



Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 12:52 pm GMT

PDB ID : 6SL1
EMDB ID : EMD-10234
Title : Structure of the open conformation of CtTel1
Authors : Jansma, M.; Eustermann, S.E.; Kostrewa, D.; Lammens, K.; Hopfner, K.P.
Deposited on : 2019-08-16
Resolution : 3.60 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

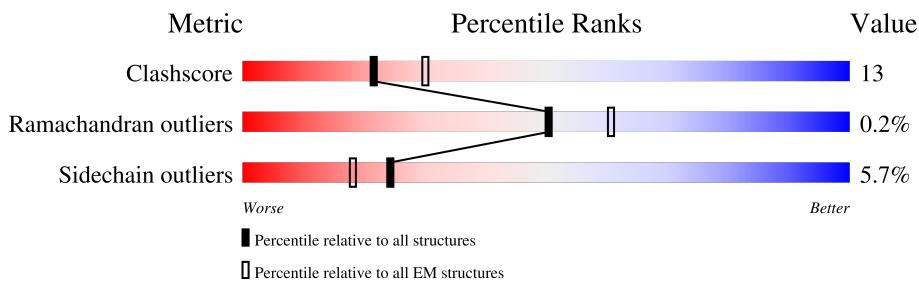
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	2944	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 21041 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 Serine/threonine-protein kinase Tell1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2652	21009	13361	3665	3888	95	0	0

There are 21 discrepancies between the modelled and reference sequences:

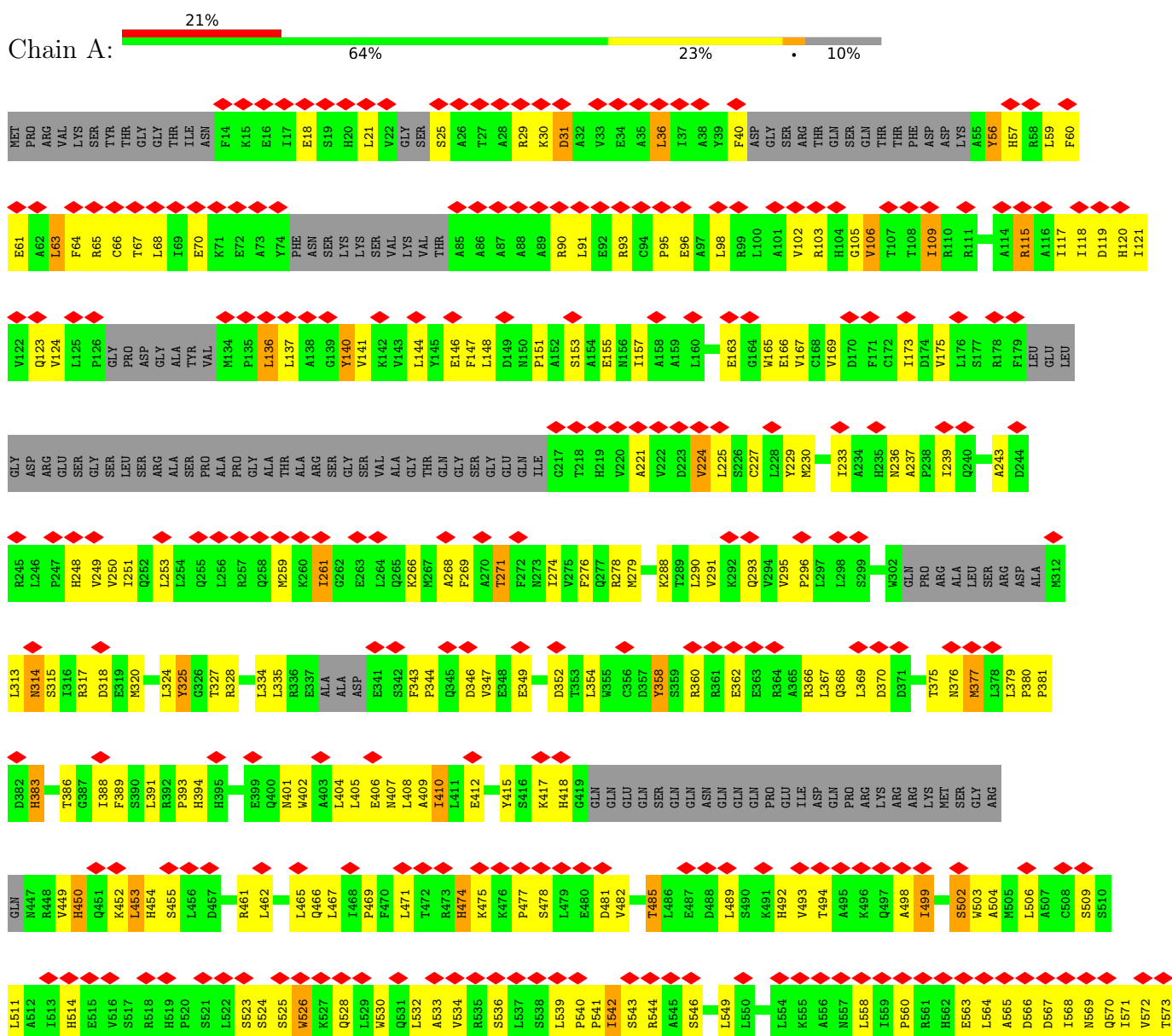
Chain	Residue	Modelled	Actual	Comment	Reference
A	1489	SER	GLU	conflict	UNP G0S4S9
A	2847	LEU	PHE	conflict	UNP G0S4S9
A	2848	TYR	-	insertion	UNP G0S4S9
A	2849	GLN	-	insertion	UNP G0S4S9
A	2850	TRP	-	insertion	UNP G0S4S9
A	2851	SER	-	insertion	UNP G0S4S9
A	2852	ILE	-	insertion	UNP G0S4S9
A	2853	SER	-	insertion	UNP G0S4S9
A	2854	PRO	-	insertion	UNP G0S4S9
A	2855	VAL	-	insertion	UNP G0S4S9
A	2856	ARG	-	insertion	UNP G0S4S9
A	2857	MET	-	insertion	UNP G0S4S9
A	2858	ALA	-	insertion	UNP G0S4S9
A	2859	LYS	-	insertion	UNP G0S4S9
A	2860	LEU	-	insertion	UNP G0S4S9
A	2861	GLN	-	insertion	UNP G0S4S9
A	2862	ASN	-	insertion	UNP G0S4S9
A	2863	ALA	-	insertion	UNP G0S4S9
A	2864	ARG	-	insertion	UNP G0S4S9
A	2865	GLU	-	insertion	UNP G0S4S9
A	2866	VAL	-	insertion	UNP G0S4S9

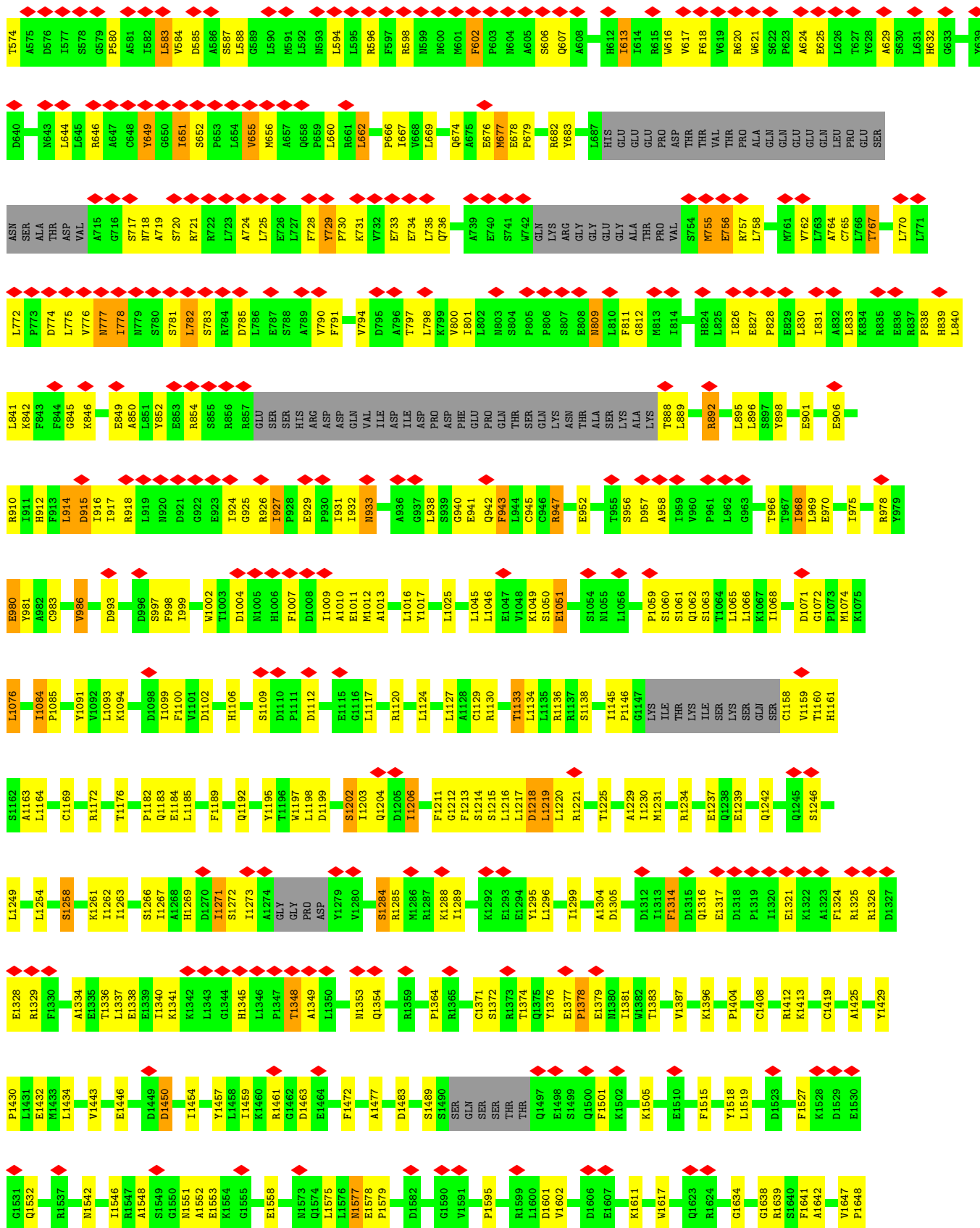
- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Serine/threonine-protein kinase Tel1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	111910	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.068	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0118	Depositor
Map size (Å)	372.768, 372.768, 372.768	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	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: AGS, MG

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	0.50	1/21421 (0.0%)	0.51	5/29018 (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	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2067	VAL	CB-CG2	-5.15	1.42	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1378	PRO	CA-N-CD	-8.88	99.07	111.50
1	A	2608	LEU	CB-CG-CD1	-5.49	101.66	111.00
1	A	1652	LEU	CA-CB-CG	5.39	127.71	115.30
1	A	2486	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	1758	GLU	C-N-CA	-5.20	108.71	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2481	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	259	MET	Peptide
1	A	474	HIS	Peptide
1	A	677	MET	Peptide

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	21009	0	21193	544	0
2	A	31	0	12	3	0
3	A	1	0	0	0	0
All	All	21041	0	21205	547	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 13.

All (547) 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:1378:PRO:HD2	1:A:1379:GLU:H	1.20	1.06
1:A:1730:TRP:HZ3	1:A:1736:PRO:HD2	1.30	0.97
1:A:1730:TRP:CZ3	1:A:1736:PRO:HD2	2.00	0.96
1:A:2647:ARG:NH2	1:A:2774:GLU:OE2	2.06	0.88
1:A:2608:LEU:HD11	1:A:2663:PHE:HD1	1.40	0.86
1:A:1698:ARG:HD2	1:A:1730:TRP:HE1	1.41	0.85
1:A:845:GLY:HA3	1:A:918:ARG:HH12	1.40	0.85
1:A:841:LEU:HD22	1:A:918:ARG:HB2	1.60	0.84
1:A:2092:GLU:HG2	1:A:2115:ARG:HH22	1.41	0.83
1:A:1378:PRO:HD2	1:A:1379:GLU:N	1.93	0.83
1:A:1651:LEU:HD13	1:A:2080:LEU:HD11	1.60	0.82
1:A:225:LEU:HD21	1:A:268:ALA:HB2	1.62	0.81
1:A:1648:PRO:HD2	1:A:2084:LEU:HD21	1.63	0.80
1:A:718:ASN:HD21	1:A:778:ILE:HG12	1.47	0.80
1:A:2498:SER:HB3	1:A:2507:TRP:CD1	2.18	0.79
1:A:776:VAL:HA	1:A:783:SER:HB2	1.63	0.79
1:A:966:THR:O	1:A:970:GLU:N	2.14	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:GLY:HA2	1:A:915:ASP:HB2	1.65	0.79
1:A:1383:THR:HG21	1:A:1732:PRO:HG3	1.67	0.76
1:A:2486:ARG:HH22	1:A:2847:LEU:HD11	1.49	0.76
1:A:2636:HIS:NE2	1:A:2831:GLU:OE2	2.18	0.76
1:A:1698:ARG:HD2	1:A:1730:TRP:NE1	2.01	0.75
1:A:324:LEU:HD23	1:A:407:ASN:HB3	1.68	0.74
1:A:2159:LEU:HG	1:A:2163:ARG:NH2	2.03	0.74
1:A:1062:GLN:NE2	1:A:1091:TYR:OH	2.21	0.74
1:A:328:ARG:NH2	1:A:678:GLU:OE1	2.22	0.72
1:A:144:LEU:HA	1:A:147:PHE:HB3	1.70	0.72
1:A:569:ASN:O	1:A:573:THR:OG1	2.06	0.72
1:A:1698:ARG:CD	1:A:1730:TRP:HE1	2.03	0.72
1:A:544:ARG:HG3	1:A:584:VAL:HG11	1.72	0.71
1:A:2608:LEU:HD11	1:A:2663:PHE:CD1	2.24	0.71
1:A:2608:LEU:CD1	1:A:2663:PHE:HD1	2.04	0.71
1:A:755:MET:SD	1:A:755:MET:N	2.63	0.71
1:A:1218:ASP:OD1	1:A:1218:ASP:N	2.21	0.70
1:A:2012:ASP:OD1	1:A:2034:SER:OG	2.10	0.70
1:A:1450:ASP:OD1	1:A:1450:ASP:N	2.25	0.70
1:A:941:GLU:OE1	1:A:941:GLU:N	2.23	0.70
1:A:2586:ALA:HB3	1:A:2592:PRO:HG2	1.71	0.70
1:A:175:VAL:HG11	1:A:224:VAL:HG21	1.74	0.70
1:A:1324:PHE:HB2	1:A:1334:ALA:HB2	1.75	0.69
1:A:1777:ILE:HD11	1:A:1808:TYR:HB2	1.74	0.69
1:A:25:SER:O	1:A:29:ARG:NH2	2.23	0.69
2:A:3001:AGS:H5'1	2:A:3001:AGS:H8	1.73	0.69
1:A:565:ALA:O	1:A:569:ASN:N	2.26	0.69
1:A:2474:THR:HG22	1:A:2655:THR:HA	1.74	0.69
1:A:1378:PRO:CD	1:A:1379:GLU:H	2.02	0.69
1:A:1730:TRP:HZ3	1:A:1736:PRO:CD	2.05	0.68
1:A:1660:TYR:CZ	1:A:1799:PRO:HG2	2.28	0.68
1:A:102:VAL:O	1:A:106:VAL:N	2.26	0.68
1:A:103:ARG:NH2	1:A:146:GLU:OE2	2.26	0.68
1:A:2443:THR:HG22	1:A:2444:LEU:H	1.59	0.68
1:A:947:ARG:NH2	1:A:993:ASP:OD2	2.25	0.68
1:A:2204:ALA:HB3	1:A:2239:GLN:HE22	1.59	0.68
1:A:31:ASP:N	1:A:31:ASP:OD1	2.26	0.67
1:A:764:ALA:O	1:A:767:THR:OG1	2.10	0.67
1:A:2092:GLU:OE2	1:A:2115:ARG:NH2	2.27	0.67
1:A:583:LEU:HB2	1:A:620:ARG:HB3	1.77	0.66
1:A:1642:ALA:O	1:A:2118:TRP:NE1	2.29	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:LEU:HD12	1:A:408:LEU:HD13	1.77	0.66
1:A:155:GLU:OE1	1:A:892:ARG:NH1	2.30	0.65
1:A:1959:ARG:NH2	1:A:1977:ASP:OD1	2.30	0.65
1:A:2471:GLY:O	1:A:2487:GLN:NE2	2.28	0.65
1:A:2792:VAL:HG23	1:A:2861:GLN:HE22	1.61	0.65
1:A:572:VAL:HG11	1:A:598:ARG:HG3	1.78	0.65
1:A:1295:TYR:HD1	1:A:1296:LEU:HD12	1.61	0.65
1:A:1647:VAL:HG12	1:A:2084:LEU:HD22	1.78	0.65
1:A:826:ILE:HG12	1:A:828:PRO:HD2	1.78	0.64
1:A:2647:ARG:HH21	1:A:2774:GLU:CD	2.00	0.64
1:A:450:HIS:HA	1:A:453:LEU:HB2	1.79	0.64
1:A:1215:SER:OG	1:A:1218:ASP:OD1	2.14	0.64
1:A:1182:PRO:HB2	1:A:1211:PHE:HA	1.80	0.64
1:A:1225:THR:HG23	1:A:1258:SER:HB3	1.79	0.64
1:A:1321:GLU:HB3	1:A:1337:LEU:HD23	1.79	0.63
1:A:1642:ALA:HB2	1:A:2088:ALA:HB1	1.79	0.63
1:A:452:LYS:HA	1:A:455:SER:HB2	1.79	0.63
1:A:1919:GLU:O	1:A:1923:ASN:ND2	2.28	0.63
1:A:669:LEU:HD22	1:A:895:LEU:HD13	1.79	0.63
1:A:1183:GLN:NE2	1:A:1212:GLY:O	2.32	0.63
1:A:2498:SER:HB3	1:A:2507:TRP:HD1	1.64	0.63
1:A:358:TYR:HE2	1:A:366:ARG:HB3	1.64	0.63
1:A:809:ASN:O	1:A:809:ASN:ND2	2.29	0.63
1:A:405:LEU:HD22	1:A:467:LEU:HD13	1.79	0.62
1:A:543:SER:O	1:A:546:SER:OG	2.15	0.62
1:A:2613:ASN:OD1	1:A:2613:ASN:N	2.30	0.62
1:A:560:PRO:HG2	1:A:563:GLU:HB2	1.82	0.62
1:A:21:LEU:HA	1:A:29:ARG:HG3	1.82	0.62
1:A:343:PHE:HB3	1:A:344:PRO:HD3	1.80	0.62
1:A:1197:TRP:NE1	1:A:1202:SER:O	2.33	0.62
1:A:2461:PRO:O	1:A:2465:MET:HG2	2.00	0.62
1:A:2486:ARG:NH2	1:A:2847:LEU:HD11	2.14	0.62
1:A:1936:ASP:OD1	1:A:1936:ASP:N	2.30	0.62
1:A:1158:CYS:SG	1:A:1159:VAL:N	2.73	0.61
1:A:568:ILE:HG12	1:A:594:LEU:HD22	1.83	0.61
1:A:717:SER:OG	1:A:721:ARG:NH1	2.33	0.61
1:A:1378:PRO:CD	1:A:1379:GLU:N	2.61	0.61
1:A:1317:GLU:OE1	1:A:1317:GLU:N	2.34	0.61
1:A:1532:GLN:HE21	1:A:1575:LEU:CD1	2.14	0.61
1:A:119:ASP:O	1:A:123:GLN:NE2	2.34	0.61
1:A:533:ALA:HA	1:A:536:SER:HB2	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:ASN:N	1:A:777:ASN:OD1	2.33	0.60
1:A:1601:ASP:OD1	1:A:1602:VAL:N	2.34	0.60
1:A:261:ILE:HD13	1:A:313:LEU:HD11	1.82	0.60
1:A:940:GLY:O	1:A:943:PHE:N	2.32	0.60
1:A:1443:VAL:HG11	1:A:1483:ASP:HB3	1.82	0.60
1:A:1860:ILE:HD13	1:A:2727:GLU:HB3	1.83	0.60
1:A:534:VAL:HG13	1:A:571:ILE:HD11	1.83	0.60
1:A:901:GLU:N	1:A:901:GLU:OE1	2.35	0.60
1:A:477:PRO:HB3	1:A:481:ASP:HB2	1.84	0.60
1:A:314:ASN:N	1:A:314:ASN:OD1	2.33	0.60
1:A:889:LEU:HG	1:A:941:GLU:HG3	1.84	0.60
1:A:2108:THR:HG22	1:A:2112:PHE:CE2	2.37	0.60
1:A:2440:ASP:OD1	1:A:2485:SER:HA	2.01	0.60
1:A:2524:ARG:HH11	1:A:2590:SER:HB2	1.67	0.59
1:A:927:ILE:HB	1:A:932:ILE:HD11	1.84	0.59
1:A:1713:LEU:O	1:A:1717:GLN:HG2	2.03	0.59
1:A:2203:ASP:OD1	1:A:2204:ALA:N	2.36	0.59
1:A:646:ARG:NH1	1:A:652:SER:O	2.35	0.59
1:A:1653:ARG:NH1	1:A:1658:GLN:OE1	2.34	0.59
1:A:498:ALA:HA	1:A:542:ILE:HG12	1.84	0.59
1:A:1329:ARG:NE	1:A:1379:GLU:OE2	2.32	0.59
1:A:1463:ASP:OD1	1:A:1518:TYR:OH	2.21	0.59
1:A:1049:LYS:O	1:A:1050:SER:OG	2.19	0.59
1:A:120:HIS:NE2	1:A:140:TYR:OH	2.36	0.58
1:A:524:SER:O	1:A:528:GLN:N	2.33	0.58
1:A:797:THR:HA	1:A:800:VAL:HG12	1.85	0.58
1:A:888:THR:OG1	1:A:889:LEU:N	2.36	0.57
1:A:124:VAL:HG11	1:A:140:TYR:HE1	1.68	0.57
1:A:540:PRO:HG2	1:A:541:PRO:HD3	1.86	0.57
1:A:1617:TRP:CZ2	1:A:1651:LEU:HD21	2.39	0.57
1:A:2443:THR:HG22	1:A:2444:LEU:N	2.18	0.57
1:A:539:LEU:O	1:A:543:SER:OG	2.15	0.57
1:A:1758:GLU:HG2	1:A:1835:ALA:HB2	1.87	0.57
1:A:2769:ASP:OD2	1:A:2772:THR:OG1	2.22	0.57
1:A:229:TYR:O	1:A:233:ILE:HG22	2.04	0.57
1:A:288:LYS:HG2	1:A:334:LEU:HD21	1.87	0.56
1:A:1109:SER:HB3	1:A:1120:ARG:HH21	1.70	0.56
1:A:1007:PHE:H	1:A:1010:ALA:HB3	1.69	0.56
1:A:1195:TYR:O	1:A:1199:ASP:HB2	2.05	0.56
1:A:1326:ARG:O	1:A:1328:GLU:N	2.36	0.56
1:A:2474:THR:CG2	1:A:2655:THR:HA	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:PHE:O	1:A:64:PHE:N	2.34	0.56
1:A:362:GLU:HA	1:A:366:ARG:HD3	1.88	0.56
1:A:772:LEU:HB3	1:A:839:HIS:HD2	1.70	0.56
1:A:157:ILE:O	1:A:165:TRP:N	2.39	0.56
1:A:926:ARG:HA	1:A:958:ALA:HB1	1.88	0.56
1:A:1192:GLN:HB2	1:A:1354:GLN:HG3	1.86	0.56
1:A:1197:TRP:HD1	1:A:1198:LEU:HD23	1.70	0.56
1:A:148:LEU:HD12	1:A:227:CYS:HB2	1.86	0.56
1:A:1124:LEU:O	1:A:1138:SER:OG	2.20	0.56
1:A:2470:THR:O	1:A:2474:THR:OG1	2.16	0.56
2:A:3001:AGS:O3A	2:A:3001:AGS:O2G	2.24	0.56
1:A:1025:LEU:HD11	1:A:1068:ILE:HG12	1.88	0.56
1:A:729:TYR:HD2	1:A:782:LEU:HG	1.71	0.55
1:A:1337:LEU:HB2	1:A:1419:CYS:SG	2.46	0.55
1:A:1237:GLU:OE2	1:A:1285:ARG:NH1	2.39	0.55
1:A:2631:GLU:OE2	1:A:2634:LYS:NZ	2.36	0.55
1:A:2439:GLN:CB	1:A:2485:SER:HB3	2.36	0.55
1:A:1068:ILE:HG22	1:A:1076:LEU:HD21	1.88	0.55
1:A:151:PRO:HB2	1:A:892:ARG:CZ	2.37	0.55
1:A:720:SER:O	1:A:724:ALA:N	2.40	0.55
1:A:1049:LYS:NZ	1:A:1051:GLU:OE1	2.39	0.55
1:A:1558:GLU:OE1	1:A:1558:GLU:N	2.23	0.55
1:A:838:PRO:O	1:A:842:LYS:N	2.31	0.55
1:A:566:ASP:HA	1:A:569:ASN:HB2	1.88	0.55
1:A:770:LEU:HD21	1:A:840:LEU:HD22	1.88	0.55
1:A:2486:ARG:HH22	1:A:2847:LEU:CD1	2.18	0.55
1:A:2843:ARG:NH2	1:A:2900:ASP:OD1	2.40	0.55
1:A:344:PRO:O	1:A:415:TYR:OH	2.25	0.54
1:A:449:VAL:O	1:A:452:LYS:N	2.33	0.54
1:A:57:HIS:NE2	1:A:61:GLU:OE2	2.40	0.54
1:A:999:ILE:HD11	1:A:1045:LEU:HD13	1.89	0.54
1:A:2162:ILE:HD11	1:A:2195:CYS:SG	2.48	0.54
1:A:1304:ALA:HB3	1:A:1736:PRO:HG3	1.89	0.54
1:A:2725:PHE:O	1:A:2735:TRP:HD1	1.90	0.54
1:A:849:GLU:HA	1:A:852:TYR:HD2	1.72	0.54
1:A:1046:LEU:HD23	1:A:1050:SER:HA	1.89	0.54
1:A:386:THR:HG23	1:A:402:TRP:CH2	2.43	0.54
1:A:827:GLU:O	1:A:830:LEU:N	2.40	0.54
1:A:1136:ARG:HH12	1:A:1192:GLN:HG2	1.73	0.54
1:A:666:PRO:HA	1:A:669:LEU:HB2	1.89	0.54
1:A:1638:GLY:CA	1:A:2087:LEU:HB3	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2616:LEU:HD22	1:A:2659:GLY:HA3	1.88	0.54
1:A:772:LEU:HD11	1:A:790:VAL:HG21	1.89	0.54
1:A:1577:ASN:HD22	1:A:1579:PRO:HD2	1.73	0.54
1:A:393:PRO:HB2	1:A:394:HIS:CD2	2.43	0.54
1:A:929:GLU:HG3	1:A:933:ASN:HD21	1.73	0.54
1:A:60:PHE:HE1	1:A:98:LEU:HD23	1.73	0.53
1:A:526:TRP:HD1	1:A:558:LEU:HD13	1.71	0.53
1:A:2606:LYS:HB2	1:A:2663:PHE:HB3	1.90	0.53
1:A:947:ARG:HH21	1:A:947:ARG:HB2	1.74	0.53
1:A:1214:SER:OG	1:A:1218:ASP:OD2	2.26	0.53
1:A:1951:ASP:OD1	1:A:1952:GLY:N	2.37	0.53
1:A:1698:ARG:HD2	1:A:1730:TRP:CE2	2.43	0.53
1:A:1639:ARG:HB2	1:A:2091:THR:HG21	1.91	0.53
1:A:998:PHE:O	1:A:1002:TRP:NE1	2.42	0.53
1:A:1340:ILE:HG12	1:A:1457:TYR:CG	2.44	0.53
1:A:1404:PRO:HB2	1:A:1446:GLU:HG2	1.91	0.53
1:A:678:GLU:O	1:A:682:ARG:N	2.41	0.53
1:A:782:LEU:HA	1:A:785:ASP:HB2	1.91	0.53
1:A:1229:ALA:HA	1:A:1262:ILE:HG12	1.90	0.53
1:A:1321:GLU:OE1	1:A:1341:LYS:NZ	2.40	0.52
1:A:59:LEU:O	1:A:63:LEU:N	2.41	0.52
1:A:572:VAL:HG21	1:A:598:ARG:HG3	1.92	0.52
1:A:617:VAL:O	1:A:621:TRP:N	2.41	0.52
1:A:649:TYR:HD2	1:A:651:ILE:HG12	1.73	0.52
1:A:482:VAL:O	1:A:485:THR:OG1	2.26	0.52
1:A:2109:LEU:HA	1:A:2112:PHE:HD2	1.75	0.52
1:A:417:LYS:HB2	1:A:475:LYS:HE3	1.91	0.52
1:A:465:LEU:HD11	1:A:504:ALA:HA	1.92	0.52
1:A:583:LEU:HD22	1:A:621:TRP:HA	1.91	0.52
1:A:314:ASN:HA	1:A:317:ARG:HB2	1.92	0.52
1:A:2033:ASP:HB3	1:A:2069:HIS:NE2	2.25	0.52
1:A:2063:LEU:O	1:A:2067:VAL:HG23	2.10	0.52
1:A:105:GLY:O	1:A:109:ILE:N	2.43	0.52
1:A:1341:LYS:HG2	1:A:1345:HIS:CD2	2.45	0.52
1:A:1202:SER:OG	1:A:1204:GLN:N	2.32	0.51
1:A:1638:GLY:HA3	1:A:2087:LEU:HB3	1.91	0.51
1:A:1100:PHE:CD2	1:A:1134:LEU:HD22	2.46	0.51
1:A:368:GLN:HB2	1:A:370:ASP:OD1	2.09	0.51
1:A:1430:PRO:O	1:A:1434:LEU:HG	2.11	0.51
1:A:1763:SER:OG	1:A:1795:GLU:OE2	2.28	0.51
1:A:2670:LEU:HD12	1:A:2768:LEU:HD11	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2486:ARG:HH12	1:A:2847:LEU:HD21	1.76	0.51
1:A:2734:GLU:O	1:A:2738:LYS:HG2	2.11	0.51
1:A:1213:PHE:CD2	1:A:1219:LEU:HB2	2.45	0.51
1:A:236:ASN:ND2	1:A:983:CYS:SG	2.84	0.51
1:A:978:ARG:HH21	1:A:981:TYR:HE2	1.59	0.51
1:A:1353:ASN:OD1	1:A:1354:GLN:N	2.43	0.51
1:A:2510:ILE:O	1:A:2514:SER:OG	2.22	0.51
1:A:98:LEU:HD13	1:A:140:TYR:CE2	2.45	0.51
1:A:1551:ASN:HD22	1:A:1553:GLU:H	1.58	0.51
1:A:2531:SER:HB3	1:A:2587:SER:HA	1.92	0.51
1:A:93:ARG:HA	1:A:96:GLU:HG3	1.93	0.51
1:A:584:VAL:H	1:A:587:SER:HB2	1.76	0.51
1:A:1698:ARG:HD2	1:A:1730:TRP:CZ2	2.46	0.51
1:A:225:LEU:HD22	1:A:253:LEU:HD13	1.93	0.50
1:A:250:VAL:HG13	1:A:268:ALA:HB1	1.92	0.50
1:A:2470:THR:HG23	1:A:2474:THR:HG21	1.92	0.50
1:A:618:PHE:O	1:A:731:LYS:NZ	2.35	0.50
1:A:1892:GLU:CD	1:A:2739:ARG:HH22	2.15	0.50
1:A:266:LYS:NZ	1:A:315:SER:HB3	2.25	0.50
1:A:354:LEU:HD22	1:A:404:LEU:HD11	1.94	0.50
1:A:274:ILE:O	1:A:278:ARG:NH1	2.44	0.50
1:A:229:TYR:CD1	1:A:271:THR:HG22	2.46	0.50
1:A:115:ARG:HA	1:A:118:ILE:HD12	1.94	0.50
1:A:938:LEU:HD22	1:A:942:GLN:HB3	1.94	0.50
1:A:1579:PRO:HG3	1:A:1684:SER:HB2	1.93	0.50
1:A:1684:SER:O	1:A:1684:SER:OG	2.23	0.50
1:A:621:TRP:O	1:A:731:LYS:NZ	2.44	0.50
1:A:1199:ASP:OD2	1:A:1234:ARG:NH1	2.44	0.50
1:A:1295:TYR:CD1	1:A:1296:LEU:HD12	2.45	0.50
1:A:1971:ASP:OD1	1:A:1972:LEU:N	2.45	0.50
1:A:466:GLN:O	1:A:469:PRO:HD2	2.12	0.49
1:A:239:ILE:O	1:A:243:ALA:N	2.44	0.49
1:A:489:LEU:O	1:A:493:VAL:HG23	2.12	0.49
1:A:1184:GLU:OE2	1:A:1184:GLU:N	2.42	0.49
1:A:1429:TYR:OH	1:A:1694:GLU:OE1	2.17	0.49
1:A:2482:VAL:O	1:A:2484:VAL:N	2.46	0.49
1:A:888:THR:HB	1:A:941:GLU:HG2	1.93	0.49
1:A:1099:ILE:O	1:A:1102:ASP:N	2.45	0.49
1:A:1653:ARG:HH22	1:A:1658:GLN:HB2	1.77	0.49
1:A:1136:ARG:HG3	1:A:1189:PHE:CE1	2.47	0.49
1:A:570:GLN:O	1:A:574:THR:N	2.39	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1013:ALA:O	1:A:1017:TYR:N	2.39	0.49
1:A:2484:VAL:HG23	1:A:2485:SER:N	2.28	0.49
1:A:1730:TRP:CD1	1:A:1730:TRP:N	2.79	0.49
1:A:2550:MET:HG2	1:A:2579:PHE:CE2	2.47	0.49
1:A:2745:THR:HG21	1:A:2774:GLU:HB2	1.94	0.49
1:A:536:SER:HA	1:A:539:LEU:HD13	1.93	0.49
1:A:293:GLN:O	1:A:296:PRO:HD2	2.13	0.49
1:A:2204:ALA:HB3	1:A:2239:GLN:NE2	2.24	0.49
1:A:933:ASN:OD1	1:A:933:ASN:N	2.43	0.48
1:A:975:ILE:O	1:A:981:TYR:HB2	2.11	0.48
1:A:358:TYR:CD2	1:A:366:ARG:HD2	2.48	0.48
1:A:2558:PRO:HB2	1:A:2660:LEU:HD23	1.96	0.48
1:A:2792:VAL:HG23	1:A:2861:GLN:NE2	2.27	0.48
1:A:449:VAL:HG13	1:A:450:HIS:H	1.79	0.48
1:A:462:LEU:HD12	1:A:465:LEU:HB3	1.94	0.48
1:A:56:TYR:H	1:A:56:TYR:HD2	1.61	0.48
1:A:95:PRO:HA	1:A:98:LEU:HD12	1.95	0.48
1:A:383:HIS:CE1	1:A:662:LEU:HD11	2.48	0.48
1:A:408:LEU:O	1:A:412:GLU:N	2.40	0.48
1:A:409:ALA:HB2	1:A:467:LEU:HD11	1.95	0.48
1:A:1242:GLN:O	1:A:1246:SER:OG	2.22	0.48
1:A:95:PRO:HA	1:A:98:LEU:HB2	1.95	0.48
1:A:584:VAL:HG22	1:A:585:ASP:H	1.78	0.48
1:A:1611:LYS:HB2	1:A:1611:LYS:HE3	1.67	0.48
1:A:18:GLU:HA	1:A:21:LEU:HG	1.96	0.48
1:A:268:ALA:O	1:A:271:THR:HG23	2.14	0.48
1:A:2221:ILE:O	1:A:2225:ARG:HG2	2.14	0.48
1:A:388:ILE:HG13	1:A:389:PHE:CD1	2.49	0.48
1:A:410:ILE:HG13	1:A:474:HIS:CE1	2.49	0.48
1:A:511:LEU:HA	1:A:514:HIS:CE1	2.49	0.48
1:A:2550:MET:HG2	1:A:2579:PHE:HE2	1.79	0.48
2:A:3001:AGS:O2B	2:A:3001:AGS:O5'	2.29	0.48
1:A:450:HIS:CE1	1:A:454:HIS:HD2	2.32	0.47
1:A:678:GLU:N	1:A:679:PRO:HD2	2.29	0.47
1:A:794:VAL:O	1:A:797:THR:OG1	2.21	0.47
1:A:1225:THR:HG22	1:A:1261:LYS:HG3	1.96	0.47
1:A:1084:ILE:N	1:A:1085:PRO:HD2	2.29	0.47
1:A:369:LEU:HD21	1:A:502:SER:HB3	1.95	0.47
1:A:646:ARG:NH1	1:A:652:SER:OG	2.45	0.47
1:A:655:VAL:HG23	1:A:656:MET:H	1.78	0.47
1:A:358:TYR:HD2	1:A:366:ARG:HD2	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ARG:HH12	1:A:462:LEU:HB3	1.80	0.47
1:A:1202:SER:OG	1:A:1203:ILE:N	2.46	0.47
1:A:2092:GLU:HG2	1:A:2115:ARG:NH2	2.21	0.47
1:A:2536:PRO:HA	1:A:2582:GLU:HA	1.97	0.47
1:A:845:GLY:HA3	1:A:918:ARG:NH1	2.19	0.47
1:A:1552:ALA:HB3	1:A:1595:PRO:HD3	1.96	0.47
1:A:2282:LYS:NZ	1:A:2287:GLU:OE1	2.39	0.47
1:A:2608:LEU:N	1:A:2608:LEU:HD12	2.30	0.47
1:A:325:TYR:OH	1:A:406:GLU:OE1	2.20	0.47
1:A:797:THR:O	1:A:801:ILE:N	2.30	0.47
1:A:2244:SER:OG	1:A:2247:ASP:OD2	2.20	0.47
1:A:173:ILE:HG23	1:A:249:VAL:HG21	1.96	0.47
1:A:465:LEU:HD21	1:A:504:ALA:HB2	1.97	0.47
1:A:917:ILE:HD13	1:A:917:ILE:HA	1.77	0.46
1:A:1348:THR:HG22	1:A:1349:ALA:H	1.78	0.46
1:A:2159:LEU:HG	1:A:2163:ARG:CZ	2.44	0.46
1:A:2319:LYS:HE3	1:A:2360:GLN:HE22	1.79	0.46
1:A:1698:ARG:HG2	1:A:1728:SER:HA	1.98	0.46
1:A:1169:CYS:O	1:A:1172:ARG:N	2.48	0.46
1:A:1197:TRP:NE1	1:A:1206:ILE:HG12	2.30	0.46
1:A:910:ARG:NH1	1:A:952:GLU:OE1	2.48	0.46
1:A:1204:GLN:HA	1:A:1216:LEU:HD21	1.96	0.46
1:A:2126:ASP:N	1:A:2126:ASP:OD1	2.47	0.46
1:A:1231:MET:SD	1:A:1239:GLU:HG3	2.56	0.46
1:A:1261:LYS:HE3	1:A:1261:LYS:HB3	1.77	0.46
1:A:2486:ARG:HH22	1:A:2847:LEU:CG	2.29	0.46
1:A:839:HIS:HA	1:A:842:LYS:HE3	1.97	0.46
1:A:141:VAL:HG13	1:A:224:VAL:HG23	1.97	0.46
1:A:978:ARG:C	1:A:980:GLU:H	2.19	0.46
1:A:1066:LEU:HB3	1:A:1106:HIS:CD2	2.51	0.46
1:A:1641:PHE:CE1	1:A:2085:GLY:HA2	2.51	0.46
1:A:2376:LEU:O	1:A:2380:ASN:ND2	2.48	0.46
1:A:36:LEU:O	1:A:40:PHE:N	2.48	0.45
1:A:889:LEU:HD22	1:A:896:LEU:HD11	1.98	0.45
1:A:1249:LEU:HD11	1:A:1254:LEU:HB2	1.97	0.45
1:A:1336:THR:HG23	1:A:1457:TYR:OH	2.16	0.45
1:A:2465:MET:HE3	1:A:2507:TRP:HE3	1.79	0.45
1:A:613:ILE:O	1:A:617:VAL:N	2.42	0.45
1:A:906:GLU:O	1:A:910:ARG:HG3	2.16	0.45
1:A:229:TYR:HB2	1:A:271:THR:HG22	1.97	0.45
1:A:896:LEU:HD23	1:A:896:LEU:HA	1.65	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2053:ASP:OD1	1:A:2053:ASP:N	2.50	0.45
1:A:526:TRP:CD1	1:A:558:LEU:HD22	2.52	0.45
1:A:570:GLN:O	1:A:574:THR:HG22	2.15	0.45
1:A:625:GLU:O	1:A:629:ALA:HB3	2.16	0.45
1:A:1943:LEU:HD13	1:A:1958:PHE:HB2	1.97	0.45
1:A:2064:LYS:HB2	1:A:2064:LYS:HE3	1.68	0.45
1:A:2825:LEU:O	1:A:2829:ARG:HG2	2.16	0.45
1:A:65:ARG:HA	1:A:68:LEU:HB2	1.99	0.45
1:A:498:ALA:O	1:A:502:SER:HB2	2.17	0.45
1:A:733:GLU:HA	1:A:736:GLN:HB3	1.99	0.45
1:A:1542:ASN:O	1:A:1546:ILE:HG23	2.17	0.45
1:A:1713:LEU:HD23	1:A:1713:LEU:HA	1.79	0.45
1:A:2530:LYS:HB2	1:A:2533:GLN:CG	2.46	0.45
1:A:2165:MET:SD	1:A:2188:LEU:HG	2.57	0.45
1:A:730:PRO:O	1:A:734:GLU:N	2.39	0.45
1:A:1387:VAL:HG11	1:A:1425:ALA:HB2	1.99	0.45
1:A:588:LEU:HD22	1:A:644:LEU:HD22	1.98	0.45
1:A:1371:CYS:HB2	1:A:1378:PRO:HB3	1.98	0.45
1:A:827:GLU:HG2	1:A:831:ILE:HD13	1.99	0.45
1:A:153:SER:O	1:A:157:ILE:HG23	2.17	0.45
1:A:539:LEU:HB2	1:A:542:ILE:O	2.15	0.45
1:A:1381:ILE:HB	1:A:1733:TYR:OH	2.17	0.45
1:A:1578:GLU:HB2	1:A:1579:PRO:HD3	1.98	0.45
1:A:2503:VAL:HG13	1:A:2506:ILE:HB	1.99	0.45
1:A:772:LEU:HB3	1:A:839:HIS:CD2	2.51	0.44
1:A:892:ARG:O	1:A:986:VAL:HG22	2.17	0.44
1:A:165:TRP:CH2	1:A:169:VAL:HG21	2.53	0.44
1:A:237:ALA:O	1:A:239:ILE:N	2.50	0.44
1:A:1049:LYS:HD2	1:A:1049:LYS:HA	1.71	0.44
1:A:1325:ARG:NH2	1:A:1338:GLU:OE2	2.37	0.44
1:A:1457:TYR:CE1	1:A:1461:ARG:HG3	2.53	0.44
1:A:1575:LEU:HD12	1:A:1575:LEU:HA	1.73	0.44
1:A:1634:GLY:CA	1:A:2067:VAL:HG21	2.48	0.44
1:A:115:ARG:NH2	1:A:163:GLU:O	2.51	0.44
1:A:137:LEU:HD12	1:A:137:LEU:HA	1.78	0.44
1:A:239:ILE:HD12	1:A:278:ARG:HD2	2.00	0.44
1:A:2329:LEU:HD11	1:A:2348:HIS:CE1	2.53	0.44
1:A:366:ARG:N	1:A:368:GLN:OE1	2.49	0.44
1:A:584:VAL:HG12	1:A:587:SER:OG	2.18	0.44
1:A:2530:LYS:HB2	1:A:2533:GLN:HG2	1.99	0.44
1:A:2660:LEU:HA	1:A:2660:LEU:HD12	1.72	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:GLU:O	1:A:91:LEU:HD11	2.18	0.44
1:A:968:ILE:H	1:A:968:ILE:HG12	1.46	0.44
1:A:1408:CYS:O	1:A:1412:ARG:HG2	2.18	0.44
1:A:1648:PRO:CD	1:A:2084:LEU:HD21	2.39	0.44
1:A:2439:GLN:HB3	1:A:2485:SER:HB3	2.00	0.44
1:A:1477:ALA:HB1	1:A:1519:LEU:HD11	1.99	0.44
1:A:602:PHE:O	1:A:606:SER:HB3	2.18	0.44
1:A:144:LEU:HD12	1:A:144:LEU:H	1.83	0.43
1:A:624:ALA:HB2	1:A:735:LEU:HD23	2.00	0.43
1:A:896:LEU:HD13	1:A:945:CYS:SG	2.58	0.43
1:A:1192:GLN:H	1:A:1354:GLN:HE21	1.65	0.43
1:A:1450:ASP:O	1:A:1454:ILE:HG13	2.18	0.43
1:A:2182:LEU:HD12	1:A:2182:LEU:HA	1.81	0.43
1:A:525:SER:HA	1:A:528:GLN:HB2	1.99	0.43
1:A:2409:GLU:O	1:A:2413:GLU:HG2	2.18	0.43
1:A:2922:ASP:O	1:A:2926:GLN:HG2	2.18	0.43
1:A:580:PRO:HB2	1:A:616:TRP:HZ2	1.82	0.43
1:A:2313:ALA:O	1:A:2317:ASN:ND2	2.51	0.43
1:A:63:LEU:O	1:A:67:THR:N	2.41	0.43
1:A:731:LYS:HA	1:A:734:GLU:HB3	1.99	0.43
1:A:772:LEU:HD21	1:A:790:VAL:HB	2.01	0.43
1:A:826:ILE:CG1	1:A:828:PRO:HD2	2.46	0.43
1:A:571:ILE:HA	1:A:574:THR:HG22	2.00	0.43
1:A:1284:SER:HB2	1:A:1288:LYS:HE2	2.00	0.43
1:A:367:LEU:H	1:A:401:ASN:ND2	2.17	0.43
1:A:540:PRO:CG	1:A:541:PRO:HD3	2.47	0.43
1:A:914:LEU:HD23	1:A:914:LEU:HA	1.73	0.43
1:A:1285:ARG:O	1:A:1289:ILE:HG12	2.19	0.43
1:A:2323:ASP:HA	1:A:2356:GLN:HE21	1.83	0.43
1:A:2471:GLY:HA3	1:A:2490:THR:HG21	1.99	0.43
1:A:2748:ALA:O	1:A:2752:LEU:HD13	2.18	0.43
1:A:165:TRP:CZ3	1:A:169:VAL:HG21	2.54	0.43
1:A:467:LEU:HG	1:A:471:LEU:HD12	2.00	0.43
1:A:765:CYS:SG	1:A:794:VAL:HG22	2.59	0.43
1:A:1634:GLY:HA3	1:A:2067:VAL:HG21	2.00	0.43
1:A:1670:SER:HB2	1:A:1804:LEU:HG	2.01	0.43
1:A:221:ALA:O	1:A:224:VAL:N	2.50	0.43
1:A:798:LEU:HD22	1:A:850:ALA:HB1	2.00	0.43
1:A:2357:GLU:OE1	1:A:2358:LEU:HD12	2.18	0.43
1:A:1617:TRP:CD1	1:A:1650:ASP:HB3	2.54	0.43
1:A:1757:LEU:HD23	1:A:1835:ALA:HB1	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2899:ALA:O	1:A:2903:ILE:HG13	2.19	0.43
1:A:36:LEU:H	1:A:36:LEU:HG	1.37	0.43
1:A:375:THR:OG1	1:A:376:ASN:N	2.52	0.43
1:A:827:GLU:HG3	1:A:925:GLY:N	2.33	0.43
1:A:1133:THR:O	1:A:1133:THR:OG1	2.31	0.43
1:A:1267:ILE:O	1:A:1271:ILE:HG23	2.19	0.43
1:A:511:LEU:HA	1:A:514:HIS:HE1	1.82	0.42
1:A:1314:PHE:CE2	1:A:1413:LYS:HG2	2.54	0.42
1:A:1324:PHE:HE1	1:A:1364:PRO:HD3	1.84	0.42
1:A:1457:TYR:CZ	1:A:1461:ARG:HG3	2.54	0.42
1:A:1641:PHE:CD2	1:A:2084:LEU:HB3	2.54	0.42
1:A:2674:LEU:HD13	1:A:2803:ASP:OD2	2.18	0.42
1:A:1374:THR:HG23	1:A:1376:TYR:HD2	1.84	0.42
1:A:2854:PRO:HA	1:A:2857:MET:HB3	2.01	0.42
1:A:349:GLU:HA	1:A:352:ASP:HB2	2.00	0.42
1:A:1489:SER:OG	1:A:1548:ALA:HB2	2.19	0.42
1:A:1432:GLU:HG2	1:A:1472:PHE:CE2	2.54	0.42
1:A:1679:LYS:O	1:A:1679:LYS:HG2	2.19	0.42
1:A:2110:ALA:O	1:A:2114:LYS:HG3	2.20	0.42
1:A:2116:SER:HB2	1:A:2171:ILE:HD11	2.02	0.42
1:A:461:ARG:HD3	1:A:492:HIS:NE2	2.35	0.42
1:A:1120:ARG:HD3	1:A:1145:ILE:HD11	2.01	0.42
1:A:1296:LEU:HA	1:A:1299:ILE:HG22	2.01	0.42
1:A:2052:LEU:HD12	1:A:2052:LEU:HA	1.77	0.42
1:A:163:GLU:HA	1:A:166:GLU:HG2	2.02	0.42
1:A:669:LEU:HA	1:A:669:LEU:HD23	1.75	0.42
1:A:827:GLU:HG3	1:A:925:GLY:H	1.85	0.42
1:A:1093:LEU:HD23	1:A:1093:LEU:HA	1.84	0.42
1:A:1146:PRO:HB3	1:A:1163:ALA:HB2	2.02	0.42
1:A:276:PHE:O	1:A:279:MET:N	2.48	0.42
1:A:1501:PHE:HE1	1:A:1505:LYS:HD2	1.84	0.42
1:A:674:GLN:O	1:A:677:MET:N	2.52	0.42
1:A:725:LEU:HB2	1:A:775:LEU:HD22	2.02	0.42
1:A:2108:THR:O	1:A:2112:PHE:CD2	2.73	0.42
1:A:2439:GLN:HA	1:A:2485:SER:HB3	2.01	0.42
1:A:2439:GLN:H	1:A:2446:GLN:NE2	2.18	0.42
1:A:2481:GLU:C	1:A:2483:ALA:H	2.21	0.42
1:A:291:VAL:O	1:A:295:VAL:HG23	2.21	0.41
1:A:346:ASP:O	1:A:349:GLU:N	2.53	0.41
1:A:756:GLU:OE1	1:A:757:ARG:N	2.53	0.41
1:A:1269:HIS:O	1:A:1272:SER:N	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1459:ILE:HD13	1:A:1515:PHE:HE1	1.83	0.41
1:A:63:LEU:HA	1:A:66:CYS:HB3	2.03	0.41
1:A:758:LEU:O	1:A:762:VAL:N	2.44	0.41
1:A:791:PHE:HB3	1:A:846:LYS:NZ	2.35	0.41
1:A:827:GLU:HB3	1:A:828:PRO:HD3	2.01	0.41
1:A:912:HIS:O	1:A:916:ILE:HB	2.20	0.41
1:A:969:LEU:HD23	1:A:1009:ILE:HD11	2.02	0.41
1:A:2035:TRP:HB2	1:A:2086:ALA:HB2	2.02	0.41
1:A:2647:ARG:HD3	1:A:2774:GLU:OE2	2.20	0.41
1:A:2799:ARG:NH1	1:A:2941:ALA:O	2.53	0.41
1:A:758:LEU:HG	1:A:762:VAL:HG23	2.00	0.41
1:A:1072:GLY:HA3	1:A:1076:LEU:HD23	2.01	0.41
1:A:1777:ILE:HD12	1:A:1780:LEU:HD12	2.03	0.41
1:A:2593:LYS:HB3	1:A:2593:LYS:HE3	1.84	0.41
1:A:30:LYS:HG3	1:A:90:ARG:HG2	2.02	0.41
1:A:64:PHE:O	1:A:68:LEU:N	2.52	0.41
1:A:290:LEU:HD12	1:A:290:LEU:HA	1.92	0.41
1:A:729:TYR:HD1	1:A:729:TYR:O	2.04	0.41
1:A:1730:TRP:N	1:A:1730:TRP:HD1	2.17	0.41
1:A:60:PHE:CE1	1:A:98:LEU:HD23	2.52	0.41
1:A:248:HIS:HA	1:A:251:ILE:HD11	2.02	0.41
1:A:466:GLN:HG2	1:A:503:TRP:CD2	2.55	0.41
1:A:678:GLU:N	1:A:679:PRO:CD	2.83	0.41
1:A:725:LEU:HD23	1:A:778:ILE:HD12	2.02	0.41
1:A:2123:ARG:HE	1:A:2123:ARG:HB2	1.62	0.41
1:A:2681:TYR:OH	1:A:2727:GLU:OE1	2.38	0.41
1:A:503:TRP:CE3	1:A:506:LEU:HD12	2.55	0.41
1:A:669:LEU:HD21	1:A:898:TYR:HB2	2.03	0.41
1:A:756:GLU:OE1	1:A:757:ARG:HG3	2.20	0.41
1:A:1059:PRO:O	1:A:1060:SER:OG	2.35	0.41
1:A:1698:ARG:NH1	1:A:1730:TRP:CZ2	2.88	0.41
1:A:2182:LEU:HD22	1:A:2217:HIS:CE1	2.56	0.41
1:A:2825:LEU:HD23	1:A:2916:VAL:HG13	2.01	0.41
1:A:568:ILE:HG23	1:A:594:LEU:HB3	2.01	0.41
1:A:775:LEU:HD23	1:A:775:LEU:HA	1.88	0.41
1:A:1686:ASP:C	1:A:1688:PHE:H	2.24	0.41
1:A:237:ALA:O	1:A:239:ILE:HG13	2.20	0.41
1:A:320:MET:H	1:A:320:MET:HG2	1.54	0.41
1:A:380:PRO:HA	1:A:381:PRO:HD3	1.93	0.41
1:A:388:ILE:HG13	1:A:389:PHE:H	1.86	0.41
1:A:809:ASN:HD21	1:A:812:GLY:HA3	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1670:SER:OG	1:A:1803:HIS:ND1	2.26	0.41
1:A:651:ILE:HG13	1:A:652:SER:H	1.85	0.41
1:A:924:ILE:H	1:A:924:ILE:HG13	1.77	0.41
1:A:1129:CYS:HB3	1:A:1176:THR:HG21	2.03	0.41
1:A:1336:THR:O	1:A:1340:ILE:HG13	2.19	0.41
1:A:1551:ASN:HD22	1:A:1553:GLU:N	2.19	0.41
1:A:2375:LYS:HG2	1:A:2414:VAL:HG21	2.03	0.41
1:A:2768:LEU:HD23	1:A:2775:VAL:HG12	2.03	0.41
1:A:377:MET:H	1:A:377:MET:HG3	1.48	0.41
1:A:478:SER:O	1:A:482:VAL:HG23	2.20	0.41
1:A:151:PRO:HB2	1:A:892:ARG:NH2	2.36	0.40
1:A:1217:LEU:O	1:A:1221:ARG:HG3	2.22	0.40
1:A:1680:SER:O	1:A:1680:SER:OG	2.38	0.40
1:A:2159:LEU:HD12	1:A:2159:LEU:HA	1.90	0.40
1:A:2557:PRO:HA	1:A:2558:PRO:HD3	1.95	0.40
1:A:462:LEU:HA	1:A:465:LEU:HB3	2.02	0.40
1:A:1046:LEU:HD11	1:A:1061:SER:O	2.21	0.40
1:A:1396:LYS:HE3	1:A:1396:LYS:HB2	1.66	0.40
1:A:1658:GLN:HG3	1:A:1661:ARG:NH2	2.37	0.40
1:A:1755:ARG:HD3	1:A:1755:ARG:HA	1.83	0.40
1:A:1916:ILE:HD12	1:A:1916:ILE:HA	1.90	0.40
1:A:2579:PHE:CE1	1:A:2595:LEU:HD23	2.56	0.40
1:A:117:ILE:O	1:A:121:ILE:HG13	2.22	0.40
1:A:391:LEU:HD13	1:A:402:TRP:CE3	2.57	0.40
1:A:530:TRP:HE1	1:A:567:ASP:CG	2.25	0.40
1:A:1117:LEU:O	1:A:1120:ARG:N	2.53	0.40
1:A:1263:ILE:HD13	1:A:1263:ILE:HA	1.79	0.40
1:A:95:PRO:HG3	1:A:136:LEU:HD12	2.03	0.40
1:A:117:ILE:O	1:A:120:HIS:HB3	2.21	0.40
1:A:367:LEU:H	1:A:401:ASN:HD22	1.70	0.40
1:A:509:SER:OG	1:A:549:LEU:HA	2.20	0.40
1:A:607:GLN:NE2	1:A:719:ALA:HB3	2.37	0.40
1:A:1217:LEU:HD23	1:A:1220:LEU:HD12	2.03	0.40
1:A:1273:ILE:HD13	1:A:1273:ILE:HA	1.95	0.40
1:A:1443:VAL:HG23	1:A:1443:VAL:O	2.21	0.40
1:A:1959:ARG:HD3	1:A:1959:ARG:HA	1.72	0.40
1:A:335:LEU:HD11	1:A:347:VAL:HG21	2.03	0.40
1:A:499:ILE:H	1:A:499:ILE:HG12	1.56	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	2612/2944 (89%)	2388 (91%)	220 (8%)	4 (0%)	47 79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2482	VAL
1	A	2483	ALA
1	A	418	HIS
1	A	1377	GLU

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	2291/2529 (91%)	2160 (94%)	131 (6%)	20 55

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASP
1	A	36	LEU
1	A	56	TYR
1	A	63	LEU
1	A	106	VAL
1	A	109	ILE
1	A	115	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	136	LEU
1	A	140	TYR
1	A	167	VAL
1	A	224	VAL
1	A	230	MET
1	A	261	ILE
1	A	269	PHE
1	A	271	THR
1	A	314	ASN
1	A	318	ASP
1	A	325	TYR
1	A	327	THR
1	A	358	TYR
1	A	360	ARG
1	A	377	MET
1	A	379	LEU
1	A	383	HIS
1	A	410	ILE
1	A	450	HIS
1	A	453	LEU
1	A	485	THR
1	A	494	THR
1	A	499	ILE
1	A	502	SER
1	A	523	SER
1	A	526	TRP
1	A	532	LEU
1	A	542	ILE
1	A	564	LEU
1	A	583	LEU
1	A	596	ARG
1	A	602	PHE
1	A	613	ILE
1	A	632	HIS
1	A	649	TYR
1	A	651	ILE
1	A	655	VAL
1	A	660	LEU
1	A	662	LEU
1	A	667	ILE
1	A	676	GLU
1	A	683	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	728	PHE
1	A	729	TYR
1	A	755	MET
1	A	756	GLU
1	A	767	THR
1	A	774	ASP
1	A	777	ASN
1	A	778	ILE
1	A	781	SER
1	A	782	LEU
1	A	809	ASN
1	A	811	PHE
1	A	833	LEU
1	A	854	ARG
1	A	892	ARG
1	A	914	LEU
1	A	915	ASP
1	A	927	ILE
1	A	931	ILE
1	A	933	ASN
1	A	943	PHE
1	A	947	ARG
1	A	956	SER
1	A	957	ASP
1	A	968	ILE
1	A	980	GLU
1	A	986	VAL
1	A	997	SER
1	A	1004	ASP
1	A	1011	GLU
1	A	1012	MET
1	A	1016	LEU
1	A	1051	GLU
1	A	1063	SER
1	A	1065	LEU
1	A	1071	ASP
1	A	1074	MET
1	A	1076	LEU
1	A	1084	ILE
1	A	1094	LYS
1	A	1112	ASP
1	A	1127	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1130	ARG
1	A	1133	THR
1	A	1160	THR
1	A	1161	HIS
1	A	1164	LEU
1	A	1185	LEU
1	A	1202	SER
1	A	1206	ILE
1	A	1218	ASP
1	A	1219	LEU
1	A	1230	ILE
1	A	1258	SER
1	A	1266	SER
1	A	1271	ILE
1	A	1284	SER
1	A	1305	ASP
1	A	1314	PHE
1	A	1316	GLN
1	A	1348	THR
1	A	1372	SER
1	A	1450	ASP
1	A	1527	PHE
1	A	1577	ASN
1	A	1654	GLU
1	A	1687	CYS
1	A	1868	ASP
1	A	2045	SER
1	A	2077	THR
1	A	2126	ASP
1	A	2247	ASP
1	A	2295	PHE
1	A	2381	TYR
1	A	2410	VAL
1	A	2547	LEU
1	A	2567	ASN
1	A	2600	THR
1	A	2637	ARG
1	A	2649	TYR
1	A	2660	LEU
1	A	2792	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	252	GLN
1	A	293	GLN
1	A	394	HIS
1	A	401	ASN
1	A	450	HIS
1	A	454	HIS
1	A	474	HIS
1	A	492	HIS
1	A	562	HIS
1	A	607	GLN
1	A	632	HIS
1	A	643	ASN
1	A	674	GLN
1	A	824	HIS
1	A	1027	ASN
1	A	1062	GLN
1	A	1106	HIS
1	A	1200	ASN
1	A	1298	ASN
1	A	1345	HIS
1	A	1354	GLN
1	A	1456	GLN
1	A	1509	GLN
1	A	1512	HIS
1	A	1532	GLN
1	A	1542	ASN
1	A	1551	ASN
1	A	1573	ASN
1	A	1574	GLN
1	A	1577	ASN
1	A	1656	GLN
1	A	1665	GLN
1	A	1844	ASN
1	A	2179	GLN
1	A	2239	GLN
1	A	2255	GLN
1	A	2317	ASN
1	A	2354	GLN
1	A	2356	GLN
1	A	2360	GLN
1	A	2446	GLN
1	A	2487	GLN
1	A	2518	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2567	ASN
1	A	2624	GLN
1	A	2641	GLN
1	A	2678	HIS
1	A	2770	HIS
1	A	2849	GLN
1	A	2861	GLN
1	A	2925	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is 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	AGS	A	3001	3	26,33,33	0.77	1 (3%)	26,52,52	1.16	2 (7%)

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	AGS	A	3001	3	-	8/17/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001	AGS	PG-S1G	2.02	1.95	1.90

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	AGS	PA-O3A-PB	-4.40	117.73	132.83
2	A	3001	AGS	C5'-C6-N6	2.16	123.64	120.35

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3001	AGS	PB-O3B-PG-O2G
2	A	3001	AGS	PB-O3B-PG-O3G
2	A	3001	AGS	C5'-O5'-PA-O3A
2	A	3001	AGS	PB-O3A-PA-O5'
2	A	3001	AGS	C5'-O5'-PA-O1A
2	A	3001	AGS	O4'-C4'-C5'-O5'
2	A	3001	AGS	PA-O3A-PB-O1B
2	A	3001	AGS	PA-O3A-PB-O2B

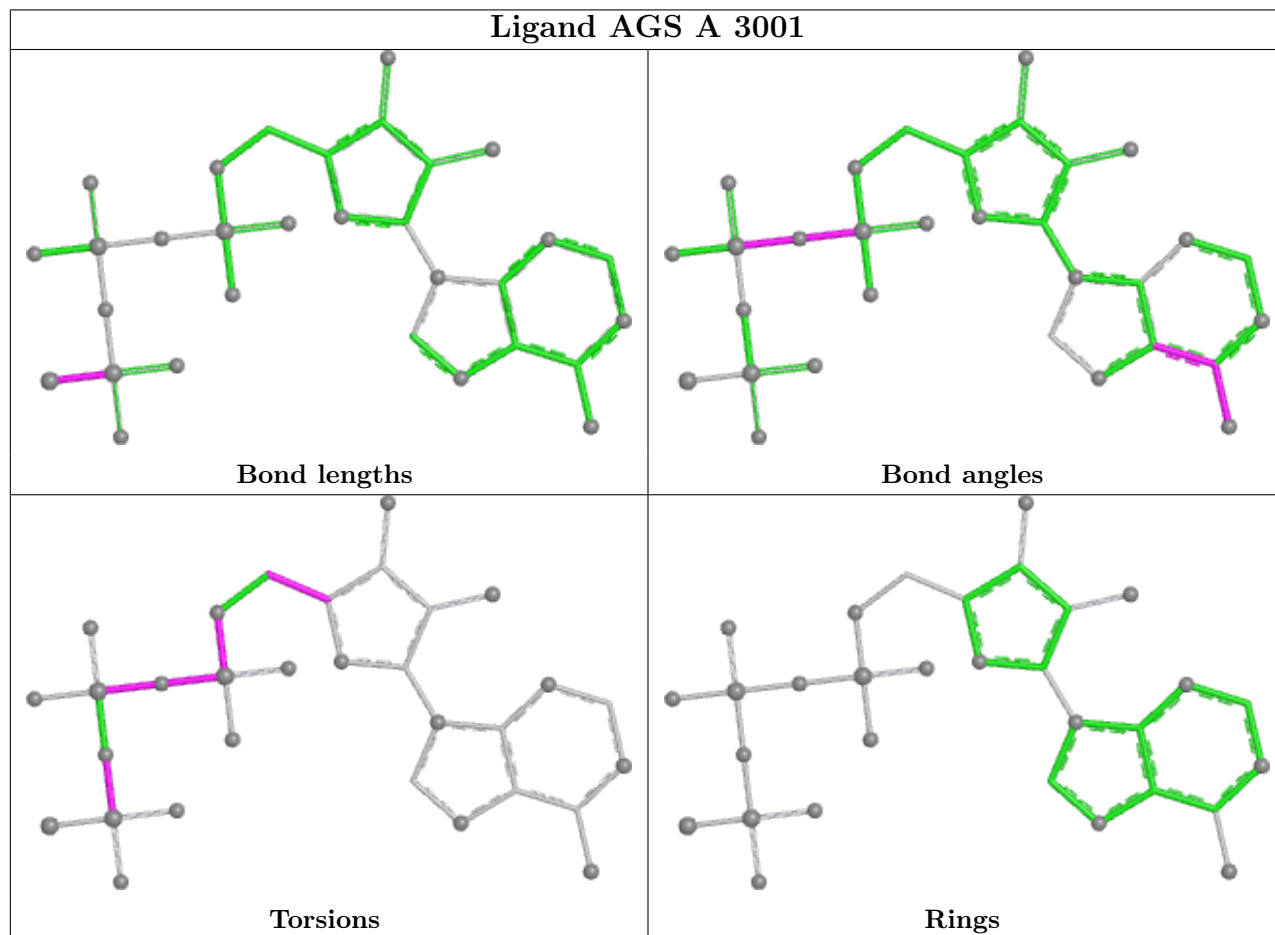
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3001	AGS	3	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.

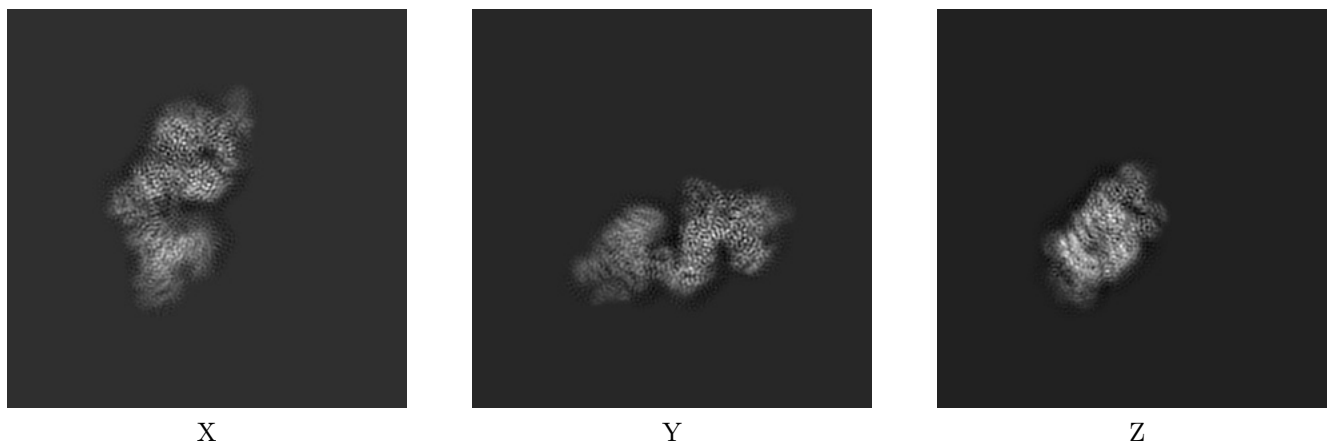
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10234. 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](#)

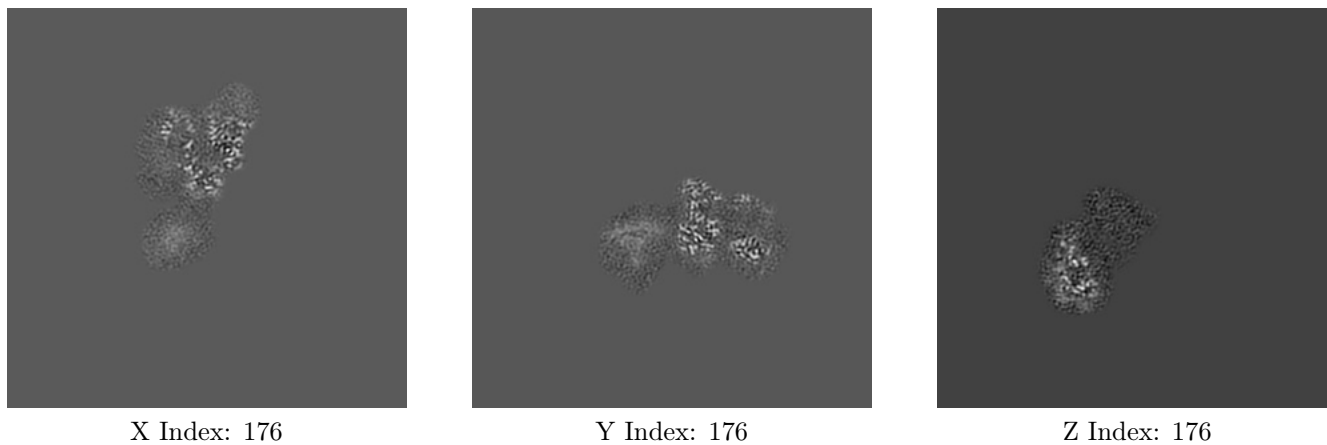
6.1.1 Primary map



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

6.2 Central slices [i](#)

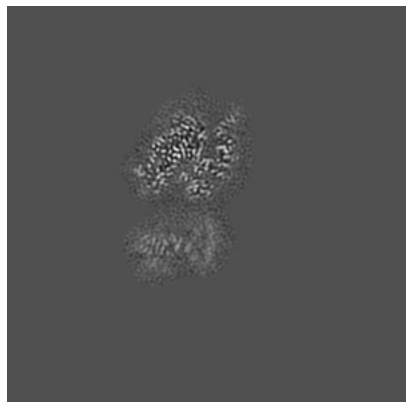
6.2.1 Primary map



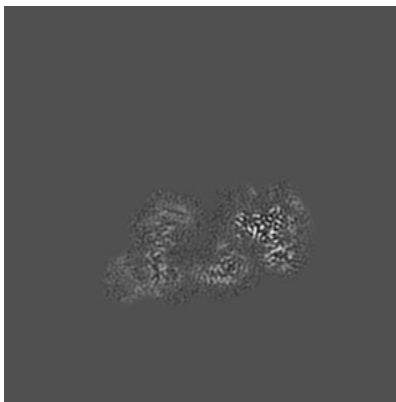
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

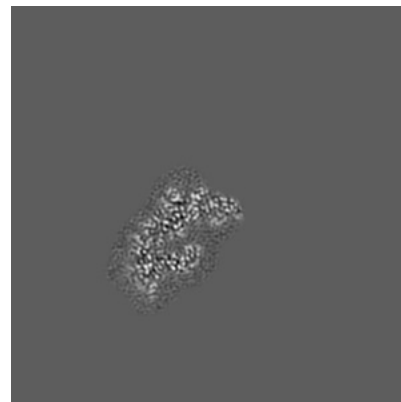
6.3.1 Primary map



X Index: 156



Y Index: 147

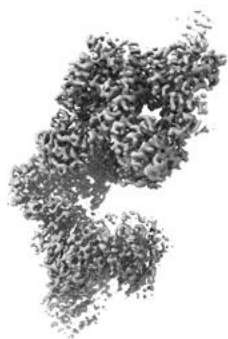


Z Index: 194

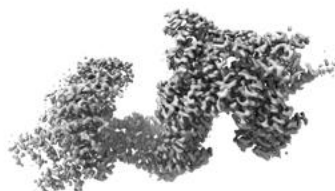
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

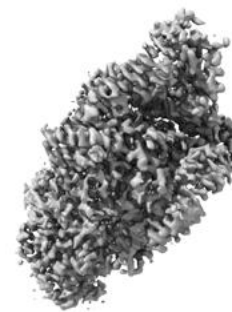
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0118. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

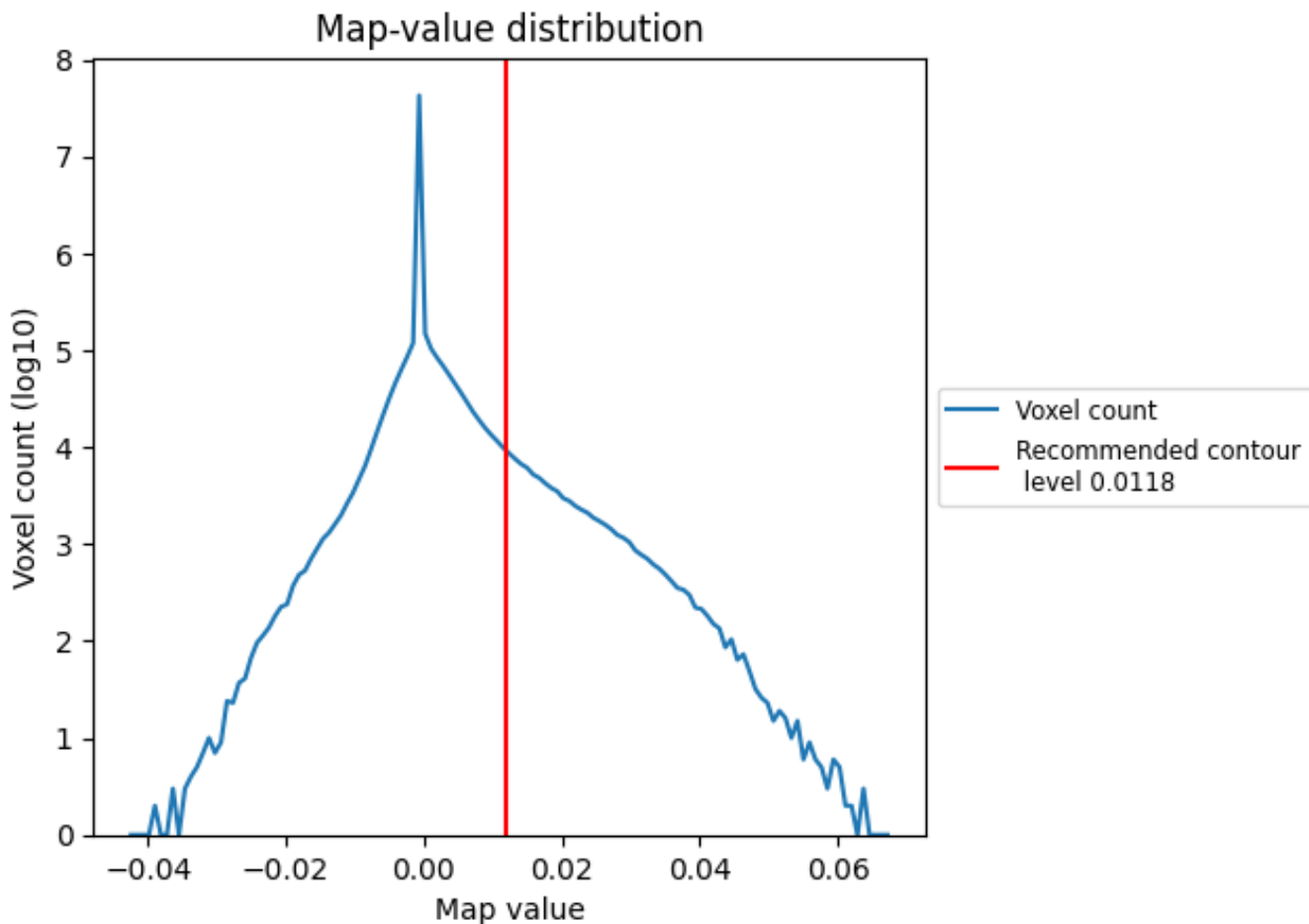
6.5 Mask visualisation

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

7 Map analysis [i](#)

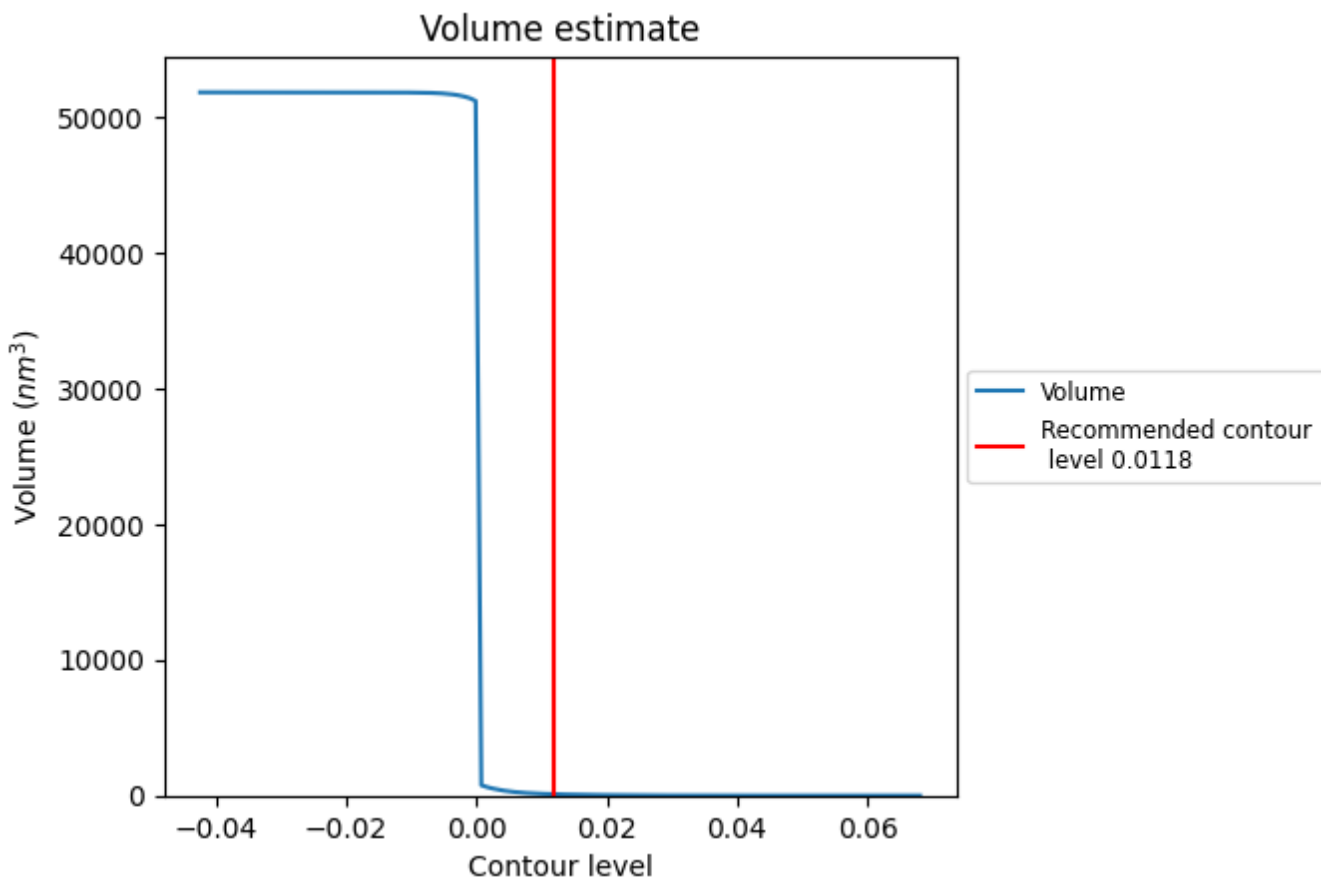
This section contains the results of statistical analysis of the map.

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.

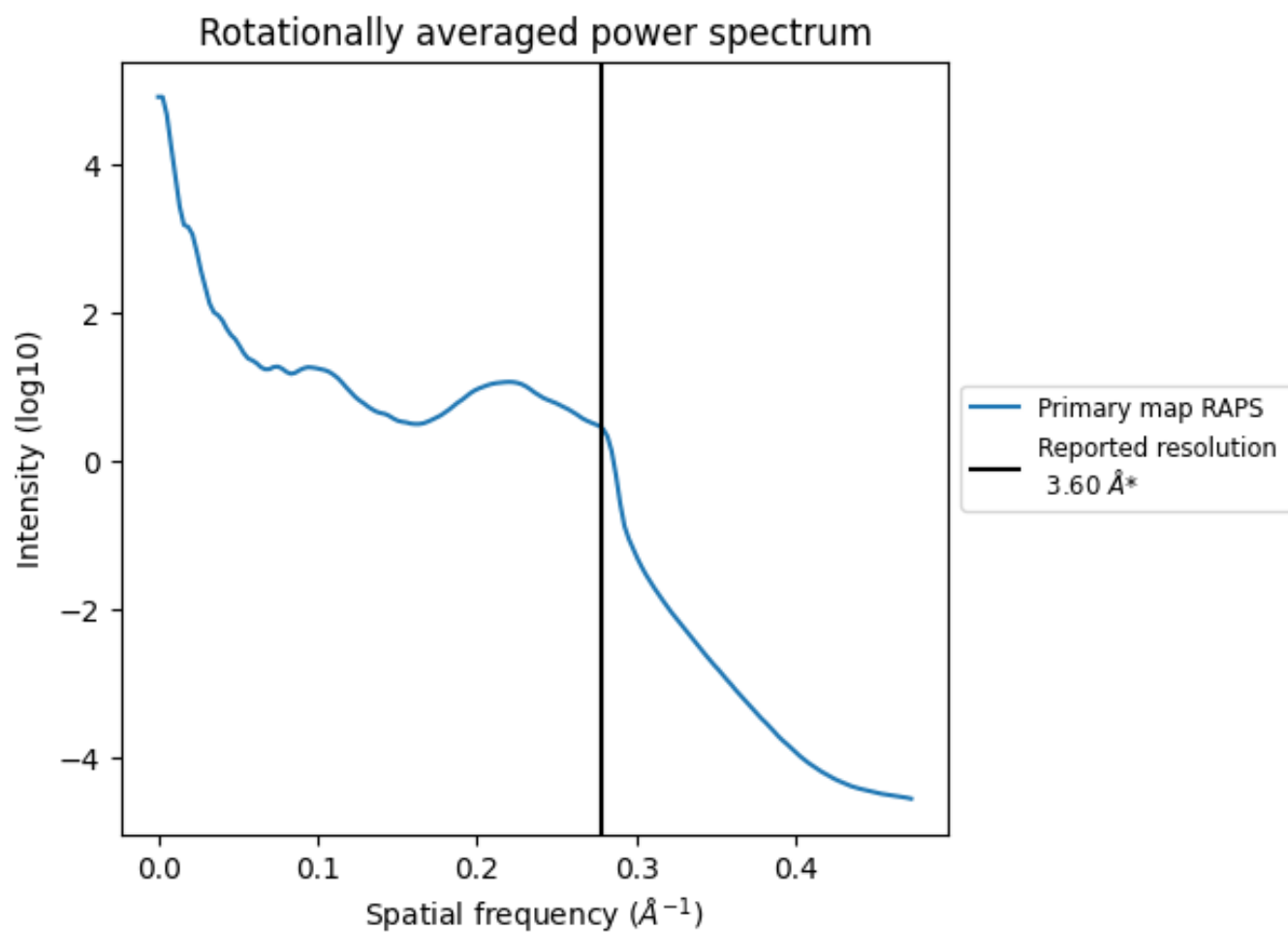
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 103 nm³; this corresponds to an approximate mass of 93 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

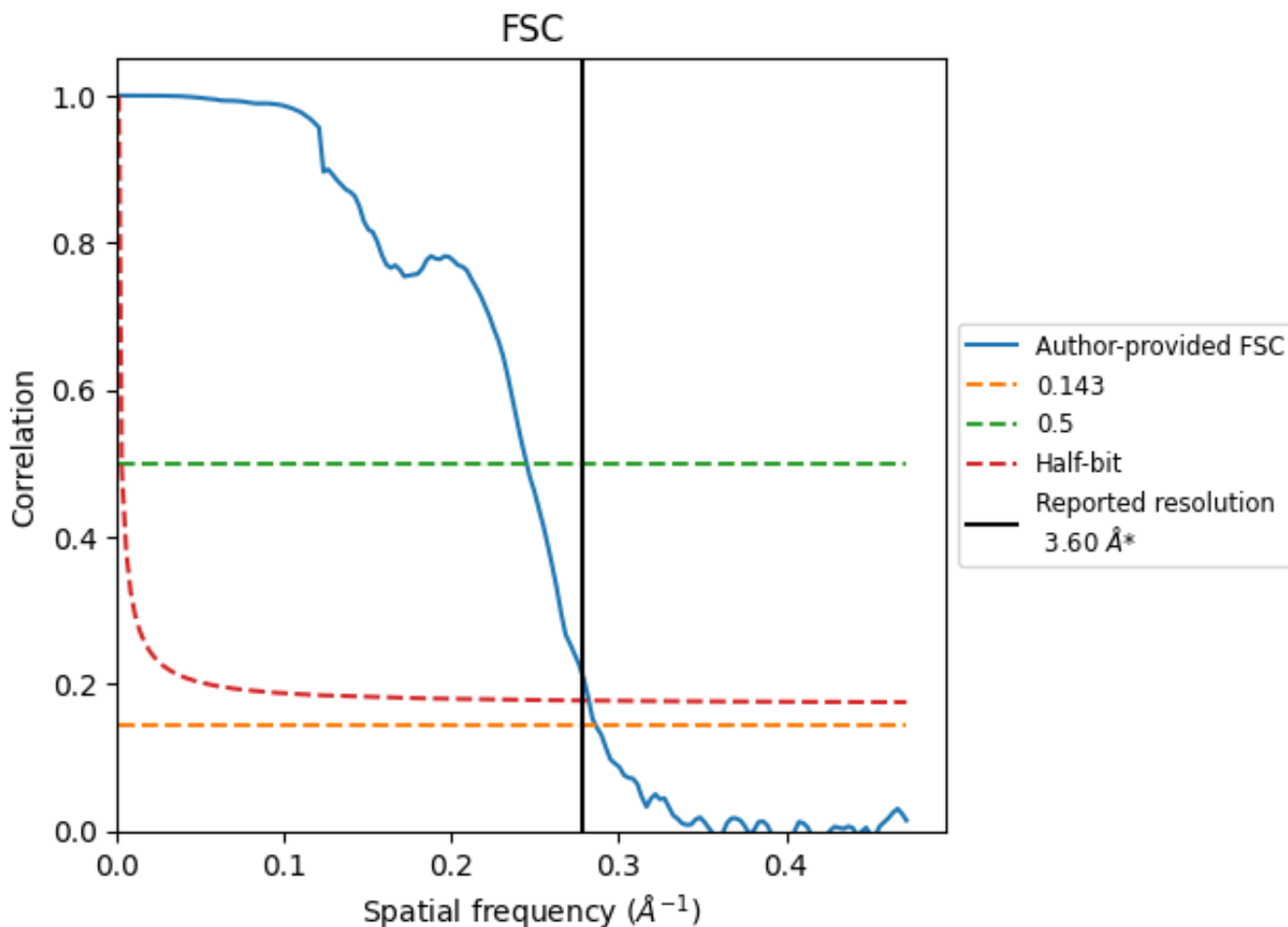


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

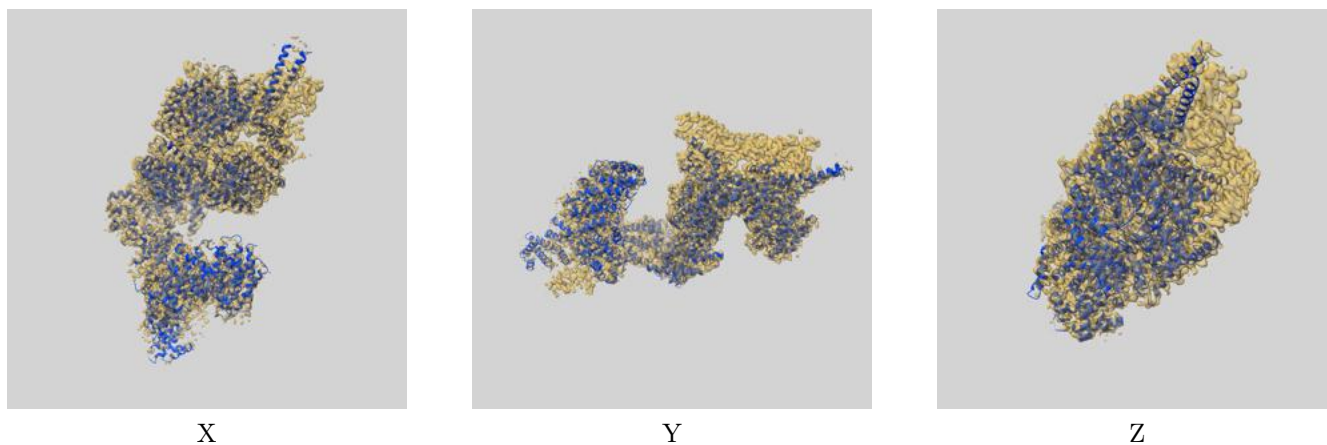
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.49	4.08	3.54
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

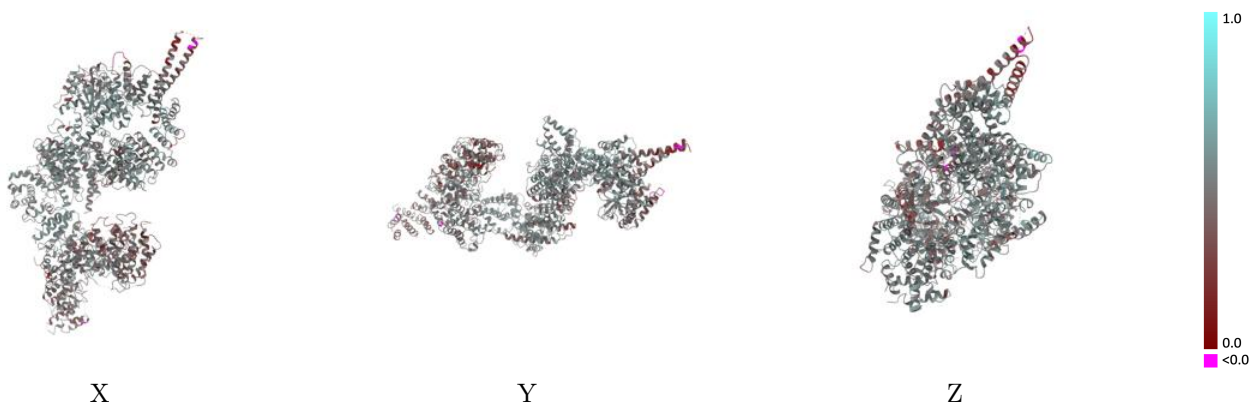
This section contains information regarding the fit between EMDB map EMD-10234 and PDB model 6SL1. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



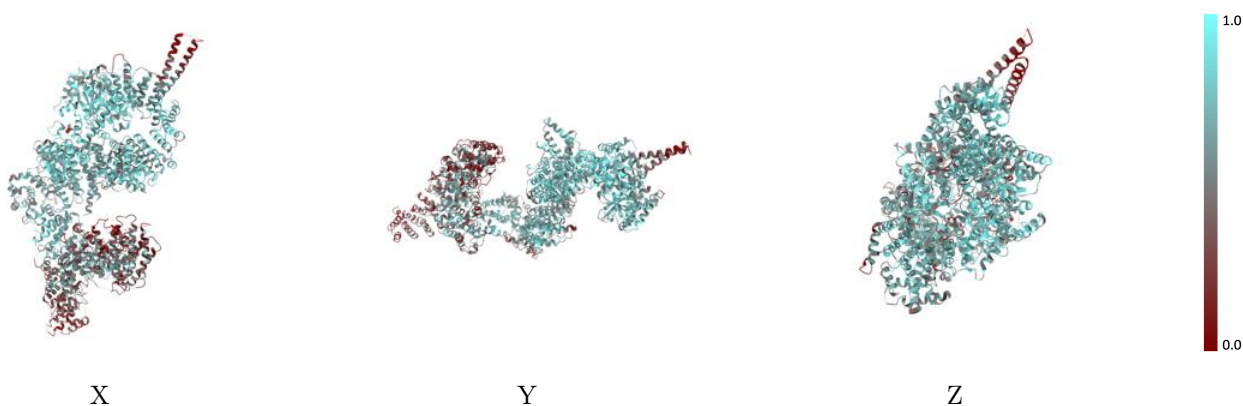
The images above show the 3D surface view of the map at the recommended contour level 0.0118 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



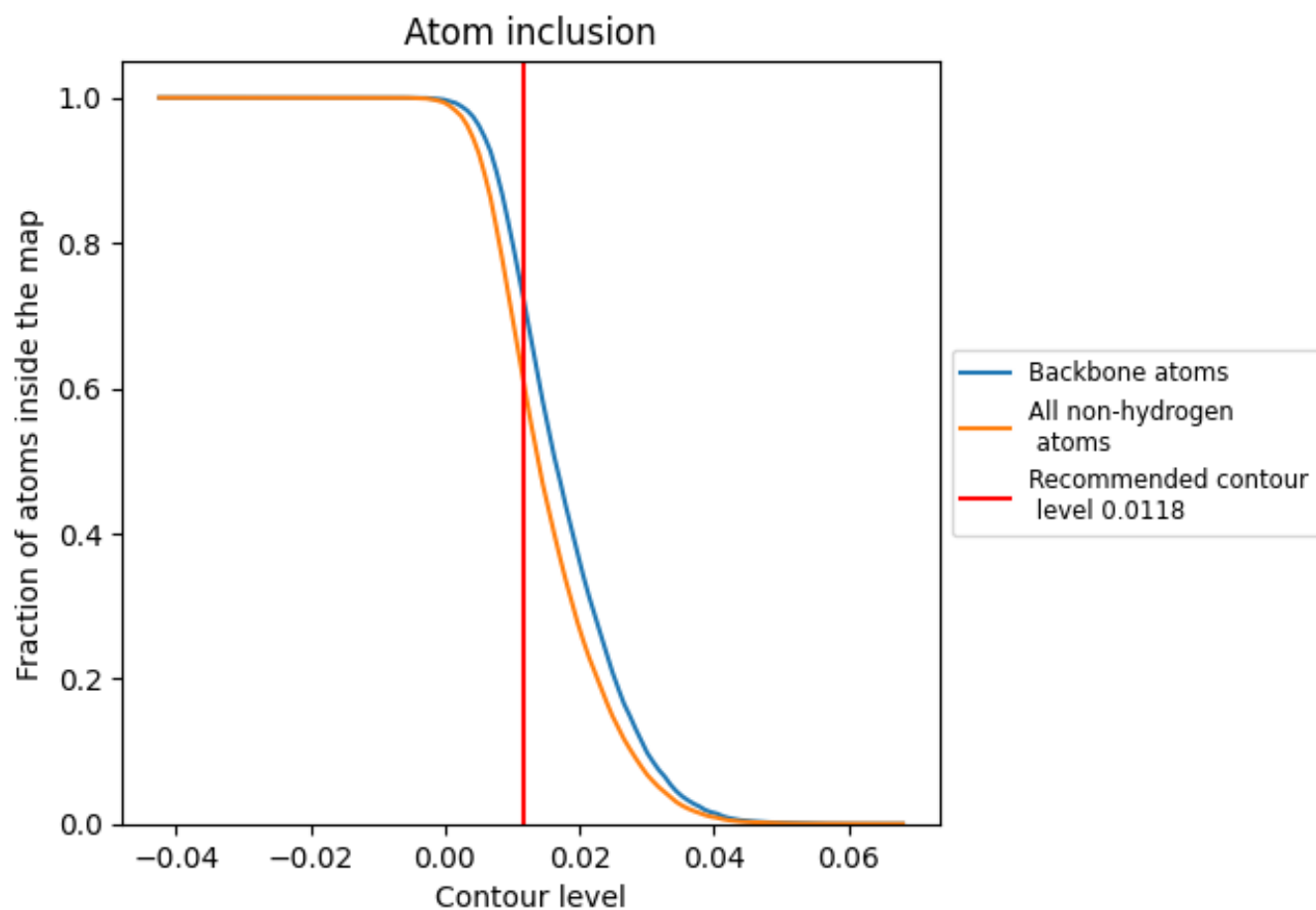
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0118).





9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.0118) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6039	 0.4720
A	 0.6039	 0.4720

