



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 09:04 AM UTC

PDB ID : 7EYE / pdb_00007eye
EMDB ID : EMD-31382
Title : Cryo-EM (SPA) structure of Nup155 N-terminus (19-863) at 5.1 Angstrom resolution
Authors : Niranjan, S.
Deposited on : 2021-05-30
Resolution : 5.10 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

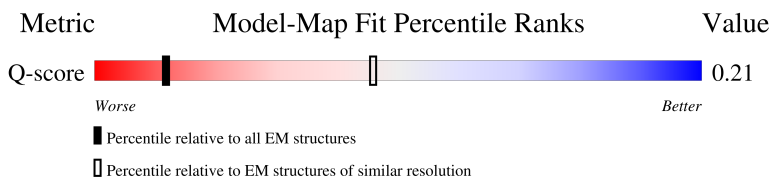
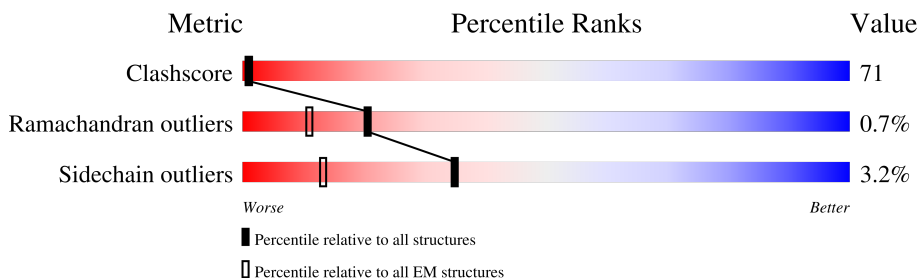
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.10 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	844 (4.60 - 5.60)

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	1114	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5426 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 G protein/GFP fusion protein,Nuclear pore complex protein Nup155.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	696	5426	3460	921	1012	33	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	SER	-	linker	UNP B7UCZ6
A	-10	GLY	-	linker	UNP B7UCZ6
A	-9	LEU	-	linker	UNP B7UCZ6
A	-8	ARG	-	linker	UNP B7UCZ6
A	-7	SER	-	linker	UNP B7UCZ6
A	-6	ARG	-	linker	UNP B7UCZ6
A	-5	ALA	-	linker	UNP B7UCZ6
A	-4	GLN	-	linker	UNP B7UCZ6
A	-3	ALA	-	linker	UNP B7UCZ6
A	-2	SER	-	linker	UNP B7UCZ6
A	-1	ASN	-	linker	UNP B7UCZ6
A	0	SER	-	linker	UNP B7UCZ6

A808	E809	Q811	R812	E813	L814	E816	Q817	L818	T821	T822	F823	K824	L826	V827	R828	R829	H830	R831	E832	L833	T834	G835	A836	L837	I838	S839	S840	L841	I842	H843	C844	Y845	D848	H849	A850	A851	V852	D853	G854	I855	S856	L857	H858	L859	Q860	D861	I862	C863																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
GLY	PHE	MET	ARG	LYS	SER	PRO	GLY	ASN	ASN	GLY	ASN	PRO	THR	GLN	GLN	MET	GLN	GLN	GLN	GLN	LEU	GLN	ARG	K766	F767	H768	E769	A770	G771	L772	S773	E774	K775	I776	S777	L778	Q779	A780	I781	Q782	L783	V784	R785	R786	K787	S788	Y789	Q790	A791	L792	A793	L794	L797	L798	C799	E800	H801	Q802	F803	T804	I805	I806	Y807																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
ARG	ILE	PHE	LYS	ILE	GLN	ASN	GLY	ASN	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88595	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 ($e^-/\text{\AA}^2$)	1.15	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	6.639	Depositor
Minimum map value	-2.914	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.144	Depositor
Recommended contour level	0.37	Depositor
Map size (Å)	197.52, 197.52, 197.52	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.823, 0.823, 0.823	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.46	0/5535	0.92	20/7507 (0.3%)

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	2

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	808	ALA	N-CA-C	8.94	124.09	111.30
1	A	807	VAL	CA-C-N	-8.16	109.46	123.25
1	A	807	VAL	C-N-CA	-8.16	109.46	123.25
1	A	272	THR	N-CA-C	8.07	120.16	111.36
1	A	276	ASP	N-CA-C	7.42	121.30	111.28
1	A	810	LEU	N-CA-C	7.02	121.79	112.25
1	A	268	LEU	N-CA-C	6.59	118.46	111.28
1	A	201	LEU	CA-C-N	6.49	126.84	119.83
1	A	201	LEU	C-N-CA	6.49	126.84	119.83
1	A	524	LEU	N-CA-C	-5.53	105.26	111.28
1	A	828	ILE	CA-C-N	-5.53	110.99	121.54
1	A	828	ILE	C-N-CA	-5.53	110.99	121.54
1	A	799	CYS	CA-C-N	5.50	131.75	122.79
1	A	799	CYS	C-N-CA	5.50	131.75	122.79
1	A	280	LEU	N-CA-C	5.15	119.53	112.68
1	A	251	CYS	CA-C-N	-5.13	113.82	122.29
1	A	251	CYS	C-N-CA	-5.13	113.82	122.29
1	A	811	GLN	N-CA-C	5.10	121.67	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	467	LEU	CA-C-N	-5.06	112.29	121.14
1	A	467	LEU	C-N-CA	-5.06	112.29	121.14

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	271	PHE	Peptide
1	A	338	VAL	Peptide

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	5426	0	5435	769	0
All	All	5426	0	5435	769	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 71.

All (769) 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:A:262:SER:CB	1:A:268:LEU:HD22	1.43	1.46
1:A:276:ASP:O	1:A:278:PRO:HD3	1.30	1.30
1:A:89:LEU:CD1	1:A:94:VAL:HG21	1.74	1.17
1:A:262:SER:HB3	1:A:268:LEU:HD22	1.16	1.16
1:A:262:SER:HB2	1:A:268:LEU:HD22	1.16	1.12
1:A:801:HIS:CD2	1:A:802:GLN:H	1.65	1.12
1:A:335:ASP:HA	1:A:338:VAL:HG22	1.22	1.11
1:A:375:PHE:H	1:A:383:ASN:HB2	1.16	1.11
1:A:262:SER:HB3	1:A:268:LEU:CD2	1.83	1.07
1:A:262:SER:CB	1:A:268:LEU:CD2	2.31	1.07
1:A:729:GLY:O	1:A:778:LEU:HD11	1.52	1.07
1:A:334:ILE:HD12	1:A:337:SER:OG	1.55	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ASP:HA	1:A:338:VAL:CG2	1.86	1.05
1:A:554:LEU:HD21	1:A:565:VAL:HG22	1.39	1.04
1:A:54:ASN:OD1	1:A:330:ILE:HG22	1.59	1.02
1:A:520:LEU:HA	1:A:523:LEU:HD12	1.42	1.00
1:A:56:THR:HG21	1:A:388:VAL:HG22	1.45	0.99
1:A:524:LEU:HD22	1:A:565:VAL:HG23	1.40	0.99
1:A:519:GLN:O	1:A:523:LEU:HG	1.62	0.98
1:A:335:ASP:CA	1:A:338:VAL:HG22	1.94	0.96
1:A:89:LEU:HD13	1:A:94:VAL:HG21	1.45	0.96
1:A:105:MET:H	1:A:118:THR:HB	1.30	0.95
1:A:262:SER:OG	1:A:268:LEU:HD13	1.65	0.94
1:A:106:MET:HG2	1:A:503:LEU:HD21	1.48	0.94
1:A:801:HIS:CG	1:A:802:GLN:H	1.85	0.93
1:A:106:MET:HA	1:A:117:LEU:HA	1.51	0.92
1:A:100:MET:HG2	1:A:120:ASP:H	1.32	0.92
1:A:375:PHE:O	1:A:376:ARG:NE	2.03	0.92
1:A:262:SER:HB2	1:A:268:LEU:CD2	1.97	0.91
1:A:89:LEU:HD13	1:A:94:VAL:CG2	2.00	0.91
1:A:123:ILE:HD13	1:A:165:LEU:HD21	1.52	0.90
1:A:393:PRO:HG2	1:A:420:MET:HB3	1.51	0.90
1:A:724:ASN:O	1:A:728:ALA:HB3	1.71	0.90
1:A:121:SER:O	1:A:122:ASP:HB3	1.70	0.89
1:A:89:LEU:CD1	1:A:94:VAL:CG2	2.50	0.89
1:A:374:PRO:HA	1:A:383:ASN:H	1.36	0.89
1:A:164:LEU:HD11	1:A:175:ILE:HG23	1.54	0.88
1:A:57:VAL:HB	1:A:390:VAL:HG12	1.56	0.87
1:A:730:GLY:HA3	1:A:778:LEU:HD12	1.55	0.87
1:A:374:PRO:HA	1:A:383:ASN:N	1.88	0.87
1:A:59:GLY:HA2	1:A:392:LEU:HD13	1.55	0.87
1:A:565:VAL:HA	1:A:568:TRP:HD1	1.41	0.86
1:A:831:LYS:HZ1	1:A:861:ASP:HB3	1.40	0.86
1:A:334:ILE:O	1:A:338:VAL:HG13	1.74	0.86
1:A:156:ILE:HG21	1:A:240:TYR:HE1	1.39	0.85
1:A:396:PHE:HZ	1:A:407:LYS:H	1.20	0.85
1:A:183:LEU:HG	1:A:197:GLY:HA3	1.58	0.85
1:A:801:HIS:CD2	1:A:802:GLN:N	2.44	0.85
1:A:464:ILE:HB	1:A:500:PHE:HE1	1.41	0.85
1:A:769:GLU:HA	1:A:772:LEU:HD13	1.58	0.85
1:A:766:LYS:HA	1:A:770:ALA:HB3	1.57	0.85
1:A:301:GLN:HG3	1:A:317:SER:HA	1.60	0.84
1:A:724:ASN:O	1:A:728:ALA:N	2.08	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ILE:HA	1:A:362:THR:HA	1.59	0.84
1:A:283:ALA:HB3	1:A:292:TYR:HB2	1.58	0.84
1:A:262:SER:HB3	1:A:268:LEU:HB2	1.59	0.84
1:A:57:VAL:HA	1:A:390:VAL:H	1.40	0.83
1:A:729:GLY:O	1:A:778:LEU:CD1	2.26	0.83
1:A:724:ASN:O	1:A:728:ALA:CB	2.27	0.82
1:A:285:ASP:HB3	1:A:290:ILE:HB	1.61	0.82
1:A:142:GLU:HB3	1:A:170:PRO:HD2	1.61	0.82
1:A:102:CYS:H	1:A:120:ASP:HB3	1.45	0.81
1:A:375:PHE:N	1:A:383:ASN:HB2	1.92	0.81
1:A:262:SER:HB3	1:A:268:LEU:CG	2.10	0.80
1:A:797:LEU:HA	1:A:800:GLU:HB2	1.63	0.80
1:A:182:ASN:HA	1:A:197:GLY:H	1.46	0.80
1:A:101:GLN:H	1:A:120:ASP:CG	1.90	0.80
1:A:229:ALA:HB1	1:A:279:ILE:HG21	1.62	0.79
1:A:123:ILE:HD12	1:A:147:VAL:HG11	1.65	0.79
1:A:54:ASN:O	1:A:57:VAL:HG22	1.83	0.78
1:A:100:MET:HG2	1:A:120:ASP:N	1.99	0.78
1:A:768:HIS:CD2	1:A:769:GLU:HG2	2.18	0.78
1:A:257:SER:HA	1:A:314:ARG:HH12	1.49	0.78
1:A:112:ILE:HD12	1:A:114:ARG:HD2	1.64	0.77
1:A:663:HIS:HA	1:A:666:ILE:HD12	1.66	0.77
1:A:818:LEU:HA	1:A:833:LEU:HD11	1.67	0.77
1:A:90:PRO:HG2	1:A:93:LEU:HD12	1.66	0.76
1:A:64:ASP:HA	1:A:396:PHE:CD2	2.20	0.76
1:A:276:ASP:O	1:A:278:PRO:CD	2.24	0.76
1:A:797:LEU:HD21	1:A:857:LEU:HD12	1.66	0.76
1:A:53:ASN:OD1	1:A:54:ASN:N	2.19	0.75
1:A:327:ALA:HA	1:A:330:ILE:CD1	2.16	0.75
1:A:726:GLN:HA	1:A:732:LEU:CD1	2.16	0.75
1:A:67:LEU:HD13	1:A:451:THR:HG21	1.68	0.75
1:A:724:ASN:CB	1:A:728:ALA:HB2	2.17	0.75
1:A:109:PHE:HB3	1:A:149:LEU:HD22	1.69	0.74
1:A:725:SER:HA	1:A:731:PRO:HB2	1.69	0.74
1:A:538:PHE:O	1:A:542:HIS:ND1	2.20	0.74
1:A:262:SER:HB3	1:A:268:LEU:CB	2.18	0.74
1:A:93:LEU:HD11	1:A:126:TRP:CD2	2.23	0.74
1:A:79:PRO:O	1:A:519:GLN:NE2	2.21	0.74
1:A:91:PRO:O	1:A:95:GLU:HG3	1.88	0.74
1:A:823:PHE:O	1:A:825:ASP:N	2.22	0.73
1:A:144:ILE:HA	1:A:168:ALA:O	1.88	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:CYS:O	1:A:384:THR:N	2.21	0.72
1:A:327:ALA:HA	1:A:330:ILE:HD12	1.69	0.72
1:A:391:ARG:NH2	1:A:447:GLU:OE1	2.22	0.72
1:A:101:GLN:N	1:A:120:ASP:OD2	2.22	0.72
1:A:521:ARG:HH11	1:A:522:HIS:HE1	1.36	0.72
1:A:233:GLY:H	1:A:277:ASP:CG	1.97	0.72
1:A:811:GLN:HG3	1:A:811:GLN:O	1.89	0.72
1:A:674:MET:HE1	1:A:714:LEU:HD11	1.71	0.72
1:A:724:ASN:HB3	1:A:728:ALA:HB2	1.72	0.72
1:A:210:THR:HA	1:A:253:LYS:HD2	1.71	0.71
1:A:720:PHE:HD2	1:A:721:LEU:HD22	1.55	0.71
1:A:276:ASP:C	1:A:278:PRO:HD3	2.15	0.71
1:A:835:GLY:HA2	1:A:838:ILE:HD12	1.70	0.71
1:A:722:ASP:OD2	1:A:786:ARG:NH1	2.23	0.71
1:A:105:MET:N	1:A:118:THR:HB	2.04	0.71
1:A:108:VAL:HG13	1:A:503:LEU:HB2	1.71	0.71
1:A:237:GLU:OE1	1:A:256:HIS:NE2	2.23	0.71
1:A:731:PRO:HD3	1:A:778:LEU:CD1	2.20	0.71
1:A:81:ILE:HG22	1:A:450:MET:HE3	1.73	0.70
1:A:520:LEU:HA	1:A:523:LEU:CD1	2.20	0.70
1:A:65:TYR:HH	1:A:432:TRP:CD1	2.09	0.70
1:A:666:ILE:HG21	1:A:781:ILE:HD13	1.74	0.70
1:A:811:GLN:O	1:A:814:LEU:N	2.24	0.70
1:A:241:GLN:CD	1:A:243:GLU:H	1.99	0.70
1:A:343:VAL:N	1:A:361:VAL:O	2.24	0.70
1:A:663:HIS:CE1	1:A:781:ILE:HD11	2.27	0.70
1:A:499:LYS:HA	1:A:512:HIS:HA	1.72	0.70
1:A:125:MET:N	1:A:135:ALA:O	2.23	0.69
1:A:373:CYS:O	1:A:383:ASN:N	2.24	0.69
1:A:93:LEU:O	1:A:97:PHE:CB	2.40	0.69
1:A:801:HIS:CG	1:A:802:GLN:N	2.50	0.69
1:A:731:PRO:HD3	1:A:778:LEU:HD13	1.73	0.69
1:A:38:ARG:NE	1:A:479:ASP:OD2	2.26	0.69
1:A:375:PHE:H	1:A:383:ASN:CB	1.98	0.69
1:A:107:GLY:HA3	1:A:116:TRP:CE2	2.27	0.69
1:A:157:PHE:CD1	1:A:161:VAL:HB	2.27	0.69
1:A:262:SER:CB	1:A:268:LEU:HD13	2.22	0.69
1:A:244:ALA:HB2	1:A:250:ARG:HE	1.55	0.69
1:A:260:SER:O	1:A:262:SER:N	2.25	0.69
1:A:110:PRO:HG3	1:A:462:SER:HB3	1.72	0.68
1:A:121:SER:O	1:A:122:ASP:CB	2.34	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ALA:HA	1:A:173:ILE:HG13	1.74	0.68
1:A:726:GLN:HA	1:A:732:LEU:HD11	1.75	0.68
1:A:77:ASN:ND2	1:A:526:SER:HB3	2.08	0.68
1:A:362:THR:HG23	1:A:368:LEU:HD11	1.75	0.68
1:A:235:LEU:N	1:A:257:SER:OG	2.26	0.68
1:A:257:SER:HA	1:A:314:ARG:HH22	1.57	0.68
1:A:429:ASP:OD2	1:A:458:SER:N	2.26	0.68
1:A:42:ASP:O	1:A:46:LEU:N	2.21	0.68
1:A:161:VAL:HG22	1:A:201:LEU:HD11	1.76	0.68
1:A:124:PHE:HD2	1:A:137:PHE:H	1.42	0.67
1:A:726:GLN:HG3	1:A:732:LEU:HD11	1.76	0.67
1:A:53:ASN:HB3	1:A:55:PRO:HD2	1.76	0.67
1:A:110:PRO:HG3	1:A:462:SER:CB	2.24	0.67
1:A:570:THR:HG22	1:A:720:PHE:HE1	1.60	0.67
1:A:342:ILE:HD11	1:A:368:LEU:HD22	1.76	0.67
1:A:279:ILE:HA	1:A:295:SER:HA	1.76	0.67
1:A:134:LEU:HB2	1:A:136:TYR:CE1	2.29	0.67
1:A:93:LEU:HG	1:A:134:LEU:HD21	1.77	0.67
1:A:478:LYS:HE2	1:A:488:VAL:HA	1.75	0.67
1:A:347:VAL:HA	1:A:358:LEU:HD12	1.76	0.66
1:A:552:LEU:HD21	1:A:717:LEU:HD13	1.76	0.66
1:A:827:VAL:HG13	1:A:828:ILE:HG23	1.76	0.66
1:A:524:LEU:HD13	1:A:554:LEU:HD13	1.77	0.66
1:A:299:VAL:HG13	1:A:319:SER:HA	1.77	0.66
1:A:93:LEU:O	1:A:97:PHE:HB2	1.94	0.66
1:A:112:ILE:O	1:A:114:ARG:HG3	1.94	0.66
1:A:334:ILE:O	1:A:337:SER:N	2.28	0.66
1:A:153:LYS:HD3	1:A:240:TYR:CE2	2.30	0.66
1:A:368:LEU:HA	1:A:390:VAL:HG23	1.77	0.66
1:A:93:LEU:HG	1:A:134:LEU:CD2	2.26	0.66
1:A:100:MET:HB2	1:A:119:ILE:HG23	1.75	0.66
1:A:259:SER:HB3	1:A:314:ARG:HD2	1.77	0.65
1:A:464:ILE:HB	1:A:500:PHE:CE1	2.28	0.65
1:A:673:ILE:HG22	1:A:710:VAL:HG13	1.79	0.65
1:A:221:THR:HG23	1:A:224:GLY:H	1.60	0.65
1:A:40:TYR:HB3	1:A:484:THR:HA	1.77	0.65
1:A:57:VAL:HA	1:A:389:HIS:HD1	1.61	0.65
1:A:478:LYS:HG2	1:A:487:PRO:O	1.97	0.65
1:A:719:GLU:OE2	1:A:723:ARG:NE	2.30	0.65
1:A:535:ILE:HA	1:A:538:PHE:HD2	1.61	0.65
1:A:554:LEU:HD22	1:A:569:ALA:HB2	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:GLY:HA2	1:A:503:LEU:HD22	1.77	0.65
1:A:125:MET:O	1:A:135:ALA:N	2.20	0.65
1:A:156:ILE:HG21	1:A:240:TYR:CE1	2.28	0.65
1:A:216:LEU:H	1:A:230:GLY:HA2	1.60	0.65
1:A:86:ARG:HB3	1:A:509:LEU:HD13	1.79	0.65
1:A:278:PRO:HG2	1:A:296:GLU:HB3	1.79	0.65
1:A:800:GLU:O	1:A:841:LEU:HD21	1.97	0.65
1:A:143:THR:O	1:A:169:THR:HA	1.96	0.64
1:A:228:LEU:N	1:A:236:TYR:O	2.30	0.64
1:A:100:MET:SD	1:A:103:ASN:N	2.70	0.64
1:A:373:CYS:N	1:A:384:THR:O	2.24	0.64
1:A:663:HIS:CE1	1:A:777:SER:HB2	2.33	0.64
1:A:278:PRO:HD2	1:A:297:LYS:HE2	1.79	0.64
1:A:524:LEU:HD22	1:A:565:VAL:CG2	2.22	0.64
1:A:260:SER:C	1:A:262:SER:H	2.06	0.64
1:A:485:ASP:OD2	1:A:486:SER:N	2.31	0.64
1:A:337:SER:O	1:A:340:LYS:HD2	1.97	0.64
1:A:431:LEU:HD11	1:A:502:LEU:HD22	1.80	0.64
1:A:174:VAL:HA	1:A:206:TYR:O	1.97	0.64
1:A:374:PRO:CA	1:A:383:ASN:H	2.10	0.64
1:A:494:MET:SD	1:A:676:ASN:ND2	2.71	0.64
1:A:278:PRO:CG	1:A:296:GLU:HB3	2.28	0.64
1:A:64:ASP:HB3	1:A:449:GLN:NE2	2.13	0.63
1:A:175:ILE:HD12	1:A:240:TYR:HB3	1.80	0.63
1:A:335:ASP:C	1:A:338:VAL:HG22	2.22	0.63
1:A:439:PHE:HZ	1:A:516:PRO:HB3	1.61	0.63
1:A:228:LEU:HB2	1:A:236:TYR:HB2	1.81	0.63
1:A:839:ALA:HA	1:A:842:ILE:HD12	1.79	0.63
1:A:28:ARG:HD2	1:A:32:ARG:NH1	2.13	0.63
1:A:54:ASN:HA	1:A:330:ILE:CG2	2.28	0.63
1:A:89:LEU:HD11	1:A:94:VAL:HG21	1.76	0.63
1:A:241:GLN:HE22	1:A:243:GLU:HB3	1.62	0.63
1:A:119:ILE:HD13	1:A:122:ASP:OD1	1.98	0.63
1:A:280:LEU:HD12	1:A:296:GLU:HA	1.81	0.63
1:A:214:TYR:CD1	1:A:231:LYS:HD2	2.33	0.63
1:A:498:LYS:O	1:A:513:LYS:N	2.25	0.63
1:A:831:LYS:NZ	1:A:861:ASP:HB3	2.13	0.63
1:A:517:VAL:HG12	1:A:550:THR:HG23	1.79	0.63
1:A:772:LEU:HD12	1:A:772:LEU:H	1.62	0.62
1:A:564:GLU:HG3	1:A:568:TRP:NE1	2.14	0.62
1:A:520:LEU:HD21	1:A:542:HIS:NE2	2.15	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ILE:HG23	1:A:302:VAL:HG13	1.81	0.62
1:A:290:ILE:HA	1:A:303:TYR:O	2.00	0.62
1:A:665:GLY:HA2	1:A:668:ILE:HD12	1.81	0.62
1:A:105:MET:O	1:A:118:THR:N	2.32	0.62
1:A:357:GLN:HG3	1:A:358:LEU:HB2	1.81	0.62
1:A:678:TRP:CZ3	1:A:827:VAL:HG21	2.34	0.62
1:A:43:LEU:HD22	1:A:46:LEU:HD12	1.82	0.62
1:A:63:MET:HE1	1:A:447:GLU:HB2	1.81	0.62
1:A:546:GLN:NE2	1:A:550:THR:OG1	2.29	0.61
1:A:106:MET:HE1	1:A:505:ALA:HA	1.83	0.61
1:A:228:LEU:O	1:A:236:TYR:N	2.26	0.61
1:A:437:ASP:O	1:A:440:PRO:HD2	2.00	0.61
1:A:442:GLN:N	1:A:442:GLN:OE1	2.32	0.61
1:A:797:LEU:O	1:A:800:GLU:C	2.43	0.61
1:A:208:LEU:HD22	1:A:251:CYS:O	2.01	0.61
1:A:479:ASP:HB2	1:A:484:THR:HB	1.83	0.61
1:A:790:GLN:NE2	1:A:860:GLN:O	2.33	0.61
1:A:801:HIS:HA	1:A:841:LEU:HD21	1.82	0.61
1:A:538:PHE:C	1:A:542:HIS:HD1	2.08	0.61
1:A:153:LYS:HD3	1:A:240:TYR:HE2	1.64	0.60
1:A:206:TYR:CZ	1:A:240:TYR:HB2	2.36	0.60
1:A:342:ILE:HG21	1:A:360:ALA:HB1	1.82	0.60
1:A:715:LYS:HD2	1:A:789:TYR:HE2	1.64	0.60
1:A:730:GLY:CA	1:A:778:LEU:HD12	2.29	0.60
1:A:798:LEU:HD12	1:A:801:HIS:HB3	1.82	0.60
1:A:80:GLU:O	1:A:514:LEU:N	2.31	0.60
1:A:725:SER:O	1:A:732:LEU:HG	2.01	0.60
1:A:68:GLN:NE2	1:A:74:SER:O	2.34	0.60
1:A:43:LEU:HA	1:A:46:LEU:HB2	1.83	0.60
1:A:80:GLU:HG2	1:A:435:ASN:HB3	1.84	0.60
1:A:787:LYS:O	1:A:787:LYS:NZ	2.25	0.60
1:A:814:LEU:HD12	1:A:817:GLN:HB2	1.83	0.60
1:A:720:PHE:O	1:A:724:ASN:ND2	2.34	0.60
1:A:288:ARG:HB2	1:A:290:ILE:HG12	1.84	0.60
1:A:669:TYR:CZ	1:A:673:ILE:HD11	2.36	0.60
1:A:54:ASN:HD21	1:A:331:ALA:C	2.09	0.60
1:A:522:HIS:O	1:A:525:VAL:HB	2.01	0.60
1:A:142:GLU:HB3	1:A:169:THR:HB	1.83	0.60
1:A:173:ILE:N	1:A:208:LEU:O	2.35	0.60
1:A:157:PHE:HD1	1:A:158:GLN:O	1.85	0.60
1:A:282:ILE:HG22	1:A:283:ALA:H	1.67	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:PHE:N	1:A:511:PHE:O	2.32	0.59
1:A:463:ALA:HB3	1:A:466:GLU:HB2	1.84	0.59
1:A:241:GLN:OE1	1:A:243:GLU:N	2.31	0.59
1:A:257:SER:HA	1:A:314:ARG:NH1	2.15	0.59
1:A:730:GLY:HA3	1:A:778:LEU:CD1	2.30	0.59
1:A:205:LEU:HB2	1:A:250:ARG:HD3	1.84	0.59
1:A:300:ILE:N	1:A:318:VAL:O	2.32	0.59
1:A:179:SER:OG	1:A:199:GLN:HB2	2.02	0.59
1:A:67:LEU:HD22	1:A:398:ALA:HB1	1.84	0.59
1:A:294:ARG:HD2	1:A:342:ILE:O	2.03	0.59
1:A:375:PHE:C	1:A:376:ARG:HE	2.04	0.59
1:A:437:ASP:HB2	1:A:447:GLU:CA	2.33	0.59
1:A:542:HIS:HB3	1:A:547:ALA:H	1.68	0.59
1:A:27:GLY:HA3	1:A:828:ILE:HG21	1.84	0.58
1:A:285:ASP:HB2	1:A:292:TYR:CE2	2.38	0.58
1:A:359:LEU:HD11	1:A:367:ARG:HD2	1.85	0.58
1:A:215:LEU:HA	1:A:230:GLY:HA3	1.86	0.58
1:A:367:ARG:HH12	1:A:447:GLU:CD	2.11	0.58
1:A:367:ARG:NH1	1:A:447:GLU:OE2	2.31	0.58
1:A:541:LEU:HB3	1:A:542:HIS:CE1	2.38	0.58
1:A:565:VAL:HA	1:A:568:TRP:CD1	2.31	0.58
1:A:100:MET:HE2	1:A:104:CYS:HB3	1.86	0.58
1:A:356:CYS:HA	1:A:371:SER:HA	1.86	0.58
1:A:43:LEU:HD21	1:A:486:SER:OG	2.02	0.58
1:A:123:ILE:HG21	1:A:167:LEU:HD21	1.86	0.58
1:A:67:LEU:HD23	1:A:400:SER:O	2.04	0.57
1:A:769:GLU:O	1:A:772:LEU:N	2.36	0.57
1:A:357:GLN:NE2	1:A:372:THR:HB	2.19	0.57
1:A:68:GLN:O	1:A:401:THR:OG1	2.21	0.57
1:A:93:LEU:HD11	1:A:126:TRP:CG	2.40	0.57
1:A:114:ARG:NH2	1:A:127:ASN:HB3	2.20	0.57
1:A:524:LEU:CD2	1:A:565:VAL:HG23	2.27	0.57
1:A:724:ASN:HB2	1:A:728:ALA:HB2	1.85	0.57
1:A:326:ALA:O	1:A:330:ILE:HG13	2.04	0.57
1:A:161:VAL:HG22	1:A:201:LEU:CD1	2.35	0.57
1:A:335:ASP:O	1:A:338:VAL:HG22	2.04	0.57
1:A:357:GLN:N	1:A:370:PHE:O	2.35	0.57
1:A:97:PHE:CG	1:A:117:LEU:HD21	2.40	0.57
1:A:165:LEU:HB2	1:A:178:LEU:HD11	1.87	0.57
1:A:278:PRO:HB2	1:A:296:GLU:HB3	1.86	0.56
1:A:357:GLN:CD	1:A:372:THR:HB	2.30	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:PHE:CE1	1:A:387:LEU:HD13	2.39	0.56
1:A:673:ILE:CG2	1:A:710:VAL:HG13	2.35	0.56
1:A:781:ILE:O	1:A:785:VAL:HG23	2.04	0.56
1:A:97:PHE:CE2	1:A:117:LEU:HD11	2.39	0.56
1:A:100:MET:SD	1:A:102:CYS:N	2.77	0.56
1:A:334:ILE:HD11	1:A:340:LYS:HD3	1.86	0.56
1:A:813:GLU:O	1:A:817:GLN:HG3	2.06	0.56
1:A:29:LEU:HD21	1:A:667:CYS:SG	2.46	0.56
1:A:61:SER:HB3	1:A:413:TYR:CB	2.36	0.56
1:A:226:ILE:O	1:A:237:GLU:HG3	2.06	0.56
1:A:257:SER:HA	1:A:314:ARG:NH2	2.21	0.56
1:A:373:CYS:C	1:A:383:ASN:H	2.14	0.56
1:A:732:LEU:O	1:A:775:LYS:NZ	2.34	0.56
1:A:150:VAL:HG23	1:A:164:LEU:HB3	1.88	0.56
1:A:262:SER:HG	1:A:268:LEU:HD13	1.71	0.56
1:A:54:ASN:OD1	1:A:330:ILE:CG2	2.45	0.56
1:A:61:SER:HB2	1:A:409:HIS:O	2.06	0.56
1:A:858:HIS:HA	1:A:861:ASP:HB2	1.87	0.56
1:A:153:LYS:HD2	1:A:153:LYS:N	2.21	0.56
1:A:200:LEU:HD12	1:A:200:LEU:O	2.06	0.56
1:A:285:ASP:HB2	1:A:292:TYR:HE2	1.71	0.55
1:A:85:ARG:O	1:A:509:LEU:HD12	2.06	0.55
1:A:463:ALA:HB3	1:A:466:GLU:CB	2.37	0.55
1:A:114:ARG:NH1	1:A:198:MET:H	2.04	0.55
1:A:114:ARG:NH1	1:A:198:MET:N	2.54	0.55
1:A:279:ILE:HD11	1:A:293:THR:HB	1.88	0.55
1:A:524:LEU:HD13	1:A:554:LEU:CD1	2.36	0.55
1:A:54:ASN:HA	1:A:330:ILE:HG21	1.88	0.55
1:A:64:ASP:N	1:A:449:GLN:OE1	2.35	0.55
1:A:440:PRO:HB3	1:A:443:LYS:HB2	1.88	0.55
1:A:715:LYS:HD2	1:A:789:TYR:CE2	2.41	0.55
1:A:437:ASP:HB2	1:A:447:GLU:HA	1.89	0.55
1:A:124:PHE:CZ	1:A:138:ASP:HB3	2.41	0.55
1:A:523:LEU:HD12	1:A:538:PHE:HE1	1.72	0.55
1:A:854:GLY:O	1:A:858:HIS:CD2	2.60	0.55
1:A:518:ASP:OD1	1:A:521:ARG:NH2	2.31	0.55
1:A:520:LEU:O	1:A:523:LEU:HB2	2.07	0.55
1:A:124:PHE:CE2	1:A:138:ASP:HB3	2.42	0.54
1:A:257:SER:CA	1:A:314:ARG:HH12	2.19	0.54
1:A:396:PHE:CE1	1:A:406:SER:HA	2.42	0.54
1:A:359:LEU:HD12	1:A:369:TYR:CZ	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:798:LEU:O	1:A:801:HIS:HB3	2.07	0.54
1:A:262:SER:CB	1:A:268:LEU:CD1	2.85	0.54
1:A:362:THR:CG2	1:A:368:LEU:HD11	2.37	0.54
1:A:163:HIS:HB2	1:A:180:TYR:HE2	1.73	0.54
1:A:221:THR:HG22	1:A:225:ARG:H	1.73	0.54
1:A:64:ASP:HA	1:A:396:PHE:CE2	2.43	0.54
1:A:40:TYR:CD2	1:A:487:PRO:HD3	2.43	0.54
1:A:396:PHE:HE1	1:A:406:SER:HA	1.72	0.54
1:A:558:THR:HG22	1:A:558:THR:O	2.07	0.54
1:A:64:ASP:HB3	1:A:449:GLN:HE22	1.73	0.54
1:A:68:GLN:NE2	1:A:76:PRO:HD3	2.22	0.54
1:A:500:PHE:HE2	1:A:513:LYS:HB2	1.73	0.54
1:A:44:SER:O	1:A:48:MET:N	2.41	0.54
1:A:214:TYR:O	1:A:230:GLY:HA3	2.08	0.54
1:A:292:TYR:CE2	1:A:347:VAL:HG13	2.43	0.54
1:A:443:LYS:HD2	1:A:446:MET:SD	2.48	0.54
1:A:350:ASN:HA	1:A:353:SER:O	2.08	0.53
1:A:489:VAL:HG22	1:A:672:ARG:HH22	1.74	0.53
1:A:670:PHE:CZ	1:A:784:LEU:HG	2.44	0.53
1:A:205:LEU:HD11	1:A:242:ALA:HA	1.90	0.53
1:A:206:TYR:CE1	1:A:241:GLN:N	2.76	0.53
1:A:724:ASN:O	1:A:728:ALA:CA	2.56	0.53
1:A:838:ILE:O	1:A:842:ILE:HG13	2.08	0.53
1:A:93:LEU:HD11	1:A:126:TRP:CE2	2.43	0.53
1:A:774:GLU:O	1:A:777:SER:OG	2.23	0.53
1:A:487:PRO:O	1:A:490:VAL:HG22	2.09	0.53
1:A:521:ARG:HH11	1:A:522:HIS:CE1	2.22	0.53
1:A:102:CYS:SG	1:A:103:ASN:ND2	2.82	0.53
1:A:153:LYS:HB2	1:A:240:TYR:OH	2.09	0.53
1:A:40:TYR:O	1:A:483:ILE:HG23	2.08	0.53
1:A:422:ALA:HA	1:A:432:TRP:CZ2	2.44	0.53
1:A:77:ASN:HD22	1:A:526:SER:HB3	1.74	0.53
1:A:93:LEU:CD1	1:A:126:TRP:CE2	2.92	0.53
1:A:372:THR:CG2	1:A:382:PRO:HG3	2.39	0.53
1:A:478:LYS:HD3	1:A:486:SER:C	2.34	0.53
1:A:787:LYS:HZ1	1:A:791:ALA:HB2	1.73	0.53
1:A:172:ASP:HA	1:A:208:LEU:C	2.34	0.53
1:A:58:SER:OG	1:A:389:HIS:HE1	1.91	0.52
1:A:93:LEU:O	1:A:97:PHE:HB3	2.08	0.52
1:A:171:VAL:O	1:A:209:PRO:HG3	2.09	0.52
1:A:523:LEU:O	1:A:526:SER:OG	2.20	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:PRO:HG2	1:A:363:HIS:HB2	1.90	0.52
1:A:334:ILE:C	1:A:338:VAL:HG13	2.33	0.52
1:A:566:SER:O	1:A:570:THR:HG23	2.09	0.52
1:A:31:ASP:OD2	1:A:35:GLN:NE2	2.43	0.52
1:A:97:PHE:CD1	1:A:117:LEU:HD21	2.45	0.52
1:A:538:PHE:O	1:A:542:HIS:N	2.42	0.52
1:A:670:PHE:CZ	1:A:674:MET:HE3	2.45	0.52
1:A:439:PHE:O	1:A:441:PHE:N	2.42	0.52
1:A:539:PHE:CE1	1:A:544:GLU:HB2	2.44	0.52
1:A:669:TYR:CD2	1:A:717:LEU:HD22	2.44	0.52
1:A:114:ARG:HH11	1:A:198:MET:N	2.06	0.52
1:A:262:SER:CB	1:A:268:LEU:CG	2.82	0.52
1:A:663:HIS:ND1	1:A:781:ILE:HD11	2.24	0.52
1:A:82:SER:HB3	1:A:514:LEU:HD11	1.91	0.52
1:A:790:GLN:CD	1:A:861:ASP:HA	2.34	0.52
1:A:814:LEU:HA	1:A:817:GLN:CD	2.35	0.52
1:A:172:ASP:HB3	1:A:207:SER:HB2	1.92	0.52
1:A:335:ASP:N	1:A:335:ASP:OD1	2.39	0.51
1:A:346:ALA:HB3	1:A:359:LEU:HD22	1.91	0.51
1:A:779:GLN:CD	1:A:782:GLN:HE21	2.19	0.51
1:A:40:TYR:CE2	1:A:486:SER:HB2	2.45	0.51
1:A:282:ILE:HG22	1:A:283:ALA:N	2.25	0.51
1:A:673:ILE:HG12	1:A:713:GLU:OE1	2.10	0.51
1:A:78:LEU:N	1:A:79:PRO:HD3	2.25	0.51
1:A:478:LYS:HD2	1:A:478:LYS:N	2.25	0.51
1:A:104:CYS:HA	1:A:118:THR:O	2.10	0.51
1:A:292:TYR:CD1	1:A:358:LEU:HD13	2.46	0.51
1:A:89:LEU:HD12	1:A:94:VAL:HG21	1.84	0.51
1:A:469:VAL:HG11	1:A:476:LEU:N	2.25	0.51
1:A:703:PRO:HG2	1:A:706:LEU:HD13	1.92	0.51
1:A:853:ASP:O	1:A:857:LEU:HG	2.11	0.51
1:A:334:ILE:HG13	1:A:338:VAL:CG1	2.40	0.51
1:A:58:SER:N	1:A:390:VAL:O	2.40	0.51
1:A:769:GLU:HA	1:A:769:GLU:OE1	2.10	0.51
1:A:428:ASN:HD21	1:A:455:ASP:HA	1.75	0.51
1:A:460:ALA:O	1:A:503:LEU:N	2.38	0.51
1:A:791:ALA:HA	1:A:794:LEU:HD12	1.93	0.51
1:A:60:MET:HB3	1:A:393:PRO:O	2.11	0.50
1:A:148:GLY:HA3	1:A:218:ILE:HG21	1.93	0.50
1:A:298:GLY:HA3	1:A:320:GLN:HB2	1.92	0.50
1:A:361:VAL:HA	1:A:366:VAL:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:SER:O	1:A:271:PHE:O	2.29	0.50
1:A:258:LYS:O	1:A:261:LEU:HG	2.11	0.50
1:A:278:PRO:CB	1:A:296:GLU:HB3	2.42	0.50
1:A:293:THR:H	1:A:300:ILE:HD12	1.77	0.50
1:A:393:PRO:HB2	1:A:420:MET:SD	2.51	0.50
1:A:480:HIS:O	1:A:480:HIS:ND1	2.44	0.50
1:A:144:ILE:HG13	1:A:169:THR:HG22	1.91	0.50
1:A:213:THR:HG22	1:A:214:TYR:O	2.11	0.50
1:A:333:THR:HG22	1:A:336:ARG:H	1.77	0.50
1:A:460:ALA:HB3	1:A:503:LEU:HB3	1.94	0.50
1:A:725:SER:HA	1:A:731:PRO:CB	2.40	0.50
1:A:200:LEU:HD12	1:A:200:LEU:C	2.37	0.50
1:A:232:ASP:HB3	1:A:234:CYS:SG	2.51	0.50
1:A:542:HIS:CD2	1:A:546:GLN:OE1	2.65	0.50
1:A:490:VAL:HA	1:A:672:ARG:NE	2.27	0.50
1:A:85:ARG:HG3	1:A:510:MET:HE2	1.93	0.50
1:A:110:PRO:HG3	1:A:462:SER:OG	2.12	0.50
1:A:123:ILE:HG23	1:A:137:PHE:HB3	1.94	0.50
1:A:269:LEU:O	1:A:269:LEU:HD12	2.12	0.50
1:A:54:ASN:CA	1:A:330:ILE:CG2	2.90	0.49
1:A:100:MET:HB2	1:A:119:ILE:CG2	2.41	0.49
1:A:147:VAL:HG12	1:A:167:LEU:HG	1.94	0.49
1:A:175:ILE:O	1:A:203:ASP:HB2	2.11	0.49
1:A:458:SER:OG	1:A:502:LEU:HD11	2.12	0.49
1:A:523:LEU:HB2	1:A:538:PHE:CZ	2.47	0.49
1:A:106:MET:HB2	1:A:117:LEU:HD13	1.92	0.49
1:A:120:ASP:N	1:A:120:ASP:OD1	2.45	0.49
1:A:669:TYR:HE2	1:A:717:LEU:HB2	1.76	0.49
1:A:86:ARG:HA	1:A:508:SER:O	2.13	0.49
1:A:118:THR:HG22	1:A:119:ILE:N	2.28	0.49
1:A:367:ARG:HH22	1:A:391:ARG:HH21	1.60	0.49
1:A:401:THR:HG23	1:A:402:VAL:N	2.28	0.49
1:A:26:ALA:HB1	1:A:784:LEU:HD22	1.94	0.49
1:A:54:ASN:CG	1:A:332:ARG:HB2	2.38	0.49
1:A:431:LEU:HD21	1:A:502:LEU:HD22	1.94	0.49
1:A:518:ASP:HA	1:A:521:ARG:NH2	2.28	0.49
1:A:83:SER:HB3	1:A:511:PHE:CZ	2.47	0.49
1:A:208:LEU:HG	1:A:209:PRO:HD2	1.93	0.49
1:A:703:PRO:HG2	1:A:706:LEU:HD22	1.93	0.49
1:A:415:LYS:HB2	1:A:420:MET:SD	2.53	0.49
1:A:714:LEU:HB3	1:A:785:VAL:HG13	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:ILE:HG22	1:A:815:GLN:NE2	2.28	0.49
1:A:814:LEU:HA	1:A:817:GLN:CG	2.43	0.49
1:A:844:CYS:SG	1:A:845:TYR:N	2.85	0.49
1:A:206:TYR:CE1	1:A:240:TYR:HB2	2.47	0.49
1:A:217:THR:HG23	1:A:281:GLN:NE2	2.28	0.49
1:A:349:GLU:OE1	1:A:349:GLU:N	2.42	0.49
1:A:258:LYS:N	1:A:314:ARG:HH22	2.11	0.49
1:A:858:HIS:O	1:A:862:ILE:N	2.35	0.49
1:A:142:GLU:HG3	1:A:170:PRO:HG2	1.95	0.49
1:A:214:TYR:CG	1:A:231:LYS:HD2	2.47	0.49
1:A:144:ILE:HG12	1:A:167:LEU:HB3	1.95	0.48
1:A:369:TYR:CE2	1:A:391:ARG:HG3	2.48	0.48
1:A:492:GLN:OE1	1:A:517:VAL:N	2.33	0.48
1:A:499:LYS:HG2	1:A:512:HIS:CG	2.48	0.48
1:A:726:GLN:HA	1:A:732:LEU:HD12	1.94	0.48
1:A:65:TYR:HB2	1:A:394:PRO:CB	2.44	0.48
1:A:393:PRO:HB3	1:A:432:TRP:CZ3	2.48	0.48
1:A:61:SER:HB2	1:A:409:HIS:HB2	1.94	0.48
1:A:81:ILE:HA	1:A:512:HIS:O	2.13	0.48
1:A:56:THR:HG22	1:A:389:HIS:HB2	1.94	0.48
1:A:61:SER:HB3	1:A:413:TYR:HB2	1.96	0.48
1:A:81:ILE:HG23	1:A:511:PHE:HD1	1.78	0.48
1:A:787:LYS:HE2	1:A:831:LYS:HD2	1.95	0.48
1:A:811:GLN:OE1	1:A:813:GLU:HG3	2.14	0.48
1:A:127:ASN:OD1	1:A:127:ASN:O	2.32	0.48
1:A:172:ASP:OD2	1:A:209:PRO:HD3	2.14	0.48
1:A:719:GLU:CD	1:A:723:ARG:HE	2.21	0.48
1:A:811:GLN:HG3	1:A:814:LEU:H	1.79	0.48
1:A:29:LEU:HD11	1:A:663:HIS:NE2	2.29	0.48
1:A:54:ASN:CA	1:A:330:ILE:HG22	2.44	0.48
1:A:173:ILE:H	1:A:208:LEU:H	1.62	0.48
1:A:206:TYR:CE2	1:A:240:TYR:CD1	3.02	0.48
1:A:787:LYS:CE	1:A:831:LYS:HD2	2.44	0.48
1:A:374:PRO:HB2	1:A:376:ARG:O	2.14	0.47
1:A:500:PHE:CE2	1:A:513:LYS:HB2	2.49	0.47
1:A:536:GLU:H	1:A:536:GLU:CD	2.22	0.47
1:A:292:TYR:CG	1:A:358:LEU:HD13	2.49	0.47
1:A:372:THR:HA	1:A:385:LEU:HA	1.96	0.47
1:A:151:LYS:HD2	1:A:221:THR:O	2.14	0.47
1:A:284:ILE:O	1:A:284:ILE:HG13	2.13	0.47
1:A:79:PRO:C	1:A:519:GLN:HE21	2.19	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ARG:C	1:A:226:ILE:HD13	2.39	0.47
1:A:237:GLU:O	1:A:253:LYS:HA	2.15	0.47
1:A:300:ILE:HG23	1:A:318:VAL:HB	1.96	0.47
1:A:330:ILE:HG22	1:A:330:ILE:O	2.13	0.47
1:A:663:HIS:ND1	1:A:777:SER:HB2	2.28	0.47
1:A:28:ARG:HD2	1:A:32:ARG:CZ	2.44	0.47
1:A:226:ILE:O	1:A:237:GLU:HA	2.15	0.47
1:A:280:LEU:H	1:A:295:SER:HA	1.80	0.47
1:A:93:LEU:HG	1:A:134:LEU:CD1	2.45	0.47
1:A:206:TYR:CZ	1:A:240:TYR:HD1	2.32	0.47
1:A:353:SER:HB3	1:A:356:CYS:O	2.15	0.47
1:A:542:HIS:HB3	1:A:547:ALA:N	2.28	0.47
1:A:57:VAL:CA	1:A:390:VAL:H	2.18	0.47
1:A:81:ILE:HD11	1:A:500:PHE:CD2	2.50	0.47
1:A:439:PHE:HE1	1:A:546:GLN:HG3	1.80	0.47
1:A:33:GLN:HB3	1:A:671:SER:OG	2.14	0.47
1:A:294:ARG:NH2	1:A:344:GLN:HA	2.29	0.47
1:A:470:ASP:OD1	1:A:470:ASP:N	2.47	0.47
1:A:57:VAL:HB	1:A:390:VAL:CG1	2.37	0.47
1:A:106:MET:SD	1:A:503:LEU:HD11	2.56	0.47
1:A:157:PHE:HB2	1:A:161:VAL:HG21	1.97	0.47
1:A:428:ASN:ND2	1:A:455:ASP:HA	2.29	0.47
1:A:517:VAL:HA	1:A:550:THR:HG23	1.97	0.47
1:A:56:THR:HG21	1:A:388:VAL:CG2	2.32	0.46
1:A:72:LEU:HG	1:A:74:SER:H	1.79	0.46
1:A:80:GLU:HG2	1:A:435:ASN:CB	2.44	0.46
1:A:100:MET:CG	1:A:120:ASP:H	2.17	0.46
1:A:335:ASP:HA	1:A:338:VAL:HG21	1.90	0.46
1:A:565:VAL:O	1:A:568:TRP:HB2	2.15	0.46
1:A:490:VAL:HG23	1:A:491:GLN:HG2	1.98	0.46
1:A:709:SER:O	1:A:713:GLU:HG3	2.15	0.46
1:A:718:GLN:HE22	1:A:782:GLN:HB2	1.80	0.46
1:A:217:THR:HG21	1:A:282:ILE:H	1.80	0.46
1:A:524:LEU:HD21	1:A:568:TRP:CB	2.46	0.46
1:A:431:LEU:O	1:A:432:TRP:HD1	1.99	0.46
1:A:535:ILE:HG21	1:A:576:TYR:CD2	2.50	0.46
1:A:806:ILE:HG22	1:A:815:GLN:CD	2.40	0.46
1:A:825:ASP:HA	1:A:829:ARG:HB2	1.96	0.46
1:A:299:VAL:HG22	1:A:319:SER:HA	1.98	0.46
1:A:468:LYS:HE3	1:A:500:PHE:CD1	2.51	0.46
1:A:173:ILE:HD13	1:A:253:LYS:HE2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:SER:HB2	1:A:468:LYS:NZ	2.30	0.46
1:A:702:VAL:HB	1:A:707:LEU:HD21	1.98	0.46
1:A:730:GLY:O	1:A:775:LYS:HG2	2.16	0.46
1:A:54:ASN:N	1:A:330:ILE:CG2	2.79	0.46
1:A:65:TYR:OH	1:A:451:THR:HG23	2.16	0.46
1:A:403:GLU:O	1:A:404:LYS:HD3	2.16	0.46
1:A:669:TYR:CE1	1:A:673:ILE:HD11	2.51	0.46
1:A:303:TYR:OH	1:A:314:ARG:NH1	2.43	0.46
1:A:323:ILE:HG23	1:A:370:PHE:CE1	2.51	0.46
1:A:798:LEU:CD1	1:A:801:HIS:ND1	2.79	0.46
1:A:812:LYS:O	1:A:815:GLN:HB3	2.16	0.46
1:A:841:LEU:HA	1:A:844:CYS:SG	2.56	0.46
1:A:112:ILE:HG21	1:A:180:TYR:CZ	2.51	0.46
1:A:294:ARG:CZ	1:A:344:GLN:HA	2.46	0.46
1:A:478:LYS:HD2	1:A:485:ASP:O	2.16	0.46
1:A:669:TYR:CE2	1:A:717:LEU:HD22	2.51	0.46
1:A:140:LEU:HD13	1:A:144:ILE:HD11	1.96	0.45
1:A:369:TYR:HE2	1:A:391:ARG:HG3	1.81	0.45
1:A:516:PRO:O	1:A:520:LEU:HD13	2.15	0.45
1:A:838:ILE:HG22	1:A:842:ILE:HD11	1.98	0.45
1:A:65:TYR:CE2	1:A:398:ALA:HB2	2.51	0.45
1:A:100:MET:CG	1:A:120:ASP:N	2.76	0.45
1:A:303:TYR:OH	1:A:314:ARG:NE	2.47	0.45
1:A:439:PHE:CE1	1:A:546:GLN:HG3	2.51	0.45
1:A:516:PRO:O	1:A:520:LEU:HB2	2.16	0.45
1:A:548:CYS:O	1:A:573:PHE:CE2	2.69	0.45
1:A:766:LYS:CA	1:A:770:ALA:HB3	2.39	0.45
1:A:821:THR:O	1:A:826:LEU:HD12	2.16	0.45
1:A:142:GLU:OE1	1:A:142:GLU:HA	2.16	0.45
1:A:292:TYR:HE1	1:A:357:GLN:HG3	1.82	0.45
1:A:299:VAL:CG1	1:A:301:GLN:HE22	2.30	0.45
1:A:856:SER:HA	1:A:859:LEU:HD12	1.98	0.45
1:A:541:LEU:HB3	1:A:542:HIS:ND1	2.31	0.45
1:A:720:PHE:CD2	1:A:721:LEU:HD22	2.44	0.45
1:A:814:LEU:HA	1:A:817:GLN:HG3	1.99	0.45
1:A:769:GLU:O	1:A:770:ALA:C	2.59	0.45
1:A:769:GLU:O	1:A:772:LEU:HB2	2.17	0.45
1:A:859:LEU:HA	1:A:863:CYS:SG	2.57	0.45
1:A:108:VAL:CG1	1:A:503:LEU:HB2	2.42	0.45
1:A:175:ILE:C	1:A:176:LEU:HD22	2.41	0.45
1:A:206:TYR:HE1	1:A:241:GLN:O	2.00	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:TYR:CD1	1:A:358:LEU:HD22	2.52	0.45
1:A:517:VAL:HA	1:A:550:THR:CG2	2.47	0.45
1:A:664:ASN:HA	1:A:667:CYS:SG	2.56	0.45
1:A:443:LYS:HB3	1:A:446:MET:HB2	1.99	0.45
1:A:517:VAL:HG11	1:A:553:ILE:HG21	1.99	0.45
1:A:770:ALA:HA	1:A:773:SER:OG	2.16	0.45
1:A:214:TYR:HB2	1:A:231:LYS:HB2	1.97	0.45
1:A:221:THR:OG1	1:A:222:ASP:N	2.50	0.45
1:A:28:ARG:HG2	1:A:28:ARG:HH21	1.81	0.45
1:A:285:ASP:N	1:A:290:ILE:O	2.32	0.45
1:A:68:GLN:HB2	1:A:72:LEU:HD22	1.99	0.45
1:A:344:GLN:O	1:A:361:VAL:N	2.33	0.45
1:A:812:LYS:HA	1:A:815:GLN:HB3	1.98	0.45
1:A:815:GLN:O	1:A:818:LEU:HB2	2.17	0.45
1:A:221:THR:CG2	1:A:225:ARG:H	2.29	0.44
1:A:464:ILE:CB	1:A:500:PHE:HE1	2.21	0.44
1:A:489:VAL:HA	1:A:516:PRO:HG2	1.99	0.44
1:A:169:THR:HB	1:A:170:PRO:HD2	2.00	0.44
1:A:488:VAL:HG11	1:A:513:LYS:NZ	2.33	0.44
1:A:523:LEU:HD12	1:A:538:PHE:CE1	2.50	0.44
1:A:119:ILE:HB	1:A:122:ASP:OD1	2.17	0.44
1:A:374:PRO:N	1:A:382:PRO:HA	2.33	0.44
1:A:726:GLN:CD	1:A:726:GLN:N	2.76	0.44
1:A:807:VAL:HA	1:A:815:GLN:OE1	2.18	0.44
1:A:818:LEU:CA	1:A:833:LEU:HD11	2.42	0.44
1:A:51:ALA:O	1:A:56:THR:OG1	2.23	0.44
1:A:151:LYS:HZ2	1:A:470:ASP:HB2	1.81	0.44
1:A:348:ILE:HA	1:A:352:GLU:OE1	2.18	0.44
1:A:359:LEU:HD12	1:A:369:TYR:CE1	2.52	0.44
1:A:478:LYS:HB2	1:A:484:THR:O	2.17	0.44
1:A:724:ASN:HB3	1:A:728:ALA:CB	2.44	0.44
1:A:138:ASP:N	1:A:138:ASP:OD1	2.49	0.44
1:A:206:TYR:OH	1:A:240:TYR:HD1	2.01	0.44
1:A:334:ILE:HG23	1:A:335:ASP:N	2.33	0.44
1:A:372:THR:HG21	1:A:382:PRO:HG3	1.99	0.44
1:A:466:GLU:OE2	1:A:467:LEU:HD23	2.18	0.44
1:A:777:SER:O	1:A:781:ILE:HG13	2.16	0.44
1:A:327:ALA:O	1:A:330:ILE:HB	2.17	0.44
1:A:663:HIS:O	1:A:666:ILE:HB	2.18	0.44
1:A:859:LEU:O	1:A:863:CYS:HB2	2.18	0.44
1:A:60:MET:CG	1:A:413:TYR:HD1	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ASN:OD1	1:A:130:ASP:HB3	2.17	0.44
1:A:397:SER:C	1:A:399:SER:H	2.26	0.44
1:A:479:ASP:CB	1:A:484:THR:HB	2.47	0.44
1:A:770:ALA:O	1:A:773:SER:HB2	2.18	0.44
1:A:802:GLN:OE1	1:A:805:ILE:HD12	2.18	0.44
1:A:329:ASN:C	1:A:331:ALA:H	2.25	0.44
1:A:471:LYS:HD2	1:A:471:LYS:HA	1.72	0.44
1:A:53:ASN:CB	1:A:55:PRO:HD2	2.44	0.43
1:A:66:PRO:O	1:A:451:THR:HB	2.19	0.43
1:A:123:ILE:O	1:A:137:PHE:HB3	2.18	0.43
1:A:321:ASN:HA	1:A:324:VAL:HG22	2.00	0.43
1:A:371:SER:O	1:A:385:LEU:HG	2.18	0.43
1:A:124:PHE:CD2	1:A:137:PHE:N	2.85	0.43
1:A:210:THR:HG21	1:A:215:LEU:HD21	1.99	0.43
1:A:299:VAL:HA	1:A:319:SER:HA	1.99	0.43
1:A:323:ILE:HG23	1:A:370:PHE:HE1	1.83	0.43
1:A:806:ILE:HD13	1:A:806:ILE:HA	1.82	0.43
1:A:364:ALA:HB2	1:A:417:ILE:HB	2.01	0.43
1:A:439:PHE:CZ	1:A:516:PRO:HB3	2.48	0.43
1:A:58:SER:CB	1:A:389:HIS:HE1	2.31	0.43
1:A:65:TYR:CD2	1:A:398:ALA:HB2	2.53	0.43
1:A:144:ILE:HG13	1:A:169:THR:CG2	2.48	0.43
1:A:175:ILE:HD13	1:A:240:TYR:CD2	2.54	0.43
1:A:26:ALA:O	1:A:30:ILE:HG12	2.19	0.43
1:A:147:VAL:HA	1:A:166:VAL:O	2.17	0.43
1:A:153:LYS:HD2	1:A:153:LYS:H	1.83	0.43
1:A:257:SER:CA	1:A:314:ARG:HH22	2.26	0.43
1:A:47:LEU:HD13	1:A:389:HIS:CD2	2.54	0.43
1:A:768:HIS:NE2	1:A:769:GLU:OE2	2.52	0.43
1:A:29:LEU:C	1:A:29:LEU:HD23	2.43	0.43
1:A:33:GLN:HG2	1:A:667:CYS:C	2.44	0.43
1:A:241:GLN:HE22	1:A:243:GLU:CB	2.27	0.43
1:A:360:ALA:HB3	1:A:368:LEU:HB2	2.01	0.43
1:A:814:LEU:O	1:A:817:GLN:HB2	2.18	0.43
1:A:114:ARG:NE	1:A:198:MET:HB2	2.33	0.43
1:A:61:SER:HB3	1:A:413:TYR:HB3	2.00	0.43
1:A:249:GLN:HB2	1:A:251:CYS:O	2.19	0.43
1:A:73:LEU:HD23	1:A:73:LEU:H	1.84	0.43
1:A:118:THR:CG2	1:A:119:ILE:N	2.82	0.43
1:A:164:LEU:HD12	1:A:165:LEU:H	1.83	0.43
1:A:107:GLY:HA3	1:A:116:TRP:CZ2	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:VAL:HA	1:A:390:VAL:N	2.20	0.42
1:A:89:LEU:HA	1:A:90:PRO:HD3	1.80	0.42
1:A:124:PHE:HE2	1:A:137:PHE:C	2.28	0.42
1:A:216:LEU:HA	1:A:216:LEU:HD23	1.81	0.42
1:A:235:LEU:HB2	1:A:257:SER:OG	2.19	0.42
1:A:294:ARG:NH2	1:A:345:ILE:HG12	2.34	0.42
1:A:337:SER:O	1:A:340:LYS:HB3	2.19	0.42
1:A:100:MET:HE2	1:A:104:CYS:CB	2.49	0.42
1:A:257:SER:CB	1:A:314:ARG:HH12	2.32	0.42
1:A:669:TYR:O	1:A:673:ILE:HG13	2.18	0.42
1:A:21:GLU:N	1:A:24:GLU:OE1	2.49	0.42
1:A:249:GLN:H	1:A:249:GLN:CD	2.27	0.42
1:A:489:VAL:HG22	1:A:672:ARG:NH2	2.35	0.42
1:A:206:TYR:CE2	1:A:240:TYR:HB2	2.54	0.42
1:A:299:VAL:HG12	1:A:301:GLN:NE2	2.34	0.42
1:A:555:ALA:O	1:A:566:SER:HB2	2.19	0.42
1:A:730:GLY:HA2	1:A:775:LYS:HG2	2.02	0.42
1:A:181:ALA:N	1:A:197:GLY:O	2.53	0.42
1:A:221:THR:HG22	1:A:225:ARG:N	2.34	0.42
1:A:265:VAL:N	1:A:266:PRO:CD	2.82	0.42
1:A:824:LYS:O	1:A:827:VAL:HG12	2.20	0.42
1:A:56:THR:HB	1:A:388:VAL:O	2.20	0.42
1:A:292:TYR:CE1	1:A:357:GLN:HG3	2.55	0.42
1:A:357:GLN:HG2	1:A:370:PHE:O	2.19	0.42
1:A:144:ILE:HG23	1:A:168:ALA:H	1.85	0.42
1:A:393:PRO:HB3	1:A:432:TRP:HZ3	1.85	0.42
1:A:552:LEU:C	1:A:552:LEU:HD23	2.45	0.42
1:A:810:LEU:O	1:A:810:LEU:HG	2.20	0.42
1:A:126:TRP:N	1:A:126:TRP:CE3	2.88	0.42
1:A:142:GLU:HG3	1:A:171:VAL:HG23	2.01	0.42
1:A:774:GLU:O	1:A:778:LEU:HG	2.20	0.42
1:A:787:LYS:HD2	1:A:787:LYS:HA	1.82	0.42
1:A:214:TYR:O	1:A:215:LEU:HD22	2.20	0.41
1:A:323:ILE:HG23	1:A:387:LEU:HD22	2.01	0.41
1:A:367:ARG:CZ	1:A:391:ARG:HD2	2.50	0.41
1:A:469:VAL:HG21	1:A:475:PRO:HA	2.02	0.41
1:A:283:ALA:HB1	1:A:347:VAL:CG2	2.50	0.41
1:A:40:TYR:CE1	1:A:438:THR:HG23	2.55	0.41
1:A:124:PHE:HB3	1:A:136:TYR:HD1	1.85	0.41
1:A:281:GLN:HB2	1:A:294:ARG:NH1	2.35	0.41
1:A:501:VAL:HG12	1:A:510:MET:HG3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:LEU:HG	1:A:833:LEU:HD11	2.01	0.41
1:A:43:LEU:HD23	1:A:485:ASP:OD1	2.19	0.41
1:A:57:VAL:HA	1:A:389:HIS:HA	2.01	0.41
1:A:153:LYS:NZ	1:A:226:ILE:HG12	2.35	0.41
1:A:182:ASN:ND2	1:A:195:SER:O	2.53	0.41
1:A:279:ILE:CD1	1:A:293:THR:HB	2.50	0.41
1:A:367:ARG:O	1:A:390:VAL:HA	2.20	0.41
1:A:492:GLN:OE1	1:A:517:VAL:HG13	2.21	0.41
1:A:674:MET:HE1	1:A:714:LEU:HD21	2.03	0.41
1:A:790:GLN:O	1:A:794:LEU:HG	2.20	0.41
1:A:469:VAL:CB	1:A:475:PRO:HA	2.50	0.41
1:A:257:SER:HA	1:A:314:ARG:CZ	2.50	0.41
1:A:360:ALA:HB3	1:A:370:PHE:HE2	1.85	0.41
1:A:427:ASP:O	1:A:457:HIS:NE2	2.54	0.41
1:A:542:HIS:HB2	1:A:547:ALA:HB2	2.02	0.41
1:A:38:ARG:HA	1:A:484:THR:HG21	2.03	0.41
1:A:38:ARG:HA	1:A:484:THR:CG2	2.50	0.41
1:A:89:LEU:HD12	1:A:94:VAL:CG2	2.42	0.41
1:A:124:PHE:CG	1:A:136:TYR:HD1	2.39	0.41
1:A:289:ASN:O	1:A:304:ASP:HA	2.21	0.41
1:A:488:VAL:HG11	1:A:513:LYS:HZ1	1.86	0.41
1:A:779:GLN:O	1:A:782:GLN:HG2	2.20	0.41
1:A:152:PRO:HB2	1:A:157:PHE:CE2	2.56	0.41
1:A:278:PRO:O	1:A:279:ILE:C	2.61	0.41
1:A:334:ILE:O	1:A:338:VAL:N	2.54	0.41
1:A:517:VAL:O	1:A:521:ARG:HB2	2.21	0.41
1:A:797:LEU:HD13	1:A:858:HIS:CE1	2.56	0.41
1:A:824:LYS:HB2	1:A:824:LYS:HE2	1.84	0.41
1:A:34:LEU:HD21	1:A:671:SER:O	2.20	0.41
1:A:78:LEU:N	1:A:79:PRO:CD	2.84	0.41
1:A:80:GLU:O	1:A:513:LYS:HA	2.21	0.41
1:A:109:PHE:CD1	1:A:149:LEU:HB2	2.56	0.41
1:A:111:PRO:HG3	1:A:467:LEU:HD12	2.03	0.41
1:A:358:LEU:O	1:A:369:TYR:HA	2.20	0.41
1:A:439:PHE:CE1	1:A:542:HIS:CD2	3.08	0.41
1:A:80:GLU:OE2	1:A:519:GLN:NE2	2.54	0.41
1:A:114:ARG:NH1	1:A:196:GLY:O	2.54	0.41
1:A:228:LEU:HD21	1:A:238:VAL:HG12	2.02	0.41
1:A:375:PHE:O	1:A:375:PHE:CG	2.73	0.41
1:A:401:THR:HG23	1:A:402:VAL:H	1.86	0.41
1:A:523:LEU:HB2	1:A:538:PHE:CE1	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:PHE:CD1	1:A:376:ARG:NE	2.89	0.40
1:A:717:LEU:O	1:A:720:PHE:HB3	2.21	0.40
1:A:520:LEU:HG	1:A:538:PHE:CD1	2.56	0.40
1:A:282:ILE:CG2	1:A:283:ALA:H	2.33	0.40
1:A:429:ASP:CG	1:A:458:SER:H	2.29	0.40
1:A:726:GLN:NE2	1:A:732:LEU:HD21	2.36	0.40
1:A:43:LEU:HB2	1:A:352:GLU:O	2.21	0.40
1:A:100:MET:HG3	1:A:119:ILE:HA	2.03	0.40
1:A:225:ARG:NH1	1:A:305:LEU:HD13	2.35	0.40
1:A:815:GLN:HA	1:A:818:LEU:HD12	2.02	0.40
1:A:26:ALA:CB	1:A:784:LEU:HB2	2.52	0.40
1:A:57:VAL:CA	1:A:389:HIS:HD1	2.29	0.40
1:A:176:LEU:HD13	1:A:176:LEU:HA	1.87	0.40
1:A:217:THR:HG21	1:A:282:ILE:HG12	2.03	0.40
1:A:278:PRO:CD	1:A:297:LYS:HE2	2.50	0.40
1:A:375:PHE:CD1	1:A:376:ARG:HG2	2.57	0.40
1:A:497:PRO:HG3	1:A:515:ARG:CD	2.51	0.40
1:A:674:MET:CE	1:A:714:LEU:HD21	2.51	0.40
1:A:766:LYS:O	1:A:770:ALA:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	682/1114 (61%)	635 (93%)	42 (6%)	5 (1%)	18 55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	LEU
1	A	277	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	824	LYS
1	A	122	ASP
1	A	265	VAL

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	603/962 (63%)	584 (97%)	19 (3%)	34	55

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	81	ILE
1	A	89	LEU
1	A	105	MET
1	A	119	ILE
1	A	121	SER
1	A	142	GLU
1	A	145	LEU
1	A	257	SER
1	A	265	VAL
1	A	271	PHE
1	A	390	VAL
1	A	402	VAL
1	A	464	ILE
1	A	802	GLN
1	A	805	ILE
1	A	806	ILE
1	A	821	THR
1	A	824	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	68	GLN
1	A	103	ASN
1	A	281	GLN
1	A	301	GLN
1	A	383	ASN
1	A	491	GLN
1	A	512	HIS
1	A	522	HIS
1	A	724	ASN
1	A	782	GLN
1	A	783	GLN
1	A	817	GLN
1	A	843	ASN
1	A	858	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.

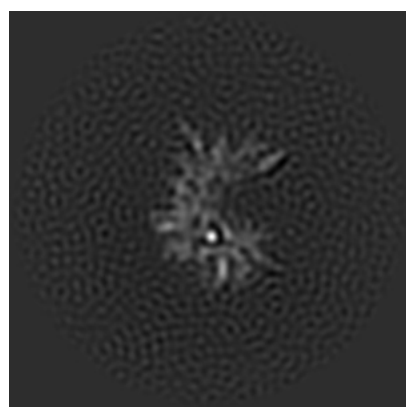
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31382. These allow visual inspection of the internal detail of the map and identification of artifacts.

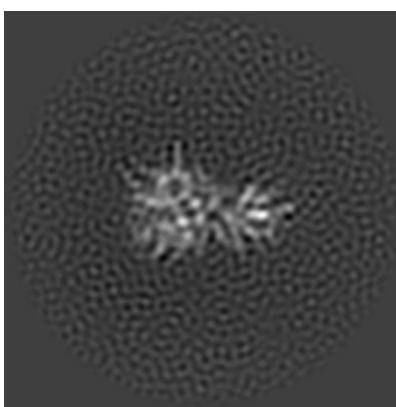
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

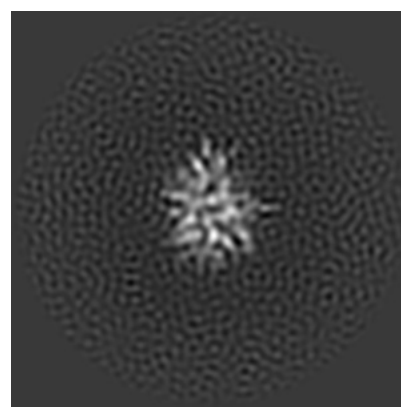
6.1.1 Primary map



X



Y

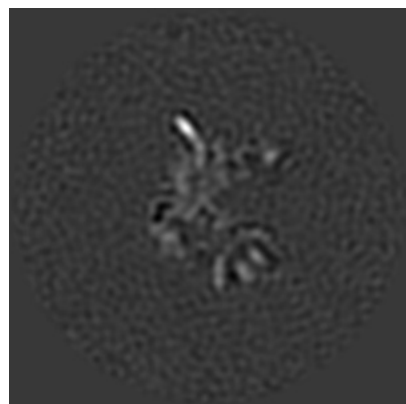


Z

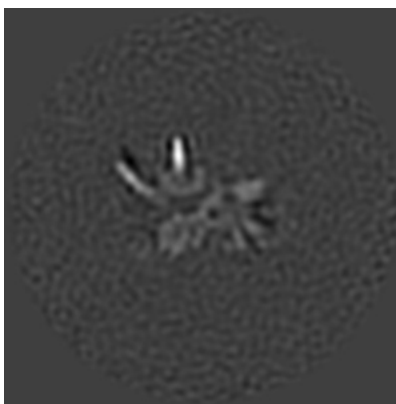
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

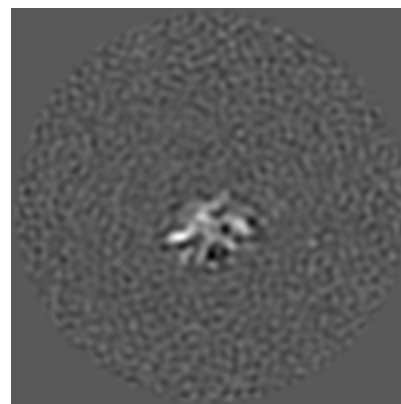
6.2.1 Primary map



X Index: 120



Y Index: 120

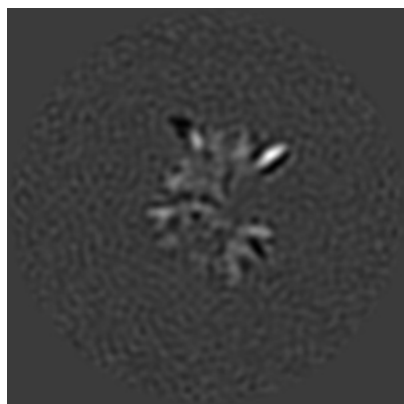


Z Index: 120

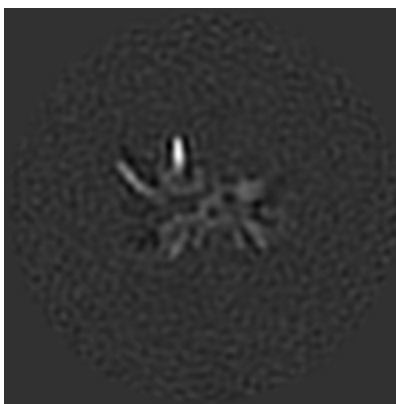
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

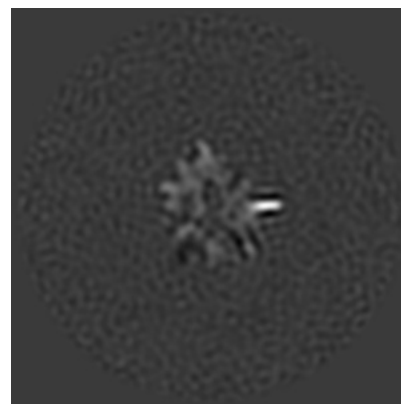
6.3.1 Primary map



X Index: 116



Y Index: 121

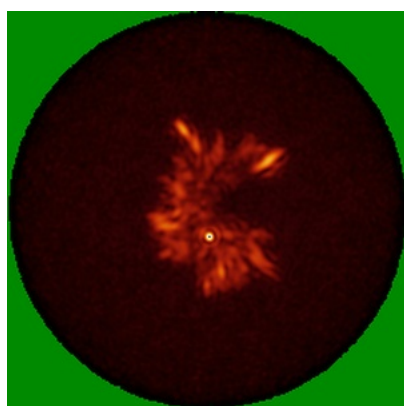


Z Index: 104

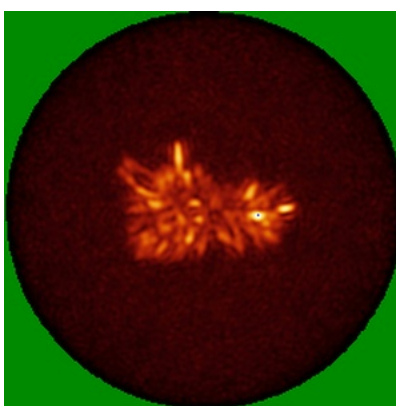
The images above show the largest variance slices of the map in three orthogonal directions.

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

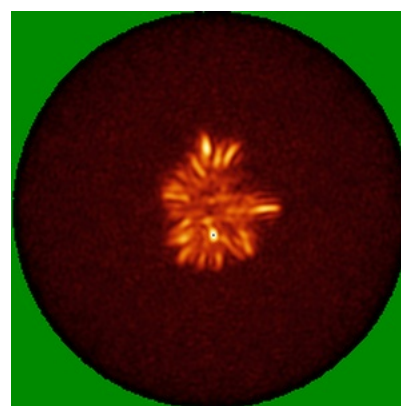
6.4.1 Primary map



X



Y

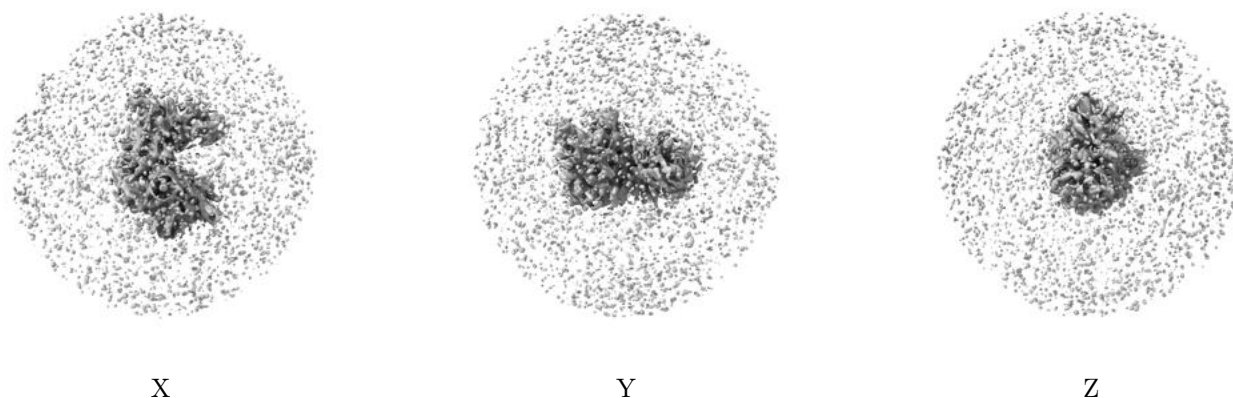


Z

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 0.37. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

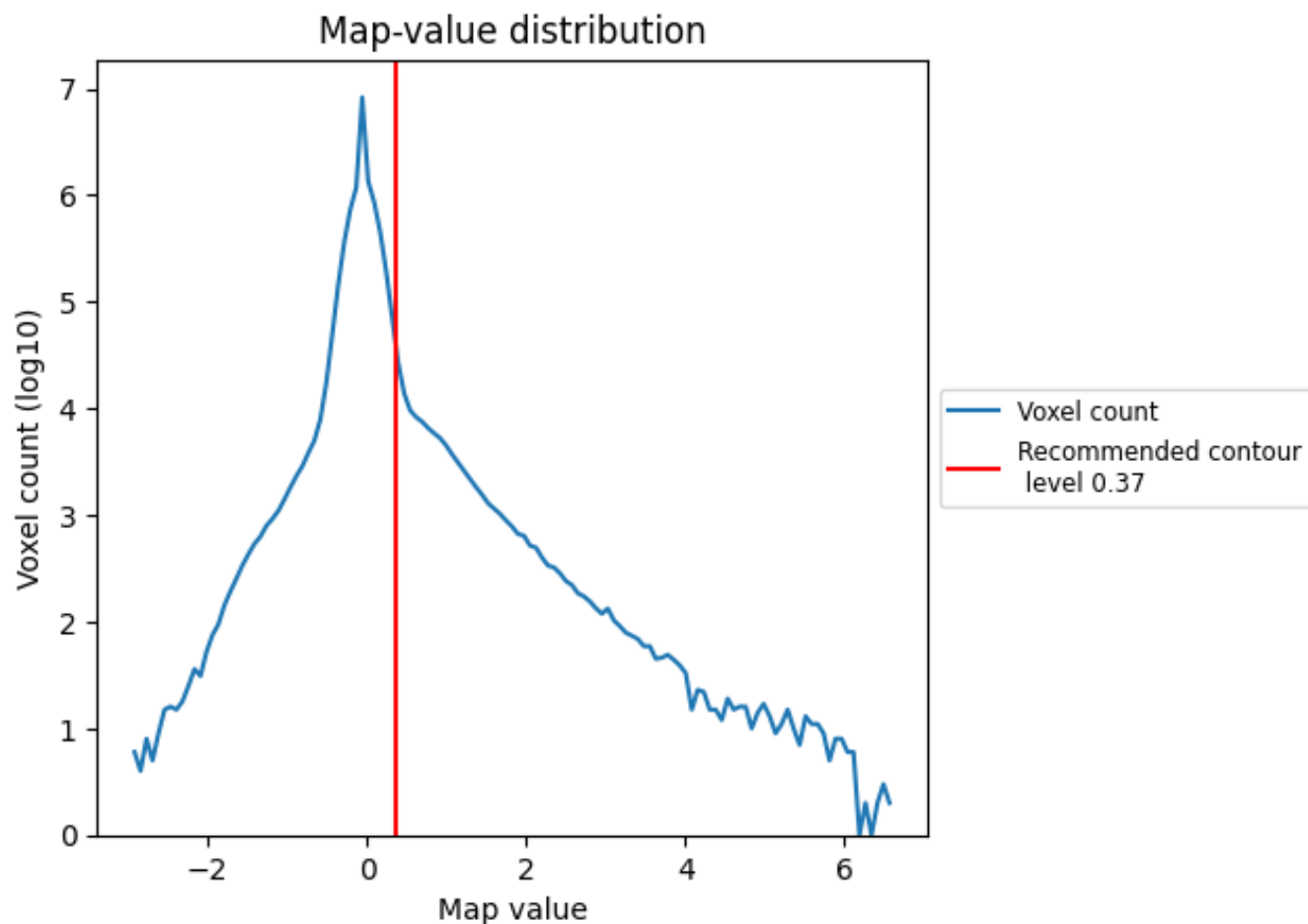
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

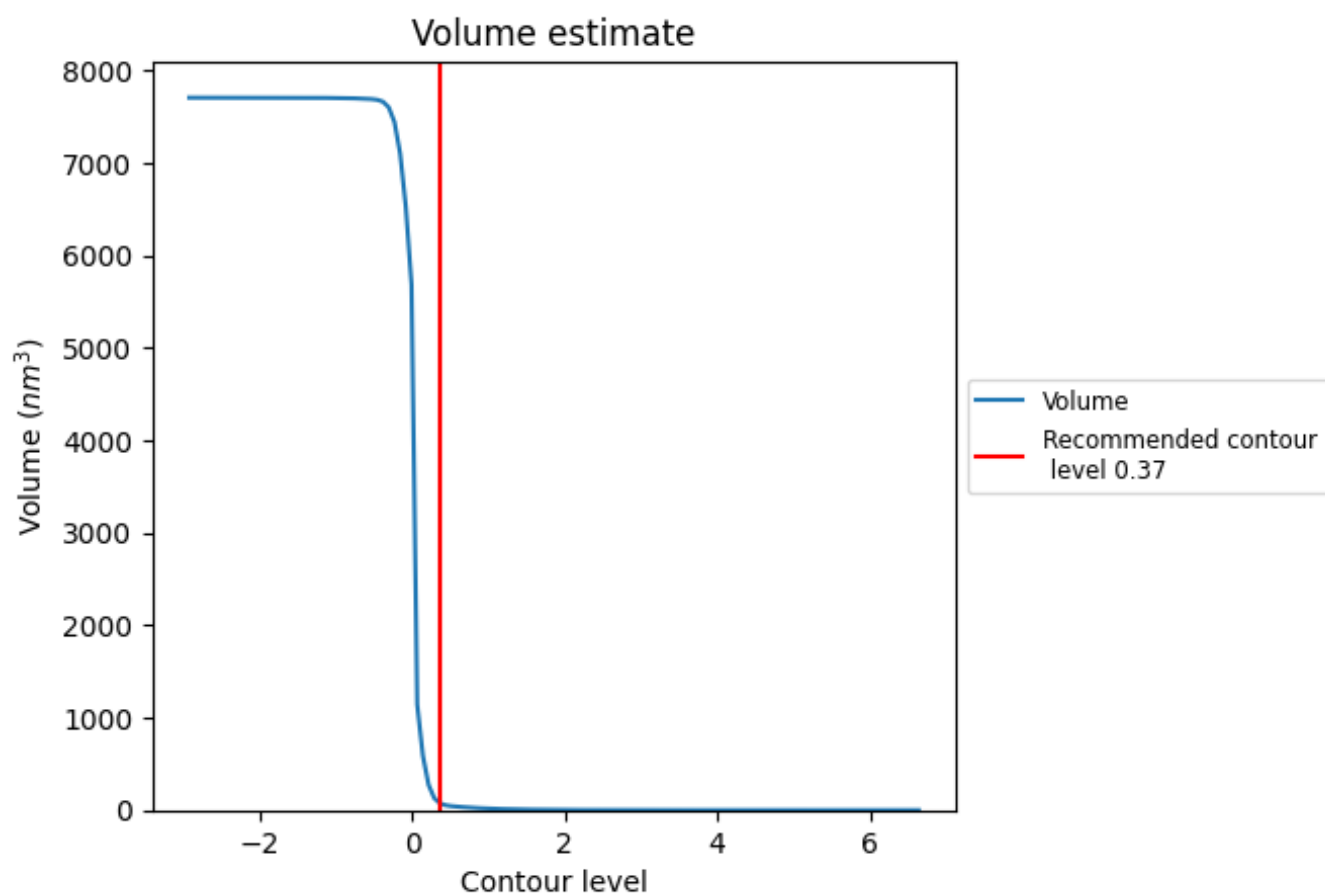
This section contains the results of statistical analysis of the map.

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.

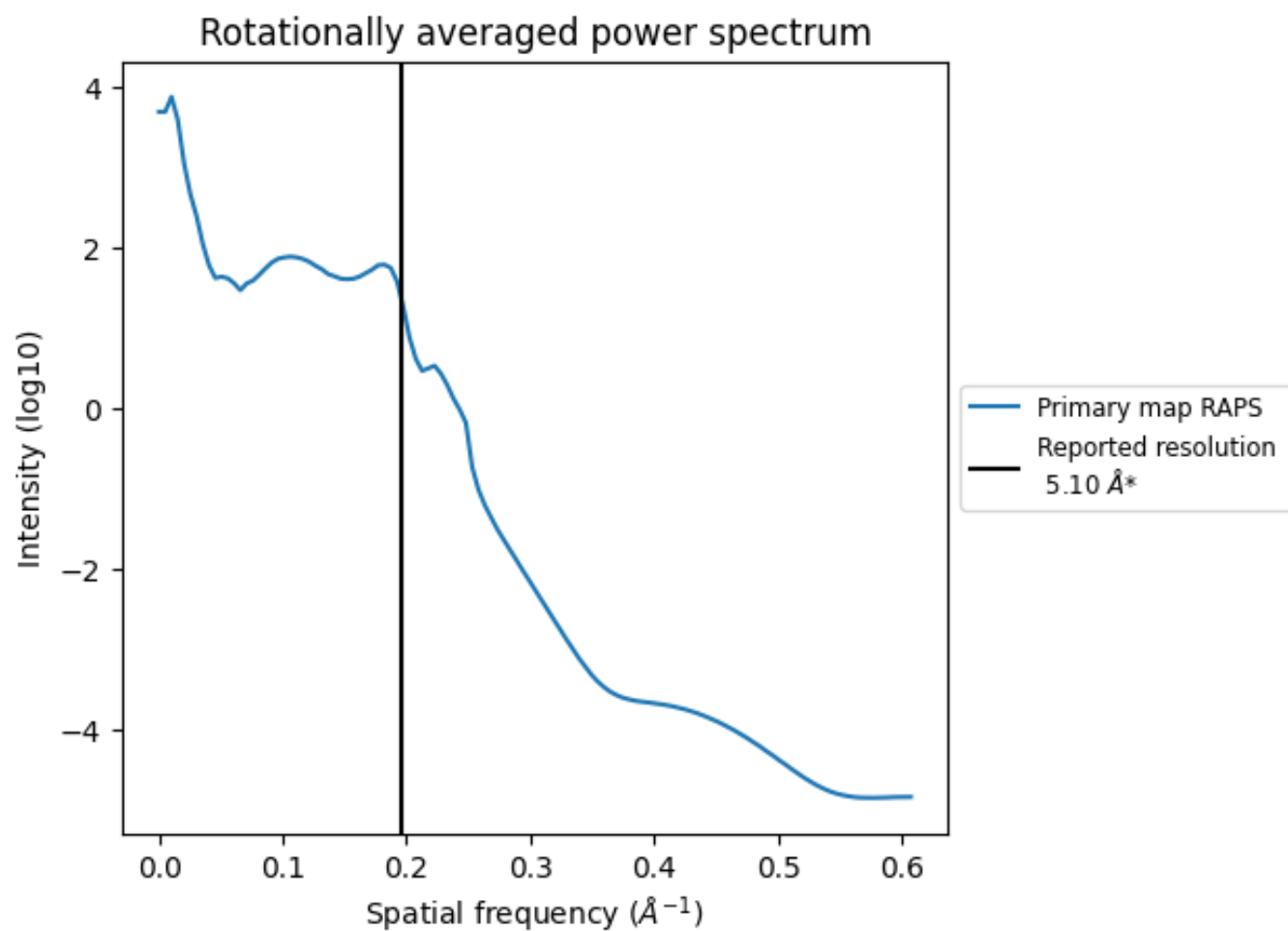
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 73 nm³; this corresponds to an approximate mass of 66 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 0.196 Å⁻¹

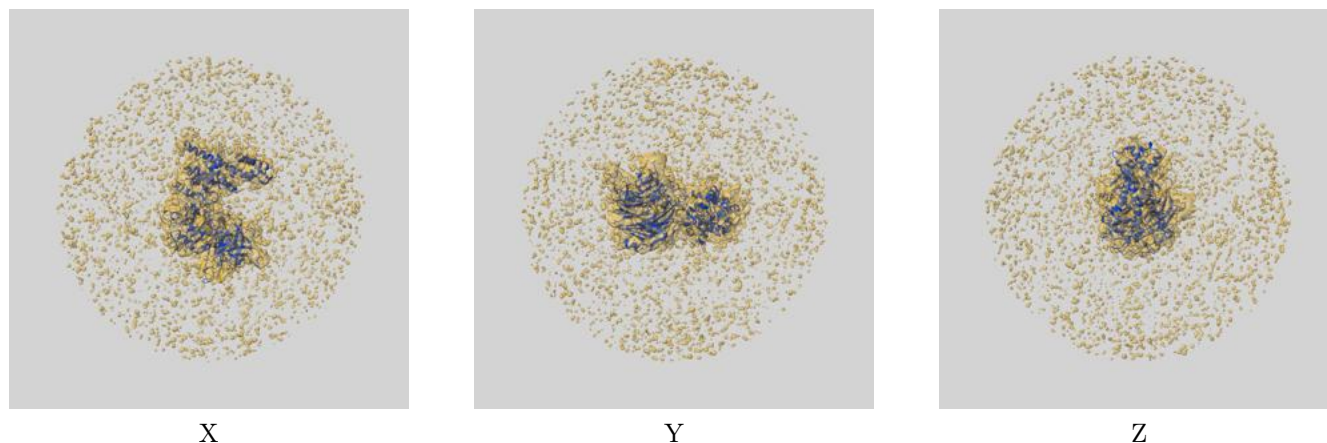
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31382 and PDB model 7EYE. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



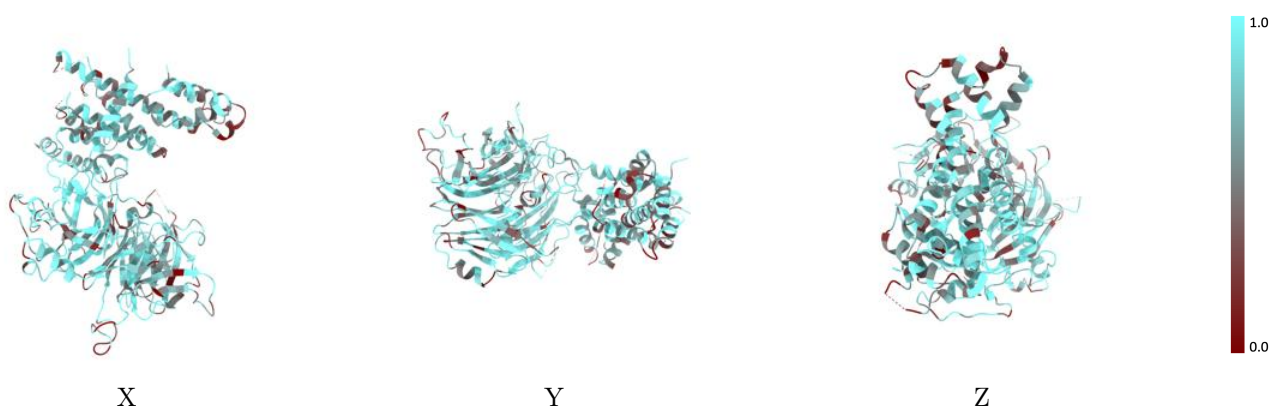
The images above show the 3D surface view of the map at the recommended contour level 0.37 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



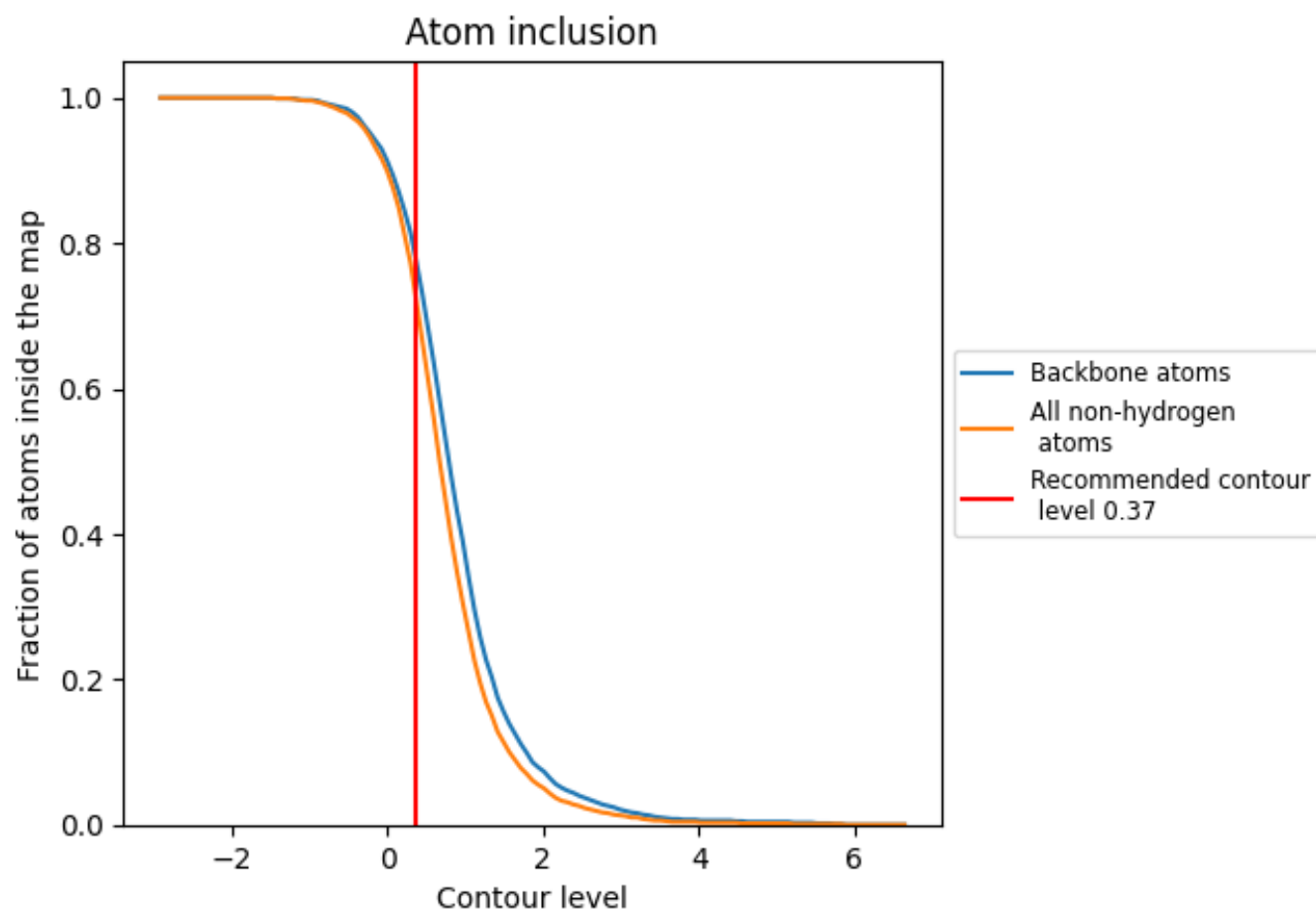
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.37).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 72% 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 (0.37) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7210	0.2100
A	0.7220	0.2100

