



Full wwPDB EM Validation Report ⓘ

Apr 29, 2026 – 02:45 am BST

PDB ID : 29HI / pdb_000029hi
EMDB ID : EMD-57180
Title : Cryo-EM structure of the CUL1-RBX1-SKP1-FBXO22 SCF ubiquitination ligase in complex with NSD2 via UNC10415667
Authors : Amann, S.J.; Robertson, K.C.; Grishkovskaya, I.; Liu, T.; James, L.I.; Brown, N.B.; Haselbach, D.
Deposited on : 2026-03-11
Resolution : 5.90 Å (reported)
Based on initial model : .

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

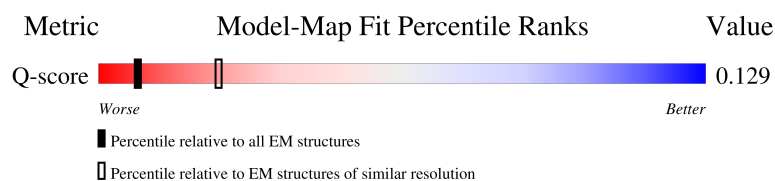
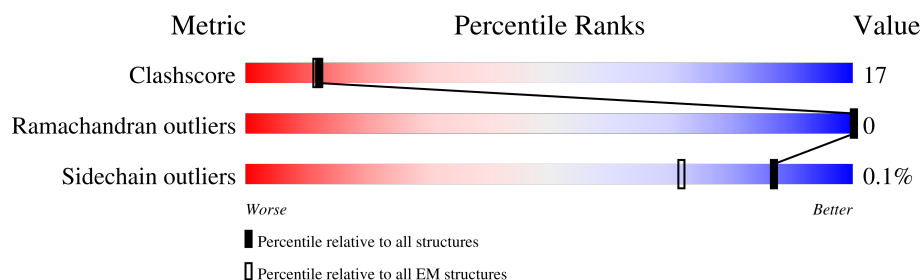
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	501 (5.40 - 6.40)

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	403	
2	B	1365	
3	C	163	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	776	
5	E	108	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	A1J21	A	501	X	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12383 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 F-box only protein 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	376	Total	C	N	O	S	0	0
			2911	1853	504	537	17		

- Molecule 2 is a protein called Histone-lysine N-methyltransferase NSD2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	136	Total	C	N	O	S	0	0
			1084	698	187	194	5		

- Molecule 3 is a protein called S-phase kinase-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	163	Total	C	N	O	S	0	0
			1308	820	211	270	7		

- Molecule 4 is a protein called Cullin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	772	Total	C	N	O	S	0	0
			6274	3969	1081	1195	29		

- Molecule 5 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	93	Total	C	N	O	S	0	0
			759	479	140	131	9		

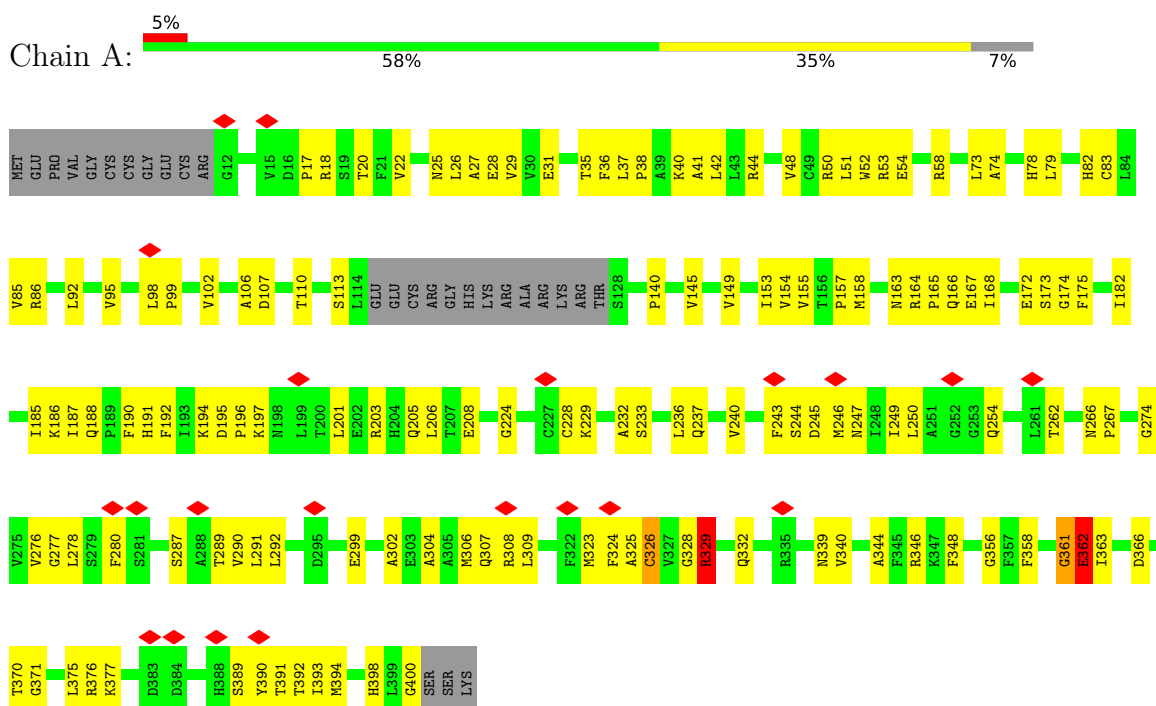
- Molecule 6 is 4-[[cyclopropyl-[({Z})-2-methyl-4-(5-oxidanylidene-2 {H}-1,4-oxazin-3-yl)but-3-enoyl]amino]methyl]- {N}]-[3-[2-[[4-(hydroxymethyl)phenyl]carbonyl-methyl-amino]ethyl]phenyl]benzamide (CCD ID: A1J21) (formula: C₃₇H₄₀N₄O₆) (labeled as "Ligand of Interest" by depositor).



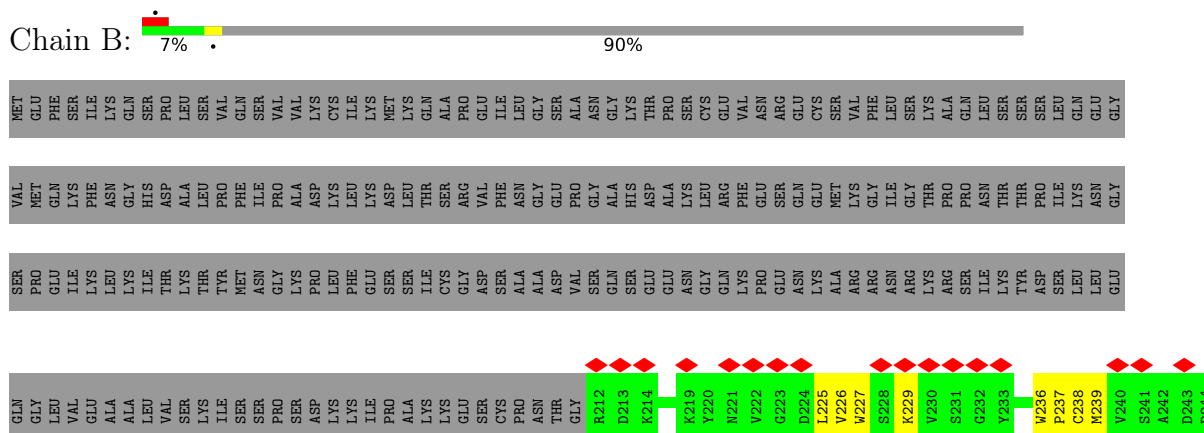
3 Residue-property plots

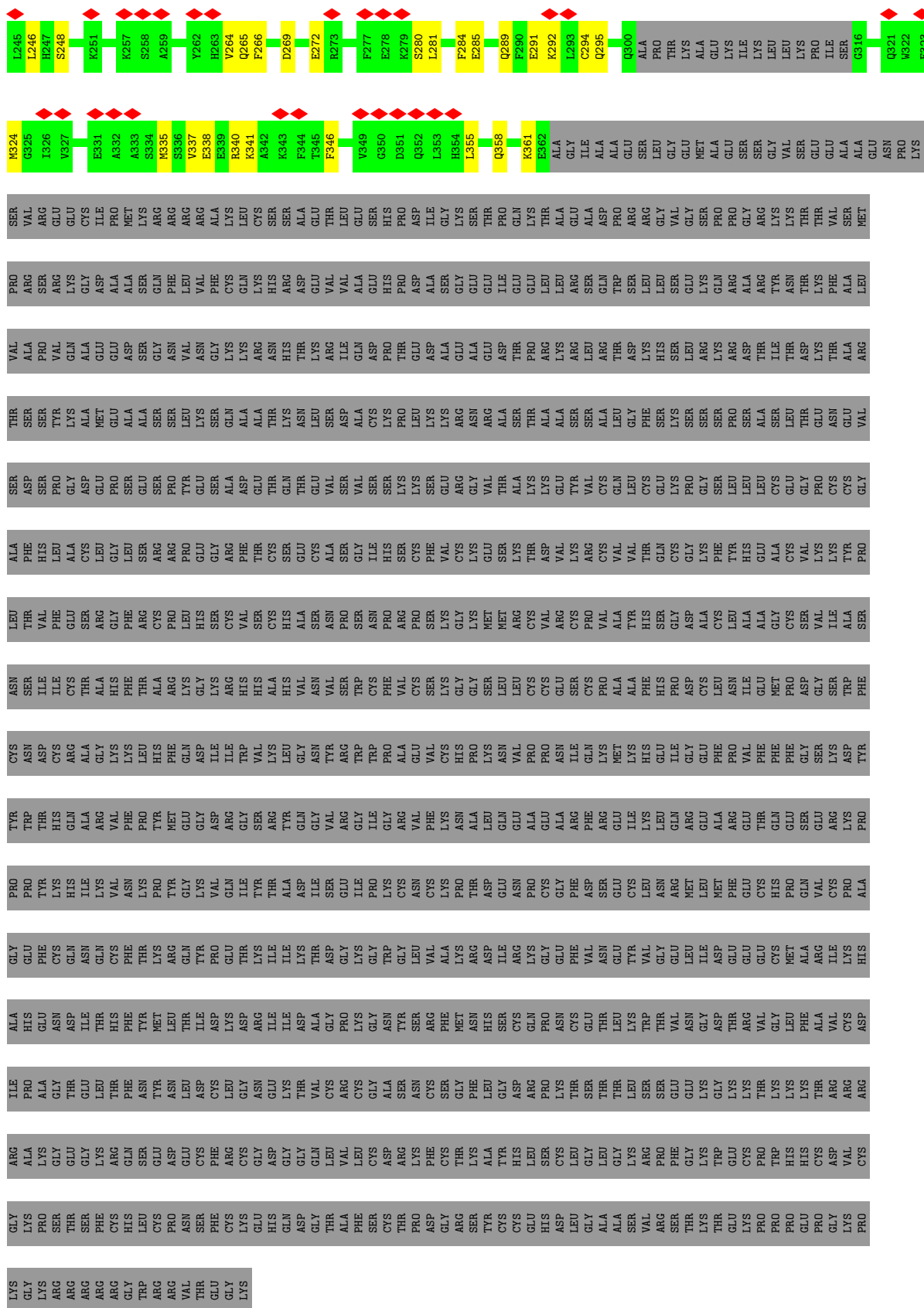
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: F-box only protein 22



• Molecule 2: Histone-lysine N-methyltransferase NSD2



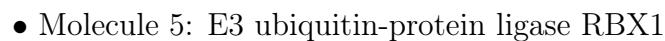


- Molecule 3: S-phase kinase-associated protein 1

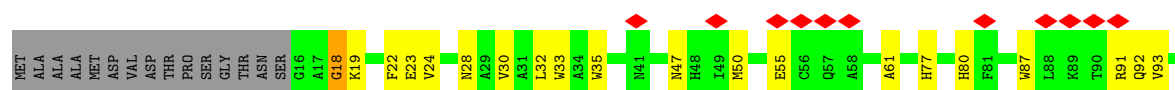
Opinion	Percentage
Doing a good job	62%
Doing a bad job	38%

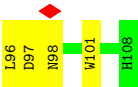


Frequency	Percentage
11%	11%
70%	70%
29%	29%



Frequency	Percentage
Daily	64%
Weekly	21%
Monthly	11%
Other	4%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47442	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.896	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	228.23999, 228.23999, 228.23999	wwPDB
Map dimensions	120, 120, 120	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.902, 1.902, 1.902	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1J21

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.28	0/2966	0.83	10/4017 (0.2%)
2	B	0.19	0/1113	0.60	0/1500
3	C	0.22	0/1331	0.67	0/1801
4	D	0.22	0/6381	0.63	2/8593 (0.0%)
5	E	0.24	0/781	0.74	2/1057 (0.2%)
All	All	0.23	0/12572	0.69	14/16968 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
5	E	0	1
All	All	0	3

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	GLU	CA-CB-CG	16.54	147.18	114.10
1	A	362	GLU	CB-CA-C	10.52	126.66	109.72
1	A	362	GLU	N-CA-CB	-7.50	98.32	110.77
4	D	625	LEU	CA-CB-CG	7.34	141.98	116.30
1	A	329	ARG	CB-CG-CD	7.32	128.13	111.30
1	A	328	GLY	CA-C-N	-7.21	108.62	121.81
1	A	328	GLY	C-N-CA	-7.21	108.62	121.81
1	A	326	CYS	CA-CB-SG	6.86	130.17	114.40
1	A	329	ARG	CG-CD-NE	6.84	127.05	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	CYS	N-CA-CB	-6.01	102.09	110.38
1	A	361	GLY	N-CA-C	-6.00	98.96	113.18
4	D	107	GLY	N-CA-C	5.71	121.03	113.37
5	E	18	GLY	CA-C-N	5.10	131.29	121.54
5	E	18	GLY	C-N-CA	5.10	131.29	121.54

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	ASP	Peptide
1	A	362	GLU	Sidechain
5	E	77	HIS	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	2911	0	2929	149	0
2	B	1084	0	1040	35	0
3	C	1308	0	1281	56	0
4	D	6274	0	6305	187	0
5	E	759	0	718	25	0
6	A	47	0	0	5	0
All	All	12383	0	12273	423	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 17.

All (423) 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)
6:A:501:A1J21:C50	6:A:501:A1J21:C51	1.78	1.54
1:A:229:LYS:HE3	2:B:272:GLU:OE1	1.38	1.21
1:A:73:LEU:HD12	1:A:166:GLN:HE22	1.33	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ARG:O	1:A:53:ARG:HG3	1.74	0.86
4:D:318:ASP:HA	4:D:321:ARG:HD2	1.57	0.86
3:C:7:GLN:HE22	3:C:11:GLY:HA2	1.41	0.84
4:D:644:LEU:HD13	4:D:651:LEU:HD11	1.59	0.84
3:C:57:LYS:HE2	3:C:103:LEU:HD13	1.60	0.84
4:D:464:LYS:HE3	4:D:703:ILE:HD11	1.58	0.84
4:D:381:VAL:HG21	4:D:395:LEU:HD11	1.60	0.83
1:A:36:PHE:HE2	3:C:120:CYS:HG	1.21	0.82
1:A:229:LYS:HE3	2:B:272:GLU:CD	2.06	0.81
4:D:151:GLU:OE1	4:D:153:ARG:HB2	1.81	0.81
4:D:278:TYR:HB2	4:D:279:LEU:HD12	1.63	0.80
6:A:501:A1J21:O38	2:B:269:ASP:CG	2.26	0.79
5:E:87:TRP:HZ3	5:E:91:ARG:HD2	1.46	0.78
1:A:186:LYS:HD3	1:A:188:GLN:HG2	1.65	0.77
4:D:352:ILE:HD11	4:D:408:VAL:HG23	1.65	0.76
4:D:431:LYS:HE2	4:D:478:ASN:HD22	1.50	0.76
2:B:225:LEU:HD23	2:B:239:MET:HE1	1.68	0.76
1:A:40:LYS:HZ3	3:C:159:TRP:CD1	2.04	0.75
1:A:74:ALA:HB2	1:A:166:GLN:HG3	1.66	0.75
1:A:362:GLU:OE1	1:A:389:SER:HA	1.87	0.75
2:B:227:TRP:HE1	2:B:289:GLN:HE21	1.31	0.75
1:A:254:GLN:HB3	1:A:361:GLY:HA3	1.69	0.74
4:D:510:ASP:HA	4:D:513:VAL:HG22	1.68	0.73
6:A:501:A1J21:O38	2:B:269:ASP:CB	2.37	0.73
3:C:24:SER:HB3	3:C:27:ILE:HG12	1.69	0.73
4:D:107:GLY:HA2	4:D:110:LEU:HD13	1.72	0.72
1:A:249:ILE:HG13	1:A:287:SER:HB3	1.72	0.70
4:D:558:GLU:O	4:D:561:ARG:HD3	1.91	0.70
6:A:501:A1J21:O38	2:B:269:ASP:HB2	1.91	0.70
4:D:362:ASP:OD1	4:D:364:LYS:HG2	1.92	0.70
2:B:335:MET:HG2	2:B:340:ARG:HB3	1.74	0.69
4:D:41:ARG:HH21	4:D:44:GLU:HG2	1.57	0.69
1:A:266:ASN:OD1	1:A:267:PRO:HD2	1.90	0.69
5:E:55:GLU:HG3	5:E:87:TRP:HE1	1.55	0.69
4:D:437:PRO:HG2	4:D:441:GLU:OE2	1.93	0.69
1:A:306:MET:HE1	1:A:348:PHE:HB2	1.73	0.68
4:D:431:LYS:HB2	4:D:473:ARG:HH21	1.58	0.68
4:D:540:LEU:HB2	5:E:32:LEU:HD23	1.73	0.68
4:D:496:CYS:SG	4:D:500:TYR:HD2	2.17	0.68
4:D:650:VAL:HG23	4:D:654:GLU:HG3	1.74	0.68
4:D:285:ASP:O	4:D:289:ARG:HG2	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:MET:HB3	1:A:356:GLY:HA3	1.75	0.67
1:A:92:LEU:O	1:A:95:VAL:HG12	1.94	0.67
1:A:240:VAL:HA	1:A:243:PHE:CE1	2.30	0.67
1:A:31:GLU:O	1:A:35:THR:HG23	1.95	0.67
5:E:18:GLY:O	5:E:19:LYS:HG2	1.94	0.66
4:D:464:LYS:CE	4:D:703:ILE:HD11	2.26	0.65
1:A:370:THR:HG22	1:A:371:GLY:H	1.61	0.65
2:B:225:LEU:HB3	2:B:284:PHE:HB3	1.76	0.65
1:A:254:GLN:H	1:A:361:GLY:HA3	1.62	0.65
4:D:350:ALA:O	4:D:353:GLU:HG3	1.96	0.65
3:C:91:GLU:HA	3:C:94:LYS:HG2	1.77	0.65
2:B:291:GLU:O	2:B:294:CYS:SG	2.46	0.64
3:C:7:GLN:NE2	3:C:11:GLY:HA2	2.13	0.64
4:D:522:LYS:O	4:D:526:THR:HG23	1.97	0.64
4:D:518:ASN:HA	4:D:521:PHE:CE2	2.33	0.64
1:A:233:SER:O	1:A:237:GLN:HG2	1.98	0.64
4:D:577:ARG:HD2	5:E:33:TRP:CD1	2.33	0.64
1:A:306:MET:HA	1:A:309:LEU:HG	1.80	0.64
1:A:361:GLY:O	1:A:362:GLU:HB2	1.97	0.63
4:D:109:ASP:OD1	4:D:110:LEU:HD12	1.97	0.63
4:D:183:VAL:O	4:D:187:ILE:HD12	1.98	0.63
1:A:157:PRO:HG2	1:A:163:ASN:HB3	1.80	0.63
3:C:43:ASP:OD1	3:C:44:PRO:HD2	1.98	0.63
4:D:275:VAL:HA	4:D:279:LEU:HD13	1.79	0.63
4:D:539:VAL:HG12	5:E:33:TRP:HE3	1.64	0.62
1:A:140:PRO:HD3	3:C:159:TRP:CZ2	2.34	0.62
1:A:155:VAL:HB	1:A:175:PHE:CZ	2.35	0.62
3:C:132:PRO:O	3:C:136:ARG:HG2	1.99	0.62
1:A:191:HIS:HE1	1:A:274:GLY:HA3	1.64	0.61
1:A:192:PHE:CE2	1:A:206:LEU:HD13	2.35	0.61
3:C:147:GLU:HA	3:C:150:GLU:HG2	1.80	0.61
1:A:309:LEU:HD21	1:A:394:MET:SD	2.41	0.61
2:B:285:GLU:H	2:B:289:GLN:HE22	1.46	0.61
3:C:85:ILE:HD12	3:C:90:GLN:HE21	1.65	0.61
4:D:759:LYS:HE3	4:D:759:LYS:HA	1.82	0.61
4:D:541:SER:H	4:D:545:TRP:HZ2	1.49	0.61
4:D:586:SER:HB3	5:E:28:ASN:O	2.01	0.61
4:D:622:VAL:HA	4:D:625:LEU:HG	1.82	0.61
3:C:54:ILE:HA	3:C:57:LYS:HZ3	1.66	0.61
4:D:430:LEU:HD21	4:D:488:MET:SD	2.40	0.60
4:D:590:LEU:HD11	4:D:608:MET:HE1	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:141:ASN:HD21	4:D:158:GLU:HB2	1.66	0.60
1:A:229:LYS:CE	2:B:272:GLU:OE1	2.32	0.60
4:D:540:LEU:HB3	4:D:545:TRP:CE2	2.37	0.60
4:D:489:ILE:HG22	4:D:493:LYS:HZ3	1.67	0.59
1:A:25:ASN:ND2	4:D:56:VAL:HG11	2.17	0.59
1:A:191:HIS:HB2	1:A:276:VAL:HG23	1.85	0.59
4:D:516:ASP:O	4:D:519:GLU:HG3	2.02	0.59
4:D:508:PHE:O	4:D:511:ILE:HG12	2.03	0.59
4:D:364:LYS:HA	4:D:425:TYR:CD1	2.38	0.58
5:E:92:GLN:HG3	5:E:101:TRP:CZ2	2.38	0.58
2:B:289:GLN:HB2	2:B:292:LYS:HE2	1.85	0.58
4:D:493:LYS:HG2	4:D:501:THR:OG1	2.04	0.58
2:B:227:TRP:HE1	2:B:289:GLN:NE2	2.01	0.58
2:B:292:LYS:O	2:B:295:GLN:HG3	2.03	0.58
4:D:243:PHE:O	4:D:246:ARG:HG2	2.03	0.58
1:A:44:ARG:HD3	3:C:132:PRO:HD3	1.86	0.57
1:A:245:ASP:O	1:A:246:MET:HE2	2.03	0.57
1:A:289:THR:HB	1:A:393:ILE:HD11	1.86	0.57
4:D:190:GLU:HG3	4:D:191:ARG:NH2	2.18	0.57
1:A:203:ARG:O	1:A:203:ARG:HD3	2.04	0.57
4:D:539:VAL:HG12	5:E:33:TRP:CE3	2.38	0.57
4:D:332:GLY:O	4:D:335:GLU:HG3	2.05	0.57
1:A:27:ALA:HB2	1:A:51:LEU:HD11	1.85	0.57
4:D:620:TYR:CE2	4:D:625:LEU:HD23	2.40	0.57
1:A:44:ARG:HH22	3:C:129:GLY:HA2	1.69	0.57
1:A:155:VAL:HB	1:A:175:PHE:CE2	2.39	0.57
5:E:87:TRP:HE3	5:E:91:ARG:HB2	1.70	0.57
4:D:134:ASN:ND2	4:D:160:TYR:HB2	2.20	0.56
4:D:620:TYR:CD2	4:D:625:LEU:HD23	2.40	0.56
1:A:110:THR:HG21	1:A:172:GLU:HG2	1.86	0.56
4:D:353:GLU:OE2	4:D:354:LYS:HG2	2.04	0.56
1:A:82:HIS:O	1:A:85:VAL:HG22	2.04	0.56
1:A:290:VAL:HA	1:A:366:ASP:HB2	1.87	0.56
5:E:92:GLN:HG3	5:E:101:TRP:HZ2	1.69	0.56
2:B:229:LYS:HB3	2:B:280:SER:HB3	1.88	0.56
4:D:642:ILE:HD11	4:D:688:MET:HE3	1.87	0.56
1:A:25:ASN:HD22	4:D:56:VAL:HG11	1.70	0.56
2:B:238:CYS:HB3	2:B:264:VAL:HB	1.87	0.56
4:D:427:ASP:CG	4:D:473:ARG:HH12	2.14	0.56
1:A:36:PHE:HE2	3:C:120:CYS:SG	2.27	0.55
1:A:164:ARG:HD3	1:A:165:PRO:O	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:453:PHE:HA	4:D:456:ILE:HD13	1.88	0.55
4:D:412:ALA:HB1	4:D:417:LYS:HD2	1.87	0.55
1:A:247:ASN:HB2	1:A:377:LYS:NZ	2.21	0.55
4:D:46:TYR:N	4:D:136:ILE:HD11	2.21	0.55
1:A:78:HIS:CD2	1:A:79:LEU:H	2.25	0.55
1:A:299:GLU:HA	1:A:302:ALA:HB3	1.88	0.55
4:D:269:LEU:HG	4:D:273:ARG:HH11	1.72	0.55
1:A:18:ARG:NH1	4:D:9:PRO:HG2	2.21	0.55
1:A:224:GLY:O	1:A:254:GLN:HG2	2.07	0.54
1:A:244:SER:HB3	1:A:250:LEU:HD21	1.89	0.54
4:D:489:ILE:HG22	4:D:493:LYS:NZ	2.22	0.54
1:A:376:ARG:N	1:A:377:LYS:HZ3	2.06	0.54
4:D:37:MET:HE2	4:D:42:TYR:HA	1.90	0.54
4:D:621:THR:HG22	4:D:668:LEU:HD23	1.90	0.54
3:C:65:HIS:CE1	3:C:68:ASP:H	2.25	0.54
1:A:254:GLN:CB	1:A:361:GLY:HA3	2.38	0.54
4:D:502:SER:HA	4:D:505:GLN:HG3	1.90	0.53
3:C:104:ILE:HG13	3:C:105:LEU:HD22	1.90	0.53
4:D:355:CYS:HB3	4:D:366:TYR:HD1	1.74	0.53
1:A:329:ARG:NH1	1:A:390:TYR:C	2.67	0.53
3:C:26:THR:HG23	3:C:111:ASP:HB3	1.90	0.53
4:D:719:MET:SD	4:D:725:LEU:HD12	2.48	0.53
4:D:364:LYS:HE3	4:D:428:SER:OG	2.08	0.53
1:A:74:ALA:H	1:A:166:GLN:NE2	2.07	0.53
4:D:452:VAL:O	4:D:456:ILE:HD12	2.09	0.53
1:A:37:LEU:HG	1:A:41:ALA:HB3	1.90	0.53
4:D:580:THR:OG1	5:E:32:LEU:HB2	2.09	0.53
1:A:20:THR:OG1	3:C:140:ASN:HB2	2.08	0.52
1:A:346:ARG:HB3	1:A:346:ARG:NH1	2.25	0.52
4:D:295:LEU:HA	4:D:298:LYS:NZ	2.24	0.52
4:D:133:LEU:O	4:D:136:ILE:HG22	2.09	0.52
1:A:26:LEU:O	1:A:29:VAL:HG22	2.09	0.52
5:E:23:GLU:HG3	5:E:24:VAL:H	1.73	0.52
1:A:323:MET:HB3	1:A:356:GLY:CA	2.40	0.52
4:D:131:LYS:HE2	4:D:131:LYS:HA	1.92	0.52
4:D:407:ALA:HA	4:D:410:LYS:HG2	1.91	0.52
1:A:17:PRO:HG2	1:A:18:ARG:HH11	1.75	0.52
4:D:313:ALA:O	4:D:314:ASP:OD1	2.28	0.52
3:C:82:THR:HG23	3:C:125:ASN:HD21	1.75	0.52
4:D:269:LEU:HG	4:D:273:ARG:NH1	2.25	0.52
4:D:445:THR:HA	4:D:448:GLN:OE1	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:285:GLU:H	2:B:289:GLN:NE2	2.08	0.51
4:D:190:GLU:HG3	4:D:191:ARG:HH22	1.75	0.51
4:D:465:PHE:HE1	4:D:696:GLN:HE21	1.59	0.51
4:D:560:GLU:HA	4:D:563:TYR:HB3	1.93	0.51
4:D:463:GLN:HG2	4:D:500:TYR:CE1	2.45	0.51
1:A:306:MET:HE3	1:A:344:ALA:O	2.09	0.51
4:D:533:LEU:HG	4:D:535:PHE:CB	2.40	0.51
4:D:533:LEU:HG	4:D:535:PHE:HB2	1.92	0.51
4:D:345:HIS:CE1	4:D:402:PHE:CD1	2.98	0.51
5:E:92:GLN:CD	5:E:101:TRP:HE1	2.19	0.51
1:A:254:GLN:H	1:A:361:GLY:CA	2.24	0.51
4:D:18:ASP:OD2	4:D:19:GLN:N	2.44	0.51
4:D:482:ASP:OD1	4:D:483:ASP:N	2.44	0.51
1:A:228:CYS:HA	1:A:232:ALA:CB	2.41	0.50
6:A:501:A1J21:O38	2:B:269:ASP:OD2	2.29	0.50
2:B:337:VAL:HA	2:B:340:ARG:HG2	1.93	0.50
5:E:87:TRP:CZ3	5:E:91:ARG:HD2	2.37	0.50
4:D:409:THR:HG23	4:D:410:LYS:HD3	1.92	0.50
4:D:335:GLU:OE2	4:D:336:LEU:HD22	2.11	0.50
3:C:23:GLN:HE22	3:C:62:CYS:HB3	1.76	0.50
1:A:145:VAL:HG12	1:A:262:THR:HG21	1.93	0.50
1:A:186:LYS:CD	1:A:188:GLN:HG2	2.40	0.50
1:A:192:PHE:HE2	1:A:206:LEU:HD13	1.77	0.50
4:D:574:HIS:CD2	4:D:577:ARG:HH21	2.30	0.50
4:D:441:GLU:HG2	4:D:442:LEU:N	2.25	0.50
4:D:518:ASN:HA	4:D:521:PHE:HE2	1.75	0.50
4:D:427:ASP:CG	4:D:469:MET:HB3	2.37	0.50
1:A:73:LEU:HD12	1:A:166:GLN:NE2	2.15	0.49
2:B:238:CYS:O	2:B:239:MET:HE2	2.11	0.49
3:C:25:VAL:HB	3:C:111:ASP:OD2	2.12	0.49
4:D:620:TYR:CZ	4:D:624:GLN:HG3	2.47	0.49
1:A:18:ARG:H	1:A:18:ARG:HD2	1.77	0.49
1:A:106:ALA:O	1:A:149:VAL:HA	2.12	0.49
1:A:240:VAL:HA	1:A:243:PHE:HE1	1.77	0.49
3:C:90:GLN:O	3:C:94:LYS:HD3	2.12	0.49
3:C:133:GLU:O	3:C:137:LYS:HG2	2.12	0.49
4:D:364:LYS:HA	4:D:425:TYR:HD1	1.76	0.49
4:D:363:PRO:HG2	4:D:364:LYS:HD3	1.93	0.49
4:D:524:HIS:HB2	4:D:569:PHE:CZ	2.47	0.49
1:A:326:CYS:HB2	1:A:362:GLU:OE2	2.13	0.49
4:D:700:HIS:HA	4:D:703:ILE:HD12	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ARG:O	1:A:377:LYS:HG3	2.12	0.49
3:C:34:LEU:HA	3:C:36:MET:HE1	1.95	0.49
4:D:508:PHE:CE1	4:D:511:ILE:HD11	2.48	0.49
3:C:28:LYS:O	3:C:32:GLU:HG3	2.13	0.49
4:D:292:GLU:O	4:D:296:ILE:HG12	2.12	0.49
4:D:460:ASP:O	4:D:463:GLN:HG3	2.13	0.49
3:C:47:LEU:HD12	3:C:109:TYR:HE2	1.78	0.49
4:D:143:HIS:HA	4:D:146:ARG:NH2	2.27	0.49
1:A:154:VAL:HG22	1:A:167:GLU:HG3	1.93	0.48
4:D:22:ASP:HA	4:D:25:ARG:NH1	2.27	0.48
4:D:758:GLU:OE1	4:D:759:LYS:HD2	2.13	0.48
4:D:168:ARG:HA	4:D:172:PHE:HB3	1.95	0.48
1:A:28:GLU:HB2	4:D:143:HIS:HD2	1.78	0.48
2:B:236:TRP:CD2	2:B:237:PRO:HD2	2.49	0.48
3:C:24:SER:CB	3:C:27:ILE:HG12	2.40	0.48
1:A:304:ALA:HB1	1:A:308:ARG:HH12	1.78	0.48
1:A:158:MET:HE3	1:A:158:MET:O	2.14	0.48
1:A:244:SER:CB	1:A:250:LEU:HD21	2.44	0.48
4:D:121:GLN:O	4:D:124:GLU:HG3	2.13	0.48
4:D:651:LEU:HB3	4:D:653:ASP:H	1.79	0.48
1:A:78:HIS:CD2	1:A:79:LEU:HD23	2.49	0.48
4:D:87:GLU:HA	4:D:90:LYS:NZ	2.28	0.48
1:A:325:ALA:HB3	1:A:358:PHE:CZ	2.49	0.48
2:B:338:GLU:O	2:B:341:LYS:HG3	2.13	0.48
4:D:406:ASN:O	4:D:409:THR:HG22	2.14	0.48
4:D:499:GLU:HG2	4:D:500:TYR:N	2.29	0.48
4:D:446:LEU:O	4:D:450:MET:HG2	2.14	0.47
4:D:427:ASP:OD1	4:D:469:MET:HB3	2.12	0.47
4:D:672:TYR:HD2	4:D:674:GLY:H	1.58	0.47
4:D:589:GLU:HG2	4:D:602:GLN:HE22	1.78	0.47
1:A:292:LEU:CB	1:A:392:THR:HB	2.45	0.47
2:B:226:VAL:HB	2:B:281:LEU:HD12	1.96	0.47
3:C:21:ALA:HA	3:C:27:ILE:HD12	1.97	0.47
3:C:154:ARG:O	3:C:154:ARG:NH1	2.47	0.47
4:D:382:MET:HG2	4:D:387:ASN:HB3	1.96	0.47
5:E:47:ASN:HD22	5:E:80:HIS:CD2	2.31	0.47
1:A:78:HIS:HE1	1:A:86:ARG:HD3	1.80	0.47
4:D:649:LEU:HD11	5:E:22:PHE:CZ	2.49	0.47
5:E:93:VAL:HA	5:E:101:TRP:HH2	1.79	0.47
4:D:220:ALA:O	4:D:221:LYS:HE2	2.15	0.47
4:D:496:CYS:SG	4:D:500:TYR:HB3	2.55	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:546:PRO:HD2	4:D:547:PHE:CD1	2.49	0.47
1:A:190:PHE:CZ	1:A:277:GLY:HA3	2.50	0.46
3:C:86:PRO:HD2	3:C:89:ASP:OD2	2.15	0.46
1:A:54:GLU:O	1:A:58:ARG:HG2	2.15	0.46
4:D:464:LYS:HG3	4:D:468:LYS:NZ	2.29	0.46
1:A:291:LEU:HD12	1:A:392:THR:O	2.16	0.46
1:A:188:GLN:O	1:A:278:LEU:HD12	2.16	0.46
1:A:324:PHE:HB2	1:A:393:ILE:HG23	1.97	0.46
1:A:78:HIS:HD2	1:A:79:LEU:H	1.62	0.46
2:B:335:MET:CG	2:B:340:ARG:HB3	2.41	0.46
4:D:238:ALA:O	4:D:241:GLU:HG3	2.15	0.46
1:A:37:LEU:HD12	1:A:38:PRO:HD2	1.97	0.46
2:B:265:GLN:NE2	2:B:266:PHE:O	2.49	0.46
1:A:102:VAL:HG13	1:A:145:VAL:HG23	1.98	0.46
4:D:266:ALA:O	4:D:270:GLU:HG2	2.16	0.46
1:A:167:GLU:CD	1:A:339:ASN:HA	2.40	0.46
1:A:28:GLU:HG3	4:D:139:TYR:OH	2.16	0.46
4:D:461:VAL:HG13	4:D:464:LYS:NZ	2.29	0.46
4:D:571:ALA:HA	4:D:574:HIS:CE1	2.51	0.45
5:E:98:ASN:O	5:E:101:TRP:HZ3	2.00	0.45
1:A:166:GLN:HA	1:A:339:ASN:ND2	2.32	0.45
1:A:323:MET:HE3	1:A:325:ALA:HB2	1.97	0.45
4:D:473:ARG:HB2	4:D:473:ARG:CZ	2.45	0.45
1:A:73:LEU:CD1	1:A:166:GLN:HE22	2.16	0.45
2:B:239:MET:HE2	2:B:239:MET:HA	1.97	0.45
3:C:124:ALA:O	3:C:127:ILE:HG22	2.16	0.45
1:A:22:VAL:HA	1:A:26:LEU:HD12	1.99	0.45
1:A:48:VAL:HG13	3:C:136:ARG:HH11	1.82	0.45
1:A:228:CYS:HA	1:A:232:ALA:HB1	1.97	0.45
3:C:18:VAL:HG22	3:C:22:LYS:NZ	2.31	0.45
4:D:463:GLN:HB3	4:D:500:TYR:CZ	2.51	0.45
2:B:246:LEU:HG	2:B:248:SER:HB3	1.99	0.45
4:D:104:LEU:HD13	4:D:171:LEU:HD12	1.99	0.45
4:D:541:SER:C	4:D:545:TRP:HE1	2.24	0.45
1:A:236:LEU:O	1:A:240:VAL:HG13	2.17	0.45
1:A:247:ASN:HB2	1:A:377:LYS:HD3	1.99	0.45
1:A:329:ARG:HH11	1:A:391:THR:HA	1.81	0.45
4:D:142:ARG:CZ	4:D:143:HIS:HE1	2.30	0.45
4:D:490:SER:HA	4:D:493:LYS:NZ	2.32	0.45
4:D:609:ALA:O	4:D:613:GLN:HG3	2.17	0.45
1:A:52:TRP:CD1	1:A:52:TRP:N	2.86	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLU:O	1:A:168:ILE:HD13	2.16	0.45
1:A:196:PRO:HG2	1:A:197:LYS:NZ	2.32	0.45
2:B:346:PHE:CD1	2:B:355:LEU:HA	2.52	0.45
4:D:367:VAL:HG11	4:D:425:TYR:CG	2.52	0.45
4:D:44:GLU:HG3	4:D:48:HIS:NE2	2.32	0.44
4:D:275:VAL:HA	4:D:279:LEU:CD1	2.47	0.44
1:A:50:ARG:HG2	1:A:50:ARG:HH11	1.82	0.44
2:B:225:LEU:CB	2:B:284:PHE:HB3	2.44	0.44
4:D:465:PHE:O	4:D:469:MET:HG2	2.17	0.44
4:D:582:LEU:HB2	5:E:30:VAL:HG13	1.98	0.44
1:A:37:LEU:HB3	1:A:42:LEU:HD13	1.98	0.44
1:A:329:ARG:NH1	1:A:390:TYR:O	2.51	0.44
4:D:366:TYR:O	4:D:370:VAL:HG23	2.17	0.44
3:C:5:LYS:HA	3:C:5:LYS:HD2	1.83	0.44
1:A:205:GLN:O	1:A:208:GLU:HG2	2.17	0.44
4:D:22:ASP:HA	4:D:25:ARG:CZ	2.48	0.44
4:D:325:LEU:O	4:D:328:ARG:HG2	2.18	0.44
1:A:292:LEU:HB2	1:A:392:THR:HB	2.00	0.44
4:D:376:LYS:HG3	4:D:377:TYR:N	2.33	0.44
1:A:299:GLU:HG3	1:A:340:VAL:CG2	2.47	0.44
5:E:96:LEU:HG	5:E:97:ASP:H	1.83	0.44
4:D:464:LYS:NZ	4:D:465:PHE:CE2	2.86	0.44
1:A:187:ILE:HD12	1:A:280:PHE:HD1	1.83	0.43
4:D:341:GLU:OE2	4:D:342:THR:HG23	2.18	0.43
4:D:496:CYS:SG	4:D:500:TYR:CD2	3.05	0.43
1:A:140:PRO:HD3	3:C:159:TRP:CH2	2.54	0.43
1:A:325:ALA:HB3	1:A:358:PHE:CE1	2.53	0.43
1:A:182:ILE:CG2	1:A:185:ILE:HB	2.48	0.43
4:D:355:CYS:HB3	4:D:366:TYR:CD1	2.51	0.43
4:D:542:SER:HA	4:D:545:TRP:CD1	2.53	0.43
1:A:28:GLU:HB2	4:D:143:HIS:CD2	2.53	0.43
3:C:22:LYS:HB3	3:C:28:LYS:HZ1	1.83	0.43
4:D:299:HIS:O	4:D:302:ILE:HG22	2.17	0.43
4:D:307:PHE:CD1	4:D:336:LEU:HD12	2.53	0.43
4:D:498:PHE:CG	4:D:499:GLU:N	2.86	0.43
4:D:503:LYS:O	4:D:507:MET:HG3	2.18	0.43
4:D:756:LEU:HB3	4:D:762:LEU:HD23	2.00	0.43
4:D:297:GLU:HG2	4:D:298:LYS:N	2.33	0.43
4:D:415:SER:O	4:D:419:PRO:HD2	2.18	0.43
4:D:275:VAL:HG23	4:D:279:LEU:HD13	2.00	0.43
4:D:507:MET:HG2	4:D:544:SER:HB3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ARG:HB3	1:A:346:ARG:CZ	2.48	0.43
4:D:431:LYS:HD2	4:D:432:LYS:H	1.84	0.43
5:E:35:TRP:O	5:E:50:MET:HE1	2.19	0.43
1:A:78:HIS:HE1	1:A:86:ARG:CD	2.32	0.42
1:A:174:GLY:C	1:A:175:PHE:CD1	2.97	0.42
1:A:186:LYS:HE3	1:A:186:LYS:HB3	1.88	0.42
1:A:306:MET:O	1:A:309:LEU:HB2	2.19	0.42
1:A:307:GLN:OE1	1:A:348:PHE:CD2	2.72	0.42
3:C:20:ILE:HA	3:C:23:GLN:CD	2.43	0.42
4:D:144:TRP:O	4:D:147:ARG:HG2	2.19	0.42
1:A:299:GLU:HG3	1:A:340:VAL:HG21	2.00	0.42
3:C:110:LEU:O	3:C:111:ASP:HB3	2.19	0.42
1:A:140:PRO:HA	3:C:159:TRP:O	2.19	0.42
1:A:153:ILE:HG13	1:A:154:VAL:N	2.33	0.42
1:A:247:ASN:H	1:A:375:LEU:HD23	1.84	0.42
4:D:100:LEU:HD12	4:D:166:THR:HG22	2.00	0.42
4:D:273:ARG:HH11	4:D:273:ARG:HG3	1.83	0.42
1:A:74:ALA:HB2	1:A:166:GLN:CG	2.42	0.42
1:A:290:VAL:HB	1:A:309:LEU:HD23	2.02	0.42
1:A:332:GLN:OE1	1:A:332:GLN:N	2.53	0.42
1:A:191:HIS:O	1:A:192:PHE:CD1	2.73	0.42
4:D:332:GLY:C	4:D:336:LEU:HD23	2.44	0.42
4:D:535:PHE:CE2	4:D:537:ILE:HB	2.53	0.42
3:C:54:ILE:HG13	3:C:57:LYS:NZ	2.34	0.42
4:D:233:GLU:OE2	4:D:283:THR:HG22	2.20	0.42
4:D:364:LYS:HD2	4:D:425:TYR:HD1	1.85	0.42
4:D:191:ARG:HA	4:D:191:ARG:NE	2.35	0.42
1:A:375:LEU:HB3	1:A:377:LYS:NZ	2.35	0.42
1:A:187:ILE:HD12	1:A:280:PHE:CD1	2.55	0.42
3:C:150:GLU:HA	3:C:153:VAL:HG22	2.00	0.42
4:D:272:GLN:HA	4:D:284:GLN:OE1	2.20	0.42
4:D:540:LEU:HD23	4:D:545:TRP:CD2	2.55	0.42
4:D:703:ILE:HD13	4:D:703:ILE:HG21	1.80	0.42
1:A:53:ARG:HD2	1:A:54:GLU:N	2.35	0.41
4:D:445:THR:O	4:D:449:VAL:HG23	2.20	0.41
4:D:498:PHE:CZ	5:E:61:ALA:HA	2.55	0.41
1:A:98:LEU:HD23	1:A:99:PRO:O	2.19	0.41
2:B:225:LEU:HD13	2:B:284:PHE:HD2	1.85	0.41
3:C:1:MET:HG2	3:C:2:PRO:O	2.20	0.41
5:E:87:TRP:CE3	5:E:91:ARG:HB2	2.52	0.41
1:A:201:LEU:HD11	1:A:206:LEU:HD21	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:376:LYS:HG3	4:D:377:TYR:HD1	1.85	0.41
3:C:101:PHE:O	3:C:104:ILE:HG12	2.20	0.41
4:D:258:THR:HG22	4:D:261:MET:HE2	2.03	0.41
4:D:343:HIS:O	4:D:347:GLN:HG2	2.20	0.41
4:D:540:LEU:HB3	4:D:545:TRP:CZ2	2.54	0.41
5:E:23:GLU:HG3	5:E:24:VAL:N	2.34	0.41
1:A:362:GLU:C	1:A:363:ILE:HD12	2.45	0.41
2:B:358:GLN:HG3	2:B:361:LYS:HE3	2.02	0.41
3:C:132:PRO:HB3	3:C:136:ARG:HH12	1.86	0.41
4:D:547:PHE:CE2	4:D:582:LEU:HD13	2.55	0.41
1:A:398:HIS:CE1	1:A:400:GLY:H	2.39	0.41
4:D:41:ARG:HH21	4:D:44:GLU:CG	2.29	0.41
4:D:41:ARG:HA	4:D:41:ARG:NE	2.36	0.41
4:D:110:LEU:HB3	4:D:114:SER:OG	2.21	0.41
4:D:117:LYS:HG3	4:D:118:PHE:N	2.36	0.41
1:A:174:GLY:O	1:A:175:PHE:CD1	2.74	0.41
3:C:64:HIS:HA	3:C:88:TRP:CZ3	2.56	0.41
3:C:154:ARG:NH1	3:C:158:GLN:HB2	2.35	0.41
4:D:364:LYS:HD2	4:D:425:TYR:CD1	2.56	0.41
4:D:638:GLN:O	4:D:641:GLN:HG2	2.21	0.41
1:A:48:VAL:HG22	3:C:132:PRO:HB3	2.02	0.41
1:A:110:THR:HA	1:A:113:SER:OG	2.20	0.41
1:A:167:GLU:OE2	1:A:339:ASN:HA	2.21	0.41
2:B:324:MET:C	2:B:324:MET:SD	3.04	0.41
2:B:337:VAL:HG12	2:B:340:ARG:HH21	1.86	0.41
3:C:6:LEU:HD13	3:C:45:VAL:HG23	2.03	0.41
3:C:18:VAL:C	3:C:22:LYS:HZ2	2.28	0.41
3:C:45:VAL:HA	3:C:46:PRO:HD3	1.67	0.41
4:D:201:ILE:HG13	4:D:202:SER:N	2.36	0.41
4:D:625:LEU:HD11	4:D:640:LEU:HD21	2.02	0.41
1:A:306:MET:SD	1:A:348:PHE:HD2	2.44	0.41
3:C:54:ILE:HA	3:C:57:LYS:NZ	2.33	0.41
1:A:83:CYS:SG	1:A:173:SER:HA	2.60	0.40
1:A:306:MET:HE2	1:A:306:MET:HB2	1.89	0.40
4:D:46:TYR:OH	4:D:139:TYR:HB2	2.21	0.40
4:D:136:ILE:HD12	4:D:136:ILE:HA	1.93	0.40
4:D:507:MET:HG2	4:D:545:TRP:CZ3	2.56	0.40
4:D:648:LEU:C	4:D:649:LEU:HD12	2.46	0.40
1:A:167:GLU:C	1:A:168:ILE:HD13	2.47	0.40
3:C:65:HIS:CG	3:C:66:LYS:N	2.89	0.40
3:C:150:GLU:O	3:C:153:VAL:HG22	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ASN:OD1	1:A:26:LEU:HG	2.22	0.40
1:A:166:GLN:HA	1:A:339:ASN:HD21	1.87	0.40
1:A:191:HIS:O	1:A:192:PHE:HD1	2.05	0.40
1:A:18:ARG:CZ	4:D:9:PRO:HG2	2.52	0.40
4:D:198:THR:HA	4:D:201:ILE:HG12	2.03	0.40
4:D:605:THR:HA	4:D:608:MET:CG	2.52	0.40
1:A:153:ILE:HG13	1:A:154:VAL:H	1.85	0.40
1:A:194:LYS:HD3	1:A:195:ASP:N	2.36	0.40
2:B:346:PHE:CE1	2:B:355:LEU:HA	2.56	0.40
3:C:105:LEU:HA	3:C:105:LEU:HD13	1.91	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	372/403 (92%)	334 (90%)	38 (10%)	0	100	100
2	B	132/1365 (10%)	128 (97%)	4 (3%)	0	100	100
3	C	161/163 (99%)	143 (89%)	18 (11%)	0	100	100
4	D	770/776 (99%)	736 (96%)	34 (4%)	0	100	100
5	E	91/108 (84%)	76 (84%)	15 (16%)	0	100	100
All	All	1526/2815 (54%)	1417 (93%)	109 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	321/344 (93%)	320 (100%)	1 (0%)	86	85
2	B	109/1173 (9%)	109 (100%)	0	100	100
3	C	150/150 (100%)	150 (100%)	0	100	100
4	D	694/698 (99%)	694 (100%)	0	100	100
5	E	79/90 (88%)	79 (100%)	0	100	100
All	All	1353/2455 (55%)	1352 (100%)	1 (0%)	87	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	329	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	A	82	HIS
1	A	144	GLN
1	A	166	GLN
1	A	257	ASN
2	B	265	GLN
3	C	7	GLN
3	C	49	ASN
4	D	8	ASN
4	D	134	ASN
4	D	308	GLN
4	D	478	ASN
4	D	520	GLN
4	D	527	ASN
4	D	602	GLN
4	D	696	GLN
5	E	104	GLN

5.3.3 RNA ⓘ

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](#)

1 ligand is modelled in this entry.

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	$\# Z > 2$
6	A1J21	A	501	-	50,51,51	6.07	33 (66%)	56,70,70	4.73	31 (55%)

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
6	A1J21	A	501	-	1/1/9/12	13/42/56/56	0/4/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	501	A1J21	C32-C33	-19.25	1.28	1.51
6	A	501	A1J21	O38-C37	15.56	1.43	1.22
6	A	501	A1J21	C37-N36	14.12	1.51	1.37
6	A	501	A1J21	C19-C18	11.99	1.59	1.39
6	A	501	A1J21	C13-N15	11.03	1.52	1.34
6	A	501	A1J21	C49-C50	10.83	1.61	1.38
6	A	501	A1J21	C42-C32	-8.60	1.42	1.54
6	A	501	A1J21	C30-N29	7.58	1.52	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	501	A1J21	O40-C39	-7.19	1.27	1.42
6	A	501	A1J21	C48-C20	-6.83	1.27	1.39
6	A	501	A1J21	C16-C17	-6.79	1.33	1.52
6	A	501	A1J21	C12-C13	6.13	1.60	1.50
6	A	501	A1J21	C39-C37	-5.46	1.43	1.51
6	A	501	A1J21	C17-C18	-5.39	1.36	1.51
6	A	501	A1J21	C50-C18	5.31	1.50	1.38
6	A	501	A1J21	C22-N21	4.95	1.48	1.35
6	A	501	A1J21	C51-N15	4.95	1.62	1.45
6	A	501	A1J21	C19-C20	-4.47	1.32	1.39
6	A	501	A1J21	C28-C27	4.46	1.59	1.51
6	A	501	A1J21	C16-N15	-4.26	1.38	1.47
6	A	501	A1J21	C32-C30	4.06	1.59	1.52
6	A	501	A1J21	C20-N21	4.00	1.49	1.41
6	A	501	A1J21	O40-C41	-3.73	1.34	1.42
6	A	501	A1J21	C24-C22	3.67	1.57	1.50
6	A	501	A1J21	C34-C33	-3.11	1.25	1.32
6	A	501	A1J21	C28-N29	3.03	1.51	1.46
6	A	501	A1J21	C11-C10	2.61	1.43	1.38
6	A	501	A1J21	C45-C43	2.51	1.54	1.48
6	A	501	A1J21	C44-C43	2.47	1.54	1.48
6	A	501	A1J21	C41-C35	2.22	1.52	1.50
6	A	501	A1J21	C47-C46	2.17	1.42	1.38
6	A	501	A1J21	C07-C09	2.17	1.59	1.51
6	A	501	A1J21	C11-C12	2.09	1.42	1.39

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	501	A1J21	C41-O40-C39	17.24	126.68	111.15
6	A	501	A1J21	C12-C13-N15	12.78	138.51	118.54
6	A	501	A1J21	O14-C13-N15	-12.22	107.67	122.41
6	A	501	A1J21	C42-C32-C33	9.96	124.21	111.14
6	A	501	A1J21	C42-C32-C30	9.07	121.80	109.21
6	A	501	A1J21	C49-C50-C18	-7.95	108.43	120.63
6	A	501	A1J21	C27-C28-N29	6.94	126.25	113.54
6	A	501	A1J21	C17-C16-N15	6.23	131.14	111.93
6	A	501	A1J21	O31-C30-C32	-5.88	114.14	122.16
6	A	501	A1J21	C28-N29-C43	-5.58	112.50	118.33
6	A	501	A1J21	C51-N15-C13	5.03	137.02	122.96
6	A	501	A1J21	C16-N15-C13	-5.00	107.21	120.32
6	A	501	A1J21	C16-C17-C18	4.62	125.36	112.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	501	A1J21	O14-C13-C12	-3.94	112.57	120.23
6	A	501	A1J21	C50-C49-C48	3.86	125.72	120.25
6	A	501	A1J21	C11-C12-C13	3.36	128.81	120.29
6	A	501	A1J21	O38-C37-N36	3.18	124.03	119.67
6	A	501	A1J21	C24-C22-N21	3.16	122.88	115.92
6	A	501	A1J21	C17-C18-C19	3.02	125.50	120.54
6	A	501	A1J21	O31-C30-N29	-3.01	116.01	121.38
6	A	501	A1J21	C52-C12-C11	-2.93	114.41	118.59
6	A	501	A1J21	C49-C48-C20	2.91	123.21	119.72
6	A	501	A1J21	O08-C07-C09	2.82	122.43	112.03
6	A	501	A1J21	C53-C52-C12	2.66	123.88	120.78
6	A	501	A1J21	O23-C22-N21	-2.58	117.82	123.71
6	A	501	A1J21	C48-C20-C19	2.53	122.66	119.65
6	A	501	A1J21	C33-C32-C30	2.51	113.96	108.31
6	A	501	A1J21	C07-C09-C10	2.48	129.22	120.88
6	A	501	A1J21	C26-C25-C24	2.30	123.45	120.78
6	A	501	A1J21	C52-C12-C13	-2.04	115.12	120.29
6	A	501	A1J21	C07-C09-C53	-2.00	114.13	120.88

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	501	A1J21	C32

All (13) torsion outliers are listed below:

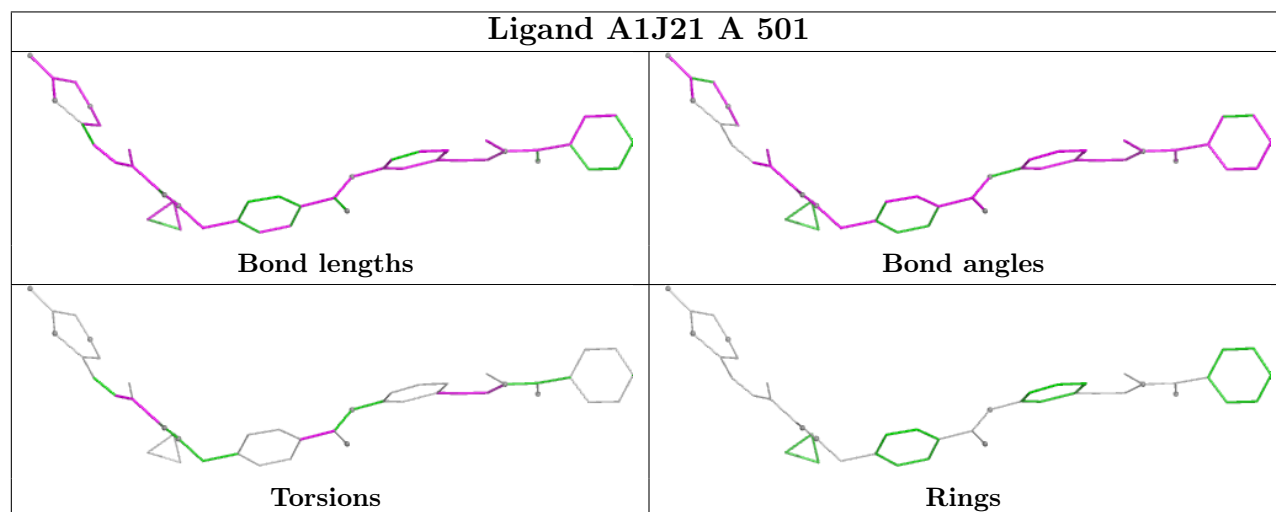
Mol	Chain	Res	Type	Atoms
6	A	501	A1J21	N15-C16-C17-C18
6	A	501	A1J21	C17-C16-N15-C13
6	A	501	A1J21	C17-C16-N15-C51
6	A	501	A1J21	N29-C30-C32-C42
6	A	501	A1J21	O31-C30-C32-C42
6	A	501	A1J21	C30-C32-C33-C34
6	A	501	A1J21	O23-C22-C24-C47
6	A	501	A1J21	N21-C22-C24-C47
6	A	501	A1J21	O23-C22-C24-C25
6	A	501	A1J21	N21-C22-C24-C25
6	A	501	A1J21	C16-C17-C18-C50
6	A	501	A1J21	C16-C17-C18-C19
6	A	501	A1J21	C42-C32-C33-C34

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	501	A1J21	5	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-57180. 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: 60



Y Index: 60



Z Index: 60

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

6.3 Largest variance slices [i](#)

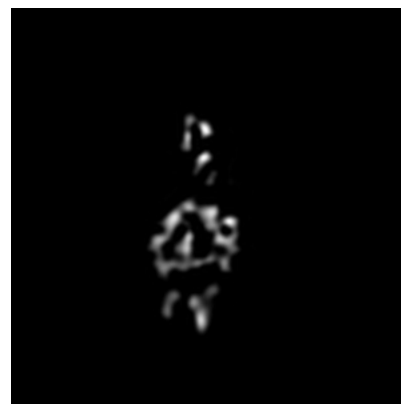
6.3.1 Primary map



X Index: 61



Y Index: 60



Z Index: 72

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

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

6.4.1 Primary map



X



Y

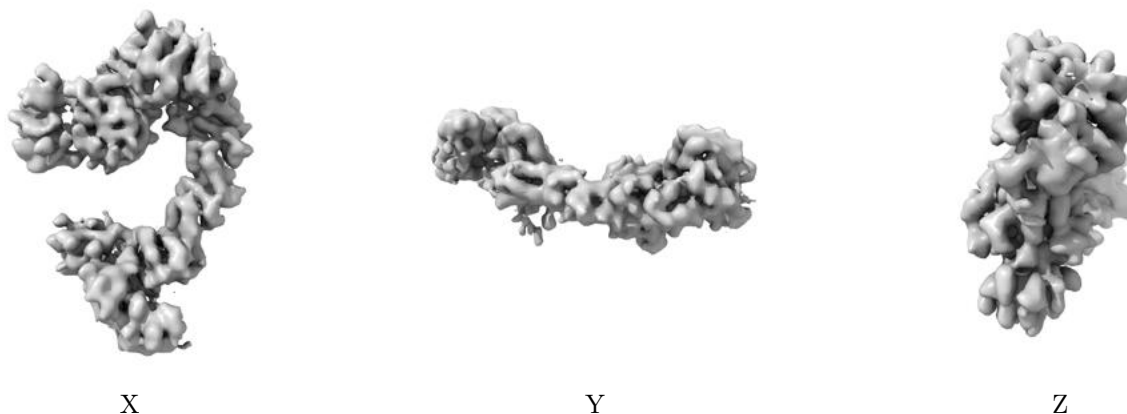


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

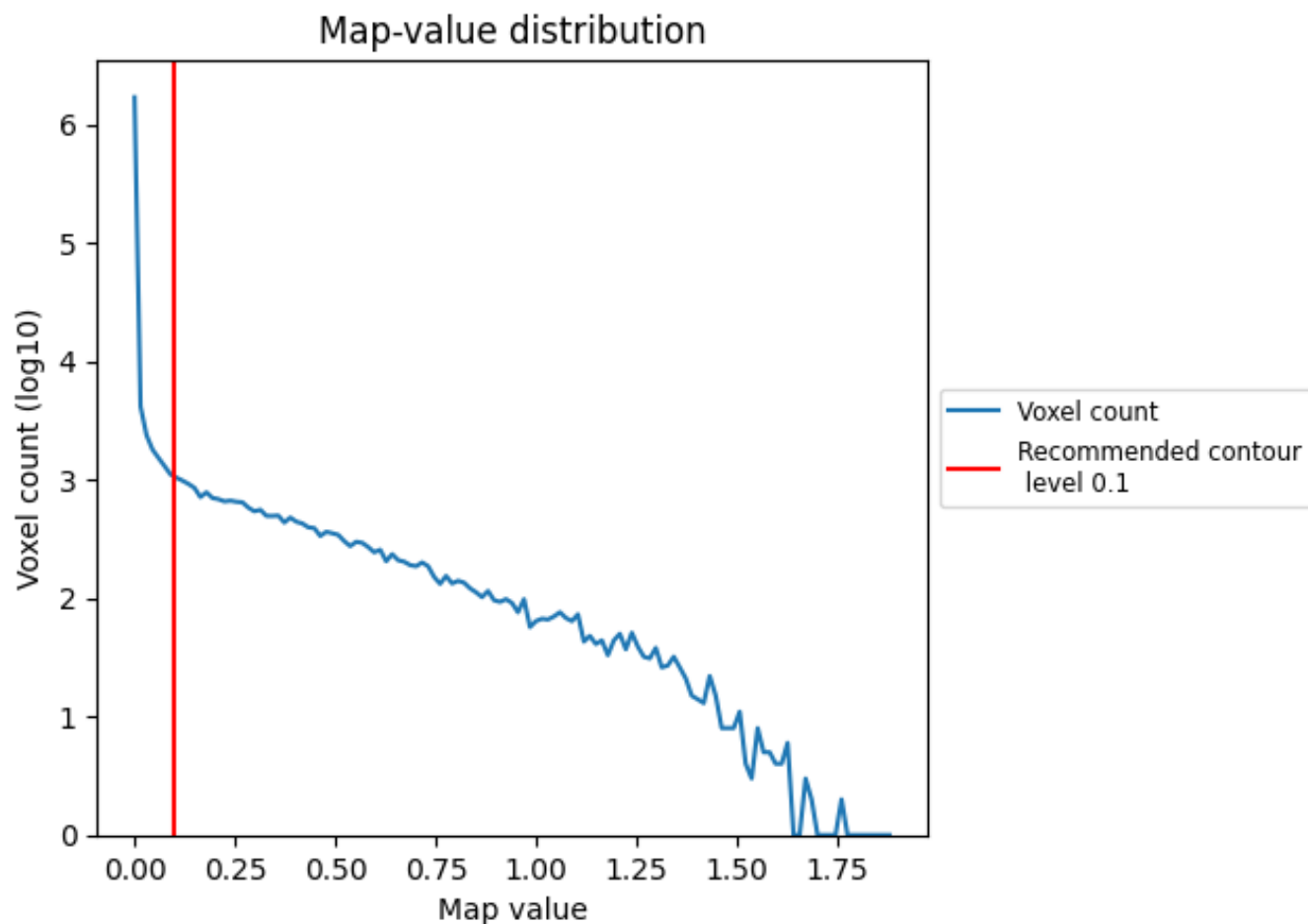
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

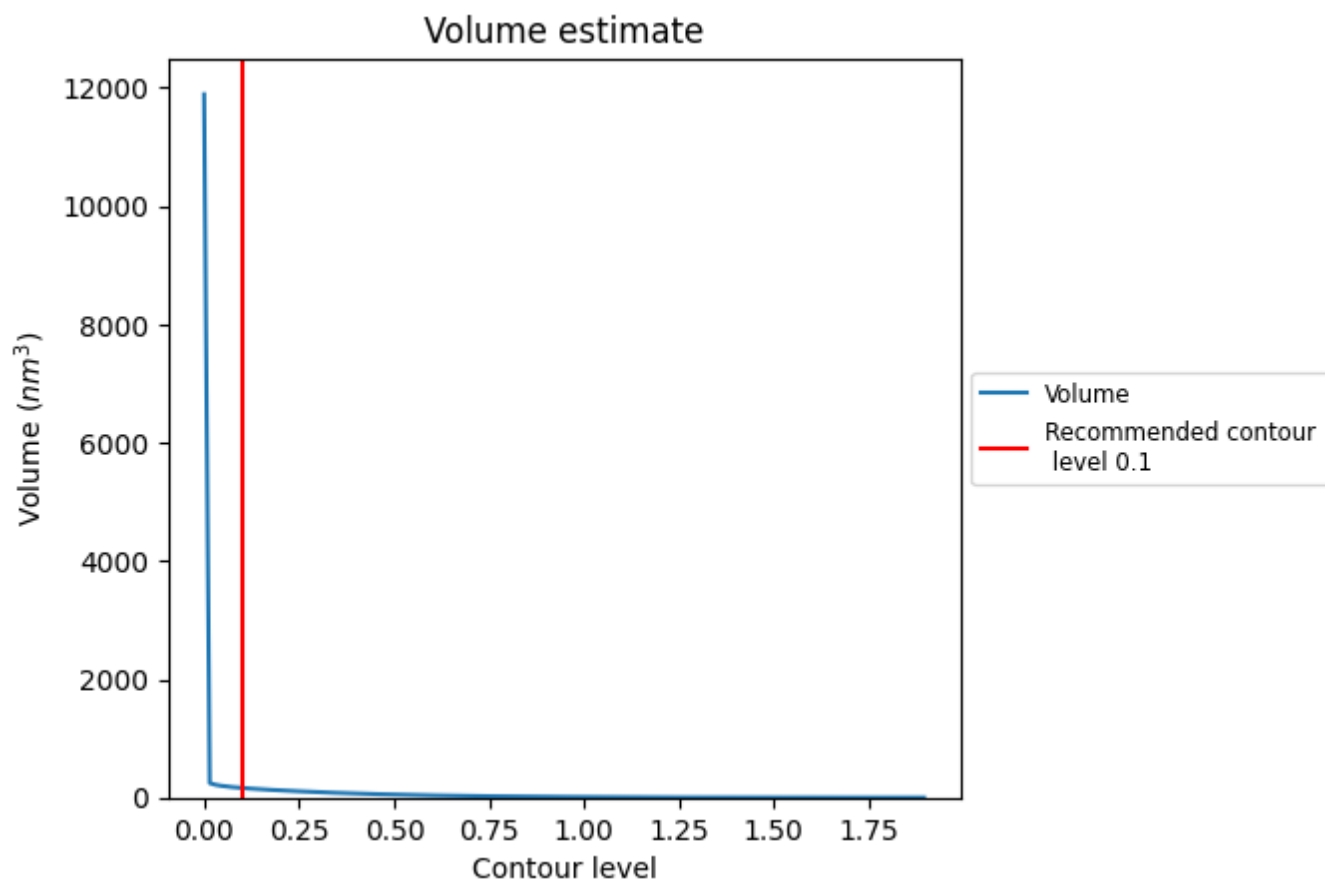
This section contains the results of statistical analysis of the map.

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.

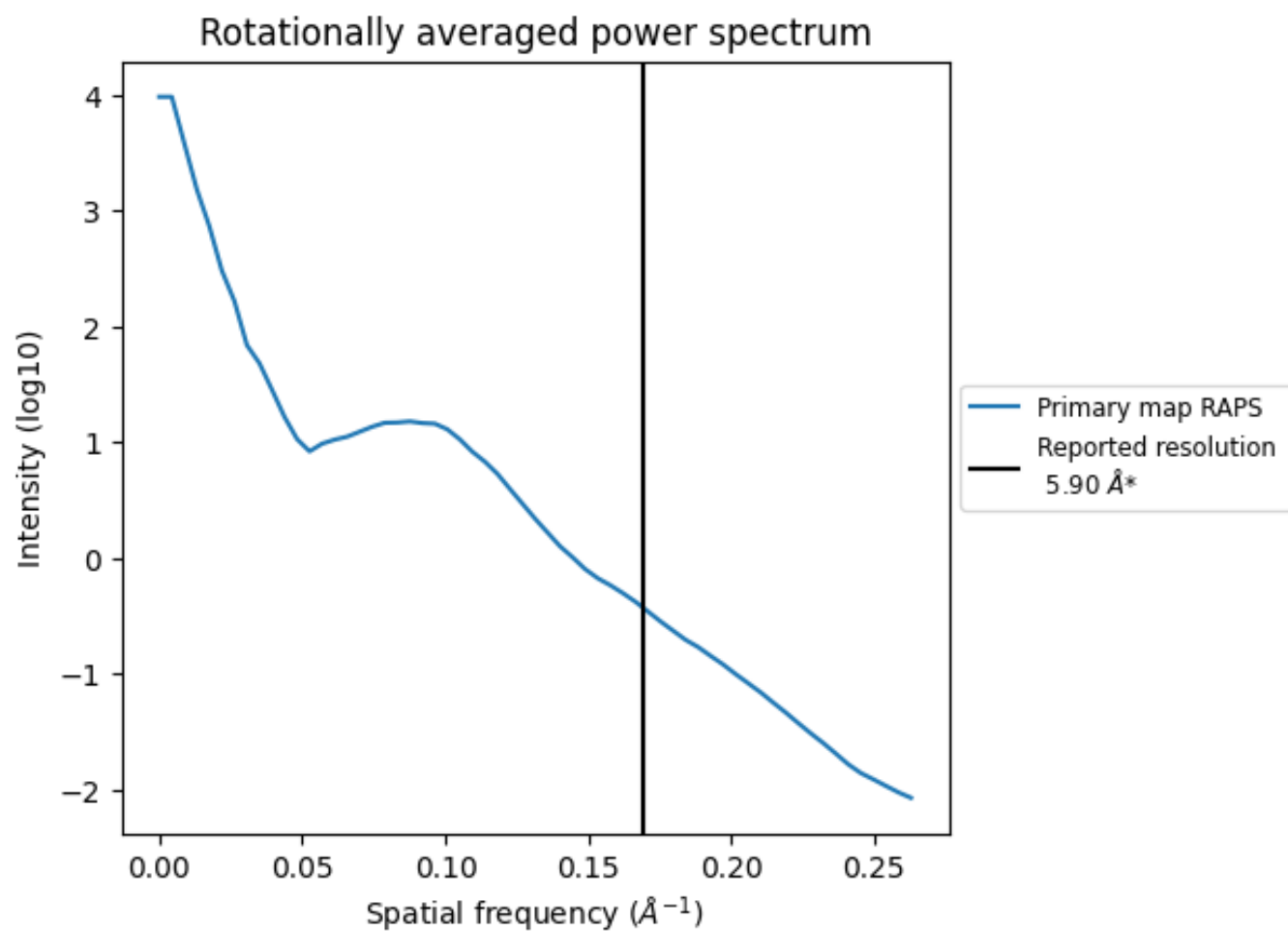
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 162 nm³; this corresponds to an approximate mass of 146 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 0.169 Å⁻¹

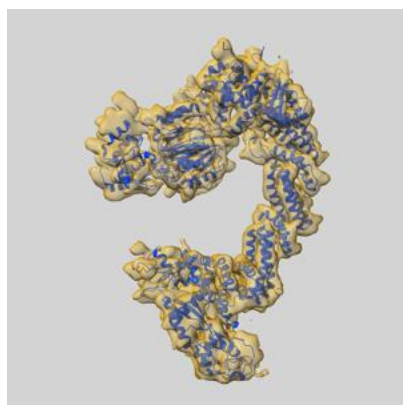
8 Fourier-Shell correlation

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

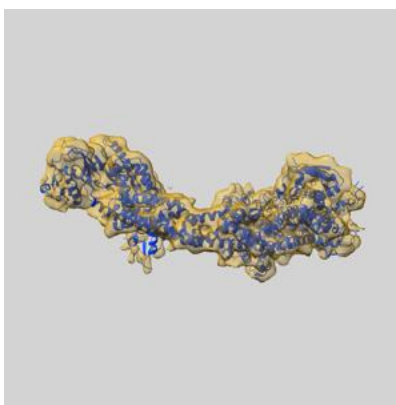
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-57180 and PDB model 29HI. Per-residue inclusion information can be found in section 3 on page 6.

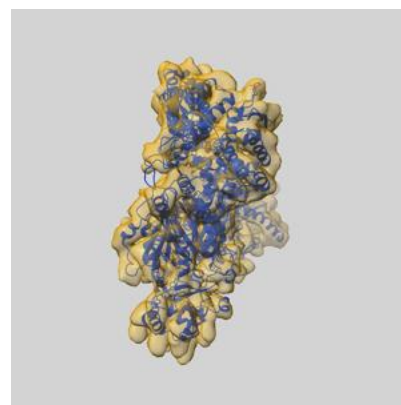
9.1 Map-model overlay [i](#)



X



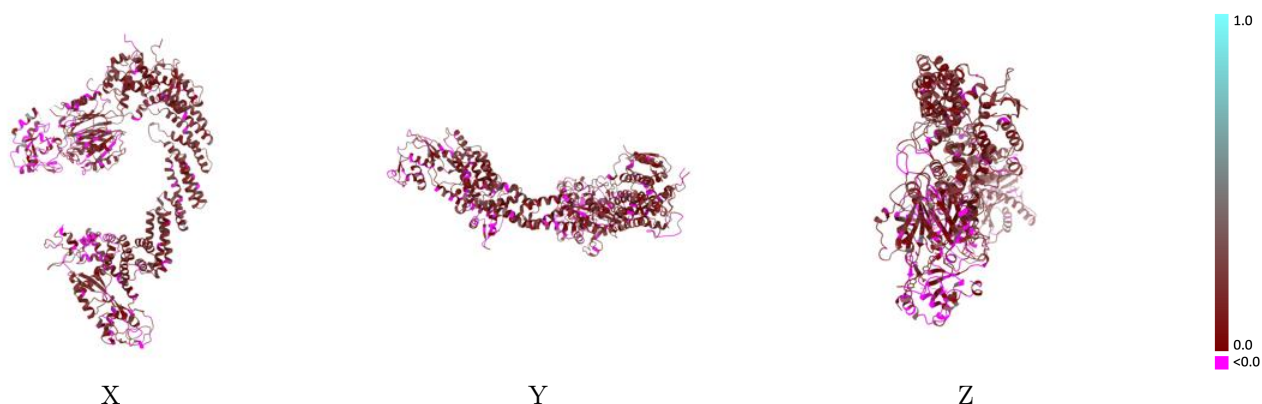
Y



Z

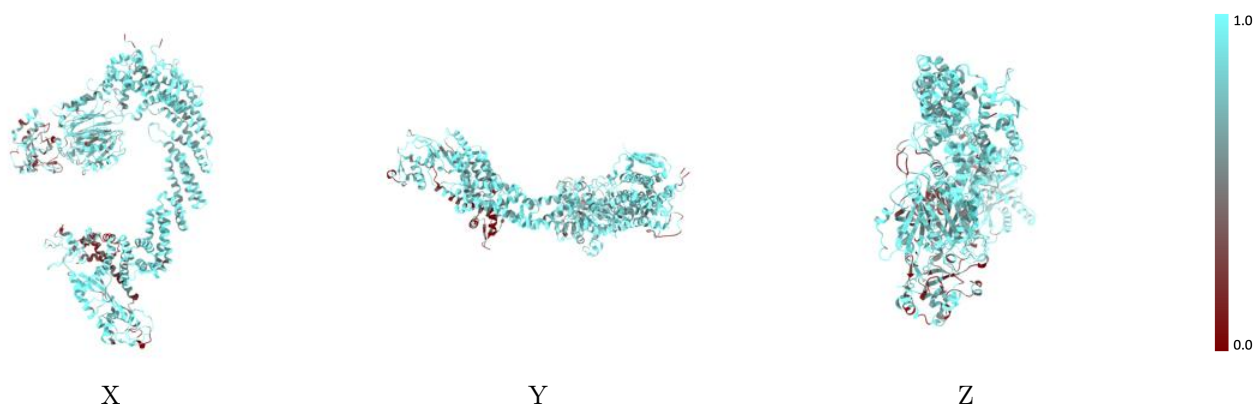
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



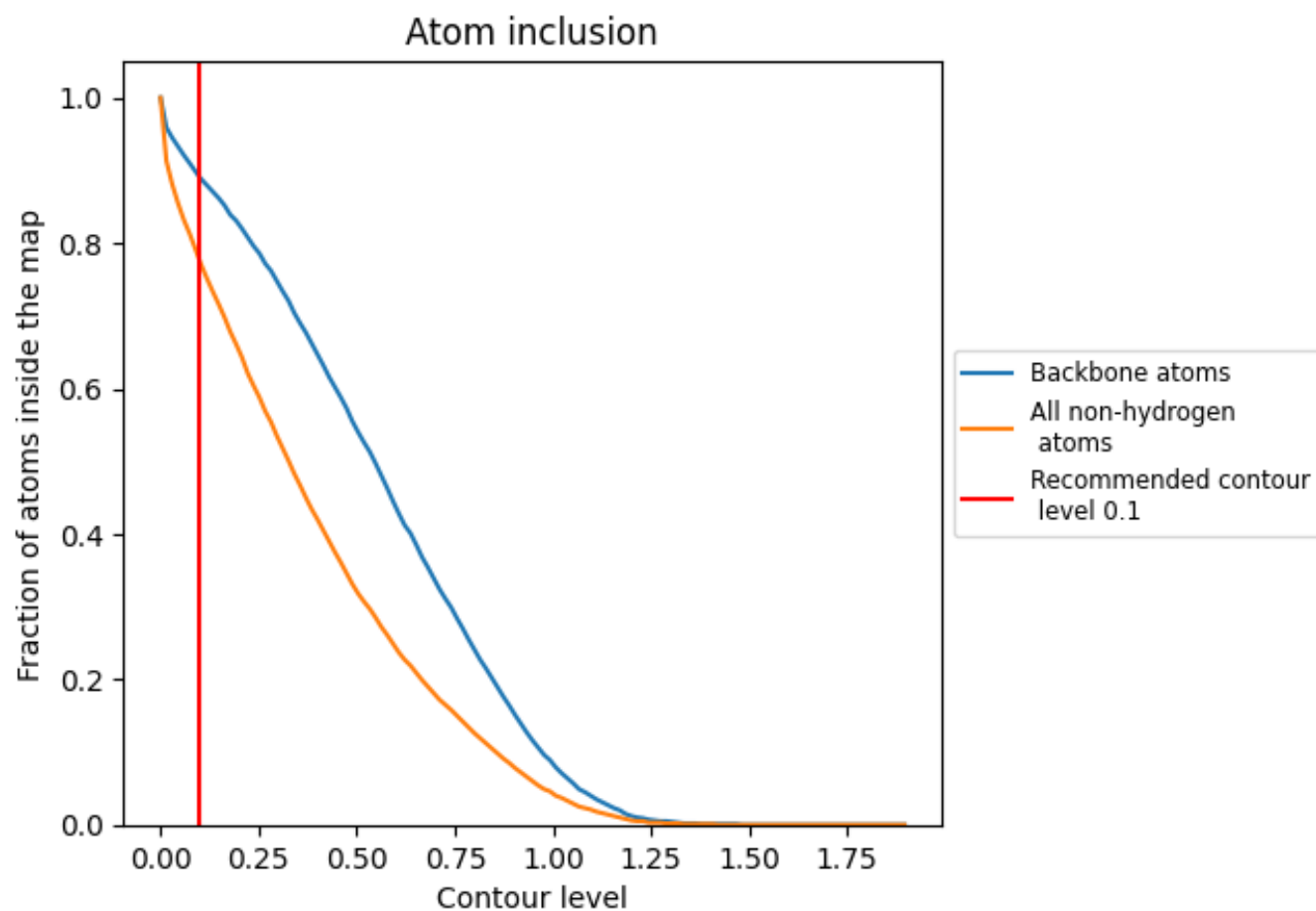
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion ⓘ



At the recommended contour level, 89% of all backbone atoms, 78% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7750	<div></div> 0.1290
A	<div></div> 0.8130	<div></div> 0.1200
B	<div></div> 0.5690	<div></div> -0.0040
C	<div></div> 0.8780	<div></div> 0.1880
D	<div></div> 0.7690	<div></div> 0.1430
E	<div></div> 0.7860	<div></div> 0.1420

