



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:49 PM UTC

PDB ID : 8S24 / pdb_00008s24
EMDB ID : EMD-19653
Title : Structure of the E3 ubiquitin ligase RNF213, determined by cryoEM
Authors : Naydenova, K.; Randow, F.
Deposited on : 2024-02-16
Resolution : 3.00 Å(reported)
Based on initial model : .

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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

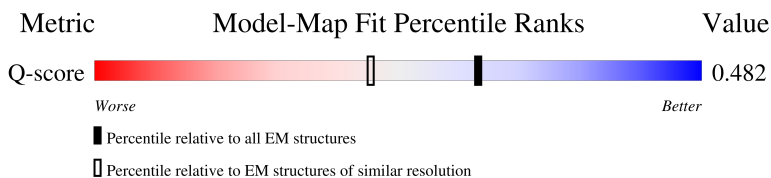
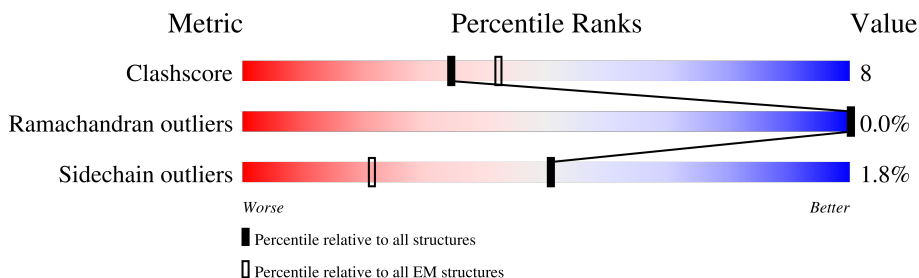
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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	5247	 66% 17% 16%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 35357 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 E3 ubiquitin-protein ligase RNF213.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4387	Total	C	N	O	S	0	0
			35324	22575	6081	6455	213		

There are 41 discrepancies between the modelled and reference sequences:

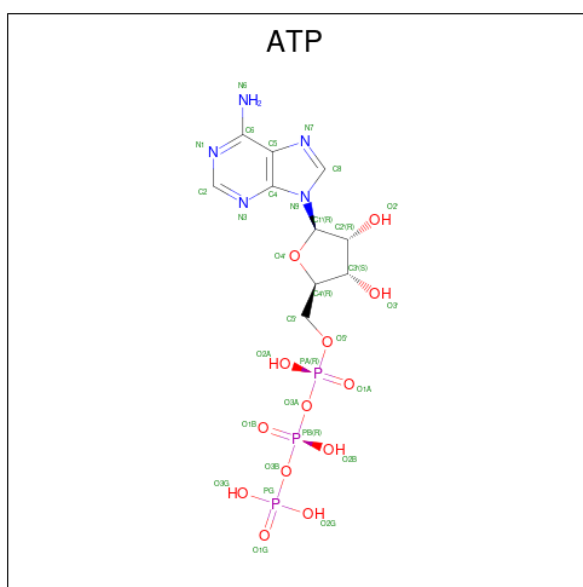
Chain	Residue	Modelled	Actual	Comment	Reference
A	-39	MET	-	initiating methionine	UNP Q63HN8
A	-38	ALA	-	expression tag	UNP Q63HN8
A	-37	SER	-	expression tag	UNP Q63HN8
A	-36	TRP	-	expression tag	UNP Q63HN8
A	-35	SER	-	expression tag	UNP Q63HN8
A	-34	HIS	-	expression tag	UNP Q63HN8
A	-33	PRO	-	expression tag	UNP Q63HN8
A	-32	GLN	-	expression tag	UNP Q63HN8
A	-31	PHE	-	expression tag	UNP Q63HN8
A	-30	GLU	-	expression tag	UNP Q63HN8
A	-29	LYS	-	expression tag	UNP Q63HN8
A	-28	GLY	-	expression tag	UNP Q63HN8
A	-27	SER	-	expression tag	UNP Q63HN8
A	-26	ALA	-	expression tag	UNP Q63HN8
A	-25	GLY	-	expression tag	UNP Q63HN8
A	-24	SER	-	expression tag	UNP Q63HN8
A	-23	ALA	-	expression tag	UNP Q63HN8
A	-22	ALA	-	expression tag	UNP Q63HN8
A	-21	GLY	-	expression tag	UNP Q63HN8
A	-20	SER	-	expression tag	UNP Q63HN8
A	-19	GLY	-	expression tag	UNP Q63HN8
A	-18	ALA	-	expression tag	UNP Q63HN8
A	-17	GLY	-	expression tag	UNP Q63HN8
A	-16	TRP	-	expression tag	UNP Q63HN8
A	-15	SER	-	expression tag	UNP Q63HN8
A	-14	HIS	-	expression tag	UNP Q63HN8
A	-13	PRO	-	expression tag	UNP Q63HN8
A	-12	GLN	-	expression tag	UNP Q63HN8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	PHE	-	expression tag	UNP Q63HN8
A	-10	GLU	-	expression tag	UNP Q63HN8
A	-9	LYS	-	expression tag	UNP Q63HN8
A	-8	GLU	-	expression tag	UNP Q63HN8
A	-7	ASN	-	expression tag	UNP Q63HN8
A	-6	LEU	-	expression tag	UNP Q63HN8
A	-5	TYR	-	expression tag	UNP Q63HN8
A	-4	PHE	-	expression tag	UNP Q63HN8
A	-3	GLN	-	expression tag	UNP Q63HN8
A	-2	ALA	-	expression tag	UNP Q63HN8
A	-1	MET	-	expression tag	UNP Q63HN8
A	0	SER	-	expression tag	UNP Q63HN8
A	1045	ASP	ASN	variant	UNP Q63HN8

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



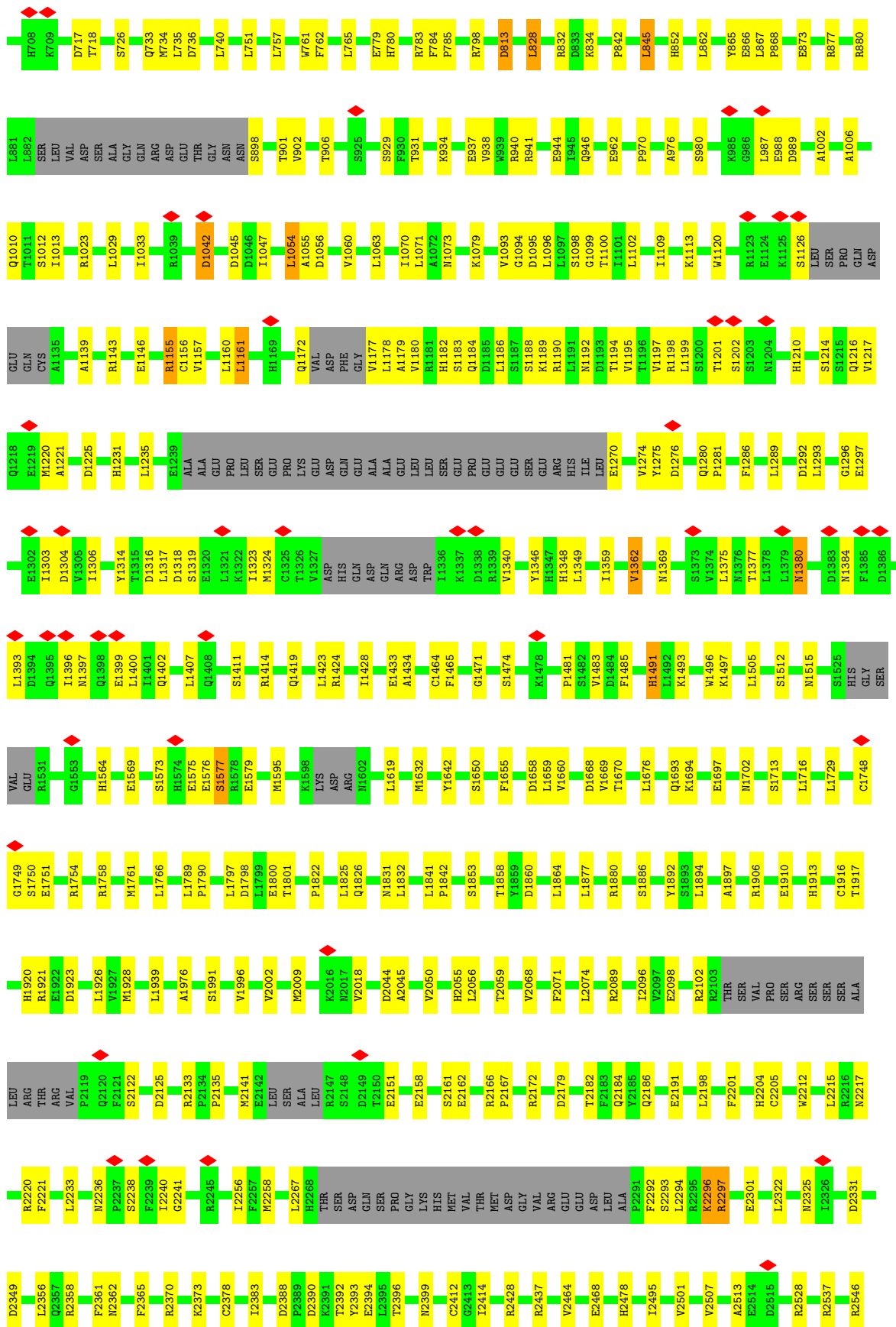
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

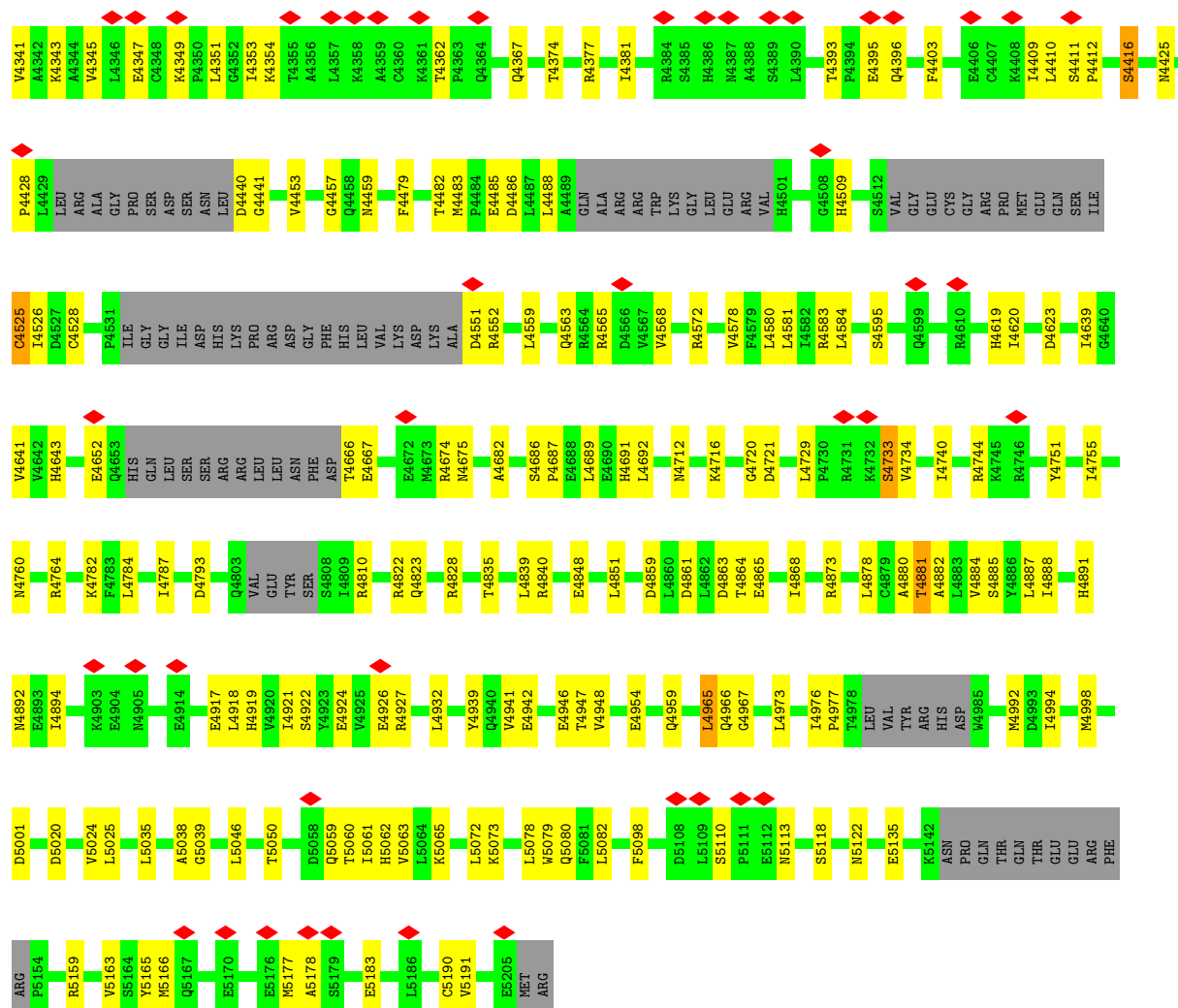
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mg	0
			1	1	

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Zn	0
			1	1	







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	143490	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	29.8	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.055	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	471.552, 471.552, 471.552	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.921, 0.921, 0.921	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, ZN

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	0.25	0/36047	0.31	0/48733

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	35324	0	35571	575	0
2	A	31	0	12	0	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
All	All	35357	0	35583	575	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 8.

All (575) 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:5061:ILE:O	1:A:5065:LYS:NZ	2.02	0.92
1:A:3979:CYS:O	1:A:3982:LYS:O	1.89	0.91
1:A:4525:CYS:SG	1:A:4526:ILE:N	2.47	0.87
1:A:1096:LEU:O	1:A:1143:ARG:NH1	2.08	0.86
1:A:687:ARG:NH2	1:A:733:GLN:OE1	2.10	0.84
1:A:1172:GLN:O	1:A:1270:GLU:N	2.10	0.84
1:A:4483:MET:O	1:A:4572:ARG:NH2	2.10	0.83
1:A:1094:GLY:O	1:A:1098:SER:OG	1.96	0.83
1:A:3381:PHE:O	1:A:3425:ARG:NH2	2.12	0.83
1:A:1023:ARG:NH2	1:A:1073:ASN:O	2.12	0.82
1:A:1155:ARG:NH2	1:A:1225:ASP:OD1	2.12	0.82
1:A:1323:ILE:HG23	1:A:1324:MET:HE3	1.60	0.82
1:A:2864:LEU:O	1:A:2878:LYS:NZ	2.12	0.81
1:A:4509:HIS:ND1	1:A:4528:CYS:SG	2.54	0.81
1:A:3654:ARG:NH2	1:A:3704:ASN:O	2.14	0.81
1:A:403:ARG:NH1	1:A:413:TRP:O	2.15	0.80
1:A:2741:THR:O	1:A:2961:LYS:NZ	2.15	0.80
1:A:4341:VAL:HG12	1:A:4353:ILE:HD12	1.63	0.80
1:A:3199:ILE:O	1:A:3208:LYS:NZ	2.15	0.80
1:A:3937:THR:HG23	1:A:3941:VAL:HG23	1.64	0.79
1:A:2694:HIS:O	1:A:2700:LYS:NZ	2.17	0.78
1:A:2172:ARG:NH2	1:A:2191:GLU:OE1	2.16	0.78
1:A:4095:LEU:O	1:A:4115:LYS:NZ	2.12	0.78
1:A:4233:ARG:NH1	1:A:4740:ILE:O	2.16	0.78
1:A:3961:GLU:N	1:A:3961:GLU:OE1	2.17	0.77
1:A:880:ARG:NH1	1:A:946:GLN:O	2.18	0.77
1:A:2158:GLU:O	1:A:2161:SER:OG	2.03	0.76
1:A:3403:ASN:OD1	1:A:3406:ARG:NE	2.20	0.75
1:A:2296:LYS:NZ	1:A:2301:GLU:OE1	2.18	0.75
1:A:4293:GLN:O	1:A:4296:SER:OG	2.05	0.74
1:A:1095:ASP:O	1:A:1099:GLY:N	2.20	0.74
1:A:587:LYS:NZ	1:A:634:GLU:OE1	2.15	0.74
1:A:1033:ILE:HD11	1:A:1060:VAL:HG21	1.68	0.74
1:A:1564:HIS:ND1	1:A:1579:GLU:OE2	2.21	0.74
1:A:4000:CYS:SG	1:A:4019:ARG:NH2	2.61	0.74
1:A:2198:LEU:HD21	1:A:2212:TRP:CH2	2.23	0.73
1:A:2631:ASP:OD2	1:A:2699:LYS:NZ	2.16	0.73
1:A:2729:GLN:NE2	1:A:2750:GLU:OE1	2.21	0.73
1:A:2548:SER:O	1:A:2552:THR:HG23	1.89	0.73
1:A:5024:VAL:HG22	1:A:5063:VAL:HG13	1.71	0.73
1:A:1694:LYS:NZ	1:A:1800:GLU:OE1	2.21	0.73
1:A:3242:LEU:HD23	1:A:3243:THR:N	2.03	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3558:MET:SD	1:A:3558:MET:N	2.62	0.73
1:A:4946:GLU:OE1	1:A:4946:GLU:N	2.22	0.73
1:A:5183:GLU:N	1:A:5183:GLU:OE1	2.22	0.73
1:A:4062:ARG:NE	1:A:4122:ASP:OD2	2.22	0.73
1:A:4393:THR:N	1:A:4396:GLN:OE1	2.22	0.73
1:A:3176:ILE:HG21	1:A:3227:ALA:HB1	1.72	0.72
1:A:3654:ARG:NH1	1:A:3706:SER:OG	2.22	0.72
1:A:3585:ARG:NH1	1:A:3669:PHE:O	2.22	0.72
1:A:1758:ARG:NH1	1:A:1761:MET:SD	2.64	0.71
1:A:684:MET:O	1:A:687:ARG:NH1	2.23	0.71
1:A:2236:ASN:OD1	1:A:2238:SER:OG	2.05	0.71
1:A:762:PHE:O	1:A:798:ARG:NH2	2.24	0.71
1:A:2365:PHE:O	1:A:2373:LYS:NZ	2.16	0.71
1:A:3585:ARG:NH2	1:A:3675:LEU:O	2.24	0.71
1:A:2122:SER:OG	1:A:2125:ASP:OD2	2.09	0.70
1:A:4425:ASN:O	1:A:4425:ASN:ND2	2.24	0.70
1:A:3843:MET:SD	1:A:3843:MET:N	2.65	0.70
1:A:1897:ALA:HB1	1:A:1939:LEU:HD23	1.72	0.70
1:A:478:ARG:NH2	1:A:498:ILE:O	2.25	0.70
1:A:976:ALA:O	1:A:980:SER:OG	2.09	0.69
1:A:1396:ILE:HG23	1:A:1397:ASN:H	1.56	0.69
1:A:4412:PRO:O	1:A:4416:SER:OG	2.11	0.69
1:A:1184:GLN:OE1	1:A:1210:HIS:NE2	2.26	0.69
1:A:2217:ASN:OD1	1:A:2220:ARG:NH2	2.26	0.69
1:A:3450:LEU:HD13	1:A:3625:TRP:CE3	2.27	0.69
1:A:642:ASP:OD1	1:A:643:TRP:N	2.26	0.69
1:A:3021:ASN:ND2	1:A:3170:GLU:OE1	2.24	0.69
1:A:1749:GLY:O	1:A:1754:ARG:NH2	2.26	0.68
1:A:2977:GLN:NE2	1:A:2978:ASP:OD1	2.27	0.68
1:A:3559:ARG:NH1	1:A:3650:GLU:OE2	2.26	0.68
1:A:3061:GLU:OE1	1:A:3061:GLU:N	2.25	0.68
1:A:3990:SER:OG	1:A:3993:GLY:N	2.27	0.68
1:A:3091:LYS:NZ	1:A:3095:GLU:OE2	2.19	0.68
1:A:862:LEU:HD11	1:A:938:VAL:HG21	1.74	0.68
1:A:3294:ASN:ND2	1:A:3454:ASP:OD2	2.26	0.68
1:A:2528:ARG:NH2	1:A:2634:SER:O	2.26	0.67
1:A:5118:SER:O	1:A:5122:ASN:ND2	2.27	0.67
1:A:2984:LEU:O	1:A:2988:SER:OG	2.09	0.67
1:A:3964:ASP:O	1:A:3967:THR:OG1	2.11	0.67
1:A:5159:ARG:HH21	1:A:5163:VAL:HG23	1.60	0.67
1:A:4187:SER:OG	1:A:4926:GLU:O	2.07	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5190:CYS:SG	1:A:5191:VAL:N	2.68	0.67
1:A:1377:THR:O	1:A:1380:ASN:ND2	2.27	0.67
1:A:3075:PRO:O	1:A:3078:GLN:NE2	2.27	0.67
1:A:1573:SER:OG	1:A:1575:GLU:OE1	2.13	0.66
1:A:2293:SER:O	1:A:2294:LEU:HD23	1.95	0.66
1:A:1402:GLN:N	1:A:1402:GLN:OE1	2.29	0.66
1:A:1569:GLU:N	1:A:1569:GLU:OE1	2.29	0.66
1:A:1913:HIS:O	1:A:1917:THR:HG23	1.96	0.66
1:A:3946:GLY:O	1:A:3949:THR:HG22	1.95	0.65
1:A:970:PRO:HB3	1:A:1002:ALA:HB1	1.77	0.65
1:A:2074:LEU:O	1:A:2089:ARG:NH1	2.29	0.65
1:A:2322:LEU:HD12	1:A:2361:PHE:CD2	2.32	0.65
1:A:620:LEU:HD13	1:A:662:LEU:CD2	2.27	0.65
1:A:2325:ASN:ND2	1:A:2331:ASP:OD2	2.29	0.65
1:A:4563:GLN:OE1	1:A:4563:GLN:N	2.30	0.65
1:A:2133:ARG:NH1	1:A:2141:MET:SD	2.70	0.64
1:A:4482:THR:HG22	1:A:4583:ARG:HG2	1.78	0.64
1:A:2044:ASP:OD1	1:A:2045:ALA:N	2.30	0.64
1:A:1892:TYR:O	1:A:1926:LEU:HD12	1.97	0.64
1:A:3980:GLU:C	1:A:3982:LYS:O	2.40	0.64
1:A:2962:MET:SD	1:A:2986:ASN:ND2	2.72	0.63
1:A:3455:VAL:O	1:A:3456:THR:HG22	1.98	0.63
1:A:1858:THR:OG1	1:A:1860:ASP:OD1	2.15	0.63
1:A:1375:LEU:HD21	1:A:1485:PHE:CZ	2.34	0.63
1:A:1186:LEU:HD23	1:A:1189:LYS:HD3	1.80	0.63
1:A:3808:GLU:N	1:A:3808:GLU:OE1	2.32	0.63
1:A:3444:ASP:OD2	1:A:3621:ARG:NH1	2.31	0.63
1:A:3450:LEU:HD12	1:A:3451:MET:N	2.14	0.63
1:A:2870:GLU:N	1:A:2870:GLU:OE1	2.32	0.62
1:A:5135:GLU:OE2	1:A:5165:TYR:OH	2.16	0.62
1:A:3742:ILE:O	1:A:3746:THR:HG23	1.98	0.62
1:A:2602:VAL:HG22	1:A:2607:LEU:HG	1.80	0.62
1:A:4782:LYS:NZ	1:A:4924:GLU:OE2	2.32	0.62
1:A:452:TYR:O	1:A:463:GLU:N	2.32	0.62
1:A:5062:HIS:ND1	1:A:5062:HIS:O	2.32	0.62
1:A:585:GLU:OE1	1:A:585:GLU:N	2.32	0.62
1:A:1375:LEU:HD11	1:A:1485:PHE:HE1	1.63	0.62
1:A:2370:ARG:NH2	1:A:2390:ASP:O	2.33	0.62
1:A:4568:VAL:HG21	1:A:4580:LEU:HD13	1.82	0.62
1:A:1318:ASP:OD2	1:A:1319:SER:N	2.33	0.61
1:A:3673:MET:SD	1:A:3673:MET:N	2.74	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2825:CYS:SG	1:A:2839:SER:OG	2.57	0.61
1:A:598:VAL:HG13	1:A:599:VAL:HG23	1.81	0.61
1:A:944:GLU:O	1:A:946:GLN:NE2	2.34	0.61
1:A:1575:GLU:OE1	1:A:1575:GLU:N	2.33	0.61
1:A:432:LEU:HD12	1:A:532:LEU:HD13	1.83	0.61
1:A:4393:THR:OG1	1:A:4395:GLU:OE2	2.18	0.60
1:A:3912:VAL:O	1:A:3916:VAL:HG23	2.02	0.60
1:A:4362:THR:O	1:A:4367:GLN:NE2	2.34	0.60
1:A:598:VAL:HG11	1:A:643:TRP:CZ2	2.37	0.60
1:A:717:ASP:OD1	1:A:718:THR:N	2.35	0.60
1:A:1297:GLU:N	1:A:1297:GLU:OE1	2.34	0.60
1:A:2618:VAL:HG11	1:A:2685:LEU:HD11	1.84	0.60
1:A:5020:ASP:O	1:A:5024:VAL:HG23	2.02	0.60
1:A:1822:PRO:HD2	1:A:1825:LEU:HD12	1.84	0.60
1:A:2221:PHE:HZ	1:A:2258:MET:HE2	1.67	0.59
1:A:4840:ARG:NH1	1:A:4859:ASP:OD1	2.35	0.59
1:A:3370:ALA:O	1:A:3373:LYS:NZ	2.35	0.59
1:A:2537:ARG:NH1	1:A:2631:ASP:O	2.35	0.59
1:A:3837:GLN:O	1:A:3841:SER:OG	2.11	0.59
1:A:5001:ASP:N	1:A:5073:LYS:O	2.36	0.59
1:A:1160:LEU:HD11	1:A:1221:ALA:HB2	1.84	0.59
1:A:4377:ARG:HA	1:A:4381:ILE:HD12	1.83	0.59
1:A:1369:ASN:N	1:A:1481:PRO:O	2.36	0.59
1:A:425:ASP:HA	1:A:431:VAL:HG23	1.85	0.59
1:A:1194:THR:OG1	1:A:1195:VAL:N	2.35	0.59
1:A:5035:LEU:O	1:A:5039:GLY:N	2.35	0.59
1:A:1433:GLU:OE1	1:A:1434:ALA:N	2.36	0.59
1:A:4485:GLU:OE2	1:A:4675:ASN:ND2	2.35	0.59
1:A:865:TYR:OH	1:A:937:GLU:OE2	2.20	0.58
1:A:2812:HIS:O	1:A:2854:LYS:NZ	2.29	0.58
1:A:779:GLU:OE1	1:A:783:ARG:NH1	2.35	0.58
1:A:1713:SER:OG	1:A:1797:LEU:O	2.16	0.58
1:A:2322:LEU:N	1:A:2362:ASN:OD1	2.36	0.58
1:A:401:PHE:HA	1:A:420:LEU:HD13	1.86	0.58
1:A:988:GLU:OE1	1:A:988:GLU:N	2.33	0.58
1:A:3368:ASN:OD1	1:A:3369:THR:N	2.34	0.58
1:A:4584:LEU:HD11	1:A:4620:ILE:HG23	1.84	0.58
1:A:1716:LEU:HD21	1:A:1729:LEU:HD11	1.86	0.58
1:A:5110:SER:OG	1:A:5113:ASN:ND2	2.36	0.58
1:A:656:ASP:OD1	1:A:657:GLU:N	2.37	0.58
1:A:1375:LEU:HD11	1:A:1485:PHE:CE1	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4483:MET:HE3	1:A:4674:ARG:HH21	1.69	0.58
1:A:1143:ARG:NH2	1:A:1198:ARG:O	2.37	0.58
1:A:2162:GLU:OE2	1:A:2166:ARG:NH1	2.34	0.58
1:A:2650:TRP:HB2	1:A:2761:LEU:HD21	1.85	0.57
1:A:3308:ASP:OD2	1:A:3311:ARG:NH1	2.37	0.57
1:A:3448:SER:OG	1:A:3451:MET:O	2.14	0.57
1:A:4325:ASP:OD1	1:A:4377:ARG:NE	2.36	0.57
1:A:1006:ALA:HB1	1:A:1013:ILE:HD11	1.85	0.57
1:A:4198:LEU:HD21	1:A:4259:TYR:HB2	1.85	0.57
1:A:2646:LYS:HG2	1:A:2761:LEU:HD22	1.86	0.57
1:A:4048:SER:O	1:A:4051:HIS:NE2	2.38	0.57
1:A:1493:LYS:O	1:A:1497:LYS:NZ	2.33	0.57
1:A:3336:GLU:O	1:A:3340:ARG:NH2	2.36	0.57
1:A:550:ASN:OD1	1:A:551:SER:N	2.39	0.56
1:A:594:LEU:O	1:A:598:VAL:HG12	2.05	0.56
1:A:2715:TYR:HA	1:A:2720:LEU:HD23	1.87	0.56
1:A:4733:SER:OG	1:A:4734:VAL:N	2.38	0.56
1:A:1198:ARG:NH1	1:A:1199:LEU:O	2.35	0.56
1:A:3274:SER:OG	1:A:3276:GLY:O	2.24	0.56
1:A:4764:ARG:NE	1:A:4954:GLU:OE2	2.31	0.56
1:A:591:TRP:CH2	1:A:630:VAL:HG11	2.40	0.56
1:A:3980:GLU:O	1:A:3982:LYS:O	2.23	0.56
1:A:3563:LEU:HD22	1:A:3653:THR:HG21	1.87	0.56
1:A:4009:CYS:HA	1:A:4015:VAL:HG12	1.87	0.56
1:A:4267:CYS:O	1:A:4276:ARG:NH1	2.36	0.56
1:A:4744:ARG:NH2	1:A:4939:TYR:OH	2.36	0.56
1:A:1054:LEU:HD23	1:A:1055:ALA:H	1.71	0.56
1:A:2850:GLU:OE2	1:A:2890:ASP:N	2.38	0.56
1:A:845:LEU:HD22	1:A:902:VAL:HG11	1.88	0.56
1:A:2240:ILE:HD12	1:A:2241:GLY:N	2.20	0.56
1:A:3941:VAL:HG23	1:A:3941:VAL:O	2.06	0.56
1:A:423:THR:HG21	1:A:434:GLU:HG3	1.88	0.55
1:A:540:ILE:O	1:A:548:ASN:ND2	2.38	0.55
1:A:5059:GLN:OE1	1:A:5059:GLN:N	2.39	0.55
1:A:428:HIS:O	1:A:430:ARG:NH2	2.39	0.55
1:A:3624:LEU:O	1:A:3628:VAL:HG23	2.06	0.55
1:A:2468:GLU:OE2	1:A:2513:ALA:N	2.38	0.55
1:A:4687:PRO:O	1:A:4691:HIS:ND1	2.39	0.55
1:A:1906:ARG:NH1	1:A:1910:GLU:OE2	2.39	0.55
1:A:3979:CYS:O	1:A:3982:LYS:C	2.50	0.55
1:A:2059:THR:O	1:A:2102:ARG:NH2	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:751:LEU:HD23	1:A:757:LEU:HD23	1.87	0.55
1:A:538:PHE:CD1	1:A:541:LEU:HD12	2.42	0.54
1:A:1991:SER:CB	1:A:1996:VAL:HG21	2.37	0.54
1:A:2184:GLN:O	1:A:2186:GLN:NE2	2.39	0.54
1:A:4266:PHE:CE1	1:A:4270:VAL:HG21	2.42	0.54
1:A:4020:CYS:SG	1:A:4021:LEU:N	2.81	0.54
1:A:5177:MET:SD	1:A:5178:ALA:N	2.81	0.54
1:A:3822:ARG:NH1	1:A:4917:GLU:OE2	2.41	0.54
1:A:1577:SER:O	1:A:1577:SER:OG	2.20	0.54
1:A:4274:TRP:CE2	1:A:4729:LEU:HD22	2.43	0.54
1:A:4341:VAL:HG12	1:A:4353:ILE:CD1	2.36	0.54
1:A:1595:MET:O	1:A:3091:LYS:NZ	2.39	0.54
1:A:3102:LEU:HD22	1:A:3105:LEU:HB2	1.90	0.54
1:A:4311:VAL:O	1:A:4311:VAL:HG13	2.07	0.54
1:A:4998:MET:HE1	1:A:5072:LEU:HB3	1.89	0.54
1:A:1396:ILE:HG23	1:A:1397:ASN:N	2.23	0.54
1:A:3535:LEU:HD21	1:A:3628:VAL:HG12	1.90	0.53
1:A:4666:THR:OG1	1:A:4667:GLU:N	2.41	0.53
1:A:637:LEU:HD22	1:A:641:LEU:HD13	1.90	0.53
1:A:2240:ILE:HD12	1:A:2241:GLY:C	2.32	0.53
1:A:3262:ALA:O	1:A:3287:TYR:OH	2.12	0.53
1:A:765:LEU:O	1:A:798:ARG:NH2	2.39	0.53
1:A:3117:ASN:OD1	1:A:3168:ARG:NH2	2.36	0.53
1:A:4102:ARG:NE	1:A:4111:CYS:SG	2.81	0.53
1:A:1380:ASN:O	1:A:1384:ASN:ND2	2.42	0.53
1:A:548:ASN:OD1	1:A:549:LEU:N	2.41	0.53
1:A:1289:LEU:HD11	1:A:1306:ILE:HD13	1.90	0.53
1:A:4086:LYS:NZ	1:A:4090:GLU:OE2	2.30	0.53
1:A:1642:TYR:O	1:A:1669:VAL:HG21	2.08	0.53
1:A:4180:ASP:OD1	1:A:4744:ARG:NH2	2.42	0.53
1:A:1275:TYR:O	1:A:1280:GLN:N	2.39	0.53
1:A:1464:CYS:O	1:A:1465:PHE:HB3	2.09	0.53
1:A:3859:ASP:OD1	1:A:3860:ALA:N	2.41	0.53
1:A:2292:PHE:CZ	1:A:2564:LEU:HD22	2.44	0.53
1:A:533:MET:HE2	1:A:559:PHE:HD2	1.73	0.53
1:A:1042:ASP:OD2	1:A:1042:ASP:N	2.41	0.53
1:A:3319:THR:OG1	1:A:3420:LEU:HD12	2.09	0.53
1:A:3837:GLN:OE1	1:A:3837:GLN:N	2.38	0.53
1:A:1177:VAL:O	1:A:1180:VAL:N	2.42	0.52
1:A:3213:SER:OG	1:A:3216:ASP:OD2	2.26	0.52
1:A:3863:ALA:O	1:A:3867:THR:HG23	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4891:HIS:HE2	1:A:4965:LEU:HD13	1.73	0.52
1:A:1655:PHE:CD1	1:A:1660:VAL:HG11	2.44	0.52
1:A:4565:ARG:NH2	1:A:4619:HIS:O	2.42	0.52
1:A:2135:PRO:HB3	1:A:2198:LEU:HD22	1.91	0.52
1:A:4921:ILE:HD11	1:A:4965:LEU:HD11	1.91	0.52
1:A:1177:VAL:HG23	1:A:1178:LEU:N	2.25	0.52
1:A:3558:MET:HE1	1:A:5038:ALA:HB3	1.90	0.52
1:A:4482:THR:HB	1:A:4559:LEU:HD11	1.91	0.52
1:A:598:VAL:HG11	1:A:643:TRP:HZ2	1.74	0.52
1:A:3240:ARG:CD	1:A:3246:LEU:HD11	2.39	0.52
1:A:2871:ASP:N	1:A:2871:ASP:OD1	2.42	0.51
1:A:2618:VAL:HG23	1:A:2707:ILE:HG13	1.91	0.51
1:A:3547:LEU:O	1:A:3548:ARG:NH1	2.40	0.51
1:A:423:THR:OG1	1:A:424:ARG:N	2.43	0.51
1:A:734:MET:HE3	1:A:734:MET:HA	1.92	0.51
1:A:2763:ILE:HG21	1:A:2898:ILE:HD12	1.93	0.51
1:A:3799:LYS:O	1:A:3802:SER:OG	2.20	0.51
1:A:4072:LEU:HD12	1:A:4076:ILE:HD12	1.91	0.51
1:A:2370:ARG:NH1	1:A:2393:TYR:O	2.43	0.51
1:A:1864:LEU:HD13	1:A:2068:VAL:HG13	1.93	0.51
1:A:3050:VAL:HG11	1:A:3176:ILE:HG12	1.93	0.51
1:A:3069:ILE:HB	1:A:3102:LEU:HD23	1.92	0.51
1:A:4153:TYR:CE1	1:A:4157:LEU:HD11	2.45	0.51
1:A:4822:ARG:NE	1:A:4823:GLN:OE1	2.34	0.51
1:A:735:LEU:HD12	1:A:736:ASP:N	2.26	0.51
1:A:1156:CYS:HB3	1:A:1221:ALA:HB1	1.92	0.50
1:A:2871:ASP:OD2	1:A:2877:LYS:NZ	2.41	0.50
1:A:4115:LYS:NZ	1:A:4118:SER:O	2.42	0.50
1:A:4395:GLU:OE1	1:A:4395:GLU:N	2.42	0.50
1:A:2055:HIS:NE2	1:A:2098:GLU:OE1	2.45	0.50
1:A:3330:CYS:SG	1:A:3346:LEU:HD22	2.51	0.50
1:A:4716:LYS:O	1:A:4720:GLY:N	2.40	0.50
1:A:1220:MET:HE1	1:A:1274:VAL:HG23	1.93	0.50
1:A:1424:ARG:O	1:A:1428:ILE:HD12	2.12	0.50
1:A:1146:GLU:HB3	1:A:1195:VAL:HG11	1.93	0.50
1:A:1877:LEU:HD23	1:A:1894:LEU:HD13	1.93	0.50
1:A:3767:TYR:OH	1:A:3815:HIS:NE2	2.39	0.50
1:A:640:SER:O	1:A:640:SER:OG	2.27	0.50
1:A:1826:GLN:N	1:A:1831:ASN:OD1	2.42	0.50
1:A:2552:THR:OG1	1:A:2555:ARG:NH2	2.45	0.50
1:A:4273:ASP:HB2	1:A:4729:LEU:HD23	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4353:ILE:HG23	1:A:4403:PHE:CE1	2.47	0.50
1:A:4891:HIS:NE2	1:A:4965:LEU:HD13	2.27	0.50
1:A:553:PHE:CE1	1:A:668:ILE:HD13	2.47	0.50
1:A:624:LEU:HD11	1:A:662:LEU:CD1	2.41	0.50
1:A:780:HIS:O	1:A:784:PHE:N	2.44	0.50
1:A:1702:ASN:O	1:A:1880:ARG:NH1	2.45	0.50
1:A:4641:VAL:HG22	1:A:4692:LEU:HD22	1.94	0.50
1:A:2233:LEU:HD23	1:A:2233:LEU:H	1.77	0.49
1:A:3880:GLN:HG3	1:A:3935:LEU:HD11	1.94	0.49
1:A:1214:SER:O	1:A:1217:VAL:N	2.45	0.49
1:A:1991:SER:HB2	1:A:1996:VAL:HG21	1.93	0.49
1:A:3240:ARG:HD3	1:A:3246:LEU:HD11	1.93	0.49
1:A:590:LEU:HD13	1:A:635:LEU:HD11	1.94	0.49
1:A:4479:PHE:HD1	1:A:4483:MET:HE1	1.77	0.49
1:A:1393:LEU:O	1:A:1396:ILE:HG22	2.12	0.49
1:A:1668:ASP:OD2	1:A:1670:THR:OG1	2.29	0.49
1:A:2296:LYS:HD2	1:A:2297:ARG:H	1.76	0.49
1:A:4921:ILE:CD1	1:A:4965:LEU:HD11	2.42	0.49
1:A:492:TRP:NE1	1:A:494:GLN:OE1	2.37	0.49
1:A:4080:ASP:OD2	1:A:4082:ALA:N	2.46	0.49
1:A:4966:GLN:NE2	1:A:4967:GLY:O	2.42	0.49
1:A:5159:ARG:NH2	1:A:5163:VAL:HG23	2.25	0.49
1:A:3547:LEU:HD23	1:A:3693:ILE:HB	1.94	0.49
1:A:751:LEU:HD21	1:A:761:TRP:CZ3	2.48	0.49
1:A:3078:GLN:N	1:A:3079:GLU:OE1	2.45	0.49
1:A:4891:HIS:NE2	1:A:4919:HIS:O	2.44	0.49
1:A:620:LEU:HD13	1:A:662:LEU:HD21	1.95	0.49
1:A:2322:LEU:HD12	1:A:2361:PHE:CE2	2.48	0.49
1:A:3242:LEU:HD23	1:A:3243:THR:H	1.78	0.49
1:A:1693:GLN:NE2	1:A:1697:GLU:OE2	2.46	0.48
1:A:765:LEU:O	1:A:798:ARG:NH1	2.47	0.48
1:A:934:LYS:O	1:A:938:VAL:HG23	2.12	0.48
1:A:2979:ILE:O	1:A:2983:VAL:HG23	2.13	0.48
1:A:4584:LEU:HD13	1:A:4623:ASP:HB3	1.95	0.48
1:A:1231:HIS:NE2	1:A:1235:LEU:HD11	2.29	0.48
1:A:3769:LYS:HD3	1:A:3784:LEU:HD21	1.95	0.48
1:A:4347:GLU:OE1	1:A:4349:LYS:HB3	2.14	0.48
1:A:4409:ILE:HG13	1:A:4410:LEU:HD12	1.95	0.48
1:A:3900:GLU:N	1:A:3900:GLU:OE1	2.47	0.48
1:A:1292:ASP:O	1:A:1296:GLY:N	2.41	0.48
1:A:4851:LEU:HD21	1:A:4878:LEU:HB3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1161:LEU:N	1:A:1161:LEU:HD23	2.29	0.48
1:A:2657:MET:HE2	1:A:2798:SER:OG	2.14	0.48
1:A:813:ASP:OD1	1:A:813:ASP:N	2.44	0.48
1:A:4810:ARG:NH2	1:A:4863:ASP:OD2	2.47	0.48
1:A:2689:ILE:HG23	1:A:2703:TYR:OH	2.14	0.47
1:A:3568:LEU:HA	1:A:3579:LEU:HD13	1.96	0.47
1:A:676:LEU:HD13	1:A:698:LEU:HA	1.94	0.47
1:A:898:SER:N	1:A:901:THR:HG1	2.13	0.47
1:A:4459:ASN:ND2	1:A:4652:GLU:OE1	2.43	0.47
1:A:4888:ILE:HG22	1:A:4892:ASN:OD1	2.13	0.47
1:A:1054:LEU:HD23	1:A:1055:ALA:N	2.29	0.47
1:A:3176:ILE:HG22	1:A:3180:LEU:HG	1.96	0.47
1:A:4219:ASN:O	1:A:4219:ASN:ND2	2.47	0.47
1:A:5025:LEU:HD13	1:A:5082:LEU:HB2	1.97	0.47
1:A:3315:PHE:HB2	1:A:3436:LEU:O	2.15	0.47
1:A:4861:ASP:OD1	1:A:4861:ASP:N	2.46	0.47
1:A:2378:CYS:O	1:A:2383:ILE:N	2.48	0.47
1:A:1789:LEU:N	1:A:1790:PRO:CD	2.77	0.47
1:A:3009:SER:OG	1:A:3010:GLU:N	2.45	0.47
1:A:3450:LEU:HD13	1:A:3625:TRP:CZ3	2.50	0.47
1:A:381:VAL:HG12	1:A:437:VAL:HG13	1.97	0.47
1:A:1359:ILE:O	1:A:1362:VAL:HG12	2.15	0.47
1:A:1576:GLU:N	1:A:1576:GLU:OE1	2.47	0.47
1:A:4012:CYS:O	1:A:4014:HIS:ND1	2.47	0.47
1:A:4440:ASP:OD1	1:A:4441:GLY:N	2.42	0.47
1:A:2495:ILE:HD11	1:A:2571:LEU:HD23	1.96	0.47
1:A:1197:VAL:CG2	1:A:1199:LEU:HD21	2.45	0.47
1:A:4198:LEU:C	1:A:4198:LEU:HD23	2.39	0.47
1:A:1483:VAL:HG23	1:A:1483:VAL:O	2.13	0.47
1:A:2204:HIS:HB3	1:A:2256:ILE:HD12	1.97	0.47
1:A:4280:VAL:HG23	1:A:4305:VAL:HG12	1.97	0.47
1:A:5025:LEU:HD11	1:A:5079:TRP:CD1	2.49	0.47
1:A:2559:ILE:HG21	1:A:2564:LEU:HD21	1.97	0.46
1:A:4835:THR:O	1:A:4839:LEU:HD23	2.16	0.46
1:A:2267:LEU:HD12	1:A:2294:LEU:HB3	1.97	0.46
1:A:2392:THR:OG1	1:A:2428:ARG:NH2	2.48	0.46
1:A:3362:VAL:HG12	1:A:3366:LEU:HD12	1.96	0.46
1:A:4994:ILE:O	1:A:4998:MET:N	2.49	0.46
1:A:1102:LEU:HD12	1:A:1188:SER:C	2.41	0.46
1:A:3408:ASN:N	1:A:3408:ASN:OD1	2.47	0.46
1:A:3947:LEU:HD11	1:A:3984:THR:HG21	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4309:ASP:OD1	1:A:4309:ASP:N	2.47	0.46
1:A:423:THR:HG21	1:A:434:GLU:CG	2.45	0.46
1:A:1139:ALA:O	1:A:1143:ARG:HG2	2.16	0.46
1:A:1216:GLN:CD	1:A:1217:VAL:HG23	2.40	0.46
1:A:1317:LEU:HD21	1:A:1340:VAL:CG2	2.46	0.46
1:A:4130:ILE:HG21	1:A:4157:LEU:HD13	1.98	0.46
1:A:1304:ASP:CG	1:A:1346:TYR:HH	2.24	0.46
1:A:1864:LEU:HD11	1:A:2071:PHE:HD2	1.81	0.46
1:A:2396:THR:OG1	1:A:2399:ASN:OD1	2.33	0.46
1:A:2733:LEU:HD22	1:A:2749:LYS:HG2	1.97	0.46
1:A:3898:SER:OG	1:A:3900:GLU:OE1	2.33	0.46
1:A:3018:ILE:HG22	1:A:3022:ILE:HD12	1.98	0.46
1:A:2002:VAL:HG22	1:A:2096:ILE:HG21	1.98	0.46
1:A:4130:ILE:HD12	1:A:4157:LEU:HD22	1.98	0.46
1:A:1632:MET:HE3	1:A:1789:LEU:HD21	1.97	0.46
1:A:2198:LEU:HD21	1:A:2212:TRP:HH2	1.74	0.46
1:A:3895:LEU:O	1:A:3898:SER:OG	2.26	0.46
1:A:1184:GLN:CD	1:A:1210:HIS:HE2	2.24	0.45
1:A:3265:ASP:OD1	1:A:3614:LEU:HD22	2.15	0.45
1:A:3346:LEU:HD12	1:A:3376:ILE:HB	1.98	0.45
1:A:495:TYR:OH	1:A:532:LEU:HB2	2.16	0.45
1:A:1471:GLY:HA3	1:A:1505:LEU:HD21	1.99	0.45
1:A:3900:GLU:OE1	1:A:3901:HIS:N	2.49	0.45
1:A:4241:ASP:OD1	1:A:4286:GLN:NE2	2.49	0.45
1:A:5166:MET:SD	1:A:5166:MET:N	2.90	0.45
1:A:1650:SER:HB3	1:A:1669:VAL:HG22	1.99	0.45
1:A:4168:THR:HG23	1:A:4740:ILE:CD1	2.46	0.45
1:A:4345:VAL:HG13	1:A:4396:GLN:HB3	1.98	0.45
1:A:5046:LEU:O	1:A:5050:THR:HG23	2.15	0.45
1:A:1054:LEU:HD22	1:A:1056:ASP:HB2	1.99	0.45
1:A:1063:LEU:C	1:A:1070:ILE:HD11	2.41	0.45
1:A:1976:ALA:HB1	1:A:2009:MET:SD	2.57	0.45
1:A:2955:ASP:OD1	1:A:3040:ARG:NH1	2.45	0.45
1:A:3000:LEU:C	1:A:3002:ASN:H	2.24	0.45
1:A:1286:PHE:CZ	1:A:1324:MET:HE1	2.52	0.45
1:A:1407:LEU:HD21	1:A:1485:PHE:CZ	2.52	0.45
1:A:1748:CYS:HB3	1:A:1801:THR:HG23	1.98	0.45
1:A:1109:ILE:O	1:A:1113:LYS:N	2.50	0.45
1:A:4581:LEU:HD11	1:A:4689:LEU:HD21	1.99	0.45
1:A:4584:LEU:HD13	1:A:4623:ASP:CG	2.42	0.45
1:A:683:CYS:H	1:A:686:THR:HG22	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3002:ASN:HB2	1:A:3003:LEU:HD22	1.98	0.45
1:A:4639:ILE:HG22	1:A:4643:HIS:CD2	2.52	0.45
1:A:3984:THR:O	1:A:3988:THR:HG22	2.17	0.45
1:A:4485:GLU:O	1:A:4486:ASP:C	2.59	0.45
1:A:852:HIS:CD2	1:A:906:THR:HG23	2.52	0.44
1:A:2009:MET:HE3	1:A:2018:VAL:HG11	1.99	0.44
1:A:3003:LEU:HB3	1:A:3004:PRO:HD2	1.99	0.44
1:A:4297:LYS:O	1:A:4303:GLN:NE2	2.47	0.44
1:A:4340:ALA:O	1:A:4343:LYS:HG3	2.17	0.44
1:A:4559:LEU:HD13	1:A:4583:ARG:NH2	2.33	0.44
1:A:3286:GLU:OE1	1:A:3290:ARG:NH1	2.50	0.44
1:A:3871:THR:O	1:A:3874:THR:OG1	2.33	0.44
1:A:1407:LEU:HD21	1:A:1485:PHE:HZ	1.83	0.44
1:A:1832:LEU:HD12	1:A:1928:MET:O	2.17	0.44
1:A:3933:VAL:HG12	1:A:3933:VAL:O	2.15	0.44
1:A:4721:ASP:OD2	1:A:4721:ASP:N	2.46	0.44
1:A:3101:LEU:HD23	1:A:3149:ILE:HB	1.99	0.44
1:A:3349:LEU:HD21	1:A:3377:PHE:HB3	2.00	0.44
1:A:3046:THR:OG1	1:A:3047:LYS:N	2.51	0.44
1:A:4751:TYR:CE2	1:A:4755:ILE:HD11	2.53	0.44
1:A:1512:SER:O	1:A:1515:ASN:N	2.50	0.44
1:A:4917:GLU:O	1:A:4918:LEU:HD12	2.16	0.44
1:A:1280:GLN:N	1:A:1281:PRO:HD2	2.32	0.44
1:A:2356:LEU:O	1:A:2358:ARG:NH1	2.51	0.44
1:A:3799:LYS:HA	1:A:3802:SER:HB3	1.99	0.44
1:A:557:GLU:HA	1:A:560:CYS:SG	2.58	0.43
1:A:1659:LEU:HD11	1:A:1761:MET:HG2	1.99	0.43
1:A:2166:ARG:HB3	1:A:2167:PRO:HD3	2.00	0.43
1:A:3167:ASN:OD1	1:A:3167:ASN:N	2.51	0.43
1:A:1318:ASP:OD2	1:A:1318:ASP:C	2.61	0.43
1:A:2133:ARG:NH2	1:A:2151:GLU:OE2	2.51	0.43
1:A:2201:PHE:O	1:A:2205:CYS:N	2.51	0.43
1:A:3000:LEU:O	1:A:3002:ASN:N	2.52	0.43
1:A:4293:GLN:NE2	1:A:4323:GLN:OE1	2.44	0.43
1:A:1094:GLY:O	1:A:1098:SER:CB	2.66	0.43
1:A:3745:GLN:O	1:A:3750:ARG:NH2	2.51	0.43
1:A:898:SER:O	1:A:902:VAL:HG23	2.18	0.43
1:A:4132:SER:HB3	1:A:4173:LEU:HD11	2.01	0.43
1:A:3195:VAL:O	1:A:3199:ILE:HG12	2.19	0.43
1:A:1414:ARG:NH1	1:A:1496:TRP:CD1	2.87	0.43
1:A:1474:SER:O	1:A:1491:HIS:NE2	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4048:SER:O	1:A:4051:HIS:CD2	2.71	0.43
1:A:987:LEU:HD22	1:A:987:LEU:N	2.34	0.43
1:A:1289:LEU:HD23	1:A:1289:LEU:O	2.19	0.43
1:A:1314:TYR:OH	1:A:1348:HIS:NE2	2.51	0.43
1:A:1886:SER:OG	1:A:1921:ARG:NH1	2.52	0.43
1:A:1920:HIS:ND1	1:A:1921:ARG:O	2.52	0.43
1:A:1798:ASP:OD1	1:A:1798:ASP:N	2.50	0.42
1:A:4188:ALA:O	1:A:4927:ARG:NH2	2.52	0.42
1:A:4351:LEU:O	1:A:4354:LYS:HB3	2.19	0.42
1:A:1916:CYS:HA	1:A:1920:HIS:CD2	2.54	0.42
1:A:4947:THR:HG22	1:A:4948:VAL:N	2.35	0.42
1:A:546:THR:HG23	1:A:547:ILE:HD12	2.01	0.42
1:A:2464:VAL:HG21	1:A:2501:VAL:HG21	2.00	0.42
1:A:3943:GLU:OE1	1:A:3943:GLU:N	2.41	0.42
1:A:4891:HIS:O	1:A:4892:ASN:C	2.61	0.42
1:A:5078:LEU:O	1:A:5079:TRP:C	2.62	0.42
1:A:940:ARG:NH2	1:A:989:ASP:OD2	2.49	0.42
1:A:3105:LEU:N	1:A:3105:LEU:HD22	2.34	0.42
1:A:3757:GLY:O	1:A:3758:GLU:C	2.62	0.42
1:A:4891:HIS:O	1:A:4894:ILE:HG22	2.19	0.42
1:A:4198:LEU:HD12	1:A:4238:ARG:HH22	1.85	0.42
1:A:633:ILE:HG22	1:A:633:ILE:O	2.19	0.42
1:A:726:SER:O	1:A:726:SER:OG	2.35	0.42
1:A:1375:LEU:HD21	1:A:1485:PHE:CE1	2.54	0.42
1:A:1419:GLN:NE2	1:A:1423:LEU:HD11	2.35	0.42
1:A:2349:ASP:OD1	1:A:2349:ASP:N	2.50	0.42
1:A:2928:VAL:HG12	1:A:2928:VAL:O	2.19	0.42
1:A:1010:GLN:N	1:A:1010:GLN:OE1	2.52	0.42
1:A:3002:ASN:C	1:A:3003:LEU:HD22	2.44	0.42
1:A:3811:LEU:N	1:A:3812:PRO:CD	2.83	0.42
1:A:4428:PRO:HB3	1:A:4595:SER:HB2	2.01	0.42
1:A:4584:LEU:HD13	1:A:4623:ASP:CB	2.50	0.42
1:A:556:PHE:CZ	1:A:633:ILE:HD11	2.54	0.42
1:A:594:LEU:HD22	1:A:643:TRP:HH2	1.85	0.42
1:A:785:PRO:HG3	1:A:834:LYS:HG3	2.02	0.42
1:A:1179:ALA:O	1:A:1183:SER:OG	2.37	0.42
1:A:2412:CYS:SG	1:A:2414:ILE:HD12	2.60	0.42
1:A:547:ILE:HG22	1:A:548:ASN:N	2.34	0.42
1:A:1276:ASP:HA	1:A:1280:GLN:HB3	2.02	0.42
1:A:2992:ASP:OD1	1:A:2992:ASP:N	2.52	0.42
1:A:3864:MET:O	1:A:3867:THR:OG1	2.38	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3950:GLU:OE1	1:A:3951:HIS:N	2.53	0.42
1:A:4343:LYS:O	1:A:4347:GLU:CG	2.68	0.42
1:A:4992:MET:N	1:A:4992:MET:SD	2.93	0.42
1:A:2783:ALA:HB2	1:A:2804:LEU:HD11	2.00	0.42
1:A:3155:ASP:OD1	1:A:3156:VAL:N	2.52	0.42
1:A:4784:LEU:HD12	1:A:4787:ILE:HD11	2.02	0.42
1:A:1093:VAL:HG21	1:A:1120:TRP:CD2	2.54	0.41
1:A:3070:PHE:HA	1:A:3105:LEU:HD21	2.02	0.41
1:A:3972:GLU:OE1	1:A:3972:GLU:N	2.52	0.41
1:A:4784:LEU:HD13	1:A:4887:LEU:HD12	2.00	0.41
1:A:5098:PHE:CD2	1:A:5191:VAL:HG13	2.55	0.41
1:A:384:HIS:HB2	1:A:495:TYR:HD1	1.84	0.41
1:A:448:ILE:O	1:A:448:ILE:HG22	2.19	0.41
1:A:1349:LEU:HD22	1:A:1400:LEU:HD13	2.02	0.41
1:A:1619:LEU:HD13	1:A:1676:LEU:HD22	2.01	0.41
1:A:4551:ASP:OD1	1:A:4552:ARG:N	2.51	0.41
1:A:4868:ILE:O	1:A:4880:ALA:HB2	2.20	0.41
1:A:867:LEU:HB2	1:A:868:PRO:HD3	2.02	0.41
1:A:1182:HIS:ND1	1:A:1182:HIS:O	2.52	0.41
1:A:1751:GLU:OE2	1:A:1754:ARG:NH1	2.53	0.41
1:A:2552:THR:HG22	1:A:2851:ASP:OD2	2.20	0.41
1:A:3275:LEU:N	1:A:3275:LEU:HD22	2.35	0.41
1:A:4153:TYR:CZ	1:A:4157:LEU:HD11	2.56	0.41
1:A:4274:TRP:CZ2	1:A:4729:LEU:HD22	2.56	0.41
1:A:828:LEU:O	1:A:832:ARG:N	2.53	0.41
1:A:2370:ARG:NE	1:A:2388:ASP:OD2	2.52	0.41
1:A:4139:LEU:HD21	1:A:4150:ILE:CD1	2.50	0.41
1:A:5079:TRP:O	1:A:5080:GLN:C	2.63	0.41
1:A:2547:VAL:CG2	1:A:2552:THR:HG22	2.49	0.41
1:A:2618:VAL:O	1:A:2707:ILE:HD11	2.20	0.41
1:A:4864:THR:HG22	1:A:4865:GLU:N	2.35	0.41
1:A:4873:ARG:HH11	1:A:4973:LEU:HD13	1.86	0.41
1:A:2383:ILE:HD11	1:A:2437:ARG:CG	2.50	0.41
1:A:3535:LEU:O	1:A:3538:SER:OG	2.32	0.41
1:A:3946:GLY:O	1:A:3947:LEU:C	2.62	0.41
1:A:628:PHE:CD2	1:A:628:PHE:C	2.99	0.41
1:A:866:GLU:OE2	1:A:941:ARG:NE	2.43	0.41
1:A:1190:ARG:NE	1:A:1192:ASN:OD1	2.54	0.41
1:A:1316:ASP:OD1	1:A:1316:ASP:N	2.53	0.41
1:A:1324:MET:HA	1:A:1324:MET:HE2	2.03	0.41
1:A:3455:VAL:HG12	1:A:3456:THR:N	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4760:ASN:O	1:A:4760:ASN:ND2	2.53	0.41
1:A:1157:VAL:O	1:A:1161:LEU:HG	2.20	0.41
1:A:2949:GLU:O	1:A:3163:ILE:HG23	2.21	0.41
1:A:1289:LEU:O	1:A:1293:LEU:HG	2.20	0.41
1:A:1658:ASP:OD1	1:A:1658:ASP:N	2.54	0.41
1:A:2394:GLU:HG3	1:A:2396:THR:HG23	2.03	0.41
1:A:2495:ILE:CD1	1:A:2571:LEU:HD23	2.51	0.41
1:A:2760:GLU:OE2	1:A:2800:LYS:N	2.53	0.41
1:A:3761:GLN:O	1:A:3762:GLU:C	2.63	0.41
1:A:3994:ILE:HG21	1:A:4058:HIS:ND1	2.36	0.41
1:A:4341:VAL:HG21	1:A:4374:THR:HB	2.02	0.41
1:A:432:LEU:C	1:A:432:LEU:HD23	2.46	0.41
1:A:842:PRO:O	1:A:845:LEU:HB2	2.21	0.41
1:A:3183:TRP:H	1:A:3183:TRP:CD1	2.39	0.41
1:A:4453:VAL:O	1:A:4457:GLY:N	2.52	0.41
1:A:873:GLU:O	1:A:877:ARG:HG2	2.21	0.40
1:A:1923:ASP:OD1	1:A:1923:ASP:N	2.50	0.40
1:A:2618:VAL:HG23	1:A:2707:ILE:CG1	2.51	0.40
1:A:4293:GLN:OE1	1:A:4712:ASN:ND2	2.54	0.40
1:A:4488:LEU:HD21	1:A:4848:GLU:HA	2.04	0.40
1:A:4932:LEU:HD11	1:A:4959:GLN:CB	2.51	0.40
1:A:594:LEU:HD21	1:A:626:VAL:HG22	2.04	0.40
1:A:1177:VAL:CG2	1:A:1178:LEU:N	2.83	0.40
1:A:2546:ARG:HD3	1:A:2848:LEU:HD23	2.02	0.40
1:A:3994:ILE:HD11	1:A:4055:ILE:HD13	2.03	0.40
1:A:4578:VAL:HG11	1:A:4682:ALA:CB	2.52	0.40
1:A:4880:ALA:O	1:A:4881:THR:C	2.65	0.40
1:A:4884:VAL:O	1:A:4885:SER:C	2.65	0.40
1:A:2179:ASP:OD1	1:A:2182:THR:HG22	2.22	0.40
1:A:3171:LYS:O	1:A:3172:HIS:CG	2.75	0.40
1:A:4941:VAL:HG12	1:A:4942:GLU:O	2.21	0.40
1:A:1071:LEU:O	1:A:1079:LYS:NZ	2.48	0.40
1:A:1841:LEU:HB2	1:A:1842:PRO:HD3	2.04	0.40
1:A:3236:ARG:NH2	1:A:3257:ILE:HD11	2.37	0.40
1:A:4793:ASP:OD2	1:A:4828:ARG:NH1	2.55	0.40
1:A:4881:THR:O	1:A:4882:ALA:C	2.64	0.40
1:A:1199:LEU:HB2	1:A:1201:THR:HG23	2.02	0.40
1:A:3291:GLN:OE1	1:A:3293:HIS:NE2	2.45	0.40
1:A:4349:LYS:O	1:A:4349:LYS:HD2	2.22	0.40
1:A:4351:LEU:O	1:A:4354:LYS:N	2.54	0.40
1:A:4976:ILE:HB	1:A:4977:PRO:HD3	2.04	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	4307/5247 (82%)	4098 (95%)	208 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2297	ARG

5.3.2 Protein sidechains [i](#)

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	3945/4653 (85%)	3873 (98%)	72 (2%)	51	77

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	381	VAL
1	A	384	HIS
1	A	479	CYS
1	A	551	SER
1	A	628	PHE
1	A	640	SER
1	A	646	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	740	LEU
1	A	813	ASP
1	A	828	LEU
1	A	845	LEU
1	A	929	SER
1	A	931	THR
1	A	962	GLU
1	A	1012	SER
1	A	1029	LEU
1	A	1042	ASP
1	A	1045	ASP
1	A	1047	ILE
1	A	1054	LEU
1	A	1100	THR
1	A	1126	SER
1	A	1155	ARG
1	A	1161	LEU
1	A	1202	SER
1	A	1303	ILE
1	A	1362	VAL
1	A	1380	ASN
1	A	1399	GLU
1	A	1411	SER
1	A	1491	HIS
1	A	1577	SER
1	A	1750	SER
1	A	1766	LEU
1	A	1853	SER
1	A	2050	VAL
1	A	2056	LEU
1	A	2215	LEU
1	A	2296	LYS
1	A	2478	HIS
1	A	2507	VAL
1	A	2607	LEU
1	A	2920	SER
1	A	2991	ASP
1	A	3042	LEU
1	A	3060	PHE
1	A	3167	ASN
1	A	3201	VAL
1	A	3223	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3312	HIS
1	A	3436	LEU
1	A	3443	ASP
1	A	3453	SER
1	A	3456	THR
1	A	3775	THR
1	A	3841	SER
1	A	3954	LEU
1	A	4116	SER
1	A	4126	LYS
1	A	4142	SER
1	A	4168	THR
1	A	4280	VAL
1	A	4284	SER
1	A	4411	SER
1	A	4416	SER
1	A	4525	CYS
1	A	4686	SER
1	A	4733	SER
1	A	4881	THR
1	A	4922	SER
1	A	4965	LEU
1	A	5060	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	428	HIS
1	A	1008	GLN
1	A	1218	GLN
1	A	1342	GLN
1	A	1347	HIS
1	A	1369	ASN
1	A	1384	ASN
1	A	1603	ASN
1	A	1679	GLN
1	A	1808	HIS
1	A	1907	GLN
1	A	1953	GLN
1	A	2186	GLN
1	A	2519	HIS
1	A	2569	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2596	GLN
1	A	2674	ASN
1	A	2876	HIS
1	A	2977	GLN
1	A	3122	HIS
1	A	3210	HIS
1	A	3222	HIS
1	A	3698	HIS
1	A	4049	GLN
1	A	4063	GLN
1	A	4151	GLN
1	A	4197	HIS
1	A	4507	ASN
1	A	4816	HIS
1	A	4905	ASN
1	A	4906	ASN
1	A	4919	HIS
1	A	5016	GLN
1	A	5113	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ATP	A	5301	3	32,33,33	1.28	5 (15%)	48,52,52	1.75	10 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	A	5301	3	-	7/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5301	ATP	C5-C4	4.07	1.46	1.39
2	A	5301	ATP	C4-N9	-2.53	1.32	1.37
2	A	5301	ATP	C8-N7	2.48	1.36	1.31
2	A	5301	ATP	C5-N7	-2.42	1.34	1.39
2	A	5301	ATP	C5-C6	2.29	1.47	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5301	ATP	C5-C4-N3	-5.15	119.63	126.72
2	A	5301	ATP	N3-C4-N9	3.97	133.91	127.17
2	A	5301	ATP	C2-N3-C4	3.59	120.59	111.83
2	A	5301	ATP	C4-C5-N7	-3.38	106.72	110.58
2	A	5301	ATP	N3-C2-N1	-3.33	123.55	128.58
2	A	5301	ATP	C4-N9-C8	3.27	109.17	105.74
2	A	5301	ATP	N9-C8-N7	-2.63	110.20	113.94
2	A	5301	ATP	C5-N7-C8	2.55	107.46	103.45
2	A	5301	ATP	C6-C5-N7	2.45	136.81	132.09
2	A	5301	ATP	C3'-C2'-C1'	2.17	105.57	101.46

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5301	ATP	C5'-O5'-PA-O1A

Continued on next page...

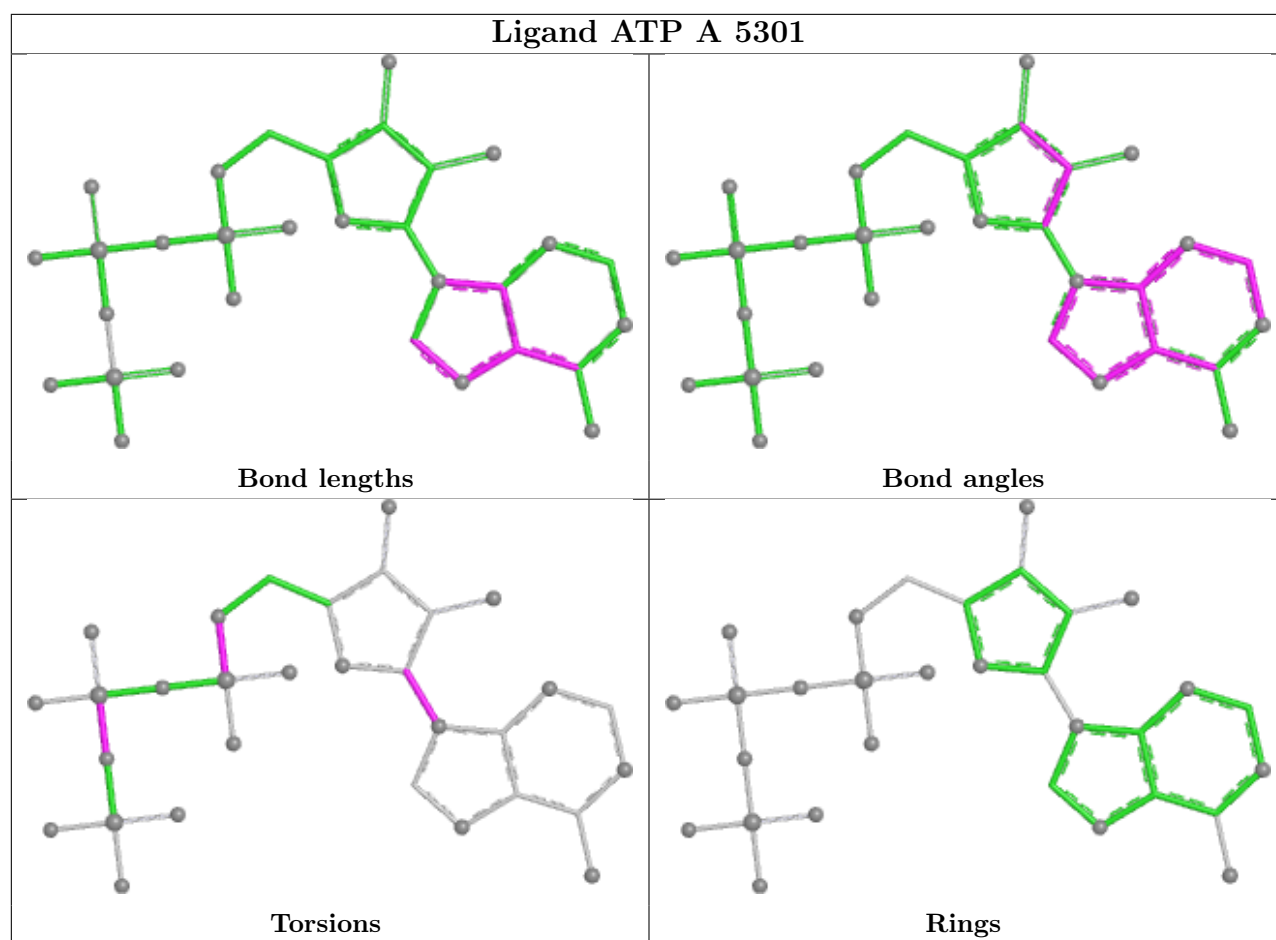
Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	5301	ATP	C5'-O5'-PA-O2A
2	A	5301	ATP	C5'-O5'-PA-O3A
2	A	5301	ATP	O4'-C1'-N9-C4
2	A	5301	ATP	PG-O3B-PB-O2B
2	A	5301	ATP	O4'-C1'-N9-C8
2	A	5301	ATP	PG-O3B-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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



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.

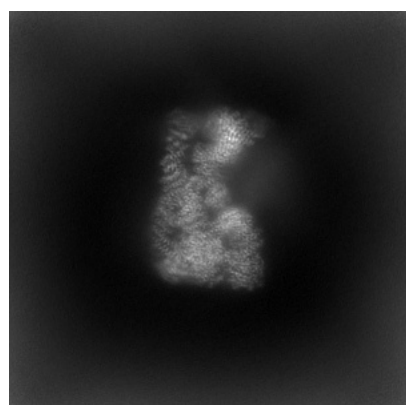
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19653. These allow visual inspection of the internal detail of the map and identification of artifacts.

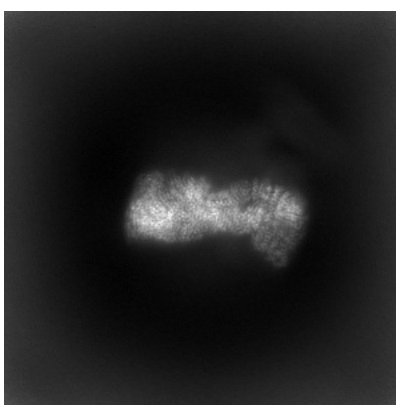
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

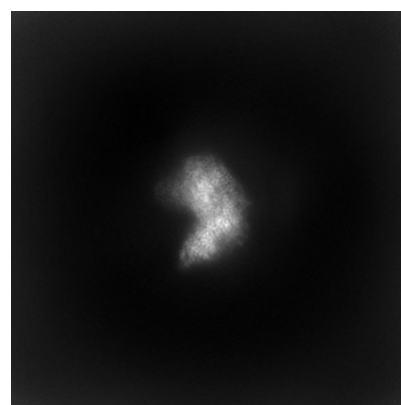
6.1.1 Primary map



X



Y

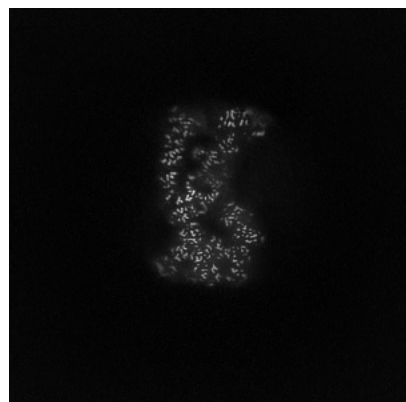


Z

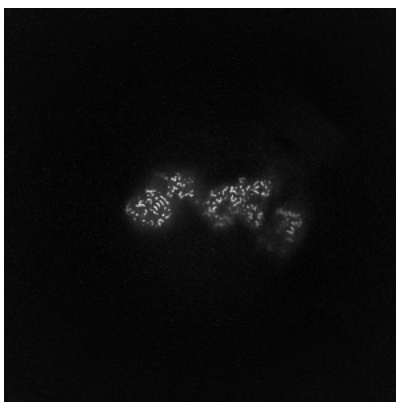
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

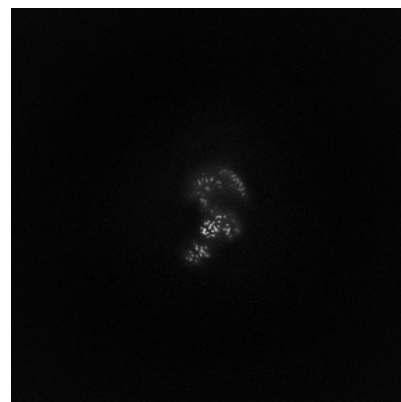
6.2.1 Primary map



X Index: 256



Y Index: 256

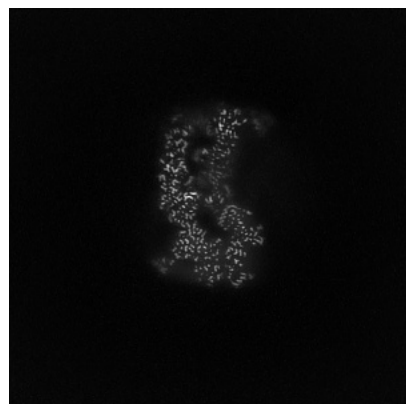


Z Index: 256

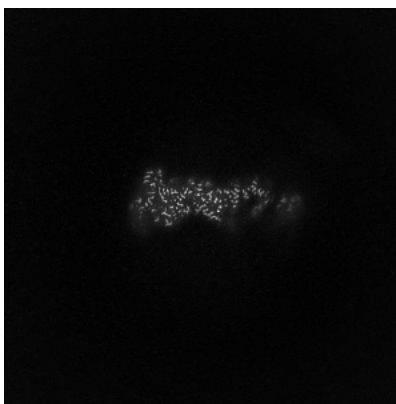
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

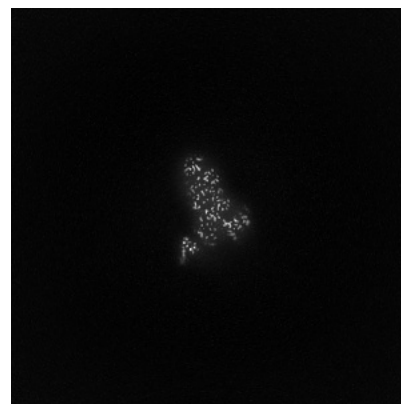
6.3.1 Primary map



X Index: 251



Y Index: 237



Z Index: 199

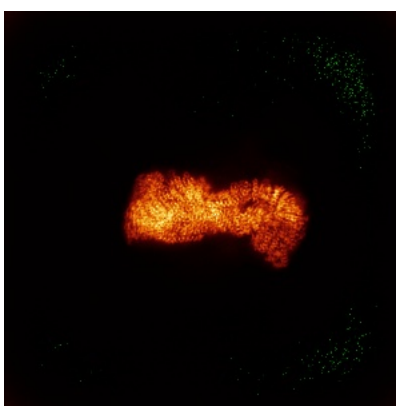
The images above show the largest variance slices of the map in three orthogonal directions.

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

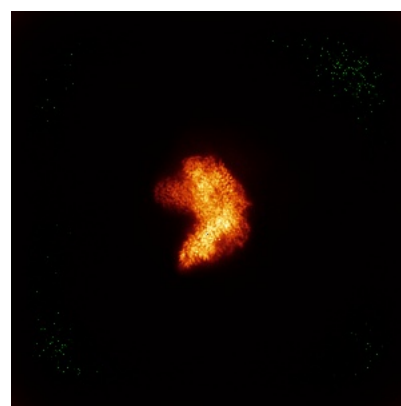
6.4.1 Primary map



X



Y

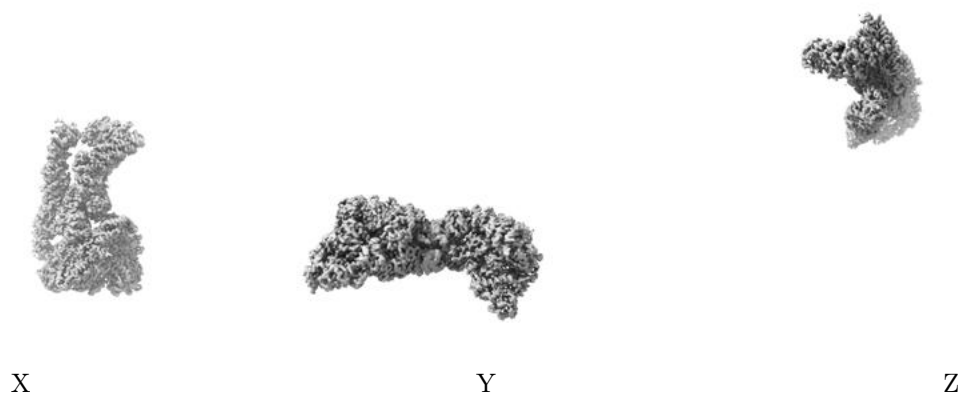


Z

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

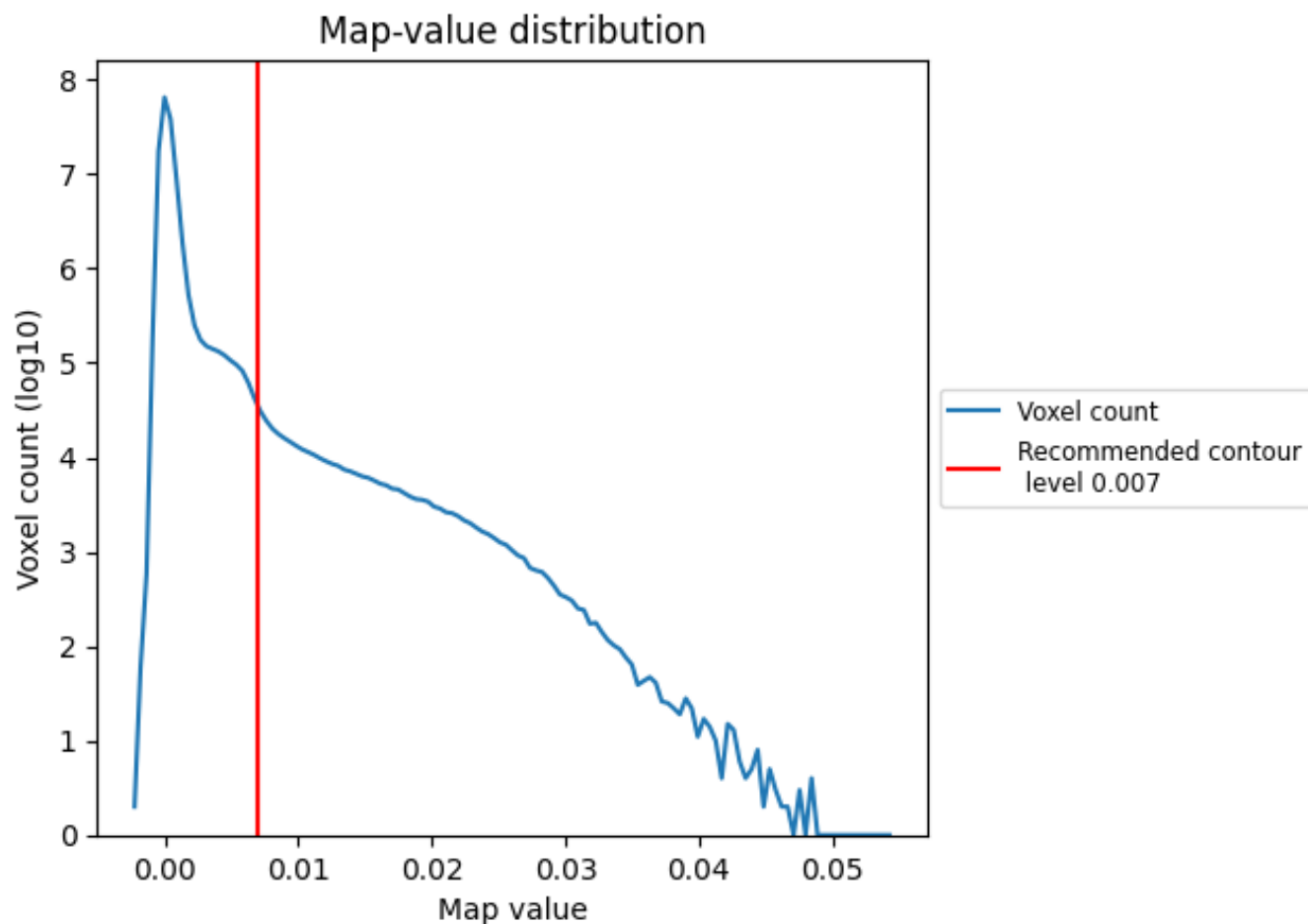
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

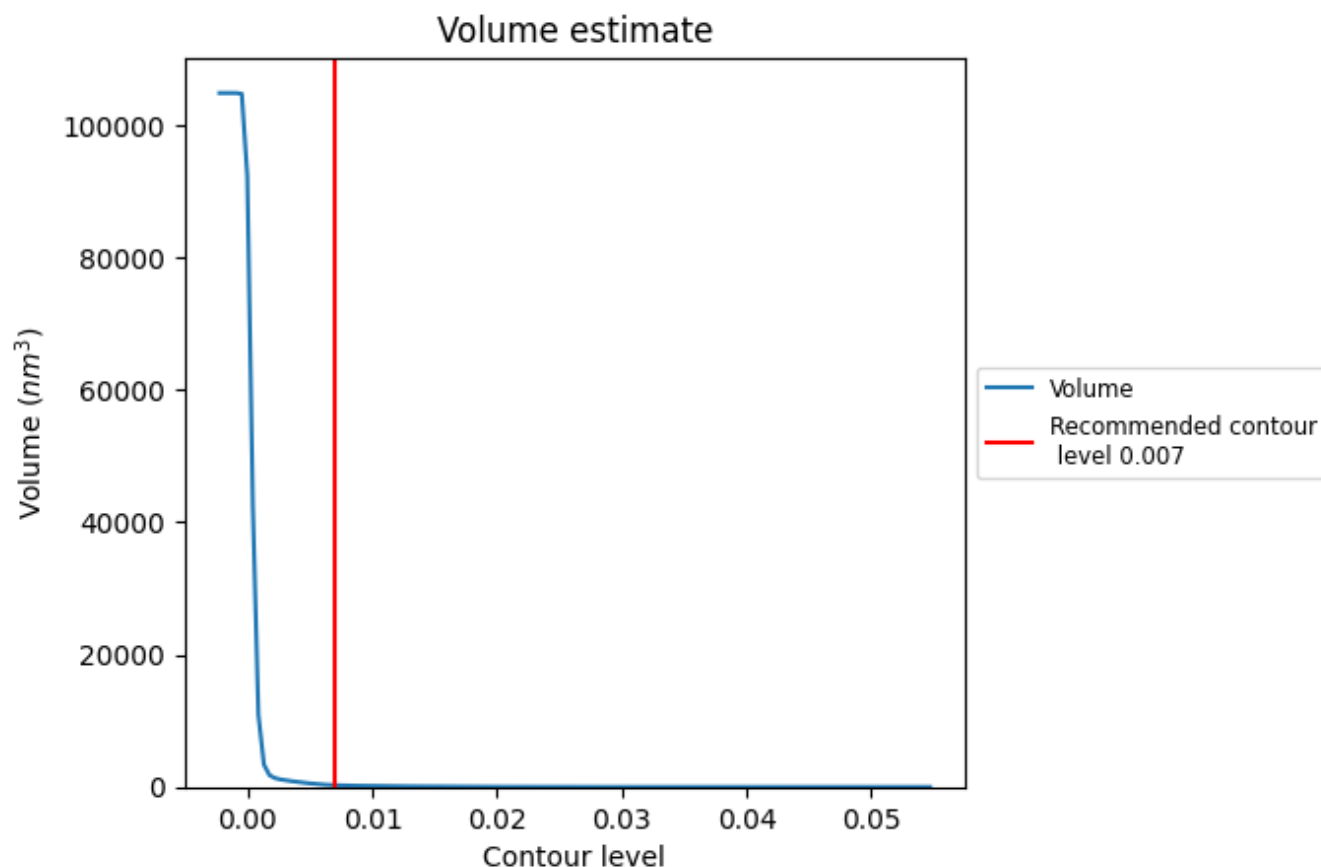
This section contains the results of statistical analysis of the map.

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.

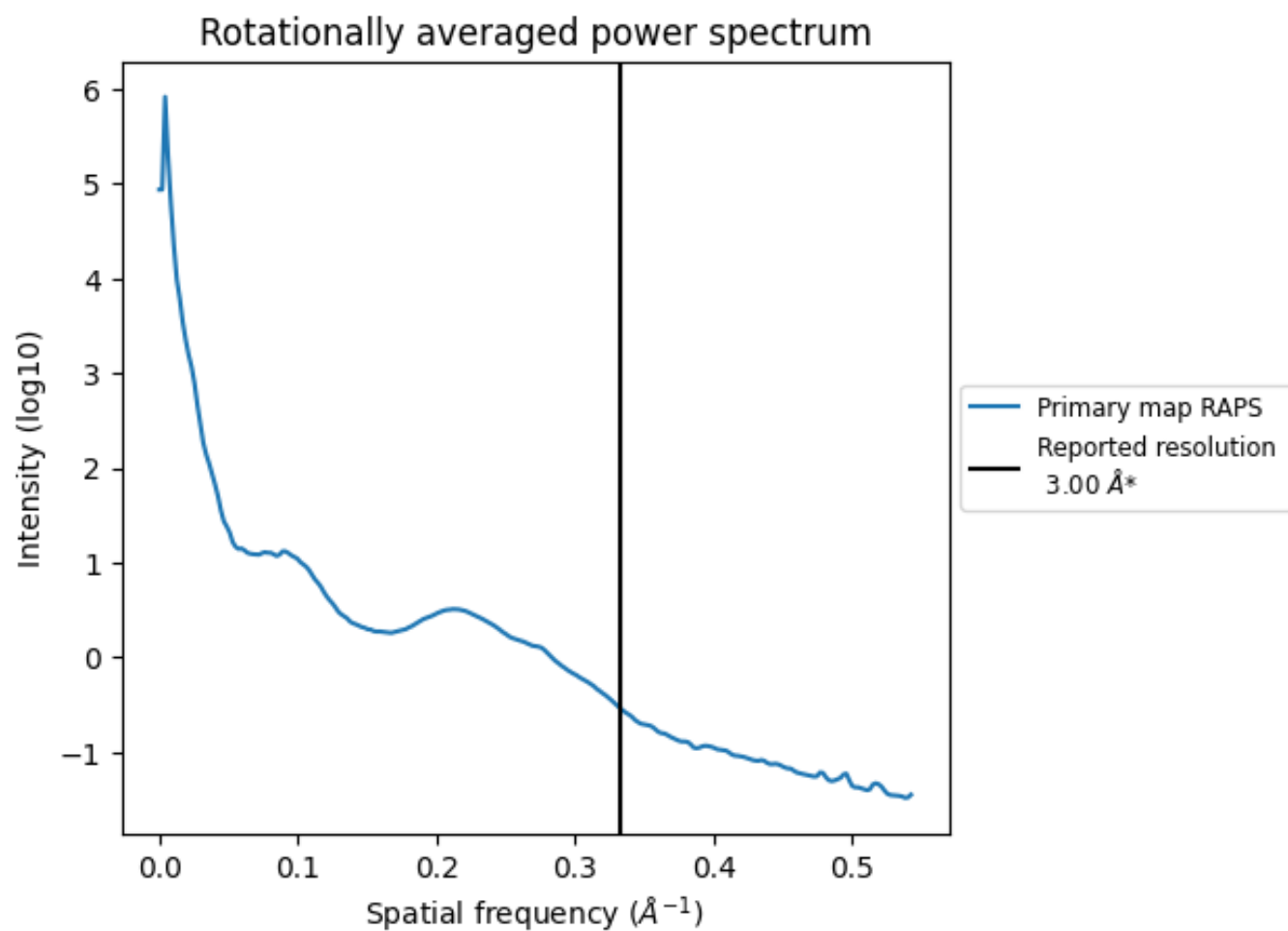
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 261 nm^3 ; this corresponds to an approximate mass of 236 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 0.333 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

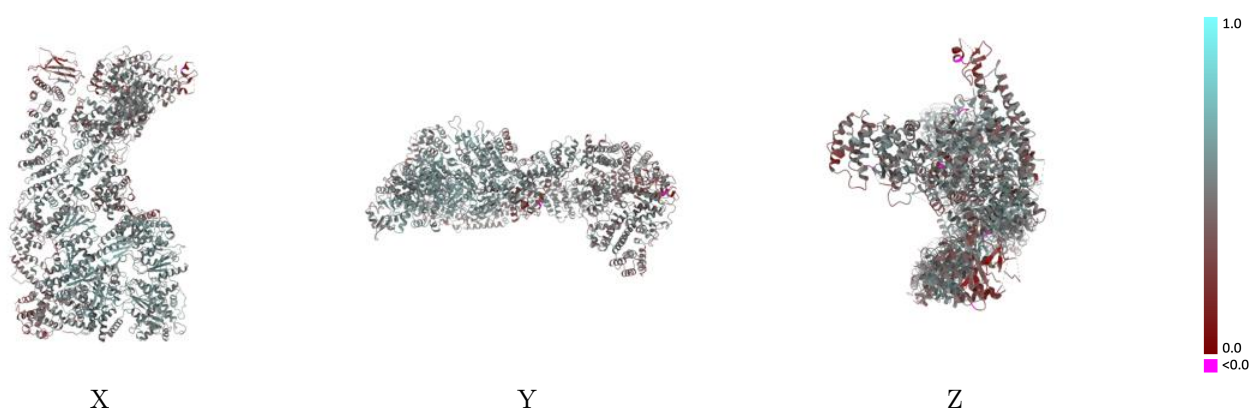
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19653 and PDB model 8S24. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

This section was not generated.

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

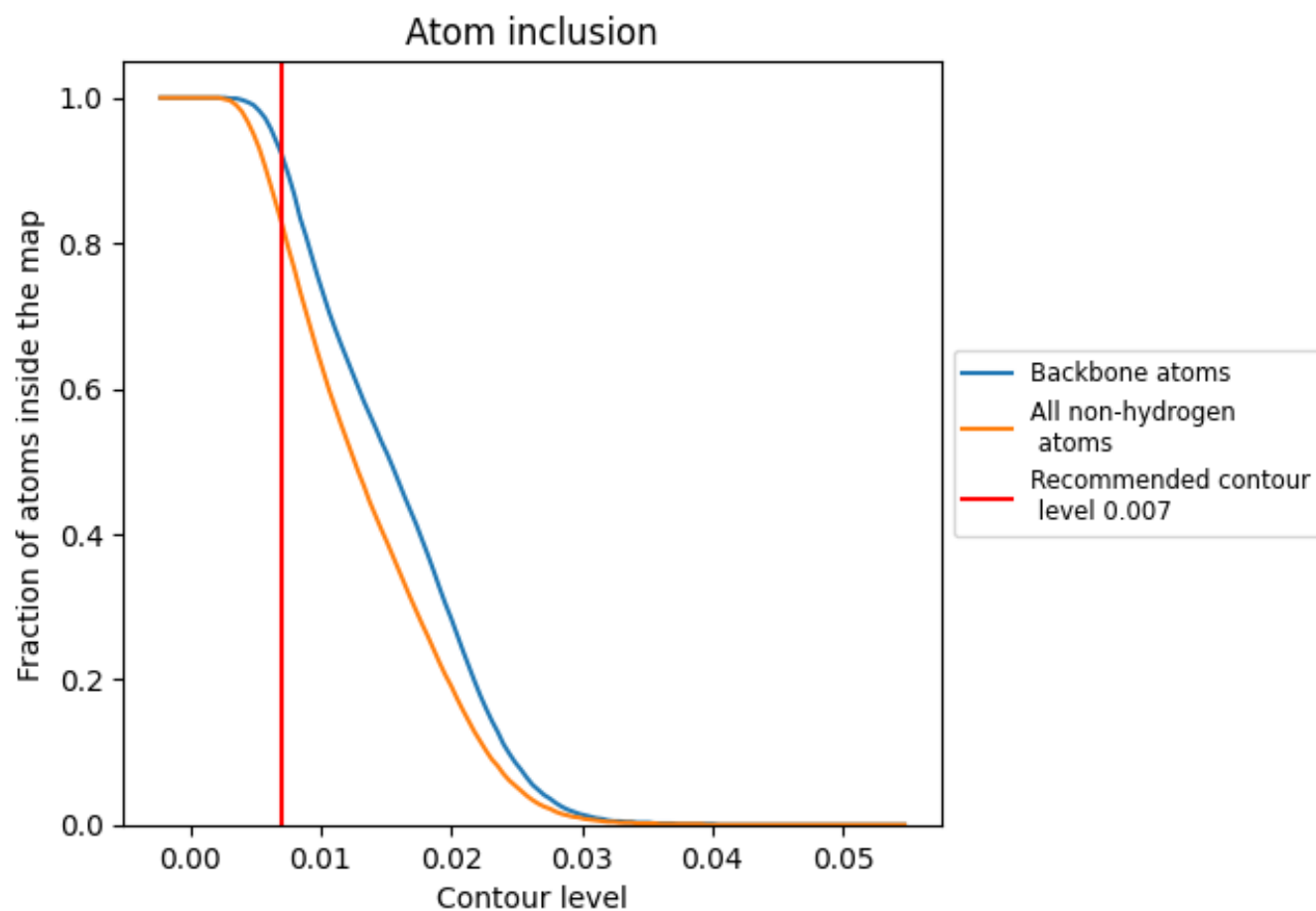


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 83% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8280	0.4820
A	0.8290	0.4820

