
1:B:640:ASP:O	1:B:725:ILE:CG2	2.58	0.52
1:D:183:SER:O	1:D:187:LEU:N	2.40	0.52
1:A:434:TYR:CG	1:A:769:TRP:CH2	2.98	0.52
1:D:602:LEU:HD21	1:D:606:ILE:HG23	1.91	0.52
1:A:183:SER:O	1:A:187:LEU:N	2.39	0.52
1:D:361:LEU:HD12	1:D:377:TRP:HB3	1.91	0.52
1:B:142:ARG:H	1:B:197:ARG:HH22	1.58	0.52
1:B:174:ARG:NH1	1:B:190:MET:SD	2.83	0.52
1:A:788:GLN:HG2	1:D:534:ILE:HD11	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:766:GLU:OE1	1:C:770:ARG:NE	2.43	0.51
1:B:767:LYS:HA	1:B:770:ARG:NE	2.25	0.51
1:B:17:PRO:O	1:B:20:GLN:NE2	2.43	0.51
1:C:548:VAL:HG12	1:C:552:ILE:HD11	0.59	0.51
1:C:665:PHE:HB3	1:C:677:TRP:HB2	1.93	0.51
1:D:339:GLN:HG2	1:D:348:VAL:HA	1.93	0.51
1:A:195:GLU:OE1	1:A:197:ARG:NH1	2.44	0.51
1:A:765:LYS:HA	1:A:769:TRP:CE3	2.46	0.51
1:B:27:HIS:CD2	1:B:271:GLU:OE1	2.64	0.51
1:C:40:ARG:NH1	1:C:44:PRO:O	2.44	0.51
1:C:136:VAL:O	1:C:140:LYS:N	2.40	0.51
1:A:477:ILE:HD11	1:A:497:ALA:HB1	1.93	0.51
1:B:415:PHE:HE1	1:B:769:TRP:HZ2	1.58	0.51
1:D:189:GLU:HA	1:D:192:ARG:HE	1.76	0.51
1:A:196:PHE:O	1:A:225:HIS:N	2.43	0.51
1:A:318:GLN:HB2	1:A:321:ARG:HE	1.76	0.51
1:D:764:MET:HA	1:D:767:LYS:HG2	1.93	0.51
1:C:419:ARG:NH2	1:C:431:PHE:O	2.43	0.51
1:D:133:LEU:HD11	1:D:166:ARG:HD3	1.93	0.51
1:D:514:ARG:HD3	1:D:699:LEU:HA	1.91	0.51
1:A:79:PHE:HA	1:A:102:ILE:HB	1.92	0.51
1:C:268:TRP:HZ2	1:C:272:ARG:C	2.00	0.51
1:A:204:HIS:HB2	1:A:236:LEU:HD11	1.91	0.51
1:D:24:ALA:O	1:D:28:ALA:HB2	2.10	0.51
1:D:324:ALA:HB3	1:D:326:ARG:HH21	1.75	0.51
1:A:177:PRO:HD3	1:A:186:LEU:HD22	1.92	0.50
1:A:24:ALA:HB3	1:A:289:MET:HE2	1.93	0.50
1:B:88:ASN:HA	1:B:91:GLN:HB3	1.92	0.50
1:A:434:TYR:CD1	1:A:769:TRP:CZ3	2.99	0.50
1:B:340:TRP:HD1	1:B:347:ILE:HD12	1.77	0.50
1:B:760:LYS:HA	1:B:763:ILE:HB	1.93	0.50
1:A:82:SER:HA	1:A:107:LYS:HD2	1.94	0.50
1:C:129:SER:HA	1:C:132:ILE:HD12	1.94	0.50
1:B:125:TYR:HA	1:B:128:LEU:HD12	1.94	0.50
1:B:208:ALA:HA	1:B:211:LEU:HD12	1.93	0.50
1:A:377:TRP:HD1	1:A:383:LEU:HD12	1.73	0.50
1:B:138:SER:O	1:B:140:LYS:NZ	2.42	0.50
1:B:268:TRP:HE3	1:B:288:MET:CE	2.25	0.50
1:D:657:LYS:HB3	1:D:689:LYS:HG2	1.94	0.50
1:A:242:ARG:HE	1:A:366:LEU:HD11	1.75	0.50
1:B:184:ARG:HH21	1:B:213:GLN:HA	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:PHE:HA	1:A:434:TYR:HB3	1.92	0.50
1:A:479:HIS:HE1	1:A:740:MET:H	1.59	0.50
1:B:13:TYR:HB2	1:B:16:GLY:H	1.77	0.50
1:D:736:ILE:HD13	1:D:752:ILE:HD11	1.93	0.50
1:B:26:GLU:OE2	1:B:54:ARG:NH2	2.44	0.49
1:D:204:HIS:HB2	1:D:233:LEU:HB2	1.94	0.49
1:A:43:LEU:HB3	1:A:46:THR:HB	1.94	0.49
1:B:3:HIS:HB3	1:B:46:THR:HG22	1.93	0.49
1:C:157:LEU:HB3	1:C:160:LEU:HD12	1.94	0.49
1:C:805:VAL:C	1:C:807:VAL:H	2.20	0.49
1:D:33:ALA:HA	1:D:48:LEU:HD23	1.95	0.49
1:C:317:LEU:HD23	1:C:323:LYS:HG2	1.94	0.49
1:C:483:LEU:HD23	1:C:748:ILE:HD11	1.94	0.49
1:D:265:VAL:HG22	1:D:288:MET:HB3	1.94	0.49
1:B:340:TRP:HB3	1:B:347:ILE:HB	1.95	0.49
1:C:349:PHE:HA	1:C:356:ARG:HA	1.94	0.49
1:D:242:ARG:HD3	1:D:370:GLY:HA3	1.93	0.49
1:B:402:ASN:HD21	1:B:448:PHE:HA	1.78	0.49
1:C:83:GLN:O	1:C:86:THR:OG1	2.24	0.49
1:C:97:LEU:HD22	1:C:317:LEU:HB3	1.95	0.49
1:C:644:ASP:HA	1:C:647:LYS:HG2	1.95	0.49
1:B:148:TYR:O	1:B:176:LEU:N	2.41	0.49
1:B:407:VAL:HG22	1:B:483:LEU:HB3	1.95	0.49
1:B:652:GLU:HB3	1:B:686:ALA:HB2	1.94	0.49
1:B:27:HIS:CD2	1:B:271:GLU:CD	2.90	0.49
1:B:254:LEU:HA	1:B:344:THR:HG22	1.94	0.49
1:C:242:ARG:HB2	1:C:366:LEU:HD11	1.94	0.49
1:A:27:HIS:HB3	1:A:268:TRP:HH2	1.78	0.49
1:C:436:ILE:HG22	1:C:440:LYS:HE3	1.95	0.49
1:C:520:ASN:C	1:C:522:SER:H	2.21	0.49
1:D:119:VAL:HG11	1:D:335:ILE:HG22	1.95	0.49
1:C:477:ILE:HG13	1:C:498:ILE:HG23	1.95	0.48
1:B:766:GLU:O	1:B:770:ARG:HG3	2.13	0.48
1:B:6:ARG:H	1:B:314:VAL:HG21	1.78	0.48
1:C:346:ARG:HH22	1:C:379:PRO:HD2	1.78	0.48
1:D:316:SER:O	1:D:321:ARG:NH1	2.47	0.48
1:B:301:ILE:HG12	1:B:340:TRP:HB2	1.94	0.48
1:B:633:GLU:O	1:B:636:GLU:HG2	2.14	0.48
1:C:142:ARG:HH22	1:C:168:ASN:HB3	1.77	0.48
1:C:233:LEU:HG	1:C:238:LEU:HD11	1.94	0.48
1:D:141:TRP:HA	1:D:197:ARG:HH11	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:LEU:HB3	1:B:241:TYR:CZ	2.49	0.48
1:D:243:TYR:HA	1:D:368:GLU:HG2	1.96	0.48
1:D:252:ARG:HB2	1:D:364:ILE:HD13	1.95	0.48
1:C:321:ARG:HH21	1:C:323:LYS:HB2	1.78	0.48
1:B:10:ILE:HG12	1:B:53:GLN:HB2	1.96	0.48
1:B:468:GLN:HE21	1:B:474:LYS:HE3	1.78	0.48
1:A:434:TYR:CD1	1:A:769:TRP:HZ3	2.32	0.48
1:C:114:LYS:NZ	1:D:57:PHE:O	2.46	0.48
1:C:438:LEU:HD13	1:C:761:LEU:HD21	1.94	0.48
1:C:478:ASP:HB2	1:C:480:LYS:HG3	1.95	0.48
1:D:135:LEU:HD13	1:D:383:LEU:HD21	1.96	0.48
1:A:742:SER:H	1:A:745:ARG:HH12	1.60	0.48
1:B:106:TRP:O	1:B:156:ARG:NH2	2.47	0.48
1:C:515:LYS:HD3	1:C:517:ASN:HD21	1.79	0.48
1:D:24:ALA:O	1:D:28:ALA:CB	2.62	0.48
1:D:328:GLY:O	1:D:332:MET:HB2	2.14	0.48
1:D:654:GLY:HA2	1:D:680:MET:HE2	1.95	0.48
1:A:33:ALA:HA	1:A:48:LEU:HD23	1.96	0.47
1:A:433:GLY:CA	1:A:768:TRP:CZ3	2.65	0.47
1:B:806:LEU:HD13	1:B:806:LEU:C	2.39	0.47
1:C:763:ILE:O	1:C:767:LYS:HB2	2.14	0.47
1:D:196:PHE:O	1:D:225:HIS:N	2.47	0.47
1:B:376:VAL:O	1:B:384:ASN:HB2	2.14	0.47
1:A:212:LYS:O	1:A:216:ALA:HB2	2.14	0.47
1:C:183:SER:OG	1:C:213:GLN:NE2	2.47	0.47
1:D:153:GLY:HA2	1:D:156:ARG:HG3	1.96	0.47
1:B:35:ILE:HA	1:B:38:ARG:HD2	1.96	0.47
1:C:183:SER:H	1:C:213:GLN:HE22	1.62	0.47
1:C:525:SER:C	1:C:527:LEU:H	2.23	0.47
1:D:416:VAL:HG22	1:D:435:CYS:HB2	1.97	0.47
1:A:519:THR:HG22	1:A:520:ASN:H	1.79	0.47
1:B:764:MET:HA	1:B:767:LYS:HB3	1.97	0.47
1:A:93:ILE:HG12	1:B:61:PHE:HB2	1.97	0.47
1:B:28:ALA:HB2	1:B:268:TRP:HZ3	1.79	0.47
1:B:261:VAL:HG22	1:B:343:LEU:HD13	1.95	0.47
1:B:507:LEU:O	1:B:732:LYS:N	2.48	0.47
1:B:749:THR:O	1:B:753:LEU:HB2	2.13	0.47
1:C:13:TYR:HB2	1:C:16:GLY:H	1.78	0.47
1:C:261:VAL:HA	1:C:343:LEU:HD22	1.96	0.47
1:B:438:LEU:HD13	1:B:761:LEU:HD21	1.97	0.47
1:B:636:GLU:OE2	1:B:636:GLU:HA	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:695:ILE:HD11	1:B:715:ILE:HG12	1.97	0.47
1:D:430:ARG:NH1	1:D:452:ILE:O	2.48	0.47
1:D:491:THR:O	1:D:495:GLU:N	2.46	0.47
1:A:652:GLU:HB2	1:A:703:TYR:HA	1.96	0.47
1:B:415:PHE:CE1	1:B:769:TRP:HZ2	2.33	0.47
1:C:364:ILE:HA	1:C:373:LYS:HA	1.97	0.47
1:D:475:GLU:O	1:D:480:LYS:N	2.48	0.47
1:B:502:LYS:HE2	1:B:752:ILE:HG12	1.97	0.47
1:D:35:ILE:O	1:D:39:ASN:N	2.40	0.47
1:D:646:ALA:HB2	1:D:676:MET:HG3	1.96	0.47
1:A:514:ARG:HA	1:A:722:LEU:HA	1.96	0.46
1:C:305:THR:HA	1:C:308:ARG:HD2	1.97	0.46
1:A:512:LEU:HD12	1:A:712:ILE:HG23	1.98	0.46
1:B:658:ASP:O	1:B:689:LYS:NZ	2.48	0.46
1:C:54:ARG:O	1:C:66:LYS:NZ	2.48	0.46
1:C:117:PHE:HA	1:C:332:MET:HE2	1.96	0.46
1:A:433:GLY:H	1:A:768:TRP:HH2	1.60	0.46
1:A:683:LYS:HD2	1:A:684:PRO:HD2	1.98	0.46
1:A:694:GLY:HA3	1:A:705:LEU:HD13	1.98	0.46
1:C:466:LYS:HD2	1:C:470:ASN:HD22	1.79	0.46
1:D:209:GLN:HA	1:D:212:LYS:HD2	1.97	0.46
1:B:507:LEU:HB2	1:B:709:SER:H	1.80	0.46
1:C:504:PHE:HE1	1:C:736:ILE:HG23	1.80	0.46
1:D:514:ARG:HD3	1:D:699:LEU:HD23	1.96	0.46
1:C:152:THR:HA	1:C:155:ILE:HD12	1.98	0.46
1:A:261:VAL:HG13	1:A:343:LEU:HD22	1.97	0.46
1:A:765:LYS:HD2	1:A:769:TRP:HE3	1.72	0.46
1:B:765:LYS:HA	1:B:769:TRP:CZ3	2.51	0.46
1:C:191:LYS:NZ	1:C:224:TYR:OH	2.45	0.46
1:C:366:LEU:HA	1:C:371:LEU:HA	1.98	0.46
1:C:680:MET:HB3	1:C:687:LEU:HG	1.98	0.46
1:D:8:GLY:HA2	1:D:51:ASP:HB3	1.97	0.46
1:A:508:GLY:HA3	1:A:728:LEU:HB3	1.98	0.46
1:B:27:HIS:HD2	1:B:271:GLU:OE1	1.98	0.46
1:B:76:VAL:HG13	1:B:314:VAL:HG13	1.98	0.46
1:B:27:HIS:HD2	1:B:271:GLU:CD	2.24	0.46
1:B:135:LEU:HG	1:B:383:LEU:HD22	1.97	0.46
1:C:134:ASP:OD2	1:C:377:TRP:NE1	2.41	0.45
1:C:515:LYS:HE3	1:C:723:THR:CB	2.46	0.45
1:C:652:GLU:HB3	1:C:703:TYR:HD1	1.81	0.45
1:A:142:ARG:HG3	1:A:169:ILE:HA	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:ASP:N	1:A:730:ASP:OD1	2.49	0.45
1:C:170:ARG:HH22	1:C:172:LYS:HB2	1.81	0.45
1:A:472:MET:HA	1:A:475:GLU:HB2	1.97	0.45
1:C:476:LEU:HD22	1:C:739:PRO:HD3	1.98	0.45
1:A:433:GLY:CA	1:A:768:TRP:CZ2	2.84	0.45
1:B:142:ARG:HH22	1:B:168:ASN:HB3	1.80	0.45
1:B:266:GLU:O	1:B:269:SER:OG	2.16	0.45
1:D:750:ILE:HA	1:D:753:LEU:HD12	1.98	0.45
1:C:194:ARG:HH12	1:C:224:TYR:HE1	1.64	0.45
1:D:502:LYS:HZ2	1:D:753:LEU:HD11	1.80	0.45
1:A:474:LYS:HA	1:A:477:ILE:HB	1.99	0.45
1:A:655:ALA:HB3	1:A:687:LEU:HD23	1.99	0.45
1:C:120:ASN:HB3	1:C:355:LEU:HB3	1.99	0.45
1:A:145:THR:HB	1:A:198:ILE:HG12	1.99	0.45
1:A:212:LYS:O	1:A:216:ALA:CB	2.65	0.45
1:D:472:MET:HE1	1:D:486:ALA:HB3	1.99	0.45
1:C:636:GLU:HB3	1:C:638:PRO:HB3	2.00	0.44
1:D:463:GLN:HA	1:D:469:TRP:HA	1.99	0.44
1:A:652:GLU:O	1:A:704:ALA:N	2.50	0.44
1:A:714:TYR:CD1	1:A:769:TRP:HD1	2.36	0.44
1:B:406:ILE:HB	1:B:482:ASP:H	1.82	0.44
1:D:146:VAL:HG12	1:D:171:LEU:HD13	1.99	0.44
1:D:309:ALA:HB1	1:D:312:MET:HE3	1.98	0.44
1:B:9:GLY:O	1:B:53:GLN:N	2.45	0.44
1:B:802:VAL:HG13	1:B:806:LEU:HB3	1.98	0.44
1:D:510:SER:HA	1:D:729:ILE:HG13	1.99	0.44
1:A:714:TYR:CD1	1:A:769:TRP:CD1	3.06	0.44
1:C:512:LEU:HD13	1:C:712:ILE:HG23	1.99	0.44
1:C:551:VAL:HG11	1:D:805:VAL:CG1	2.48	0.44
1:D:765:LYS:O	1:D:769:TRP:HB2	2.17	0.44
1:A:119:VAL:HG11	1:A:335:ILE:HG22	1.99	0.44
1:B:250:GLY:N	1:B:364:ILE:O	2.50	0.44
1:B:317:LEU:HD23	1:B:323:LYS:HE2	1.98	0.44
1:C:92:SER:OG	1:D:59:ASP:OD1	2.36	0.44
1:C:268:TRP:HD1	1:C:288:MET:HA	1.83	0.44
1:C:329:GLY:O	1:C:332:MET:HB2	2.17	0.44
1:C:439:LEU:HD22	1:C:485:VAL:HG11	2.00	0.44
1:C:514:ARG:HD3	1:C:699:LEU:HA	2.00	0.44
1:D:439:LEU:HD22	1:D:485:VAL:HG11	1.99	0.44
1:C:5:ILE:O	1:C:49:THR:OG1	2.31	0.44
1:D:184:ARG:HA	1:D:187:LEU:HB2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:ASP:OD1	1:A:381:ASP:N	2.50	0.44
1:A:764:MET:O	1:A:768:TRP:HD1	1.99	0.44
1:B:330:ARG:O	1:B:333:ASN:HB2	2.18	0.44
1:C:551:VAL:CG1	1:D:805:VAL:HG13	2.48	0.44
1:D:53:GLN:HE21	1:D:70:GLN:HG3	1.83	0.44
1:D:532:PRO:HA	1:D:535:TRP:HD1	1.83	0.44
1:C:10:ILE:HG12	1:C:53:GLN:HB2	1.99	0.43
1:C:120:ASN:O	1:C:356:ARG:N	2.43	0.43
1:D:694:GLY:HA3	1:D:705:LEU:HD13	2.00	0.43
1:A:124:ASP:HA	1:A:355:LEU:HD21	2.00	0.43
1:D:512:LEU:HB3	1:D:705:LEU:HB3	2.00	0.43
1:A:434:TYR:CG	1:A:769:TRP:HH2	2.35	0.43
1:C:321:ARG:HE	1:C:323:LYS:HB2	1.84	0.43
1:B:718:ARG:HH12	1:B:769:TRP:HA	1.83	0.43
1:C:87:THR:HG21	1:C:107:LYS:HE2	2.01	0.43
1:A:258:ASN:HD22	1:A:261:VAL:HG23	1.83	0.43
1:B:174:ARG:HD3	1:B:186:LEU:HD11	2.00	0.43
1:C:126:ALA:O	1:C:130:HIS:ND1	2.52	0.43
1:C:194:ARG:HD2	1:C:194:ARG:HA	1.71	0.43
1:C:645:LEU:HA	1:C:648:GLN:HE21	1.83	0.43
1:D:718:ARG:CZ	1:D:771:GLY:N	2.71	0.43
1:D:406:ILE:HG23	1:D:453:ARG:HH11	1.83	0.43
1:A:114:LYS:NZ	1:B:14:ALA:O	2.51	0.43
1:C:40:ARG:HD2	1:C:44:PRO:HA	2.00	0.43
1:B:27:HIS:NE2	1:B:271:GLU:HB3	2.33	0.43
1:A:313:THR:OG1	1:A:325:TRP:NE1	2.47	0.43
1:B:629:PHE:O	1:B:633:GLU:HG3	2.19	0.43
1:D:184:ARG:HA	1:D:187:LEU:HD12	2.01	0.43
1:D:305:THR:HA	1:D:308:ARG:HG2	2.00	0.43
1:B:142:ARG:H	1:B:197:ARG:NH2	2.17	0.43
1:B:240:PRO:HA	1:B:243:TYR:HD2	1.83	0.43
1:B:680:MET:HG2	1:B:687:LEU:HD21	2.01	0.43
1:C:708:GLU:OE2	1:C:734:TYR:OH	2.36	0.43
1:A:403:ARG:NH2	1:A:744:TYR:OH	2.52	0.42
1:C:473:VAL:HG13	1:C:498:ILE:HG12	2.02	0.42
1:D:657:LYS:HA	1:D:662:MET:HG3	2.00	0.42
1:A:254:LEU:HB3	1:A:256:VAL:HG23	2.02	0.42
1:B:5:ILE:O	1:B:49:THR:OG1	2.36	0.42
1:C:330:ARG:O	1:C:333:ASN:HB2	2.19	0.42
1:A:414:PRO:HG3	1:A:769:TRP:CG	2.46	0.42
1:C:26:GLU:HG2	1:C:52:ILE:HD13	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:439:LEU:HB2	1:C:485:VAL:HG21	2.00	0.42
1:C:470:ASN:HA	1:C:474:LYS:HE3	2.00	0.42
1:A:764:MET:HG2	1:A:768:TRP:CD1	2.55	0.42
1:B:331:PHE:O	1:B:335:ILE:N	2.50	0.42
1:C:155:ILE:HG12	1:D:151:SER:HB3	2.02	0.42
1:C:765:LYS:HD2	1:C:769:TRP:CG	2.55	0.42
1:D:185:PRO:HA	1:D:188:LYS:HD2	2.01	0.42
1:B:326:ARG:HH11	1:B:327:PHE:HA	1.84	0.42
1:D:150:ASP:OD1	1:D:150:ASP:N	2.52	0.42
1:A:738:THR:HG21	1:A:745:ARG:HB2	2.02	0.42
1:A:760:LYS:HA	1:A:763:ILE:HD12	2.01	0.42
1:C:183:SER:O	1:C:187:LEU:N	2.51	0.42
1:D:42:LEU:HD21	1:D:303:SER:HB3	2.02	0.42
1:A:514:ARG:HD3	1:A:699:LEU:HA	2.01	0.42
1:C:552:ILE:C	1:C:554:ARG:N	2.77	0.42
1:C:685:SER:O	1:C:697:ARG:NH1	2.47	0.42
1:D:512:LEU:HD22	1:D:705:LEU:HD23	2.00	0.42
1:A:657:LYS:HB2	1:A:687:LEU:HB3	2.02	0.42
1:A:670:ILE:HB	1:A:673:PHE:HD2	1.85	0.42
1:B:106:TRP:HB3	1:B:156:ARG:HE	1.84	0.42
1:C:184:ARG:HG2	1:C:187:LEU:HD12	2.02	0.42
1:C:185:PRO:HA	1:C:188:LYS:HD2	2.00	0.42
1:A:413:GLU:HA	1:A:414:PRO:HA	1.90	0.41
1:B:58:HIS:H	1:B:83:GLN:HG3	1.85	0.41
1:B:662:MET:HG2	1:B:677:TRP:HZ3	1.85	0.41
1:C:405:LEU:HD12	1:C:448:PHE:HB2	2.01	0.41
1:C:514:ARG:NH1	1:C:699:LEU:O	2.53	0.41
1:C:738:THR:HG21	1:C:745:ARG:HA	2.00	0.41
1:D:695:ILE:HG23	1:D:722:LEU:HD21	2.02	0.41
1:A:765:LYS:HA	1:A:769:TRP:HE3	1.83	0.41
1:C:206:MET:HE3	1:C:210:ILE:HD11	2.02	0.41
1:A:134:ASP:C	1:A:383:LEU:CD2	2.93	0.41
1:C:414:PRO:HG2	1:C:769:TRP:CD1	2.55	0.41
1:B:13:TYR:CE2	1:B:54:ARG:HD3	2.55	0.41
1:A:337:GLU:HA	1:A:351:LYS:HE3	2.03	0.41
1:A:434:TYR:HA	1:A:768:TRP:CD1	2.55	0.41
1:C:665:PHE:HA	1:C:668:SER:HB3	2.01	0.41
1:A:434:TYR:N	1:A:768:TRP:CE2	2.88	0.41
1:D:656:VAL:HG21	1:D:707:MET:HE3	2.01	0.41
1:A:184:ARG:HB2	1:A:213:GLN:HG2	2.03	0.41
1:A:462:ALA:N	1:A:470:ASN:OD1	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:SER:HB2	1:D:650:LYS:HG3	2.03	0.41
1:A:790:ILE:HG22	1:A:793:ILE:HB	2.02	0.41
1:B:116:THR:O	1:B:336:LYS:NZ	2.42	0.41
1:B:198:ILE:H	1:B:226:PHE:HD1	1.69	0.41
1:C:234:TYR:HD2	1:C:287:VAL:HG22	1.86	0.41
1:C:697:ARG:HG2	1:C:703:TYR:CG	2.55	0.41
1:D:60:SER:O	1:D:64:THR:OG1	2.33	0.41
1:D:406:ILE:O	1:D:482:ASP:N	2.54	0.41
1:B:58:HIS:NE2	1:B:83:GLN:OE1	2.53	0.41
1:B:297:ASP:OD2	1:B:343:LEU:N	2.45	0.41
1:C:446:LEU:HD12	1:C:448:PHE:HE1	1.85	0.41
1:B:613:PHE:O	1:B:617:ILE:HG12	2.21	0.41
1:B:670:ILE:H	1:B:670:ILE:HG13	1.57	0.41
1:C:764:MET:HE3	1:C:764:MET:HB2	1.92	0.41
1:D:27:HIS:HB3	1:D:268:TRP:HH2	1.85	0.41
1:D:514:ARG:HA	1:D:722:LEU:HA	2.03	0.41
1:D:638:PRO:O	1:D:640:ASP:N	2.54	0.41
1:A:148:TYR:O	1:A:176:LEU:N	2.48	0.41
1:A:226:PHE:HB2	1:A:248:LEU:HD12	2.02	0.41
1:A:36:ILE:O	1:A:40:ARG:NH2	2.38	0.40
1:A:145:THR:HG23	1:A:172:LYS:HB2	2.04	0.40
1:C:265:VAL:HG22	1:C:288:MET:HB3	2.02	0.40
1:D:65:LYS:HA	1:D:65:LYS:HD2	1.88	0.40
1:D:519:THR:OG1	1:D:520:ASN:N	2.54	0.40
1:D:511:ILE:HG13	1:D:729:ILE:HD11	2.02	0.40
1:D:755:LEU:O	1:D:759:ASP:N	2.55	0.40
1:A:305:THR:HA	1:A:308:ARG:HG2	2.04	0.40
1:B:13:TYR:HE2	1:B:54:ARG:HD3	1.87	0.40
1:B:35:ILE:HD11	1:B:296:TYR:HE1	1.85	0.40
1:D:603:SER:O	1:D:606:ILE:HG13	2.21	0.40
1:A:15:ASP:HB2	1:A:19:ALA:HB2	2.04	0.40
1:A:417:MET:N	1:A:432:GLU:O	2.53	0.40
1:A:434:TYR:HA	1:A:768:TRP:CE2	2.56	0.40
1:B:253:ILE:HG12	1:B:344:THR:HB	2.02	0.40
1:C:181:ASP:HB3	1:C:209:GLN:HG2	2.03	0.40
1:C:455:VAL:HG13	1:C:458:GLY:H	1.86	0.40
1:D:643:ASP:HA	1:D:672:THR:HG21	2.03	0.40
1:D:602:LEU:HB3	1:D:603:SER:H	1.72	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	705/832 (85%)	650 (92%)	54 (8%)	1 (0%)	48	83
1	B	705/832 (85%)	652 (92%)	47 (7%)	6 (1%)	14	51
1	C	705/832 (85%)	652 (92%)	46 (6%)	7 (1%)	12	49
1	D	705/832 (85%)	656 (93%)	47 (7%)	2 (0%)	36	72
All	All	2820/3328 (85%)	2610 (93%)	194 (7%)	16 (1%)	23	59

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	637	SER
1	B	638	PRO
1	D	807	VAL
1	B	351	LYS
1	B	517	ASN
1	B	603	SER
1	C	521	PRO
1	C	793	ILE
1	D	603	SER
1	A	43	LEU
1	C	553	ALA
1	C	526	PHE
1	B	43	LEU
1	C	806	LEU
1	C	485	VAL
1	C	638	PRO

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	619/715 (87%)	609 (98%)	10 (2%)	55	70
1	B	619/715 (87%)	614 (99%)	5 (1%)	73	80
1	C	618/715 (86%)	606 (98%)	12 (2%)	50	67
1	D	619/715 (87%)	608 (98%)	11 (2%)	51	68
All	All	2475/2860 (86%)	2437 (98%)	38 (2%)	55	72

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	PRO
1	A	100	PRO
1	A	119	VAL
1	A	136	VAL
1	A	161	ILE
1	A	221	THR
1	A	381	ASP
1	A	409	THR
1	A	698	THR
1	A	805	VAL
1	B	221	THR
1	B	511	ILE
1	B	532	PRO
1	B	602	LEU
1	B	807	VAL
1	C	4	VAL
1	C	119	VAL
1	C	173	ILE
1	C	248	LEU
1	C	270	MET
1	C	317	LEU
1	C	364	ILE
1	C	507	LEU
1	C	522	SER
1	C	523	VAL
1	C	552	ILE
1	C	619	ILE
1	D	78	ILE
1	D	87	THR
1	D	152	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	348	VAL
1	D	507	LEU
1	D	527	LEU
1	D	551	VAL
1	D	602	LEU
1	D	603	SER
1	D	806	LEU
1	D	807	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	108	HIS
1	A	109	HIS
1	A	175	GLN
1	A	213	GLN
1	A	258	ASN
1	A	300	HIS
1	A	311	GLN
1	A	315	ASN
1	A	479	HIS
1	A	690	ASN
1	A	696	GLN
1	A	754	GLN
1	B	20	GLN
1	B	45	ASN
1	B	103	GLN
1	B	113	ASN
1	B	247	ASN
1	B	255	ASN
1	B	350	ASN
1	B	402	ASN
1	B	428	ASN
1	B	468	GLN
1	B	717	GLN
1	C	3	HIS
1	C	18	ASN
1	C	53	GLN
1	C	58	HIS
1	C	70	GLN
1	C	95	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	108	HIS
1	C	175	GLN
1	C	213	GLN
1	C	247	ASN
1	C	311	GLN
1	C	322	HIS
1	C	339	GLN
1	C	402	ASN
1	C	470	ASN
1	D	20	GLN
1	D	45	ASN
1	D	95	ASN
1	D	204	HIS
1	D	209	GLN
1	D	225	HIS
1	D	315	ASN
1	D	320	HIS
1	D	322	HIS
1	D	517	ASN
1	D	696	GLN
1	D	721	ASN
1	D	754	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

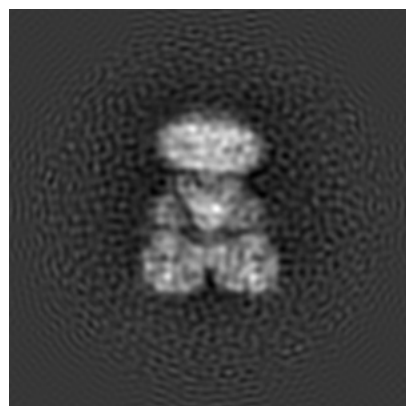
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0839. These allow visual inspection of the internal detail of the map and identification of artifacts.

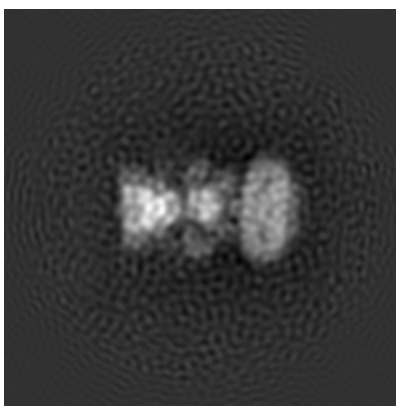
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

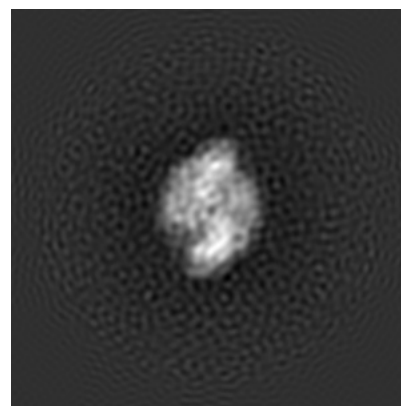
6.1.1 Primary map



X

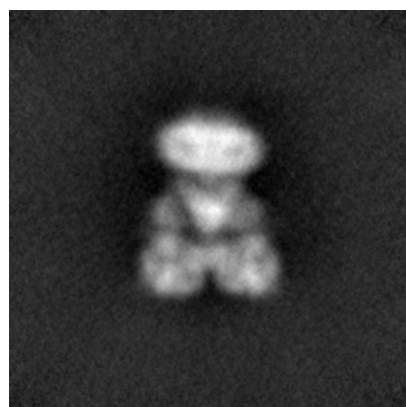


Y

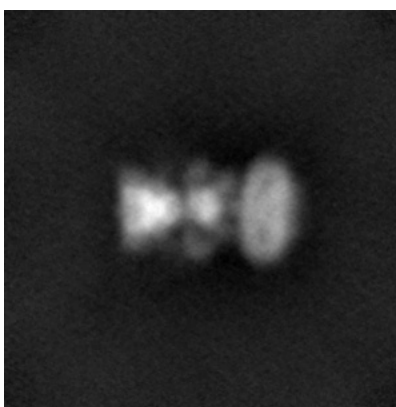


Z

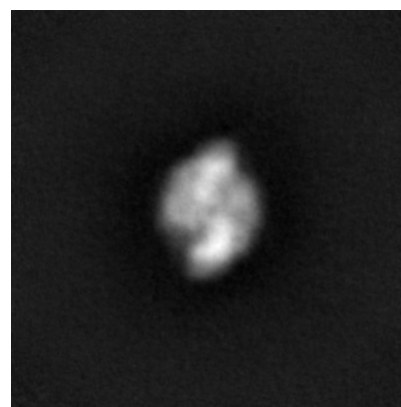
6.1.2 Raw map



X



Y

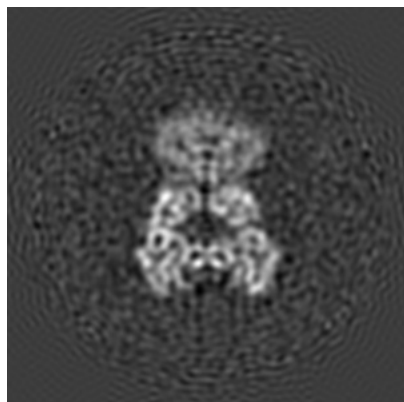


Z

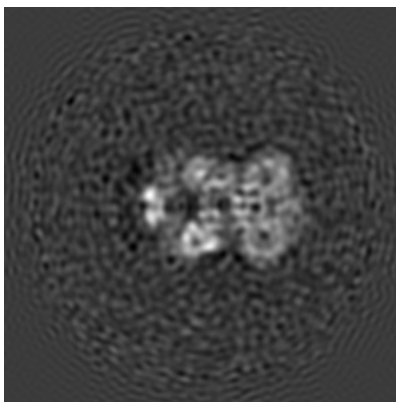
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

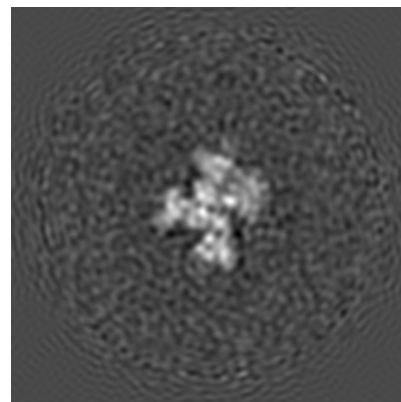
6.2.1 Primary map



X Index: 165

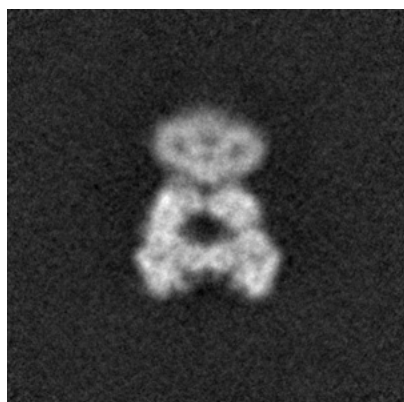


Y Index: 165

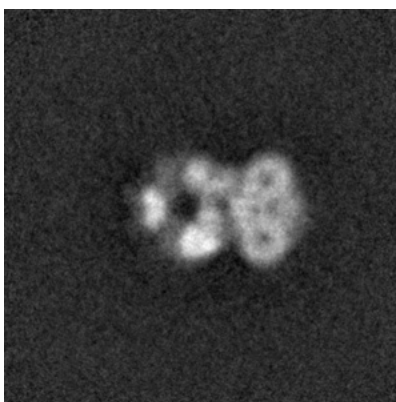


Z Index: 165

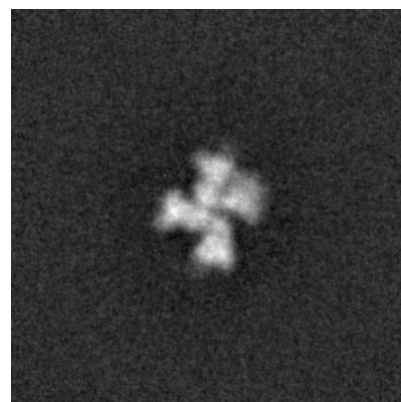
6.2.2 Raw map



X Index: 165



Y Index: 165

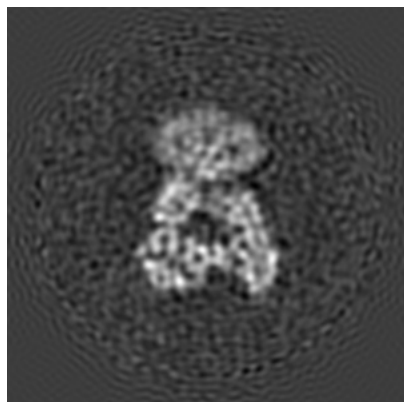


Z Index: 165

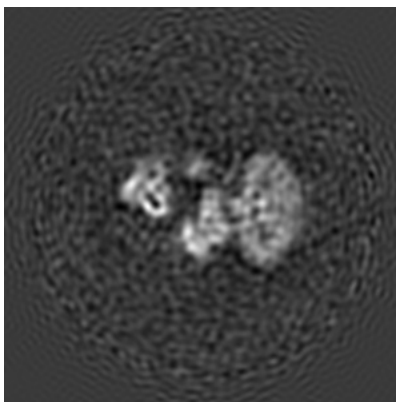
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

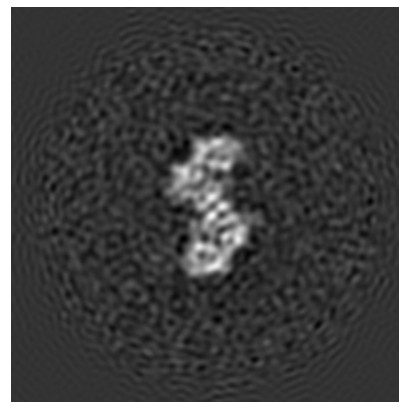
6.3.1 Primary map



X Index: 170

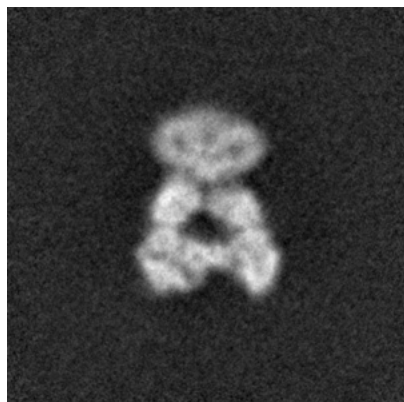


Y Index: 157

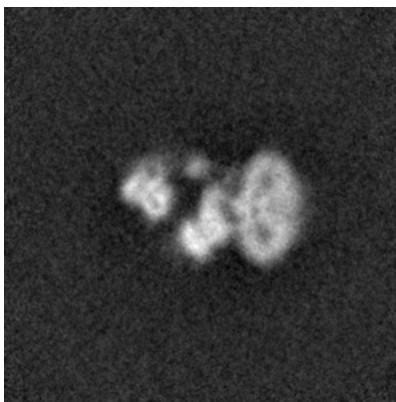


Z Index: 118

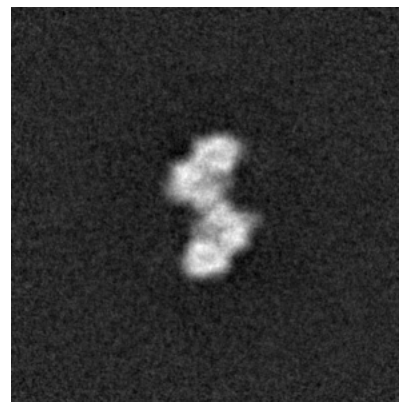
6.3.2 Raw map



X Index: 169



Y Index: 157

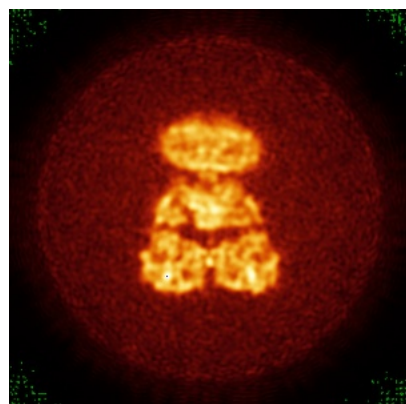


Z Index: 117

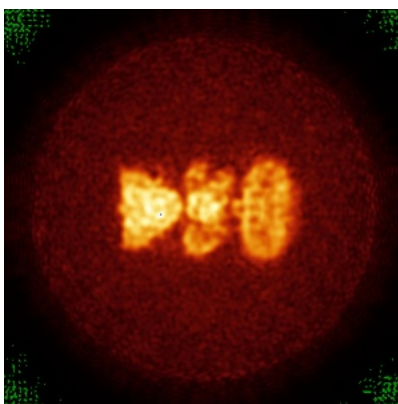
The images above show the largest variance slices of the map in three orthogonal directions.

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

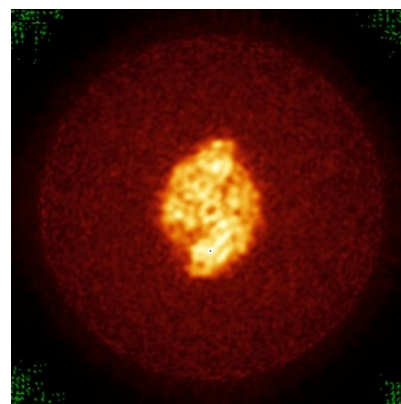
6.4.1 Primary map



X



Y

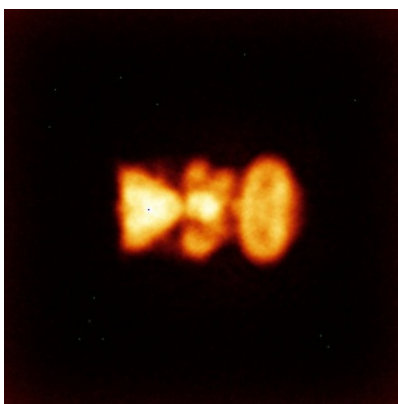


Z

6.4.2 Raw map



X



Y

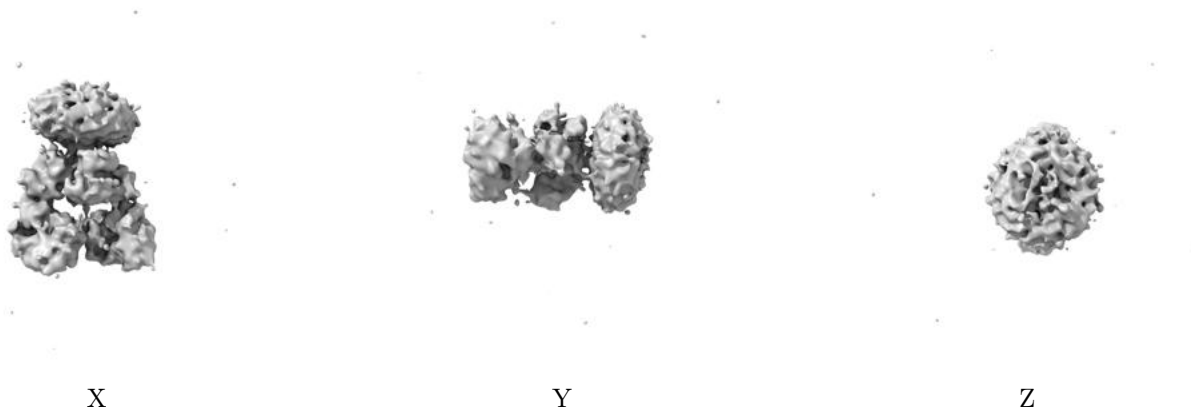


Z

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.

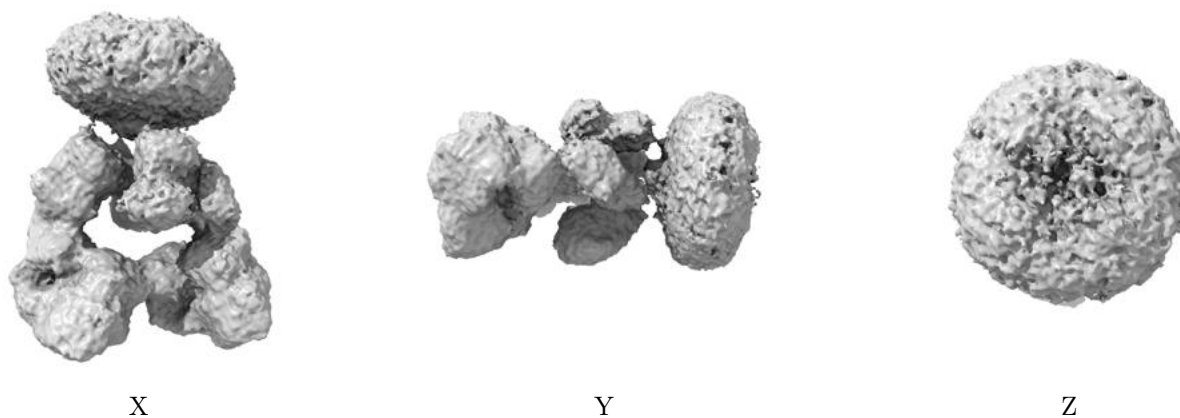
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.936. 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.

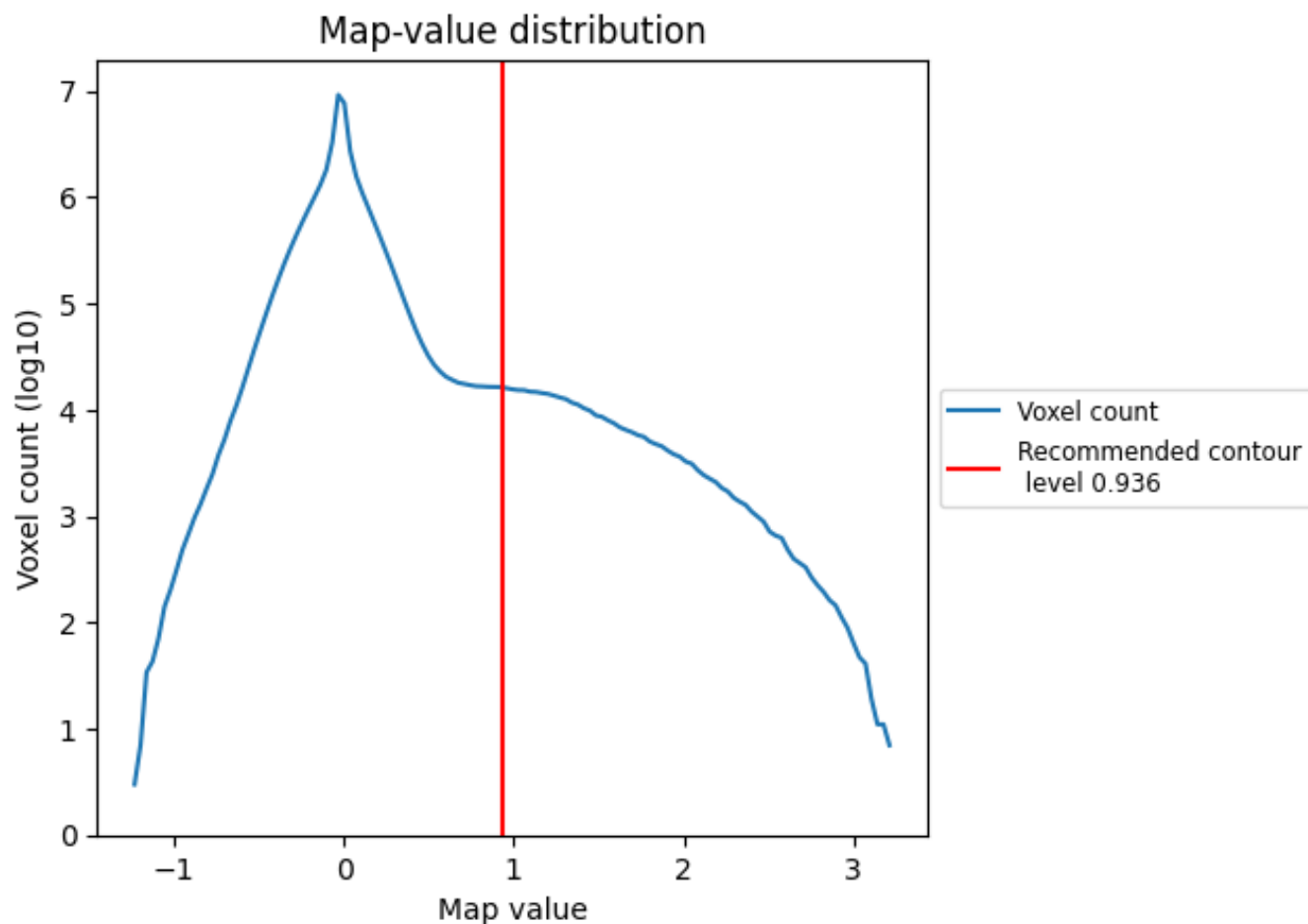
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

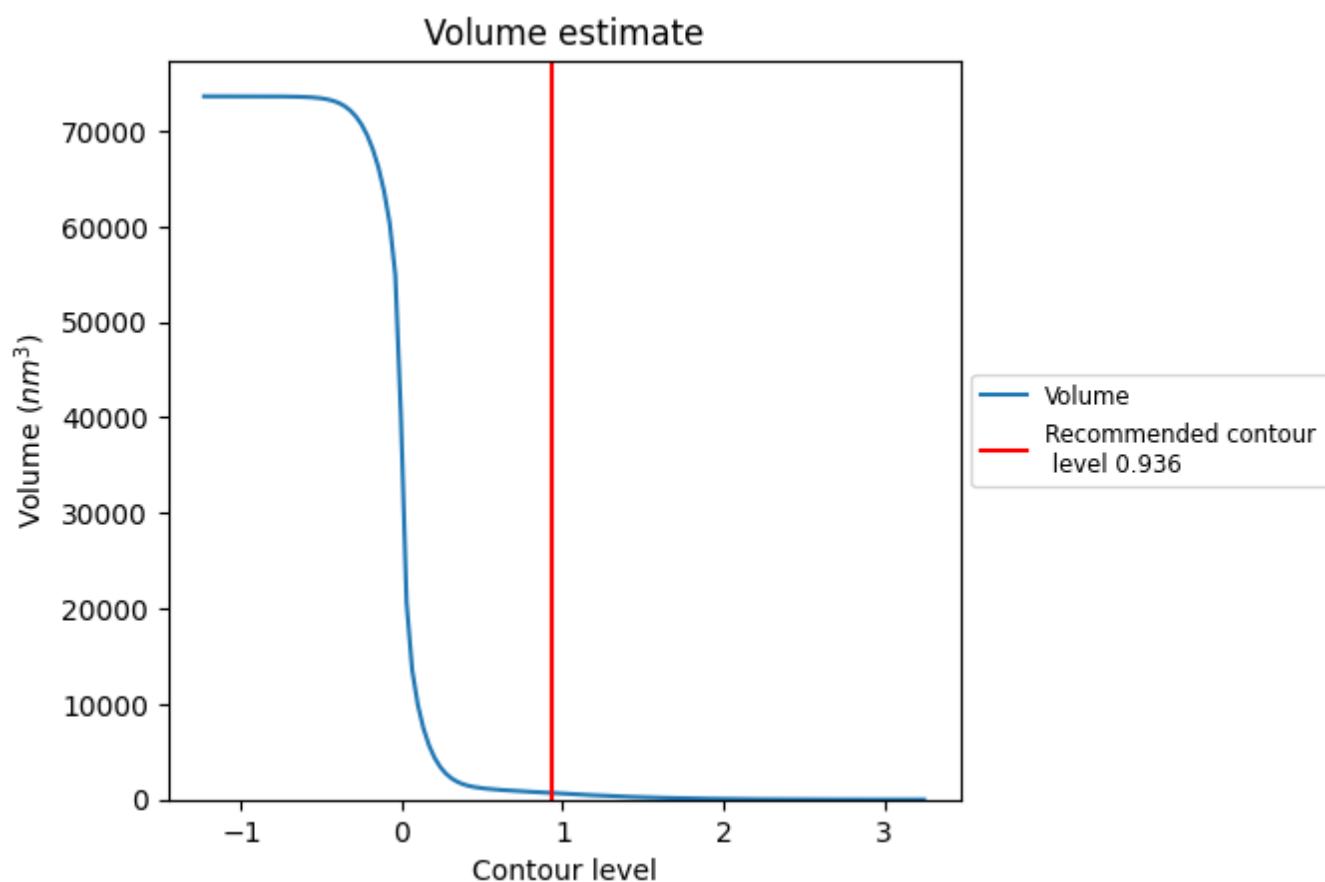
This section contains the results of statistical analysis of the map.

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.

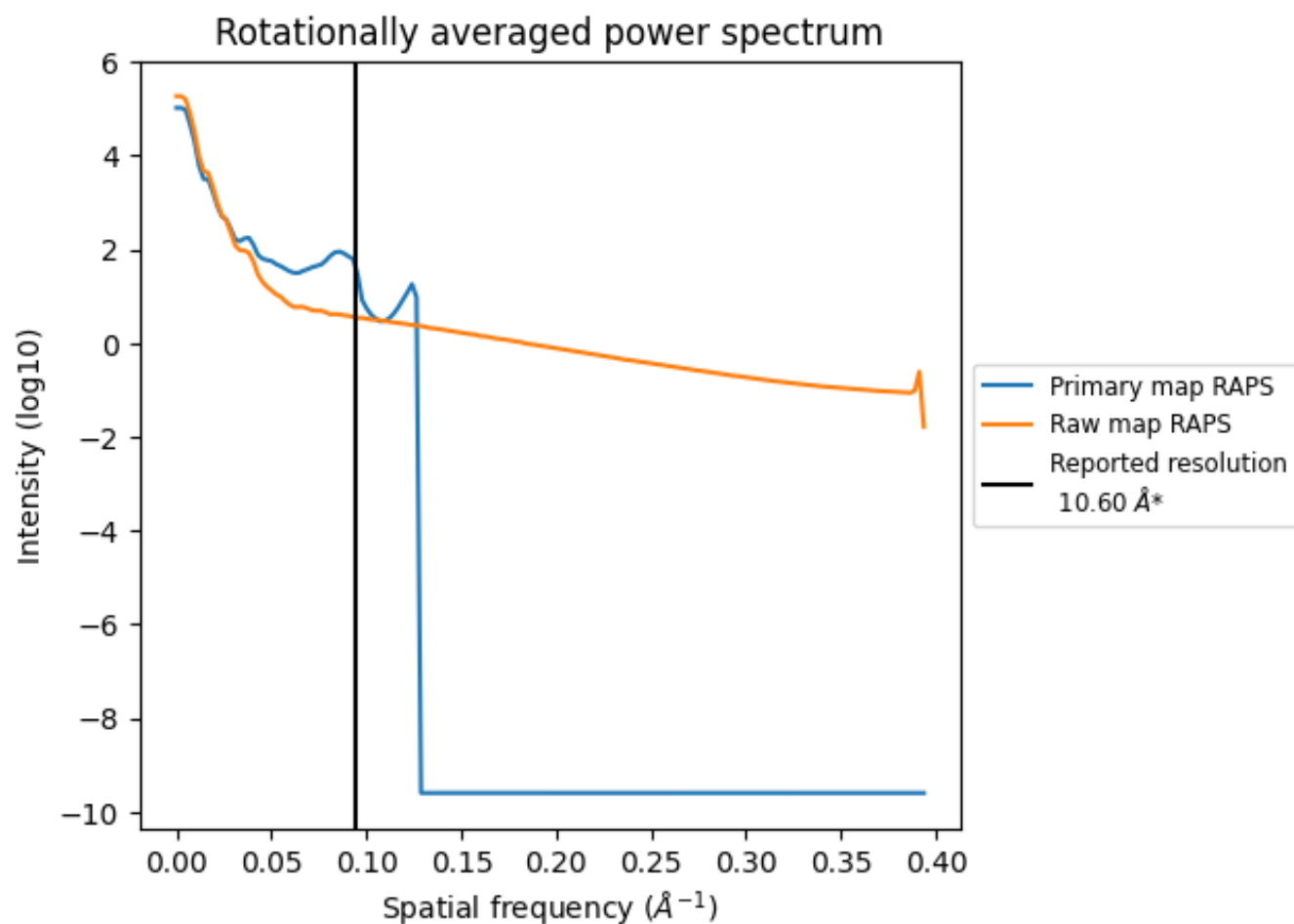
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 683 nm³; this corresponds to an approximate mass of 617 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 ⓘ

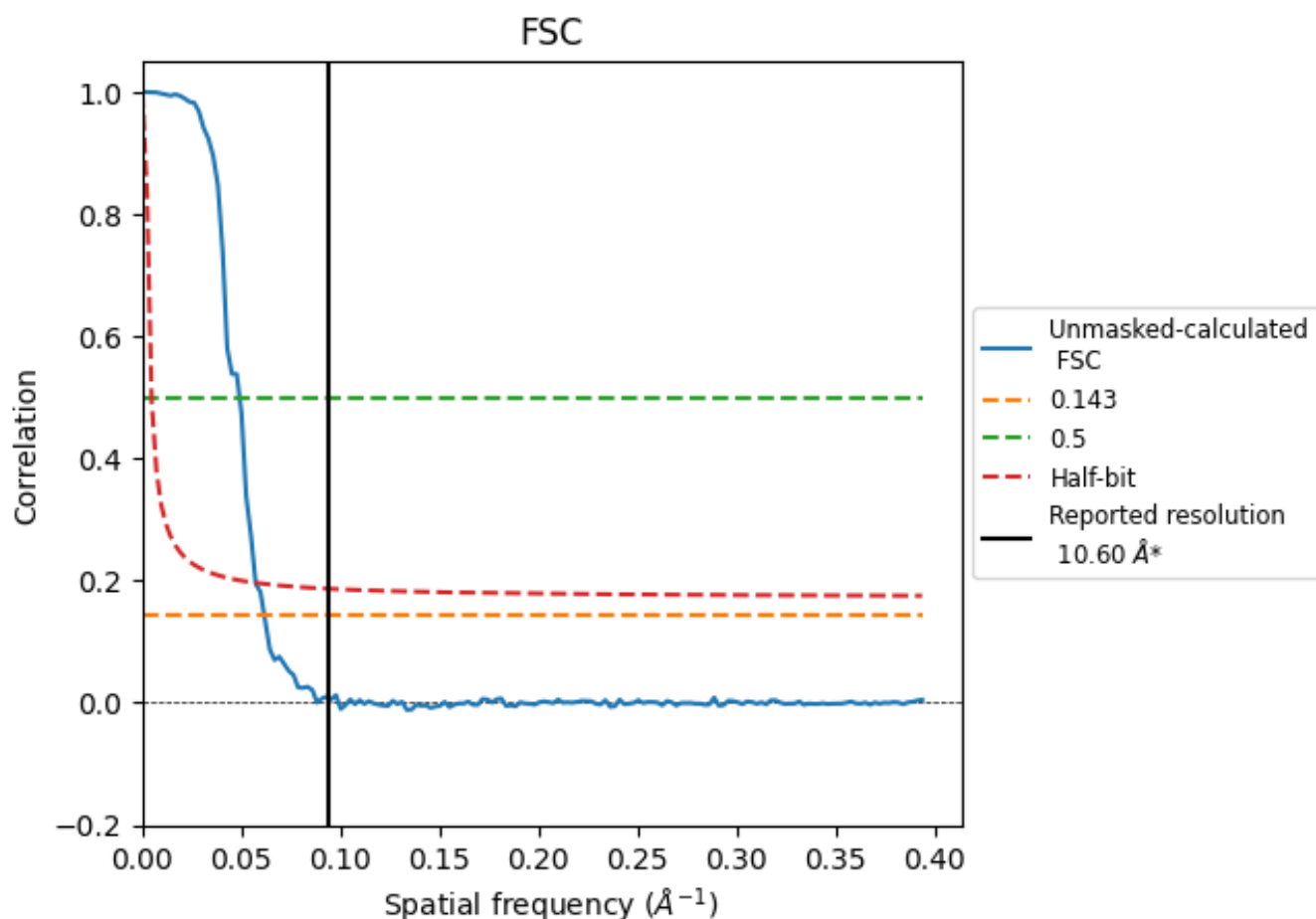


*Reported resolution corresponds to spatial frequency of 0.094 Å⁻¹

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 0.094 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

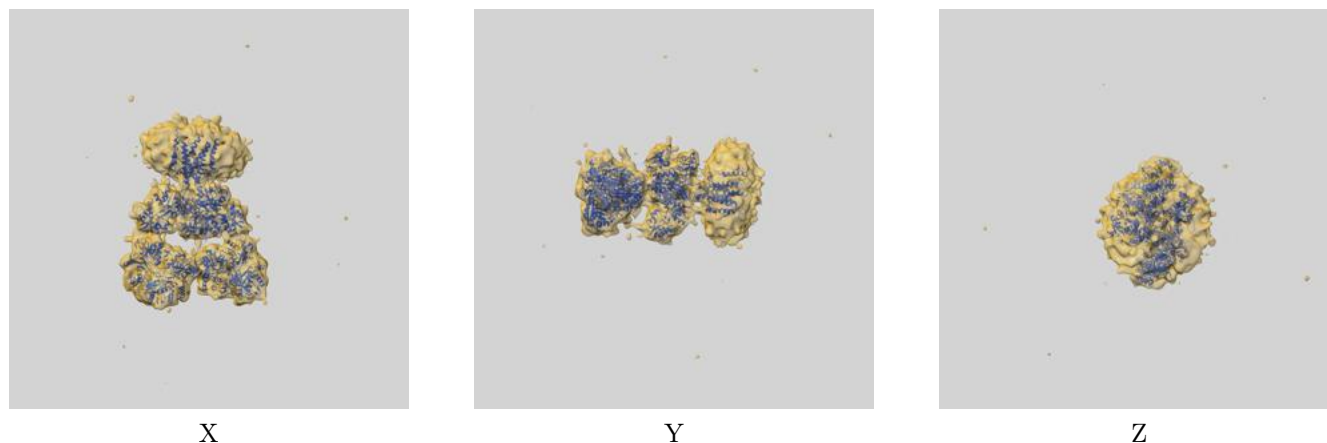
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	16.23	20.33	17.48

*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 16.23 differs from the reported value 10.6 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0839 and PDB model 6L6F. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



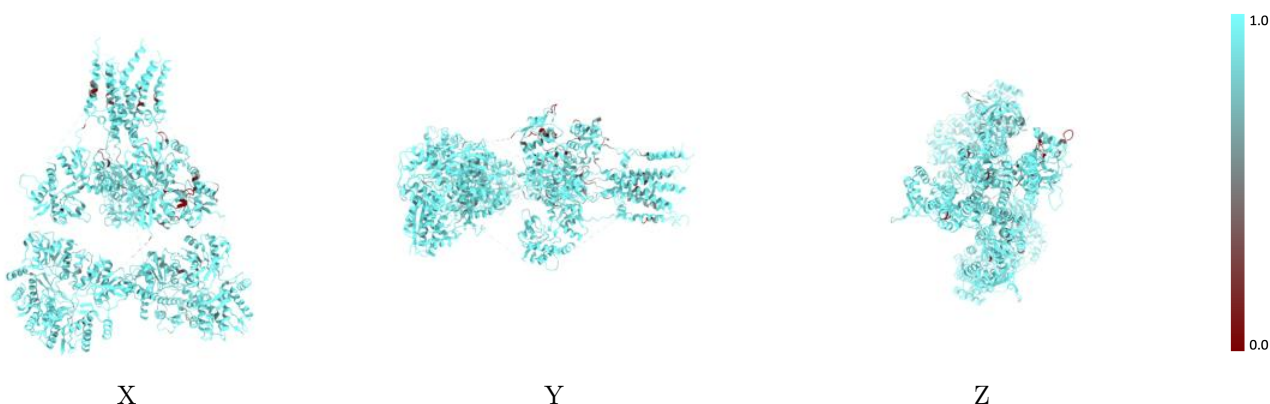
The images above show the 3D surface view of the map at the recommended contour level 0.936 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



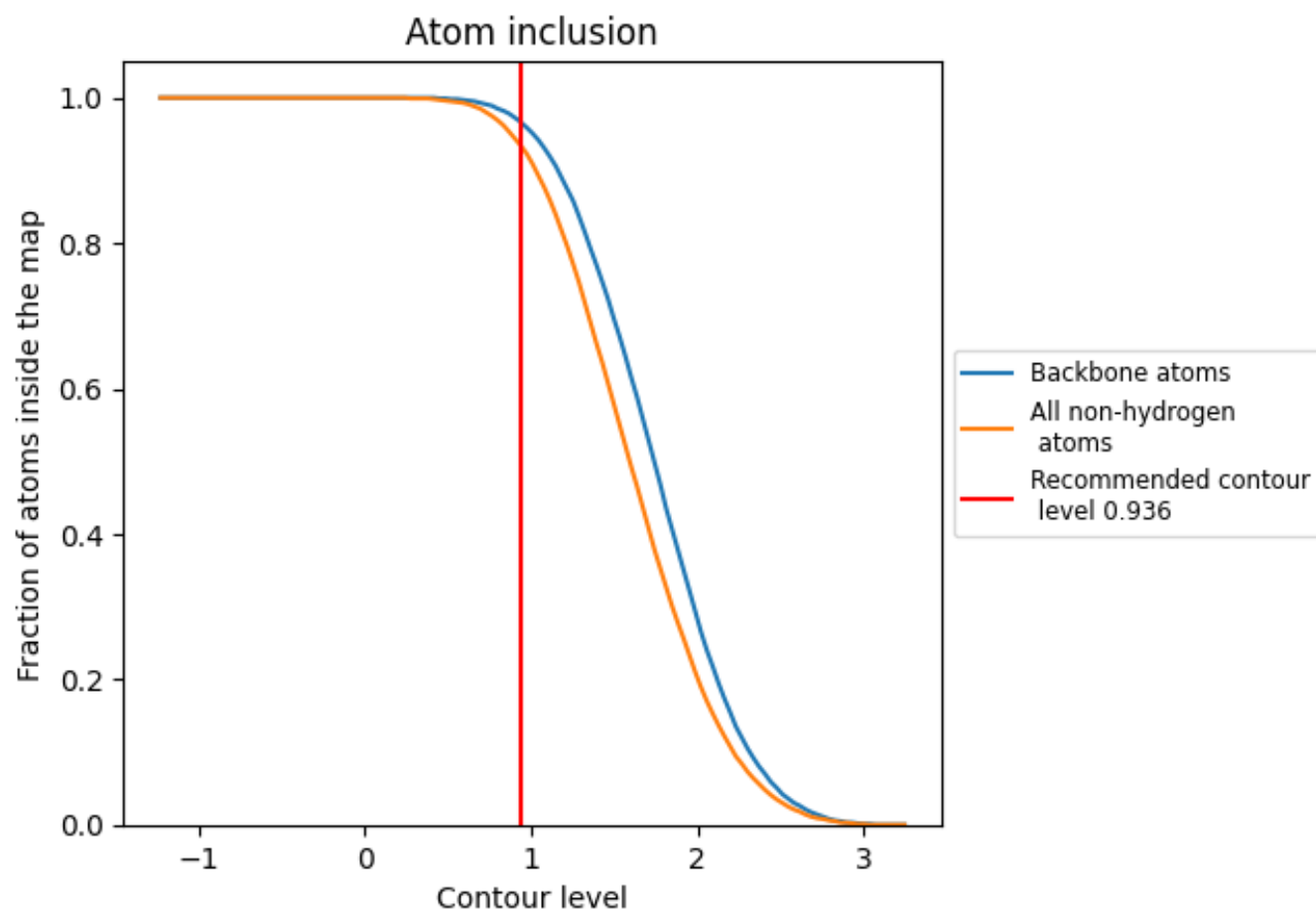
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.936).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 94% 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 (0.936) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9350	0.1340
A	0.9490	0.1360
B	0.9070	0.1340
C	0.9320	0.1300
D	0.9510	0.1370

