



## Full wwPDB EM Validation Report ⓘ

Apr 14, 2025 – 11:00 am BST

PDB ID : 9G08 / pdb\_00009g08  
EMDB ID : EMD-50913  
Title : Structure of human RNF213 bound to the secreted effector IpaH1.4 from *Shigella flexneri*  
Authors : Naydenova, K.; Randow, F.  
Deposited on : 2024-07-07  
Resolution : 3.30 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](mailto: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.dev117  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

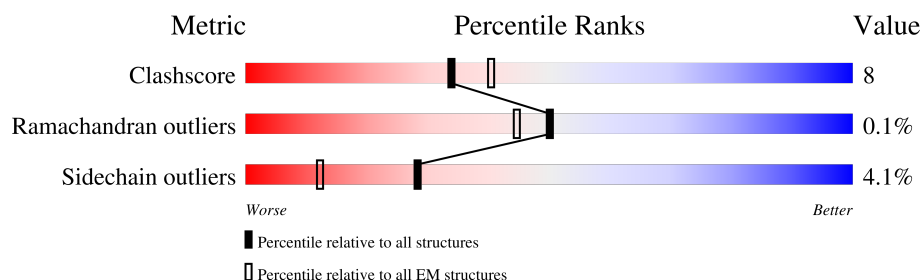
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	<div> <div>7%</div> <div>68%</div> <div>17%</div> <div>•</div> <div>14%</div> </div>
2	B	575	<div> <div>8%</div> <div>27%</div> <div>14%</div> <div>•</div> <div>59%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 77075 atoms, of which 38644 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	4529	Total	C	H	N	O	S	0	0
			73234	23323	36721	6289	6681	220		

There are 40 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...*

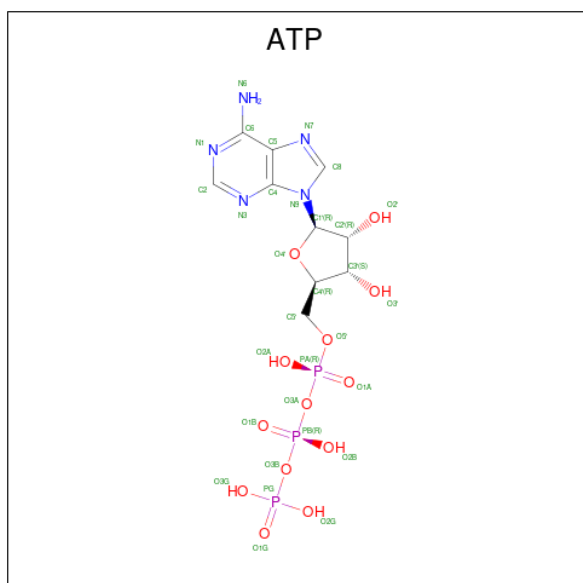
Continued from previous page...

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

- Molecule 2 is a protein called E3 ubiquitin-protein ligase IpaH1.4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O	S	
2	B	237	3794	1205	1911	322	349	7	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).

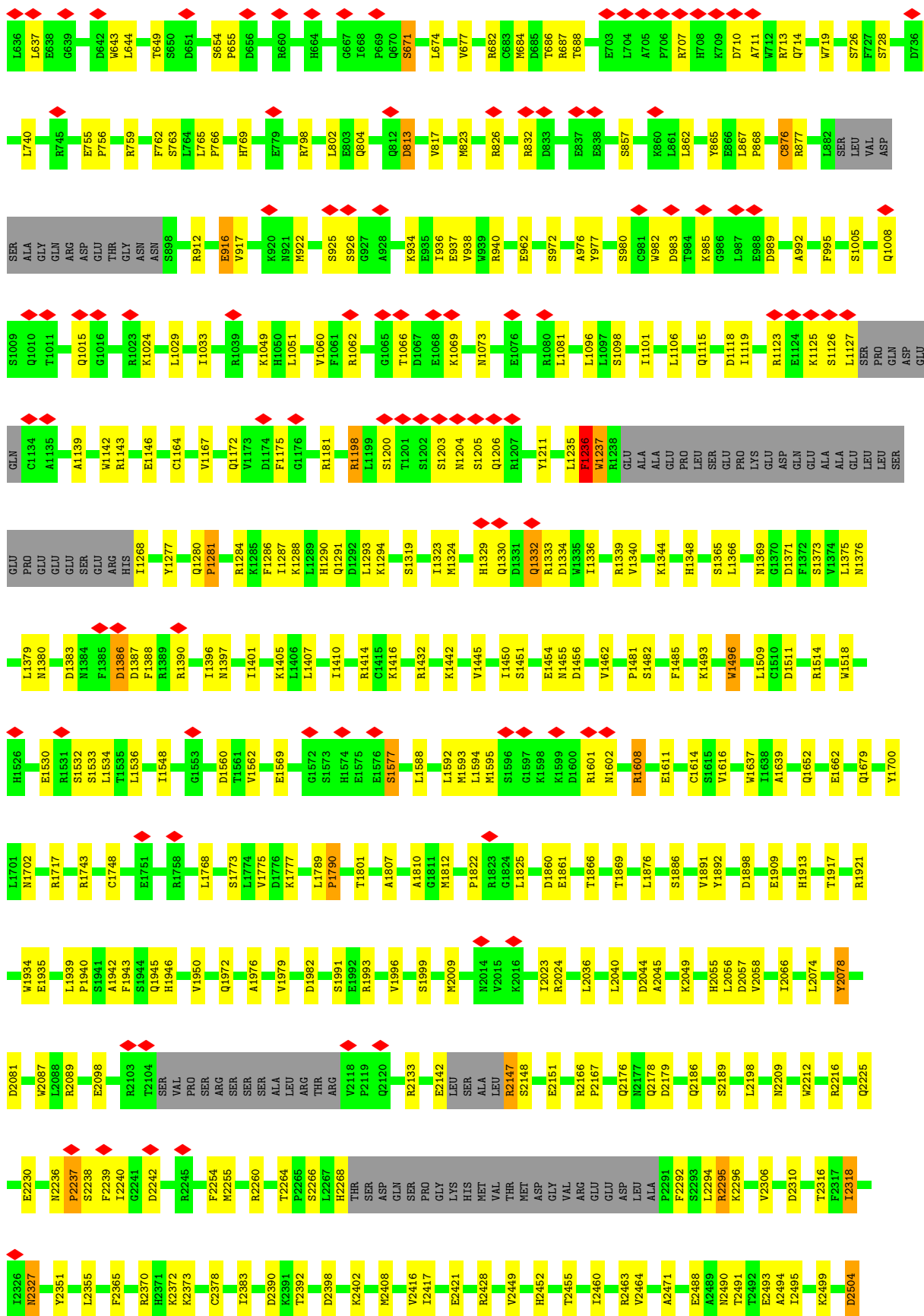


Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Mg 1	0

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	A	3	Total 3	Zn 3	0











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

LEU
ALA
LEU
ARG
LEU
SER
GLU
ASN
GLY
SER
ASN
HIS
ILE
ALA

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	334921	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 ( $e^-/\text{\AA}^2$ )	32	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	8.673	Depositor
Minimum map value	0.000	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.103	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	471.552, 471.552, 471.552	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.228, 1.228, 1.228	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, 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	0.33	0/37285	0.47	0/50439
2	B	0.28	0/1927	0.52	1/2629 (0.0%)
All	All	0.33	0/39212	0.48	1/53068 (0.0%)

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	3
2	B	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	42	LEU	CA-CB-CG	8.03	133.76	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2237	PRO	Peptide
1	A	4981	TYR	Peptide
1	A	580	GLN	Peptide
2	B	120	PHE	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	36513	36721	36694	561	0
2	B	1883	1911	1910	62	0
3	A	31	12	12	1	0
4	A	1	0	0	0	0
5	A	3	0	0	0	0
All	All	38431	38644	38616	619	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 (619) 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:1511:ASP:OD1	1:A:1514:ARG:NH1	1.93	1.02
1:A:5061:ILE:O	1:A:5065:LYS:NZ	2.05	0.89
1:A:1198:ARG:NH1	1:A:1200:SER:OG	2.06	0.89
1:A:386:ILE:HD11	1:A:529:ALA:HB2	1.55	0.88
1:A:4817:SER:O	1:A:4822:ARG:NH2	2.05	0.88
1:A:4132:SER:OG	1:A:4177:CYS:SG	2.33	0.87
1:A:2365:PHE:O	1:A:2373:LYS:NZ	2.09	0.86
1:A:4036:LEU:HD22	2:B:175:LEU:HD13	1.56	0.85
1:A:4941:VAL:HG22	1:A:4947:THR:HG22	1.56	0.84
1:A:4901:LEU:O	1:A:4903:LYS:NZ	2.10	0.84
1:A:2074:LEU:O	1:A:2089:ARG:NH2	2.10	0.83
1:A:4176:ASN:OD1	1:A:4744:ARG:NE	2.10	0.83
1:A:916:GLU:OE2	1:A:916:GLU:N	2.13	0.81
1:A:2260:ARG:O	1:A:2264:THR:OG1	1.98	0.81
1:A:1594:LEU:O	1:A:3091:LYS:NZ	2.12	0.81
2:B:97:GLU:OE1	2:B:99:ARG:NH2	2.14	0.81
1:A:3117:ASN:OD1	1:A:3168:ARG:NE	2.14	0.80
1:A:1181:ARG:NH2	1:A:1211:TYR:O	2.16	0.79
1:A:4016:HIS:NE2	1:A:4032:CYS:SG	2.56	0.79
2:B:78:LEU:O	2:B:101:ASN:ND2	2.15	0.79
1:A:3006:ALA:O	1:A:3009:SER:OG	2.01	0.79
1:A:2142:GLU:OE1	1:A:2147:ARG:NH2	2.18	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4015:VAL:O	1:A:4016:HIS:ND1	2.19	0.76
1:A:1118:ASP:OD2	1:A:1119:ILE:N	2.19	0.76
1:A:3103:LEU:O	1:A:3105:LEU:N	2.19	0.75
1:A:4592:LEU:O	1:A:4595:SER:OG	2.05	0.74
1:A:4194:GLU:OE2	1:A:4238:ARG:NH1	2.21	0.74
1:A:2166:ARG:NH2	1:A:2230:GLU:OE1	2.20	0.74
1:A:4406:GLU:N	1:A:4406:GLU:OE2	2.21	0.74
2:B:67:ILE:HD12	2:B:68:CYS:N	2.03	0.74
1:A:4941:VAL:CG2	1:A:4947:THR:HG22	2.18	0.73
1:A:545:ASP:OD1	1:A:547:ILE:HG22	1.88	0.73
2:B:213:MET:SD	2:B:215:ARG:N	2.61	0.73
1:A:3674:LEU:O	1:A:3714:LYS:NZ	2.19	0.72
1:A:3941:VAL:HG12	1:A:4057:LYS:CD	2.18	0.72
1:A:4031:ILE:HG22	1:A:4039:LEU:HB2	1.71	0.72
1:A:5043:ASN:O	1:A:5071:GLN:NE2	2.23	0.71
1:A:3645:ARG:O	1:A:3697:ASN:ND2	2.22	0.71
1:A:4784:LEU:HD21	1:A:4884:VAL:HA	1.72	0.71
1:A:1822:PRO:HD2	1:A:1825:LEU:HD12	1.71	0.71
1:A:2975:SER:N	1:A:2978:ASP:OD2	2.24	0.71
1:A:4810:ARG:NH2	1:A:4863:ASP:OD1	2.23	0.71
1:A:3941:VAL:HG12	1:A:4057:LYS:HD3	1.73	0.70
1:A:456:ASN:OD1	1:A:459:SER:N	2.24	0.70
1:A:2268:HIS:O	1:A:2295:ARG:NH2	2.24	0.70
1:A:3069:ILE:HG22	1:A:3105:LEU:CD1	2.21	0.70
1:A:3345:THR:HG21	1:A:3365:CYS:SG	2.30	0.70
1:A:1375:LEU:HD21	1:A:1485:PHE:CZ	2.27	0.70
1:A:543:THR:OG1	1:A:548:ASN:OD1	2.07	0.70
1:A:2176:GLN:OE1	1:A:2178:GLN:NE2	2.25	0.69
2:B:122:GLN:OE1	2:B:142:LYS:NZ	2.22	0.69
1:A:1768:LEU:O	1:A:1777:LYS:NZ	2.26	0.68
1:A:2618:VAL:CG2	1:A:2707:ILE:HG23	2.24	0.68
1:A:386:ILE:HD12	1:A:498:ILE:HD13	1.74	0.68
1:A:1913:HIS:O	1:A:1917:THR:HG23	1.92	0.68
1:A:4965:LEU:O	1:A:4966:GLN:NE2	2.27	0.67
1:A:1280:GLN:OE1	1:A:1284:ARG:NE	2.28	0.67
1:A:1886:SER:OG	1:A:1921:ARG:NH2	2.28	0.67
1:A:2549:MET:O	1:A:2555:ARG:NH2	2.28	0.67
1:A:2370:ARG:NH1	1:A:2390:ASP:O	2.28	0.67
1:A:585:GLU:OE2	1:A:585:GLU:N	2.27	0.67
2:B:97:GLU:OE2	2:B:117:HIS:ND1	2.27	0.66
1:A:1332:GLN:O	1:A:1334:ASP:N	2.28	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3095:GLU:OE1	1:A:3141:ARG:NH1	2.28	0.66
1:A:4000:CYS:SG	1:A:4005:LYS:NZ	2.68	0.66
2:B:213:MET:HE3	2:B:216:ALA:HB2	1.76	0.66
1:A:3242:LEU:HD12	1:A:3243:THR:N	2.11	0.66
1:A:1029:LEU:HD11	1:A:1060:VAL:HG22	1.79	0.65
1:A:3948:VAL:O	1:A:3952:VAL:HG23	1.97	0.65
1:A:4036:LEU:HD22	2:B:175:LEU:CD1	2.25	0.65
1:A:925:SER:O	1:A:972:SER:OG	2.12	0.65
1:A:4784:LEU:HD22	1:A:4887:LEU:HD23	1.77	0.65
1:A:5001:ASP:OD2	1:A:5002:SER:N	2.30	0.65
2:B:48:TRP:O	2:B:58:ARG:NH2	2.30	0.65
1:A:4744:ARG:NH1	1:A:4939:TYR:OH	2.30	0.65
1:A:3717:ASP:OD2	1:A:4796:LYS:NZ	2.21	0.64
1:A:2392:THR:OG1	1:A:2428:ARG:NH1	2.30	0.64
1:A:719:TRP:O	1:A:759:ARG:NH2	2.30	0.64
1:A:4133:VAL:HG22	1:A:4938:GLN:NE2	2.13	0.64
1:A:530:ALA:HB3	1:A:590:LEU:HD21	1.79	0.64
1:A:1387:ASP:OD1	1:A:1388:PHE:N	2.30	0.63
1:A:1569:GLU:OE2	1:A:1577:SER:N	2.31	0.63
2:B:60:ILE:HA	2:B:63:ASN:OD1	1.99	0.63
1:A:1942:ALA:O	1:A:1945:GLN:NE2	2.32	0.63
1:A:3863:ALA:O	1:A:3867:THR:HG23	1.99	0.63
1:A:2618:VAL:HG23	1:A:2707:ILE:HG23	1.80	0.63
2:B:213:MET:CE	2:B:216:ALA:HB2	2.28	0.63
2:B:158:VAL:O	2:B:161:ASN:ND2	2.32	0.62
1:A:535:ASP:OD1	1:A:535:ASP:N	2.28	0.62
1:A:976:ALA:O	1:A:980:SER:OG	2.17	0.62
1:A:1235:LEU:O	1:A:1237:TRP:N	2.33	0.62
1:A:2133:ARG:NE	1:A:2151:GLU:OE1	2.31	0.62
1:A:2490:ASN:HA	1:A:2495:ILE:HD12	1.81	0.62
1:A:2268:HIS:O	1:A:2268:HIS:ND1	2.33	0.61
1:A:4584:LEU:HD11	1:A:4620:ILE:HG23	1.82	0.61
1:A:1976:ALA:O	1:A:1979:VAL:HG22	2.01	0.60
1:A:4565:ARG:NH1	1:A:4623:ASP:OD1	2.33	0.60
1:A:411:SER:OG	1:A:414:ASP:OD2	2.20	0.60
1:A:426:LEU:HD13	1:A:432:LEU:HB2	1.84	0.60
1:A:3964:ASP:O	1:A:3967:THR:OG1	2.18	0.60
1:A:379:VAL:HG23	1:A:441:LYS:HA	1.83	0.60
1:A:4035:CYS:SG	1:A:4037:THR:OG1	2.54	0.60
1:A:1548:ILE:HG23	1:A:1562:VAL:CG1	2.31	0.60
1:A:2186:GLN:O	1:A:2189:SER:OG	2.17	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:TYR:O	1:A:478:ARG:HB2	2.01	0.59
1:A:2539:GLU:OE2	1:A:2562:ARG:NH1	2.35	0.59
1:A:4062:ARG:NE	1:A:4122:ASP:OD2	2.36	0.59
1:A:2044:ASP:OD1	1:A:2045:ALA:N	2.35	0.59
1:A:2055:HIS:NE2	1:A:2098:GLU:OE1	2.36	0.59
1:A:619:LYS:NZ	1:A:649:THR:O	2.35	0.59
1:A:4781:VAL:HG13	1:A:4887:LEU:CD1	2.33	0.59
1:A:4485:GLU:OE2	1:A:4572:ARG:NH1	2.33	0.58
1:A:4979:LEU:HD23	1:A:4980:VAL:H	1.68	0.58
2:B:55:GLY:O	2:B:57:GLN:NE2	2.36	0.58
1:A:4781:VAL:HG13	1:A:4887:LEU:HD13	1.84	0.58
1:A:737:THR:HG1	1:A:769:HIS:CD2	2.22	0.58
1:A:4871:PRO:HD2	1:A:4973:LEU:HD11	1.84	0.58
1:A:2783:ALA:HB2	1:A:2804:LEU:HD11	1.86	0.58
1:A:5120:PHE:O	1:A:5124:THR:OG1	2.12	0.58
1:A:407:GLU:HB2	1:A:449:PRO:HD2	1.86	0.57
1:A:4130:ILE:HD11	1:A:4163:ILE:HD11	1.86	0.57
1:A:498:ILE:HG21	1:A:500:TYR:CZ	2.38	0.57
1:A:740:LEU:HD23	1:A:765:LEU:HD23	1.86	0.57
1:A:2602:VAL:O	1:A:2606:SER:N	2.35	0.57
1:A:1982:ASP:OD1	1:A:1982:ASP:N	2.35	0.57
1:A:3989:LEU:HD13	1:A:4057:LYS:HB2	1.85	0.57
1:A:4505:CYS:SG	1:A:4507:ASN:N	2.76	0.57
2:B:42:LEU:HA	2:B:45:TRP:CE3	2.39	0.57
1:A:386:ILE:HD12	1:A:498:ILE:CD1	2.35	0.57
1:A:398:HIS:HB3	1:A:455:TYR:O	2.05	0.57
1:A:1455:ASN:OD1	1:A:1456:ASP:N	2.38	0.57
1:A:637:LEU:HD11	1:A:644:LEU:HD23	1.85	0.57
1:A:3175:ASP:OD1	1:A:3176:ILE:N	2.38	0.57
2:B:252:ARG:O	2:B:255:GLN:HG3	2.05	0.57
1:A:2928:VAL:HG12	1:A:2932:PHE:CE1	2.39	0.57
2:B:213:MET:SD	2:B:214:ASN:N	2.78	0.57
1:A:1386:ASP:O	1:A:1390:ARG:NE	2.38	0.57
1:A:1860:ASP:OD1	1:A:1861:GLU:N	2.38	0.57
1:A:3265:ASP:OD2	1:A:3269:ARG:NH2	2.37	0.57
1:A:4584:LEU:CD1	1:A:4620:ILE:HG23	2.35	0.56
1:A:633:ILE:HG22	1:A:633:ILE:O	2.05	0.56
1:A:2236:ASN:ND2	1:A:2237:PRO:O	2.39	0.56
1:A:3045:LEU:HD22	1:A:3157:VAL:HG21	1.87	0.56
1:A:630:VAL:HG21	1:A:637:LEU:HD21	1.88	0.56
1:A:977:TYR:O	1:A:1024:LYS:NZ	2.31	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4024:TRP:NE1	1:A:4029:GLN:O	2.39	0.56
1:A:4445:GLU:OE1	1:A:4643:HIS:NE2	2.38	0.56
2:B:206:LEU:HB3	2:B:226:LEU:HD22	1.88	0.56
1:A:3997:CYS:N	1:A:4002:GLY:O	2.35	0.56
1:A:531:ALA:O	1:A:535:ASP:OD1	2.24	0.56
1:A:4276:ARG:NE	1:A:4304:TRP:O	2.37	0.56
2:B:53:THR:OG1	2:B:84:LYS:NZ	2.36	0.56
1:A:3990:SER:O	1:A:3993:GLY:N	2.35	0.56
1:A:940:ARG:HH12	1:A:992:ALA:HB2	1.69	0.56
1:A:1376:ASN:O	1:A:1380:ASN:N	2.35	0.56
1:A:3941:VAL:HG12	1:A:4057:LYS:HD2	1.87	0.56
1:A:4888:ILE:HG12	1:A:4969:PRO:HG2	1.89	0.55
2:B:89:LEU:HB3	2:B:90:PRO:HD2	1.88	0.55
1:A:491:ASP:O	1:A:558:GLN:NE2	2.39	0.55
1:A:3069:ILE:HG22	1:A:3105:LEU:HD12	1.87	0.55
1:A:3087:ILE:HG12	1:A:3133:LEU:HD23	1.88	0.55
1:A:3982:LYS:HA	1:A:4061:PHE:CE1	2.43	0.54
1:A:3202:LYS:HG2	1:A:3270:LEU:HD21	1.89	0.54
1:A:4139:LEU:HB3	1:A:4181:SER:HB2	1.89	0.54
1:A:4387:ASN:HB3	1:A:4390:LEU:HD13	1.88	0.54
2:B:64:ARG:O	2:B:67:ILE:HG13	2.08	0.54
2:B:103:LEU:O	2:B:122:GLN:N	2.36	0.54
1:A:3556:ARG:NH2	1:A:3703:GLU:OE2	2.36	0.54
1:A:3709:VAL:HG23	1:A:3766:CYS:HB3	1.90	0.54
1:A:1051:LEU:O	1:A:1115:GLN:NE2	2.38	0.54
1:A:2787:GLN:O	1:A:2791:ALA:N	2.41	0.54
1:A:1293:LEU:O	1:A:1339:ARG:NE	2.40	0.54
1:A:674:LEU:O	1:A:677:VAL:HG12	2.08	0.53
1:A:2225:GLN:HB3	1:A:2255:MET:SD	2.48	0.53
1:A:1530:GLU:O	1:A:1532:SER:OG	2.27	0.53
2:B:223:LEU:HD22	2:B:226:LEU:HD21	1.90	0.53
1:A:3072:SER:O	1:A:3078:GLN:NE2	2.42	0.53
1:A:3806:GLU:OE2	1:A:3806:GLU:N	2.42	0.53
1:A:936:ILE:HG22	1:A:985:LYS:HE2	1.91	0.52
1:A:1235:LEU:O	1:A:1237:TRP:CD1	2.63	0.52
1:A:3102:LEU:HD12	1:A:3150:VAL:HG22	1.92	0.52
1:A:4980:VAL:O	1:A:4985:TRP:HA	2.08	0.52
1:A:414:ASP:OD2	1:A:415:SER:N	2.42	0.52
1:A:813:ASP:OD2	1:A:813:ASP:N	2.40	0.52
1:A:1407:LEU:HD12	1:A:1410:ILE:HD12	1.91	0.52
1:A:1909:GLU:OE2	1:A:5207:ARG:NH1	2.41	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4019:ARG:NH1	1:A:4020:CYS:SG	2.82	0.52
1:A:4906:ASN:OD1	1:A:4906:ASN:N	2.42	0.52
2:B:83:LEU:N	2:B:101:ASN:OD1	2.34	0.52
1:A:595:LYS:O	1:A:599:VAL:HG13	2.10	0.52
1:A:630:VAL:HG21	1:A:637:LEU:CD2	2.40	0.52
1:A:2575:LEU:O	1:A:2579:VAL:HG23	2.08	0.52
1:A:3450:LEU:HD12	1:A:3451:MET:N	2.25	0.52
1:A:3456:THR:HG22	1:A:3456:THR:O	2.10	0.52
2:B:45:TRP:NE1	2:B:88:ASP:O	2.37	0.52
2:B:96:LEU:HG	2:B:98:ILE:HG23	1.92	0.52
1:A:4854:ASP:OD2	1:A:4854:ASP:N	2.42	0.52
1:A:940:ARG:NH1	1:A:992:ALA:HB2	2.25	0.52
1:A:2598:VAL:O	1:A:2602:VAL:HG23	2.10	0.52
1:A:2918:CYS:HG	1:A:2932:PHE:HZ	1.57	0.52
1:A:408:PHE:HD1	1:A:448:ILE:HG21	1.74	0.52
2:B:260:GLY:O	2:B:262:ASP:N	2.43	0.52
1:A:3422:ARG:NE	1:A:3618:GLY:O	2.36	0.51
1:A:3585:ARG:NH1	1:A:3675:LEU:O	2.39	0.51
1:A:4781:VAL:HG22	1:A:4887:LEU:CD1	2.40	0.51
2:B:61:ALA:HB2	2:B:81:LEU:HD12	1.92	0.51
1:A:3458:LEU:CD2	1:A:3466:LEU:HD21	2.40	0.51
1:A:1548:ILE:HD11	1:A:1616:VAL:HG13	1.93	0.51
1:A:2610:ASN:OD1	1:A:2613:ARG:NH2	2.41	0.51
1:A:2729:GLN:NE2	1:A:2750:GLU:OE1	2.43	0.51
1:A:561:PHE:O	1:A:565:GLN:NE2	2.43	0.51
1:A:1005:SER:O	1:A:1008:GLN:HG3	2.11	0.51
1:A:4795:VAL:O	1:A:4799:GLN:N	2.43	0.51
1:A:4976:ILE:N	1:A:4977:PRO:CD	2.74	0.51
1:A:762:PHE:O	1:A:798:ARG:NH1	2.44	0.51
1:A:3379:THR:HG23	1:A:3418:THR:HG23	1.93	0.51
1:A:379:VAL:HG11	1:A:482:ILE:HD13	1.92	0.51
1:A:940:ARG:NH2	1:A:985:LYS:HB2	2.25	0.51
1:A:3086:ASN:O	1:A:3090:VAL:HG23	2.11	0.51
1:A:1652:GLN:NE2	1:A:1662:GLU:OE1	2.44	0.50
1:A:867:LEU:HB2	1:A:868:PRO:HD3	1.94	0.50
1:A:406:GLU:HA	1:A:409:GLY:O	2.10	0.50
1:A:1291:GLN:O	1:A:1294:LYS:HG2	2.11	0.50
1:A:1401:ILE:O	1:A:1405:LYS:HG3	2.10	0.50
1:A:813:ASP:O	1:A:817:VAL:HG23	2.12	0.50
1:A:4080:ASP:OD1	1:A:4082:ALA:N	2.44	0.50
1:A:568:ILE:O	1:A:573:ALA:HA	2.12	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3536:LEU:O	1:A:3540:VAL:HG23	2.12	0.50
1:A:4324:MET:HA	1:A:4709:ILE:HD11	1.92	0.50
1:A:4458:GLN:N	1:A:4653:GLN:OE1	2.40	0.50
1:A:3908:LEU:O	1:A:3912:VAL:HG23	2.12	0.49
1:A:4143:PHE:CZ	1:A:4223:VAL:HG12	2.47	0.49
1:A:4582:ILE:HG23	1:A:4677:TRP:HZ3	1.77	0.49
1:A:684:MET:O	1:A:687:ARG:NH2	2.45	0.49
1:A:2452:HIS:H	1:A:2455:THR:HG1	1.60	0.49
1:A:4050:ALA:O	1:A:4053:GLU:HG3	2.12	0.49
1:A:876:CYS:SG	1:A:877:ARG:N	2.86	0.49
1:A:2254:PHE:CE2	1:A:2306:VAL:HG23	2.47	0.49
1:A:3038:GLU:OE1	1:A:3127:LYS:NZ	2.45	0.49
1:A:3268:VAL:HG11	1:A:3604:LEU:HD23	1.94	0.49
1:A:3589:PHE:HB2	1:A:3635:LEU:HD13	1.94	0.49
1:A:4377:ARG:HD3	1:A:4381:ILE:HD12	1.95	0.49
1:A:2417:ILE:HD13	1:A:2578:LEU:HB2	1.94	0.49
1:A:4665:ASP:OD2	1:A:4666:THR:N	2.45	0.49
1:A:1939:LEU:N	1:A:1940:PRO:HD2	2.28	0.49
1:A:1536:LEU:HD23	1:A:1588:LEU:HD13	1.95	0.49
1:A:443:HIS:CG	1:A:448:ILE:HD11	2.48	0.49
1:A:710:ASP:OD1	1:A:713:ARG:NE	2.43	0.49
1:A:1943:PHE:O	1:A:1946:HIS:N	2.46	0.49
1:A:538:PHE:O	1:A:541:LEU:HG	2.13	0.48
1:A:1679:GLN:HG3	1:A:1775:VAL:HG13	1.95	0.48
1:A:1976:ALA:HB1	1:A:2009:MET:SD	2.53	0.48
1:A:2975:SER:O	1:A:2979:ILE:HD12	2.13	0.48
1:A:3743:PHE:O	1:A:3746:THR:OG1	2.20	0.48
1:A:3864:MET:SD	1:A:3919:GLN:NE2	2.86	0.48
1:A:862:LEU:HD11	1:A:938:VAL:HG21	1.94	0.48
1:A:1414:ARG:HD3	1:A:1496:TRP:CE2	2.49	0.48
1:A:1614:CYS:SG	1:A:3081:THR:HG21	2.53	0.48
1:A:2058:VAL:HG11	1:A:2066:ILE:HD13	1.94	0.48
1:A:1493:LYS:O	1:A:1496:TRP:HB2	2.13	0.48
1:A:4668:LEU:HD22	1:A:4674:ARG:HA	1.94	0.48
1:A:2788:GLY:O	1:A:2797:ARG:HA	2.14	0.48
1:A:3307:ALA:HB1	1:A:3314:ILE:HD13	1.93	0.48
1:A:4827:ASN:O	1:A:4831:VAL:HG23	2.13	0.48
1:A:1123:ARG:HD3	1:A:1123:ARG:C	2.34	0.48
1:A:1482:SER:O	1:A:1482:SER:OG	2.30	0.48
1:A:5164:SER:O	1:A:5168:THR:HG23	2.14	0.48
1:A:1993:ARG:NH1	1:A:2209:ASN:O	2.44	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2266:SER:O	1:A:2296:LYS:HB3	2.13	0.48
1:A:552:PHE:CE2	1:A:625:ILE:HG23	2.49	0.48
1:A:1096:LEU:HD12	1:A:1101:ILE:HD13	1.96	0.48
1:A:1548:ILE:HG23	1:A:1562:VAL:HG12	1.95	0.48
2:B:252:ARG:O	2:B:256:GLN:NE2	2.47	0.48
1:A:542:GLN:N	1:A:542:GLN:OE1	2.45	0.48
1:A:1294:LYS:HB2	1:A:1330:GLN:NE2	2.29	0.48
1:A:2216:ARG:HD2	3:A:5301:ATP:H1'	1.96	0.48
1:A:479:CYS:SG	1:A:569:TYR:HB2	2.54	0.48
1:A:1407:LEU:CD1	1:A:1410:ILE:HD12	2.44	0.48
1:A:5072:LEU:O	1:A:5075:THR:OG1	2.22	0.48
1:A:671:SER:OG	1:A:674:LEU:HB3	2.14	0.47
1:A:4979:LEU:HD22	1:A:4981:TYR:HB3	1.95	0.47
1:A:3643:ILE:O	1:A:3648:ASN:ND2	2.45	0.47
1:A:401:PHE:CE2	1:A:455:TYR:HB2	2.49	0.47
1:A:498:ILE:HG21	1:A:500:TYR:CE1	2.49	0.47
1:A:671:SER:OG	1:A:671:SER:O	2.26	0.47
1:A:3612:ASP:O	1:A:3616:GLU:HG3	2.14	0.47
1:A:4390:LEU:H	1:A:4390:LEU:HD12	1.79	0.47
1:A:4781:VAL:HG22	1:A:4887:LEU:HD13	1.96	0.47
1:A:2023:ILE:HD12	1:A:2056:LEU:CD2	2.45	0.47
1:A:4136:LYS:NZ	1:A:4937:CYS:O	2.42	0.47
1:A:4871:PRO:HA	1:A:4877:GLY:O	2.14	0.47
2:B:166:LEU:HD11	2:B:178:VAL:HG11	1.97	0.47
1:A:711:ALA:O	1:A:714:GLN:N	2.43	0.47
1:A:2416:VAL:HG12	1:A:2521:ILE:HG23	1.97	0.47
1:A:4277:VAL:HG13	1:A:4717:ILE:HG23	1.96	0.47
1:A:532:LEU:HA	1:A:535:ASP:OD1	2.15	0.47
1:A:2147:ARG:HG2	1:A:2147:ARG:HH21	1.80	0.47
1:A:4788:LEU:HD12	1:A:4915:VAL:HG11	1.95	0.47
1:A:1344:LYS:O	1:A:1348:HIS:ND1	2.41	0.47
1:A:2650:TRP:NE1	1:A:2760:GLU:HG2	2.29	0.47
1:A:2924:VAL:HG13	1:A:2967:ALA:HB3	1.96	0.47
1:A:2959:LEU:O	1:A:2963:VAL:HG23	2.14	0.47
1:A:3546:MET:O	1:A:3693:ILE:N	2.37	0.47
1:A:1369:ASN:N	1:A:1481:PRO:O	2.40	0.47
1:A:2488:GLU:O	1:A:2491:THR:OG1	2.19	0.47
1:A:3102:LEU:HG	1:A:3148:LEU:HD11	1.97	0.47
1:A:556:PHE:CZ	1:A:629:VAL:HG13	2.50	0.47
1:A:1029:LEU:CD1	1:A:1060:VAL:HG22	2.45	0.47
1:A:1743:ARG:NH2	1:A:1812:MET:SD	2.88	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1935:GLU:HG2	1:A:1940:PRO:HB2	1.97	0.47
1:A:3707:ASN:N	1:A:3707:ASN:OD1	2.48	0.46
1:A:3054:ILE:HD12	1:A:3054:ILE:H	1.79	0.46
1:A:4486:ASP:OD1	1:A:4552:ARG:NH1	2.47	0.46
1:A:3045:LEU:CD2	1:A:3157:VAL:HG21	2.44	0.46
1:A:4390:LEU:HD12	1:A:4390:LEU:N	2.30	0.46
1:A:4578:VAL:HG11	1:A:4682:ALA:CB	2.45	0.46
2:B:45:TRP:CZ3	2:B:65:LEU:HB3	2.50	0.46
1:A:2398:ASP:O	1:A:2402:LYS:HG3	2.16	0.46
1:A:3068:ILE:CG2	1:A:3103:LEU:HD22	2.46	0.46
2:B:49:GLU:O	2:B:52:GLY:N	2.41	0.46
2:B:213:MET:CG	2:B:233:LEU:HD13	2.46	0.46
1:A:382:PHE:CD2	1:A:436:ILE:CD1	2.98	0.46
1:A:582:ARG:CZ	1:A:582:ARG:HB3	2.45	0.46
1:A:983:ASP:C	1:A:985:LYS:H	2.18	0.46
1:A:2372:LYS:HE2	1:A:2372:LYS:HA	1.96	0.46
1:A:4031:ILE:HD11	2:B:215:ARG:CD	2.45	0.46
1:A:4840:ARG:NH2	1:A:4857:SER:O	2.48	0.46
1:A:382:PHE:CE1	1:A:491:ASP:OD2	2.69	0.46
1:A:802:LEU:HD22	1:A:817:VAL:HG22	1.98	0.46
1:A:823:MET:SD	1:A:826:ARG:NH1	2.89	0.46
1:A:1069:LYS:O	1:A:1073:ASN:ND2	2.41	0.46
1:A:2166:ARG:HB3	1:A:2167:PRO:HD3	1.97	0.46
2:B:76:LEU:HD12	2:B:77:ASN:H	1.79	0.46
2:B:231:LEU:HD23	2:B:268:ILE:CD1	2.46	0.46
1:A:5132:GLU:OE1	1:A:5169:LYS:NZ	2.43	0.46
1:A:5140:LYS:O	1:A:5146:THR:OG1	2.31	0.46
1:A:532:LEU:O	1:A:535:ASP:OD1	2.33	0.46
1:A:4427:VAL:HG12	1:A:4428:PRO:O	2.16	0.46
2:B:166:LEU:CD1	2:B:178:VAL:HG11	2.46	0.46
1:A:425:ASP:OD2	1:A:426:LEU:N	2.49	0.45
2:B:133:LEU:HD23	2:B:153:LEU:HD13	1.98	0.45
1:A:1015:GLN:HA	1:A:1015:GLN:OE1	2.15	0.45
1:A:2402:LYS:HE2	1:A:2582:PHE:CD1	2.51	0.45
1:A:2460:ILE:O	1:A:2464:VAL:HG23	2.16	0.45
1:A:3563:LEU:CD2	1:A:3653:THR:HG21	2.46	0.45
1:A:4637:GLU:O	1:A:4641:VAL:HG23	2.15	0.45
2:B:86:LEU:HD22	2:B:89:LEU:HD11	1.98	0.45
1:A:4961:VAL:HG22	1:A:4965:LEU:HD12	1.98	0.45
2:B:59:ASN:O	2:B:63:ASN:OD1	2.34	0.45
1:A:1287:ILE:HD13	1:A:1329:HIS:NE2	2.31	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1700:TYR:CE2	1:A:1807:ALA:HA	2.52	0.45
1:A:3728:TYR:CD2	1:A:4820:GLY:HA2	2.52	0.45
1:A:1330:GLN:O	1:A:1330:GLN:HG3	2.17	0.45
1:A:1593:MET:HG3	1:A:3084:CYS:HB3	1.99	0.45
1:A:3937:THR:HG21	1:A:3945:GLN:HA	1.99	0.45
1:A:409:GLY:O	1:A:411:SER:N	2.49	0.45
1:A:1608:ARG:O	1:A:1611:GLU:HG2	2.16	0.45
1:A:4136:LYS:NZ	1:A:4180:ASP:OD2	2.46	0.45
1:A:4782:LYS:O	1:A:4785:PRO:HD2	2.16	0.45
1:A:4835:THR:HG22	1:A:4883:LEU:HD11	1.97	0.45
2:B:61:ALA:HB2	2:B:81:LEU:CD1	2.47	0.45
1:A:682:ARG:O	1:A:686:THR:OG1	2.33	0.45
1:A:2871:ASP:N	1:A:2871:ASP:OD1	2.49	0.45
1:A:3937:THR:HA	1:A:3941:VAL:HG22	1.99	0.45
1:A:4173:LEU:HD12	1:A:4939:TYR:HB2	1.98	0.45
1:A:4791:GLN:HG2	1:A:4871:PRO:HG3	1.98	0.45
1:A:5160:ASP:OD2	1:A:5161:THR:N	2.50	0.45
1:A:1702:ASN:O	1:A:1876:LEU:HD22	2.16	0.45
1:A:4133:VAL:HG22	1:A:4938:GLN:HE22	1.81	0.45
1:A:982:TRP:O	1:A:985:LYS:HG3	2.17	0.45
1:A:3890:SER:HA	1:A:3920:TRP:CZ2	2.51	0.45
1:A:4983:HIS:CD2	1:A:4983:HIS:H	2.34	0.45
2:B:63:ASN:O	2:B:66:LYS:HG3	2.17	0.45
1:A:865:TYR:CG	1:A:938:VAL:HG22	2.52	0.45
1:A:2421:GLU:OE1	1:A:2566:TYR:OH	2.32	0.45
1:A:2686:MET:SD	1:A:2721:LEU:HB3	2.56	0.45
1:A:3811:LEU:N	1:A:3812:PRO:CD	2.80	0.45
1:A:4346:LEU:HD12	1:A:4347:GLU:HG2	1.98	0.45
1:A:1069:LYS:HE3	1:A:1069:LYS:HA	1.99	0.44
1:A:1454:GLU:HB3	1:A:1595:MET:SD	2.57	0.44
1:A:3799:LYS:HG2	1:A:3813:TRP:CE2	2.52	0.44
1:A:4930:THR:HB	1:A:4931:PRO:HD3	1.98	0.44
2:B:78:LEU:HD11	2:B:89:LEU:HD13	1.99	0.44
2:B:213:MET:HG3	2:B:233:LEU:HD13	1.99	0.44
1:A:526:LYS:HE2	1:A:579:LEU:HD21	1.99	0.44
1:A:2198:LEU:HD21	1:A:2212:TRP:CH2	2.52	0.44
1:A:4428:PRO:HB2	1:A:4595:SER:HB2	1.99	0.44
1:A:401:PHE:HB2	1:A:453:VAL:HG23	1.99	0.44
1:A:1950:VAL:HG12	1:A:1950:VAL:O	2.17	0.44
1:A:2504:ASP:OD1	1:A:2504:ASP:N	2.50	0.44
1:A:3066:PRO:CG	1:A:3101:LEU:HD13	2.47	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3870:LEU:HD11	1:A:3889:LEU:HD12	1.99	0.44
1:A:3997:CYS:O	1:A:4001:LEU:N	2.44	0.44
1:A:4428:PRO:O	1:A:4429:LEU:HB3	2.18	0.44
1:A:568:ILE:HD13	1:A:568:ILE:H	1.83	0.44
1:A:1991:SER:HB2	1:A:1996:VAL:HG21	1.98	0.44
1:A:3709:VAL:HG23	1:A:3766:CYS:CB	2.47	0.44
1:A:4784:LEU:CB	1:A:4887:LEU:HD22	2.47	0.44
1:A:1898:ASP:HB2	1:A:1934:TRP:HB3	1.99	0.44
1:A:2078:TYR:HA	1:A:2087:TRP:O	2.17	0.44
1:A:4780:LEU:CD2	1:A:4835:THR:HG23	2.48	0.44
1:A:545:ASP:CG	1:A:547:ILE:HG22	2.38	0.44
1:A:1375:LEU:HD21	1:A:1485:PHE:CE1	2.52	0.44
1:A:2715:TYR:HA	1:A:2720:LEU:HD23	1.99	0.44
1:A:5174:LEU:HD22	1:A:5174:LEU:H	1.82	0.44
2:B:157:ARG:HA	2:B:177:VAL:HB	2.00	0.44
1:A:519:ARG:HA	1:A:522:LEU:HD12	1.99	0.44
1:A:1379:LEU:O	1:A:1383:ASP:OD2	2.36	0.44
1:A:2292:PHE:HZ	1:A:2564:LEU:HD22	1.81	0.44
1:A:2968:LYS:NZ	1:A:3035:GLU:OE2	2.51	0.44
2:B:76:LEU:HG	2:B:77:ASN:N	2.33	0.44
2:B:252:ARG:HA	2:B:255:GLN:CG	2.48	0.44
1:A:1386:ASP:O	1:A:1390:ARG:NH1	2.50	0.44
1:A:2471:ALA:HB1	1:A:2516:SER:O	2.17	0.44
1:A:2894:MET:CE	1:A:2899:PHE:HB2	2.48	0.44
1:A:3455:VAL:HG12	1:A:3456:THR:N	2.33	0.44
1:A:4983:HIS:CD2	1:A:4983:HIS:N	2.85	0.44
1:A:476:VAL:HG22	1:A:477:ASN:N	2.33	0.44
1:A:2327:ASN:N	1:A:2327:ASN:OD1	2.51	0.44
1:A:2316:THR:HG22	1:A:2318:ILE:HD11	2.00	0.43
1:A:2962:MET:HE2	1:A:2982:ALA:HA	1.99	0.43
1:A:3054:ILE:HD12	1:A:3054:ILE:N	2.33	0.43
1:A:3394:ALA:O	1:A:3398:VAL:HG23	2.18	0.43
1:A:4795:VAL:HG22	1:A:4974:LYS:CG	2.47	0.43
2:B:259:THR:O	2:B:261:PRO:HD3	2.18	0.43
1:A:4582:ILE:HG12	1:A:4681:ILE:HG21	1.99	0.43
1:A:5140:LYS:O	1:A:5146:THR:CB	2.66	0.43
1:A:5144:PRO:HA	1:A:5147:GLN:HG2	2.00	0.43
1:A:588:ARG:HG3	1:A:589:TYR:N	2.33	0.43
1:A:1789:LEU:N	1:A:1790:PRO:CD	2.81	0.43
1:A:2805:VAL:HB	1:A:2825:CYS:SG	2.59	0.43
1:A:4962:SER:OG	1:A:4963:ARG:HD2	2.18	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5174:LEU:HD22	1:A:5174:LEU:N	2.32	0.43
1:A:862:LEU:CD1	1:A:938:VAL:HG21	2.49	0.43
1:A:1146:GLU:OE2	1:A:1198:ARG:N	2.50	0.43
1:A:2686:MET:O	1:A:2686:MET:HE2	2.18	0.43
1:A:4756:VAL:HG13	1:A:4761:GLY:HA3	1.99	0.43
2:B:143:ILE:HG21	2:B:146:LEU:HD23	1.99	0.43
1:A:2179:ASP:O	1:A:2179:ASP:OD2	2.37	0.43
1:A:4979:LEU:HD23	1:A:4980:VAL:N	2.33	0.43
1:A:1290:HIS:CD2	1:A:1330:GLN:HB3	2.54	0.43
1:A:3405:ILE:O	1:A:3405:ILE:HG22	2.18	0.43
1:A:4029:GLN:HG2	2:B:238:PHE:CD2	2.53	0.43
1:A:4143:PHE:CE1	1:A:4223:VAL:HG12	2.53	0.43
1:A:4172:MET:SD	1:A:4740:ILE:HA	2.59	0.43
1:A:1451:SER:OG	1:A:1518:TRP:NE1	2.46	0.43
1:A:2239:PHE:O	1:A:2239:PHE:CG	2.72	0.43
1:A:2351:TYR:CZ	1:A:2355:LEU:HD11	2.54	0.43
1:A:2861:HIS:HB3	1:A:2862:PRO:HD3	2.00	0.43
1:A:2991:ASP:OD1	1:A:2992:ASP:N	2.52	0.43
1:A:4009:CYS:C	1:A:4010:LEU:HD12	2.38	0.43
1:A:4130:ILE:HD13	1:A:4170:LEU:HD13	2.00	0.43
1:A:4347:GLU:OE1	1:A:4347:GLU:HA	2.19	0.43
1:A:4871:PRO:HG2	1:A:4973:LEU:HG	2.01	0.43
2:B:112:MET:O	2:B:114:LYS:N	2.52	0.43
1:A:1445:VAL:HG13	1:A:1462:VAL:CG1	2.49	0.43
1:A:2240:ILE:C	1:A:2240:ILE:HD12	2.38	0.43
1:A:2783:ALA:HB2	1:A:2804:LEU:CD1	2.47	0.43
1:A:3270:LEU:HD13	1:A:3280:ALA:HB2	2.01	0.43
1:A:4973:LEU:HD13	1:A:4974:LYS:HG3	1.99	0.43
1:A:2147:ARG:HG3	1:A:2148:SER:H	1.84	0.43
1:A:2979:ILE:O	1:A:2983:VAL:HG23	2.19	0.43
1:A:3195:VAL:O	1:A:3199:ILE:HG12	2.19	0.43
1:A:4071:ASP:OD2	1:A:4958:ARG:NH1	2.52	0.43
1:A:4661:LEU:O	1:A:4662:LEU:HD13	2.19	0.43
1:A:407:GLU:HB2	1:A:449:PRO:CD	2.48	0.42
2:B:153:LEU:O	2:B:173:LEU:HD12	2.19	0.42
2:B:248:GLY:HA2	2:B:251:MET:CE	2.48	0.42
1:A:737:THR:HG21	1:A:766:PRO:HG3	2.01	0.42
1:A:937:GLU:CG	1:A:985:LYS:NZ	2.82	0.42
1:A:2024:ARG:NH2	1:A:2057:ASP:OD2	2.50	0.42
1:A:4114:THR:HG21	1:A:4129:VAL:O	2.18	0.42
2:B:42:LEU:HA	2:B:45:TRP:CD2	2.54	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:GLU:N	1:A:463:GLU:OE1	2.53	0.42
1:A:530:ALA:CB	1:A:590:LEU:HD21	2.49	0.42
1:A:1164:CYS:HA	1:A:1167:VAL:HG22	2.00	0.42
1:A:519:ARG:O	1:A:523:VAL:HG23	2.20	0.42
1:A:1866:THR:N	1:A:1869:THR:OG1	2.46	0.42
1:A:4639:ILE:HG22	1:A:4643:HIS:CD2	2.54	0.42
1:A:654:SER:HB2	1:A:655:PRO:CD	2.50	0.42
1:A:1062:ARG:O	1:A:1066:THR:HG23	2.19	0.42
1:A:2036:LEU:HD23	1:A:2081:ASP:HB3	2.01	0.42
1:A:2650:TRP:CE2	1:A:2760:GLU:HG2	2.55	0.42
1:A:3673:MET:SD	1:A:3674:LEU:N	2.92	0.42
1:A:4016:HIS:CD2	1:A:4032:CYS:SG	3.13	0.42
1:A:4487:LEU:HD21	1:A:4571:ASP:OD2	2.19	0.42
1:A:420:LEU:CD2	1:A:435:GLY:HA3	2.50	0.42
1:A:626:VAL:O	1:A:630:VAL:HG23	2.19	0.42
1:A:1943:PHE:CD1	1:A:1943:PHE:N	2.88	0.42
1:A:3838:VAL:HG21	1:A:3866:CYS:SG	2.60	0.42
1:A:4761:GLY:O	1:A:4765:VAL:N	2.42	0.42
1:A:4761:GLY:HA2	1:A:4765:VAL:HG22	2.00	0.42
2:B:175:LEU:HD11	2:B:177:VAL:HG23	2.01	0.42
1:A:912:ARG:O	1:A:916:GLU:OE2	2.38	0.42
1:A:1608:ARG:HH21	1:A:1608:ARG:HG2	1.85	0.42
1:A:3237:GLN:O	1:A:3240:ARG:NE	2.48	0.42
1:A:3299:PHE:CZ	1:A:3440:VAL:HG21	2.55	0.42
1:A:4009:CYS:HG	1:A:4051:HIS:CE1	2.38	0.42
1:A:4042:GLU:HA	1:A:4042:GLU:OE1	2.20	0.42
1:A:4342:ALA:O	1:A:4345:VAL:HG12	2.20	0.42
1:A:934:LYS:O	1:A:938:VAL:HG23	2.20	0.42
1:A:2493:GLU:C	1:A:2495:ILE:H	2.23	0.42
1:A:2949:GLU:HB2	1:A:3163:ILE:HD13	2.00	0.42
1:A:3187:ILE:O	1:A:3191:LEU:HD23	2.19	0.42
1:A:3859:ASP:OD1	1:A:3860:ALA:N	2.53	0.42
1:A:398:HIS:CB	1:A:455:TYR:O	2.67	0.42
1:A:566:PRO:HG2	1:A:576:TRP:CE3	2.55	0.42
1:A:1277:TYR:O	1:A:1281:PRO:HD2	2.20	0.42
1:A:1396:ILE:O	1:A:1397:ASN:HB3	2.20	0.42
1:A:4871:PRO:HG2	1:A:4973:LEU:CG	2.50	0.42
1:A:4905:ASN:N	1:A:4905:ASN:OD1	2.52	0.42
2:B:38:ASN:HB3	2:B:69:LEU:HD21	2.02	0.42
1:A:1126:SER:C	1:A:1127:LEU:HD22	2.41	0.42
1:A:1861:GLU:O	1:A:1892:TYR:HA	2.18	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2237:PRO:O	1:A:2238:SER:C	2.58	0.42
1:A:4173:LEU:CD1	1:A:4939:TYR:HB2	2.50	0.42
1:A:4781:VAL:HG12	1:A:4920:VAL:HB	2.01	0.42
1:A:4973:LEU:HD22	1:A:4973:LEU:HA	1.89	0.42
1:A:983:ASP:O	1:A:985:LYS:N	2.53	0.41
1:A:3992:PHE:HD1	1:A:3992:PHE:O	2.03	0.41
1:A:1033:ILE:HG22	1:A:1081:LEU:HD12	2.02	0.41
1:A:2449:VAL:HG22	1:A:2463:ARG:HH21	1.85	0.41
1:A:2740:LYS:HB2	1:A:2920:SER:OG	2.20	0.41
1:A:2906:ASN:OD1	1:A:2908:THR:N	2.50	0.41
1:A:3453:SER:HB2	1:A:3529:ILE:HG23	2.01	0.41
1:A:3997:CYS:SG	1:A:3999:ILE:HB	2.60	0.41
1:A:4004:ALA:HA	1:A:4017:CYS:SG	2.60	0.41
1:A:4910:VAL:HB	1:A:4968:LYS:O	2.20	0.41
1:A:4932:LEU:CD2	1:A:4956:ILE:HG23	2.49	0.41
1:A:443:HIS:HB3	1:A:448:ILE:HD11	2.02	0.41
1:A:637:LEU:HD11	1:A:644:LEU:CD2	2.48	0.41
1:A:1106:LEU:HD11	1:A:1143:ARG:HB2	2.03	0.41
1:A:1514:ARG:HD2	1:A:2790:ALA:O	2.20	0.41
1:A:2594:ILE:O	1:A:2598:VAL:HG23	2.20	0.41
1:A:3269:ARG:NH2	1:A:3608:ALA:O	2.52	0.41
1:A:4846:ASN:OD1	1:A:4846:ASN:N	2.54	0.41
2:B:56:GLU:OE1	2:B:58:ARG:NH1	2.46	0.41
2:B:172:GLU:OE1	2:B:192:LYS:NZ	2.45	0.41
1:A:1534:LEU:HD23	1:A:1592:LEU:HD23	2.02	0.41
1:A:3000:LEU:O	1:A:3003:LEU:O	2.38	0.41
1:A:3450:LEU:HD12	1:A:3450:LEU:C	2.40	0.41
2:B:78:LEU:HD22	2:B:83:LEU:HD12	2.03	0.41
1:A:1371:ASP:OD1	1:A:1373:SER:N	2.46	0.41
1:A:1601:ARG:NE	1:A:1601:ARG:HA	2.36	0.41
1:A:2378:CYS:O	1:A:2383:ILE:N	2.46	0.41
1:A:2643:ARG:O	1:A:2647:VAL:HG23	2.21	0.41
1:A:3764:LEU:HD23	1:A:3792:TRP:CZ3	2.55	0.41
1:A:408:PHE:HD2	1:A:417:ILE:HD13	1.86	0.41
1:A:430:ARG:NE	1:A:528:ILE:HD11	2.35	0.41
1:A:916:GLU:OE2	1:A:916:GLU:CA	2.69	0.41
1:A:2690:GLY:HA2	1:A:2694:HIS:HB3	2.02	0.41
1:A:4346:LEU:HD12	1:A:4347:GLU:N	2.35	0.41
1:A:5049:TYR:CD1	1:A:5053:ILE:HD12	2.56	0.41
1:A:426:LEU:CB	1:A:430:ARG:HB2	2.51	0.41
1:A:765:LEU:O	1:A:798:ARG:NH1	2.46	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1366:LEU:HD22	1:A:1432:ARG:NH1	2.35	0.41
1:A:1383:ASP:OD2	1:A:1383:ASP:N	2.52	0.41
1:A:4132:SER:O	1:A:4136:LYS:HG2	2.21	0.41
2:B:41:TYR:HB3	2:B:45:TRP:CZ2	2.55	0.41
1:A:1236:PHE:O	1:A:1237:TRP:HB3	2.20	0.41
1:A:1319:SER:O	1:A:1323:ILE:HG13	2.20	0.41
1:A:3341:ALA:HB1	1:A:3342:PRO:HD2	2.03	0.41
1:A:3692:TYR:HB2	1:A:4978:THR:O	2.21	0.41
1:A:4114:THR:HG22	1:A:4115:LYS:N	2.36	0.41
1:A:4422:LEU:HD23	1:A:4427:VAL:HG21	2.02	0.41
1:A:755:GLU:N	1:A:756:PRO:HD2	2.36	0.41
1:A:862:LEU:HD13	1:A:917:VAL:HG11	2.03	0.41
1:A:1172:GLN:O	1:A:1268:ILE:HG23	2.21	0.41
1:A:1286:PHE:CZ	1:A:1324:MET:HG2	2.55	0.41
1:A:1637:TRP:CZ2	1:A:1639:ALA:HB2	2.56	0.41
1:A:2036:LEU:O	1:A:2040:LEU:HG	2.20	0.41
1:A:2694:HIS:NE2	1:A:2700:LYS:HB3	2.36	0.41
1:A:2955:ASP:OD1	1:A:3040:ARG:NH2	2.47	0.41
1:A:3132:GLY:HA3	1:A:3137:ARG:HH21	1.85	0.41
1:A:3176:ILE:HG21	1:A:3227:ALA:HB1	2.03	0.41
1:A:3359:LEU:HD21	1:A:3397:SER:HB3	2.03	0.41
1:A:4571:ASP:OD1	1:A:4571:ASP:N	2.53	0.41
1:A:4980:VAL:O	1:A:4981:TYR:O	2.39	0.41
1:A:5047:ASN:OD1	1:A:5048:VAL:N	2.53	0.41
1:A:5137:ILE:HG12	1:A:5190:CYS:SG	2.61	0.41
1:A:937:GLU:HG2	1:A:985:LYS:HZ1	1.86	0.41
1:A:977:TYR:CE2	1:A:1024:LYS:HB3	2.55	0.41
1:A:1139:ALA:HA	1:A:1142:TRP:CE3	2.56	0.41
1:A:1388:PHE:CE2	1:A:1396:ILE:HG23	2.56	0.41
1:A:1450:ILE:HG23	1:A:1530:GLU:HA	2.03	0.41
1:A:3109:TYR:O	1:A:3113:TYR:N	2.54	0.41
1:A:3019:LYS:HB2	1:A:3059:PHE:CE1	2.57	0.40
1:A:4385:SER:O	1:A:4391:HIS:NE2	2.48	0.40
1:A:5124:THR:CG2	1:A:5125:GLY:N	2.83	0.40
1:A:1891:VAL:HG12	1:A:1892:TYR:N	2.36	0.40
1:A:2372:LYS:HA	1:A:2372:LYS:CE	2.51	0.40
1:A:2490:ASN:ND2	1:A:2525:ASN:O	2.53	0.40
1:A:2842:VAL:HA	1:A:2882:VAL:O	2.21	0.40
1:A:2861:HIS:HB3	1:A:2862:PRO:CD	2.51	0.40
1:A:3538:SER:OG	1:A:3629:GLN:NE2	2.44	0.40
1:A:4344:ALA:O	1:A:4348:CYS:N	2.53	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4791:GLN:HE21	1:A:4880:ALA:HB1	1.86	0.40
1:A:5190:CYS:SG	1:A:5191:VAL:N	2.93	0.40
2:B:46:SER:O	2:B:49:GLU:HB3	2.21	0.40
2:B:226:LEU:HD23	2:B:226:LEU:HA	1.95	0.40
1:A:2929:GLN:HA	1:A:2932:PHE:CD2	2.56	0.40
1:A:3827:ASN:OD1	1:A:3892:PRO:HB3	2.21	0.40
1:A:4789:ALA:O	1:A:4793:ASP:OD2	2.38	0.40
1:A:726:SER:O	1:A:726:SER:OG	2.36	0.40
1:A:1454:GLU:HG3	1:A:1533:SER:OG	2.21	0.40
1:A:1700:TYR:CZ	1:A:1810:ALA:CB	3.05	0.40
1:A:1748:CYS:SG	1:A:1801:THR:HG23	2.62	0.40
1:A:2591:LYS:NZ	1:A:2617:GLU:OE2	2.42	0.40
1:A:2701:ASP:OD1	1:A:2704:ARG:NH1	2.54	0.40
1:A:2825:CYS:HB3	1:A:2879:VAL:HG11	2.02	0.40
1:A:3563:LEU:HD22	1:A:3653:THR:HG21	2.02	0.40
1:A:3813:TRP:CE3	1:A:3816:LEU:HD12	2.57	0.40
1:A:4980:VAL:O	1:A:4985:TRP:N	2.55	0.40
1:A:1336:ILE:O	1:A:1340:VAL:HG23	2.22	0.40
1:A:2978:ASP:OD1	1:A:2979:ILE:N	2.54	0.40
1:A:3423:VAL:HG21	1:A:5018:TYR:CB	2.51	0.40
1:A:4008:VAL:N	1:A:4016:HIS:O	2.48	0.40
1:A:4784:LEU:HD22	1:A:4887:LEU:CD2	2.48	0.40
1:A:4972:SER:O	1:A:4973:LEU:HD23	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4479/5247 (85%)	4245 (95%)	228 (5%)	6 (0%)	48	76
2	B	235/575 (41%)	203 (86%)	32 (14%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4714/5822 (81%)	4448 (94%)	260 (6%)	6 (0%)	50 76

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1236	PHE
1	A	1333	ARG
1	A	3104	ASN
1	A	4981	TYR
1	A	1602	ASN
1	A	2494	ALA

### 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	4076/4653 (88%)	3910 (96%)	166 (4%)	26 54
2	B	216/501 (43%)	207 (96%)	9 (4%)	25 53
All	All	4292/5154 (83%)	4117 (96%)	175 (4%)	28 54

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	388	SER
1	A	397	LEU
1	A	402	ILE
1	A	403	ARG
1	A	406	GLU
1	A	412	LYS
1	A	415	SER
1	A	438	CYS
1	A	442	LYS
1	A	445	ASP
1	A	459	SER
1	A	461	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	477	ASN
1	A	484	SER
1	A	489	SER
1	A	496	TYR
1	A	497	ASP
1	A	501	MET
1	A	519	ARG
1	A	520	LYS
1	A	522	LEU
1	A	541	LEU
1	A	545	ASP
1	A	568	ILE
1	A	581	TYR
1	A	643	TRP
1	A	671	SER
1	A	688	THR
1	A	707	ARG
1	A	728	SER
1	A	763	SER
1	A	804	GLN
1	A	813	ASP
1	A	832	ARG
1	A	857	SER
1	A	876	CYS
1	A	916	GLU
1	A	922	MET
1	A	926	SER
1	A	962	GLU
1	A	989	ASP
1	A	995	PHE
1	A	1049	LYS
1	A	1098	SER
1	A	1125	LYS
1	A	1175	PHE
1	A	1198	ARG
1	A	1203	SER
1	A	1204	ASN
1	A	1205	SER
1	A	1206	GLN
1	A	1236	PHE
1	A	1237	TRP
1	A	1281	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1288	LYS
1	A	1332	GLN
1	A	1365	SER
1	A	1386	ASP
1	A	1416	LYS
1	A	1442	LYS
1	A	1496	TRP
1	A	1509	LEU
1	A	1560	ASP
1	A	1577	SER
1	A	1608	ARG
1	A	1717	ARG
1	A	1773	SER
1	A	1790	PRO
1	A	1972	GLN
1	A	1999	SER
1	A	2049	LYS
1	A	2078	TYR
1	A	2147	ARG
1	A	2242	ASP
1	A	2294	LEU
1	A	2295	ARG
1	A	2310	ASP
1	A	2318	ILE
1	A	2327	ASN
1	A	2408	MET
1	A	2499	LYS
1	A	2504	ASP
1	A	2506	MET
1	A	2554	ASP
1	A	2580	TRP
1	A	2599	GLN
1	A	2604	SER
1	A	2606	SER
1	A	2609	GLU
1	A	2618	VAL
1	A	2640	ASP
1	A	2776	SER
1	A	2868	CYS
1	A	2870	GLU
1	A	2896	ARG
1	A	3082	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	3129	VAL
1	A	3133	LEU
1	A	3152	GLU
1	A	3155	ASP
1	A	3240	ARG
1	A	3245	GLU
1	A	3312	HIS
1	A	3319	THR
1	A	3421	SER
1	A	3447	ARG
1	A	3451	MET
1	A	3454	ASP
1	A	3553	SER
1	A	3665	TRP
1	A	3737	LYS
1	A	3780	THR
1	A	3835	TYR
1	A	3854	CYS
1	A	3898	SER
1	A	3899	ASP
1	A	3956	ASP
1	A	3991	ARG
1	A	3992	PHE
1	A	4005	LYS
1	A	4009	CYS
1	A	4014	HIS
1	A	4028	GLU
1	A	4034	TYR
1	A	4035	CYS
1	A	4072	LEU
1	A	4077	CYS
1	A	4126	LYS
1	A	4193	ASP
1	A	4219	ASN
1	A	4300	ARG
1	A	4309	ASP
1	A	4348	CYS
1	A	4371	PHE
1	A	4398	GLU
1	A	4406	GLU
1	A	4407	CYS
1	A	4505	CYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	4555	THR
1	A	4570	CYS
1	A	4572	ARG
1	A	4657	SER
1	A	4659	ARG
1	A	4660	ARG
1	A	4686	SER
1	A	4704	SER
1	A	4733	SER
1	A	4745	LYS
1	A	4774	LYS
1	A	4784	LEU
1	A	4807	SER
1	A	4846	ASN
1	A	4851	LEU
1	A	4859	ASP
1	A	4887	LEU
1	A	4905	ASN
1	A	4922	SER
1	A	4972	SER
1	A	4973	LEU
1	A	4979	LEU
1	A	4983	HIS
1	A	5002	SER
1	A	5036	SER
1	A	5103	SER
1	A	5181	PHE
1	A	5190	CYS
2	B	39	GLU
2	B	42	LEU
2	B	48	TRP
2	B	59	ASN
2	B	66	LYS
2	B	184	ASP
2	B	228	GLU
2	B	255	GLN
2	B	263	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	597	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	921	ASN
1	A	1574	HIS
1	A	1698	HIS
1	A	1804	HIS
1	A	2569	HIS
1	A	3285	GLN
1	A	4081	ASN
1	A	4458	GLN
1	A	4663	ASN
1	A	4983	HIS
2	B	160	ASN
2	B	220	ASN
2	B	256	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 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	$\# Z  > 2$
3	ATP	A	5301	-	26,33,33	0.84	1 (3%)	31,52,52	1.60	6 (19%)

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
3	ATP	A	5301	-	-	6/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5301	ATP	C5-C4	2.06	1.46	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5301	ATP	PB-O3B-PG	-3.71	120.11	132.83
3	A	5301	ATP	PA-O3A-PB	-3.37	121.25	132.83
3	A	5301	ATP	N3-C2-N1	-3.09	123.86	128.68
3	A	5301	ATP	C3'-C2'-C1'	2.86	105.29	100.98
3	A	5301	ATP	C4-C5-N7	-2.36	106.94	109.40
3	A	5301	ATP	C1'-N9-C4	-2.08	122.99	126.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5301	ATP	C5'-O5'-PA-O2A
3	A	5301	ATP	PG-O3B-PB-O2B
3	A	5301	ATP	PG-O3B-PB-O1B
3	A	5301	ATP	C5'-O5'-PA-O3A
3	A	5301	ATP	O4'-C4'-C5'-O5'
3	A	5301	ATP	C5'-O5'-PA-O1A

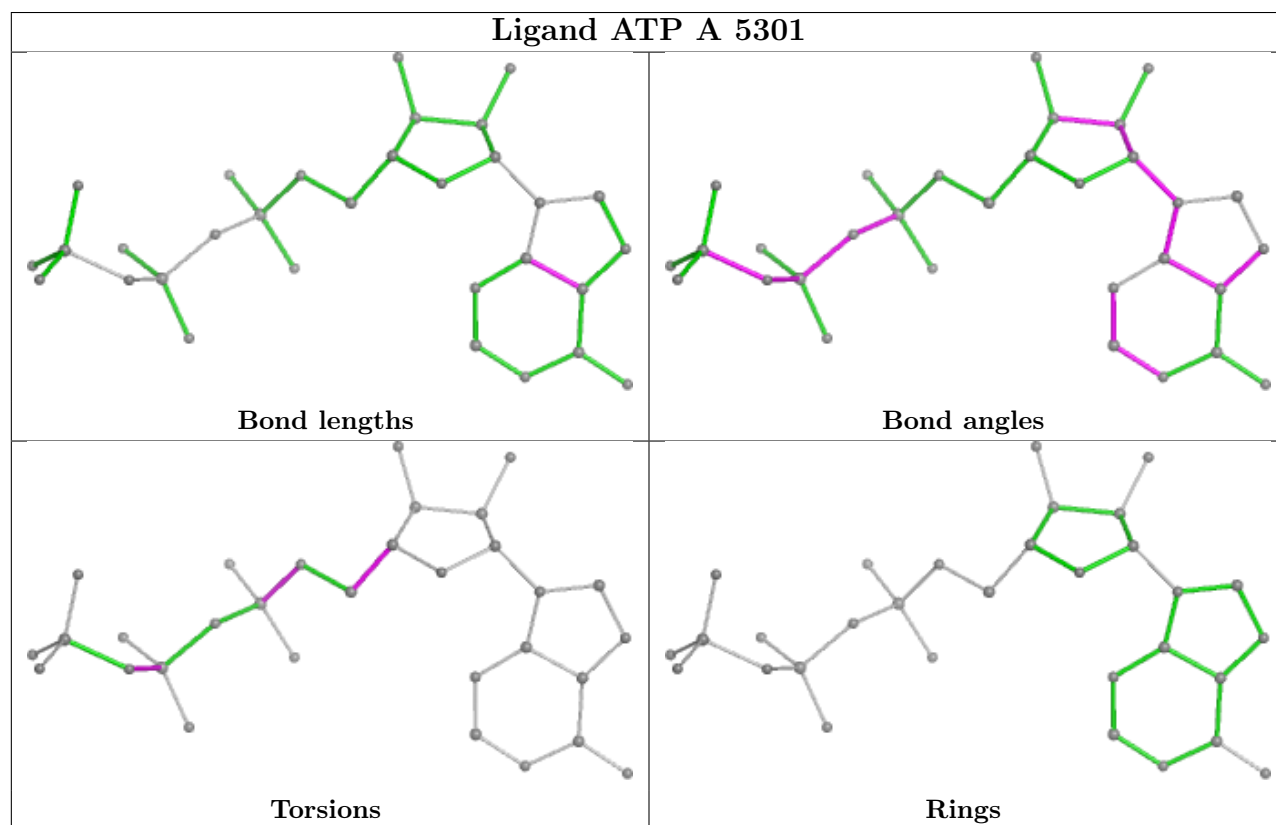
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5301	ATP	1	0

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.

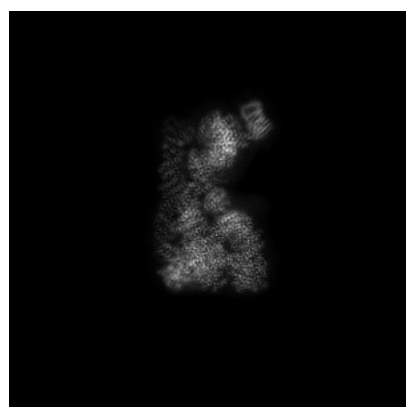
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50913. These allow visual inspection of the internal detail of the map and identification of artifacts.

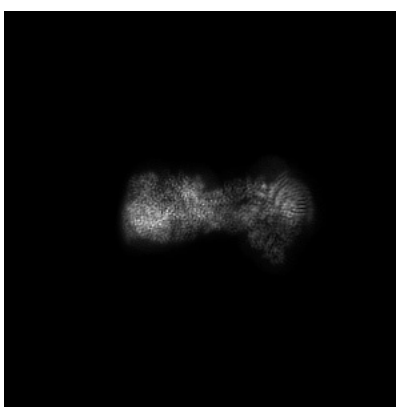
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

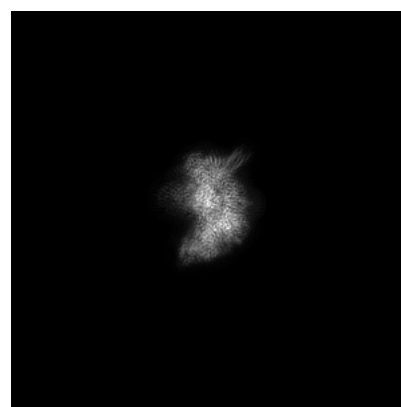
#### 6.1.1 Primary map



X



Y

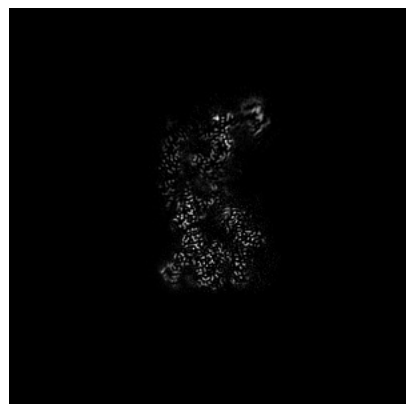


Z

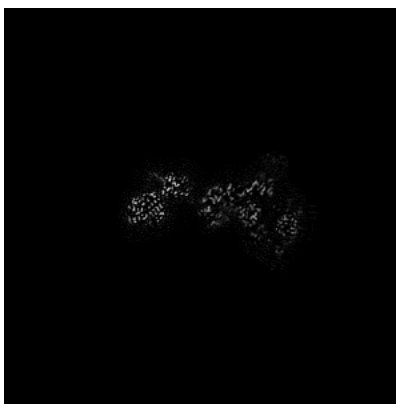
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

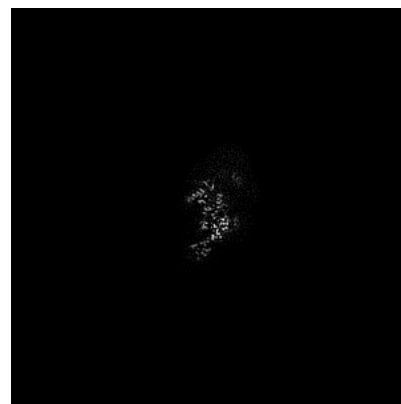
#### 6.2.1 Primary map



X Index: 192



Y Index: 192

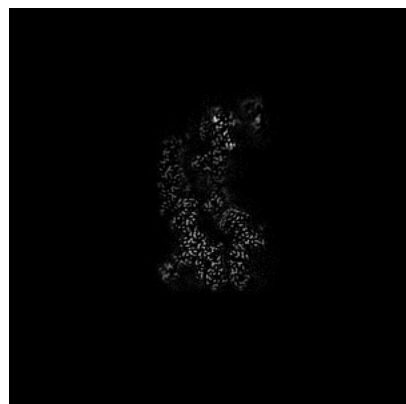


Z Index: 192

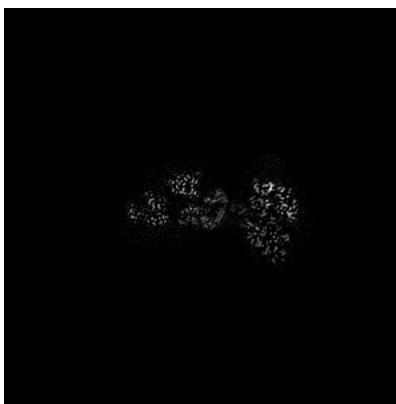
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

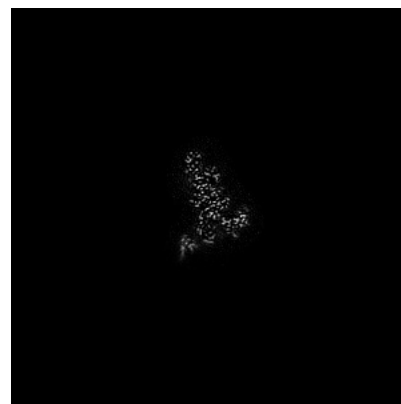
### 6.3.1 Primary map



X Index: 189



Y Index: 205

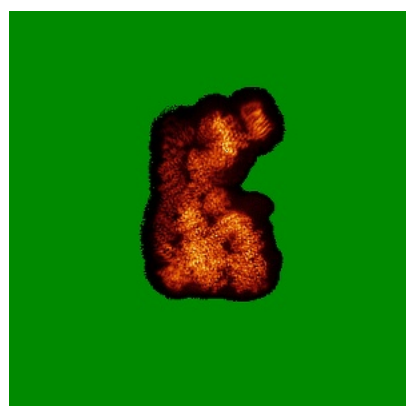


Z Index: 144

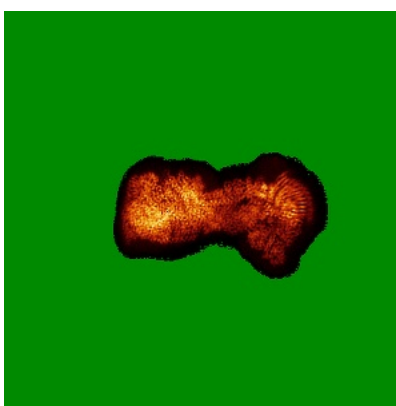
The images above show the largest variance slices of the map in three orthogonal directions.

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

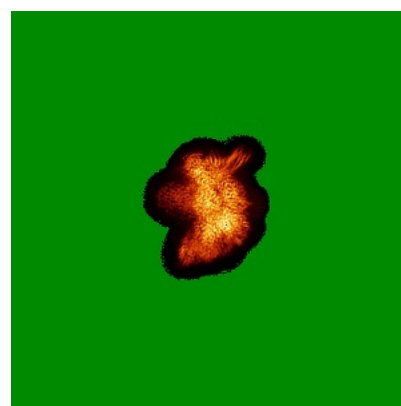
### 6.4.1 Primary map



X



Y



Z

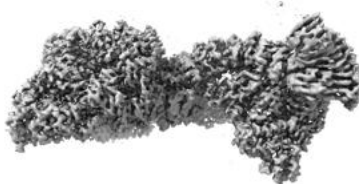
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

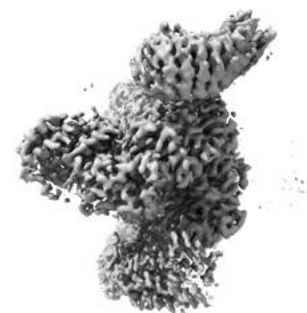
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

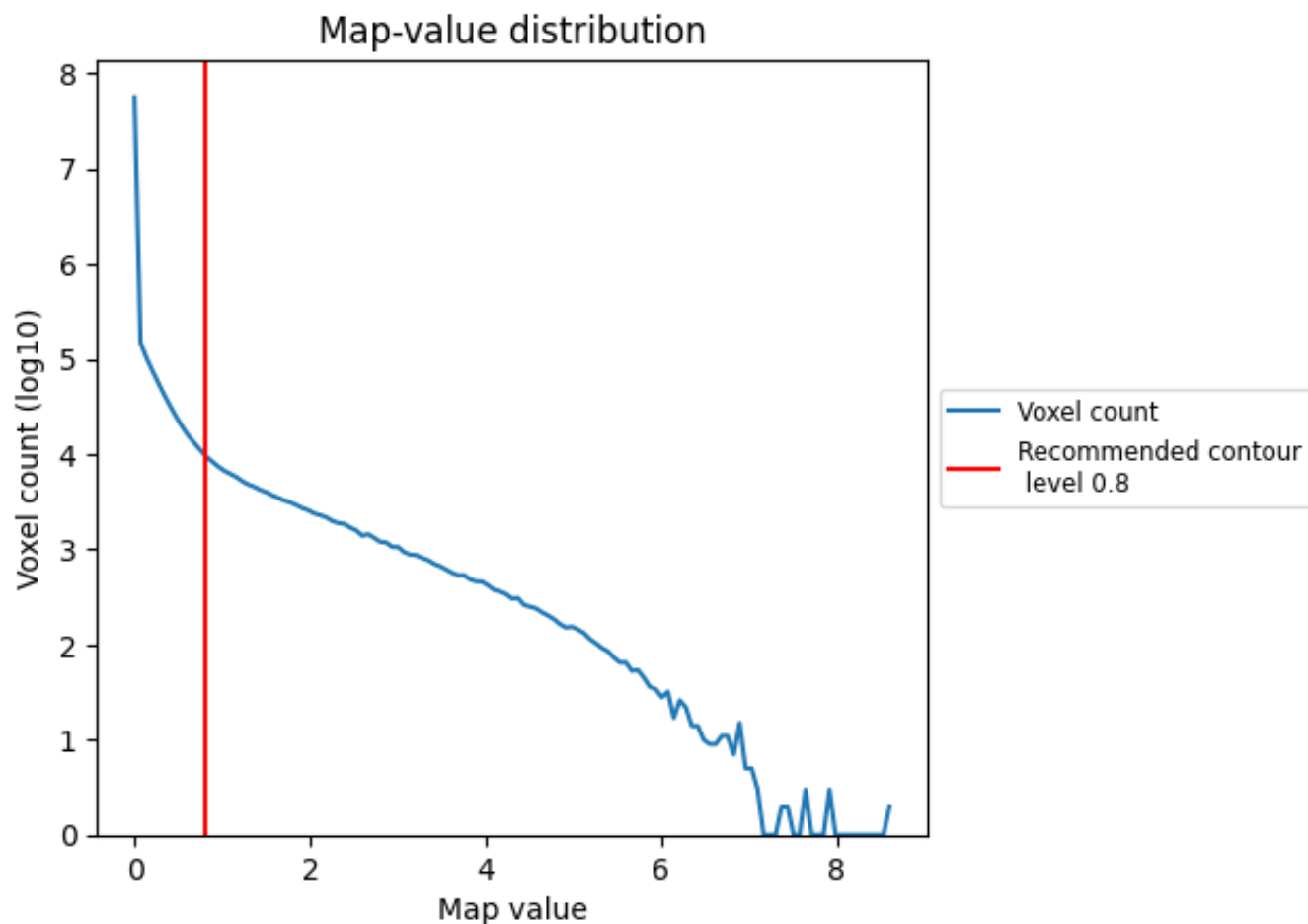
## 6.6 Mask visualisation [i](#)

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.

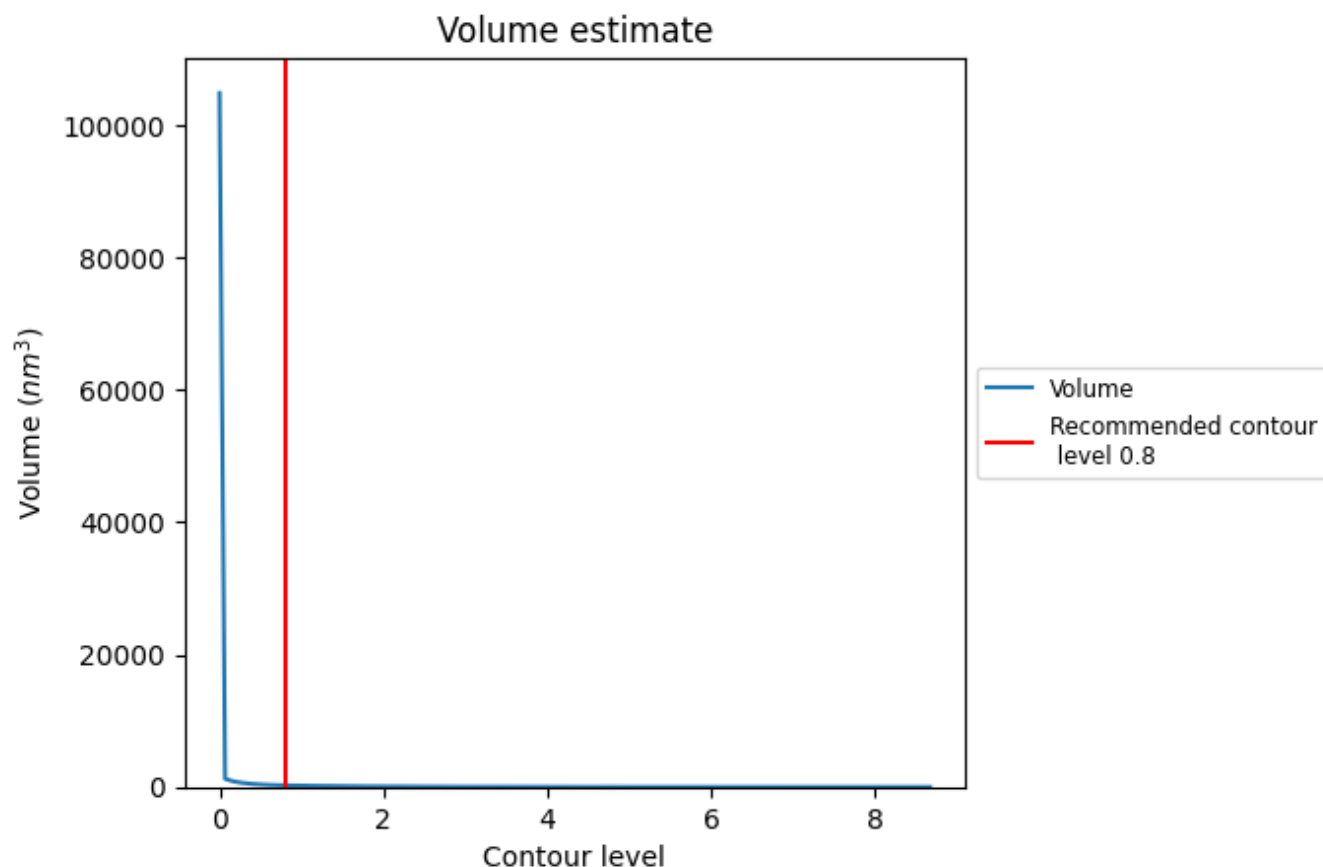
### 7.1 Map-value distribution [i](#)



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.



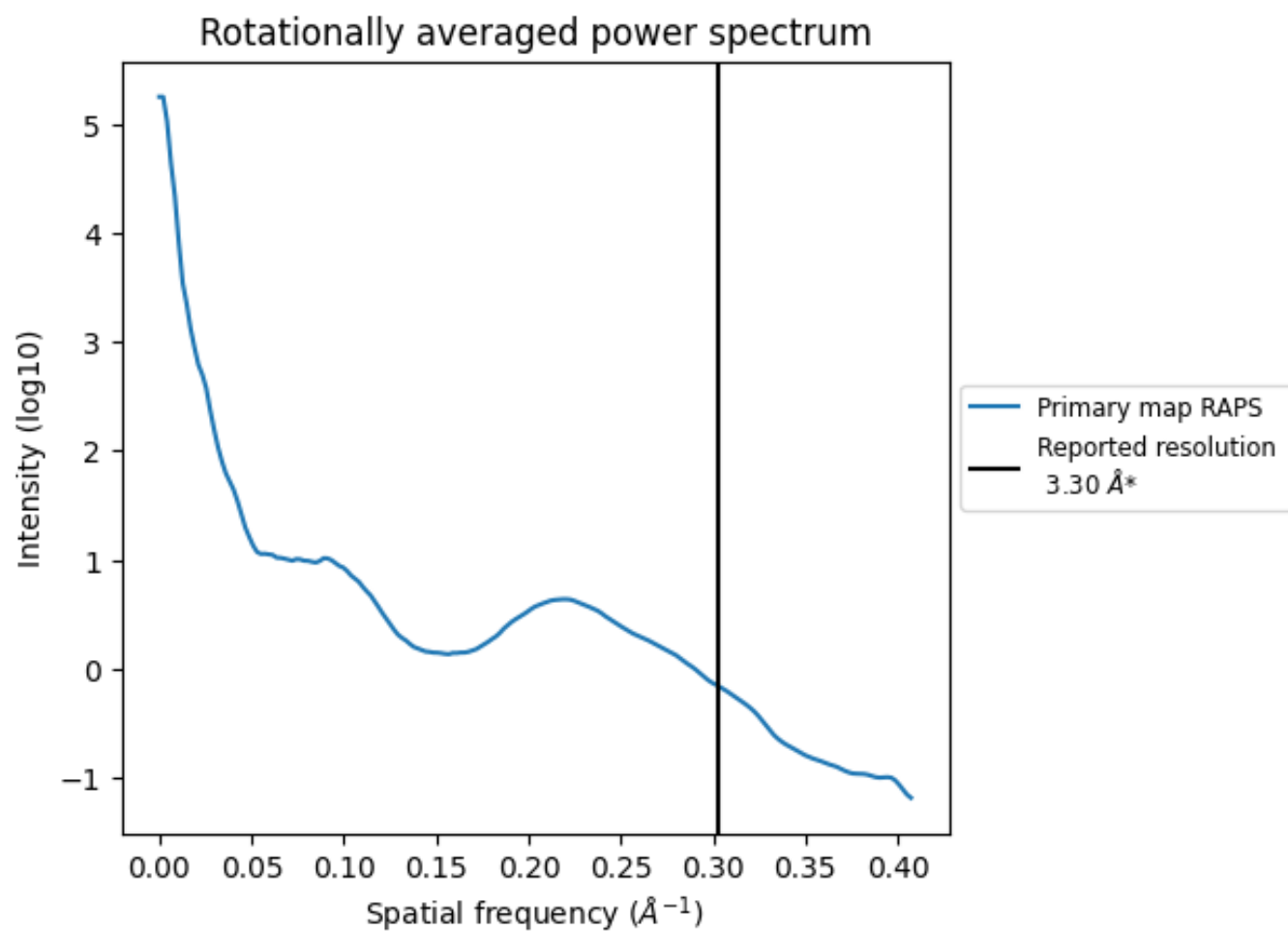
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 241  $\text{nm}^3$ ; this corresponds to an approximate mass of 218 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 0.303 Å<sup>-1</sup>

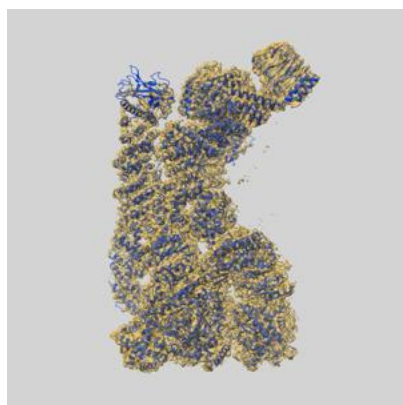
## 8 Fourier-Shell correlation ⓘ

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

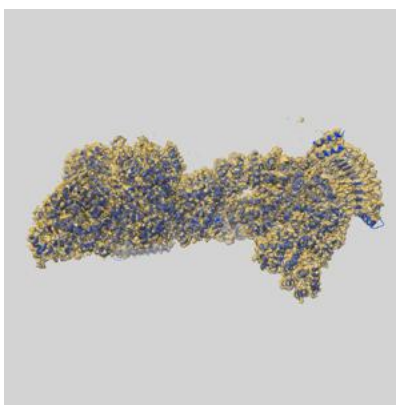
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50913 and PDB model 9G08. Per-residue inclusion information can be found in section [3](#) on page [6](#).

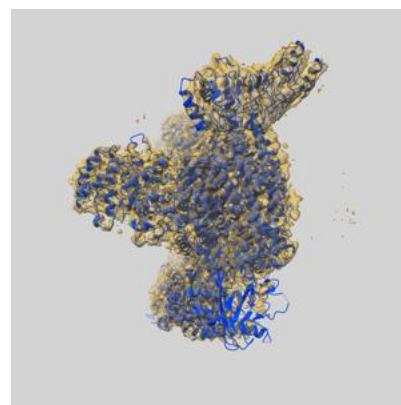
### 9.1 Map-model overlay [i](#)



X



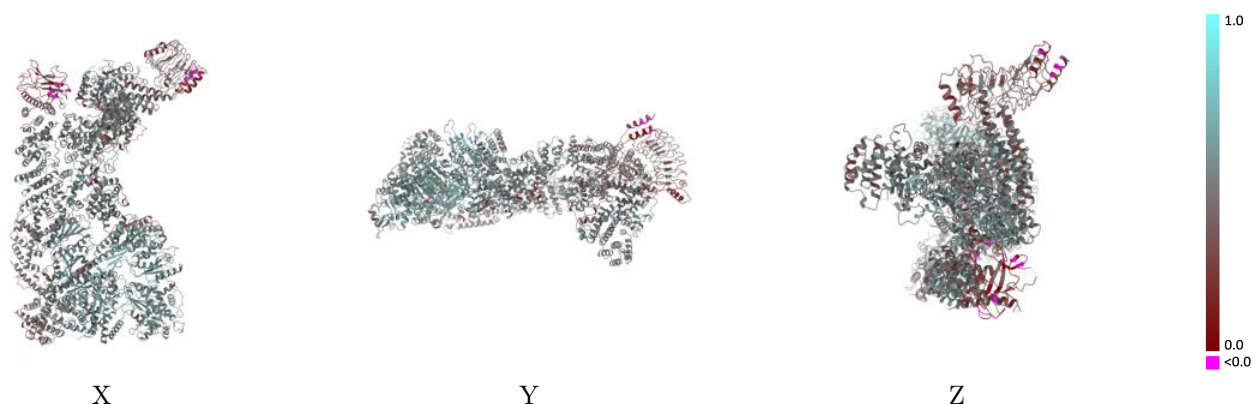
Y



Z

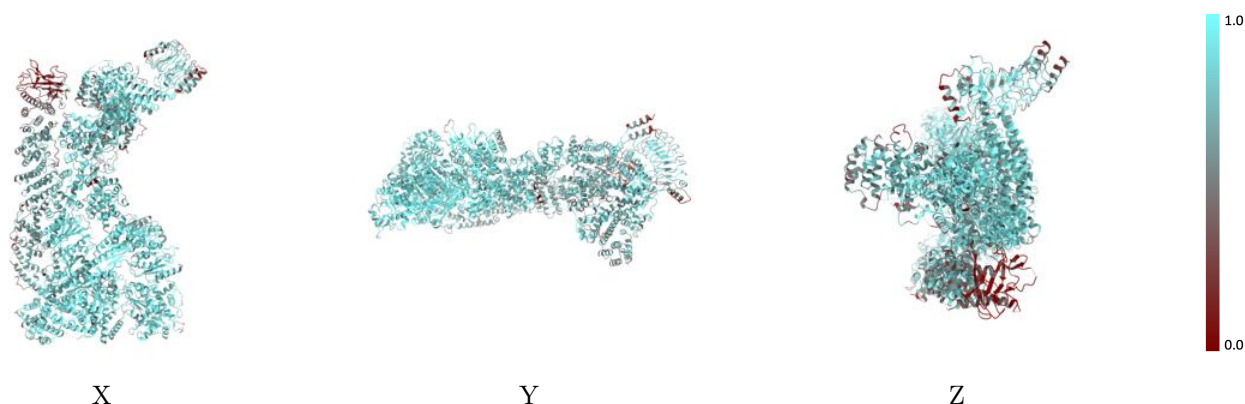
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



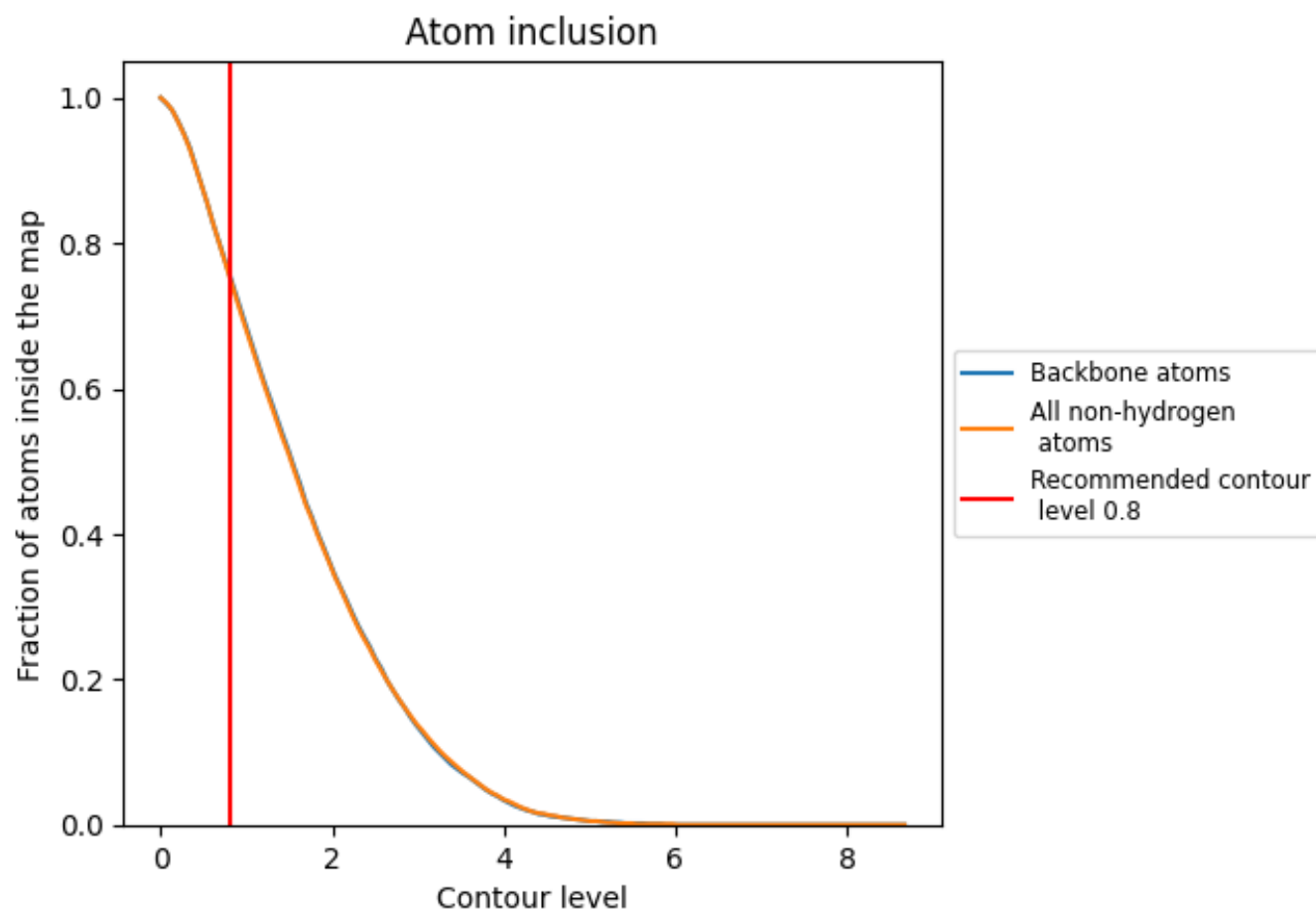
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 76% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7550	<div></div> 0.4850
A	<div></div> 0.7710	<div></div> 0.4940
B	<div></div> 0.6110	<div></div> 0.3240

