



Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 03:52 pm BST

PDB ID : 7B5L
EMDB ID : EMD-12037
Title : Ubiquitin ligation to F-box protein substrates by SCF-RBR E3-E3 super-assembly: NEDD8-CUL1-RBX1-SKP1-SKP2-CKSHS1-Cyclin A-CDK2-p27-UBE2L3 Ub ARIH1. Transition State 1
Authors : Horn-Ghetko, D.; Prabu, J.R.; Schulman, B.A.
Deposited on : 2020-12-04
Resolution : 3.80 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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

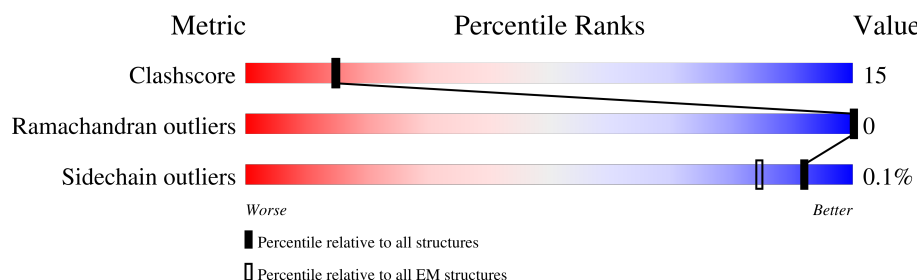
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	C	776	<div> <div>10%</div> <div>64%</div> <div>27%</div> <div>9%</div> </div>
2	H	557	<div> <div>5%</div> <div>59%</div> <div>17%</div> <div>24%</div> </div>
3	T	424	<div> <div>7%</div> <div>50%</div> <div>25%</div> <div>24%</div> </div>
4	K	73	<div> <div>•</div> <div>56%</div> <div>38%</div> <div>5%</div> </div>
5	S	163	<div> <div>7%</div> <div>59%</div> <div>25%</div> <div>•</div> <div>15%</div> </div>
6	U	75	<div> <div>•</div> <div>63%</div> <div>37%</div> </div>
7	N	76	<div> <div>63%</div> <div>58%</div> <div>42%</div> </div>
8	R	108	<div> <div>55%</div> <div>20%</div> <div>25%</div> </div>

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Mol	Chain	Length	Quality of chain
9	D	154	<div><div><div></div><div></div><div></div></div><div>36%64%34%</div></div>
10	L	298	<div><div><div></div><div></div><div></div></div><div>42%64%31%5%</div></div>
11	Y	432	<div><div><div></div><div></div><div></div></div><div>46%34%24%41%</div></div>
12	P	198	<div><div><div></div><div></div><div></div></div><div>34%18%20%61%</div></div>

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 21529 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 Cullin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	706	Total	C	N	O	S	0	0
			5752	3658	982	1085	27		

- Molecule 2 is a protein called E3 ubiquitin-protein ligase ARIH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	423	Total	C	N	O	S	0	0
			3472	2194	606	628	44		

- Molecule 3 is a protein called S-phase kinase-associated protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	321	Total	C	N	O	S	0	0
			2536	1613	436	471	16		

- Molecule 4 is a protein called Cyclin-dependent kinases regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	69	Total	C	N	O	S	0	0
			598	387	102	106	3		

- Molecule 5 is a protein called S-phase kinase-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	138	Total	C	N	O	S	0	0
			1097	697	179	217	4		

- Molecule 6 is a protein called Polyubiquitin-C.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	U	75	Total	C	N	O	0	0
			594	374	104	116		

- Molecule 7 is a protein called NEDD8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	76	Total	C	N	O	S	0	0
			599	378	104	115	2		

- Molecule 8 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	81	Total	C	N	O	S	0	0
			677	433	124	111	9		

- Molecule 9 is a protein called Ubiquitin-conjugating enzyme E2 L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	151	Total	C	N	O	S	0	0
			1209	773	209	223	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	17	ALA	CYS	engineered mutation	UNP P68036
D	137	ALA	CYS	engineered mutation	UNP P68036

- Molecule 10 is a protein called Cyclin-dependent kinase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	284	Total	C	N	O	P S	0	0
			2279	1481	388	402	1 7		

- Molecule 11 is a protein called Cyclin-A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	253	Total	C	N	O	S	0	0
			2046	1328	332	375	11		

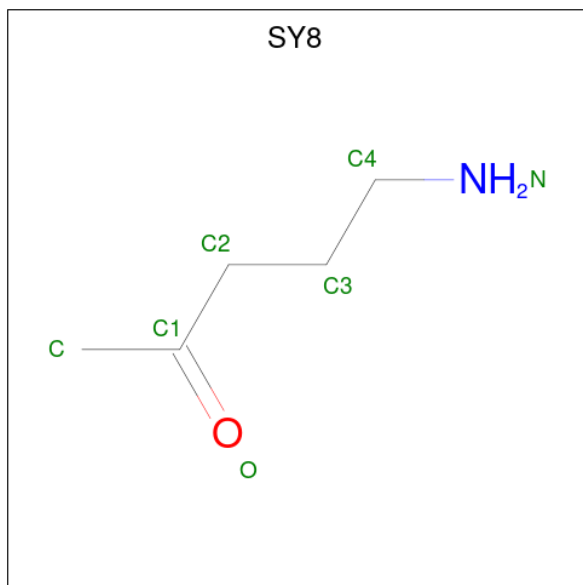
- Molecule 12 is a protein called Cyclin-dependent kinase inhibitor 1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	77	Total	C	N	O	P S	0	0
			654	407	117	126	1 3		

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
13	H	6	Total	Zn	0
			6	6	
13	R	3	Total	Zn	0
			3	3	

- Molecule 14 is 5-azanylpentan-2-one (three-letter code: SY8) (formula: C₅H₁₁NO).

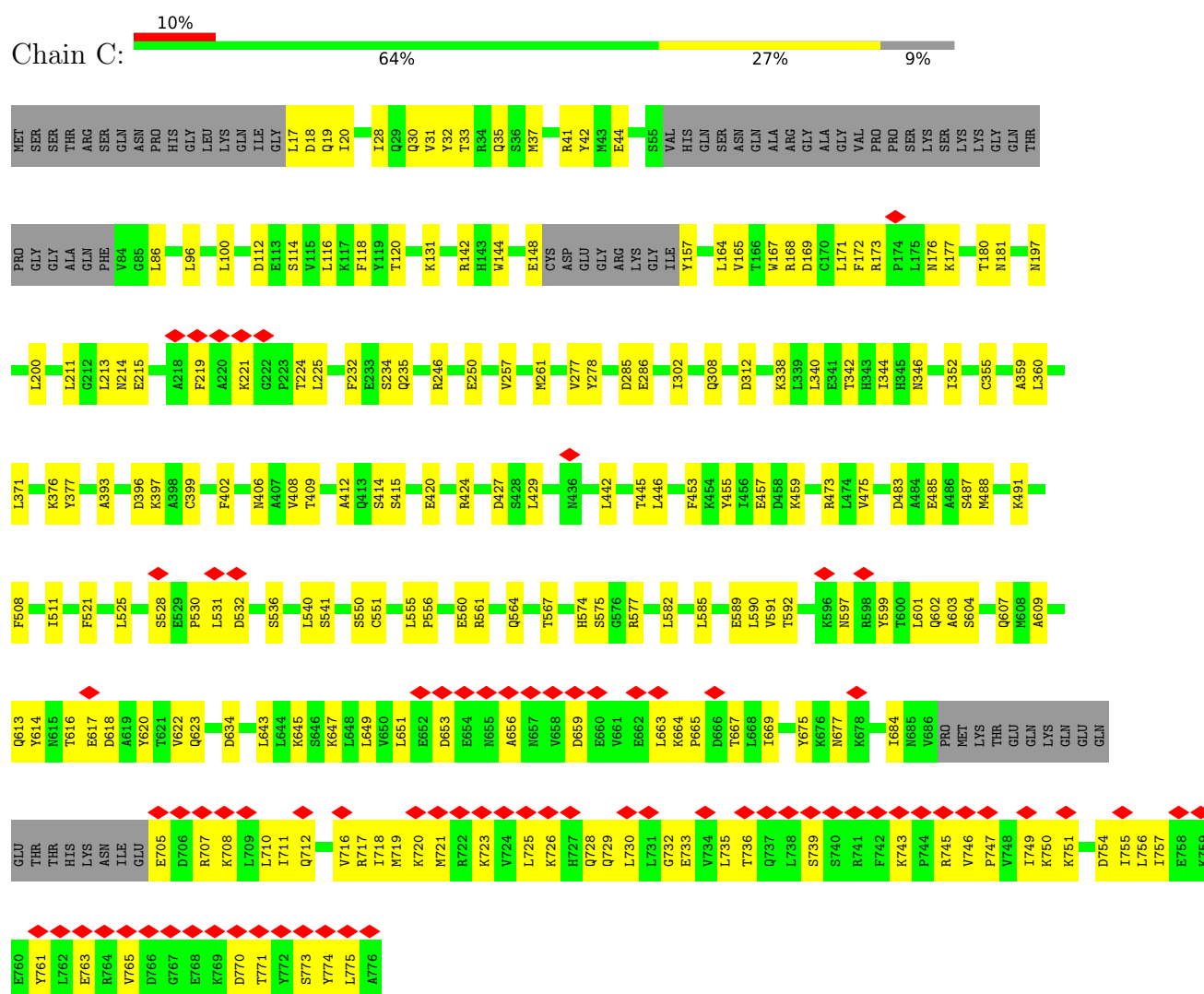


Mol	Chain	Residues	Atoms				AltConf
14	U	1	Total	C	N	O	0
			7	5	1	1	

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.

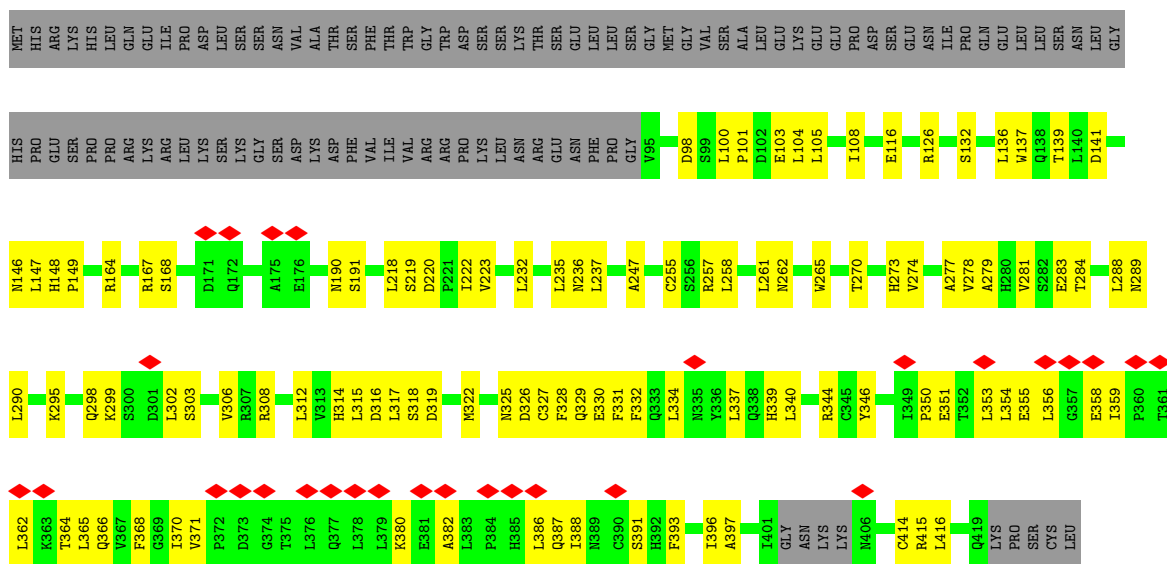
• Molecule 1: Cullin-1



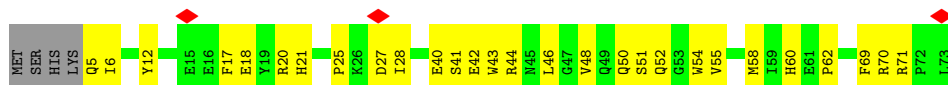
• Molecule 2: E3 ubiquitin-protein ligase ARIH1



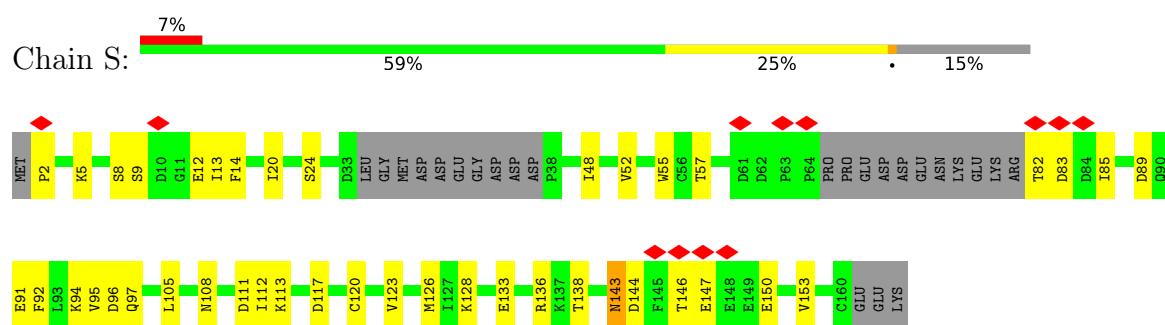
- Molecule 3: S-phase kinase-associated protein 2



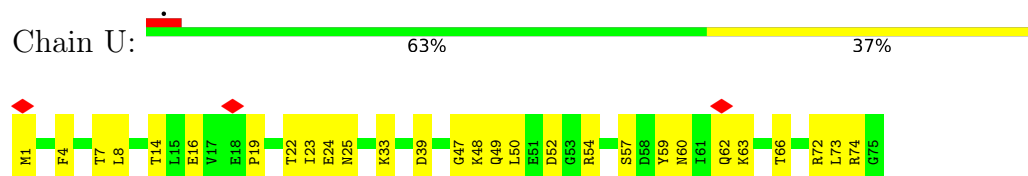
- Molecule 4: Cyclin-dependent kinases regulatory subunit 1



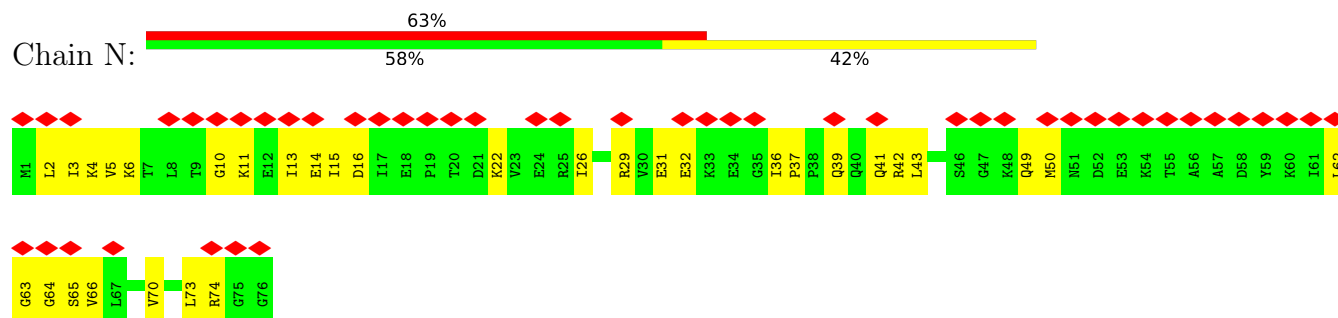
- Molecule 5: S-phase kinase-associated protein 1



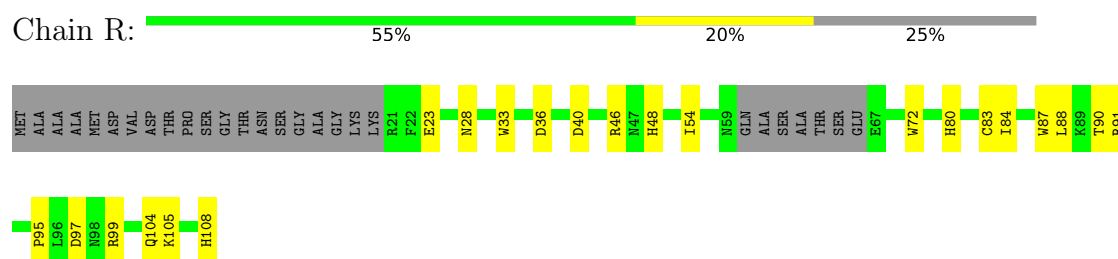
- Molecule 6: Polyubiquitin-C



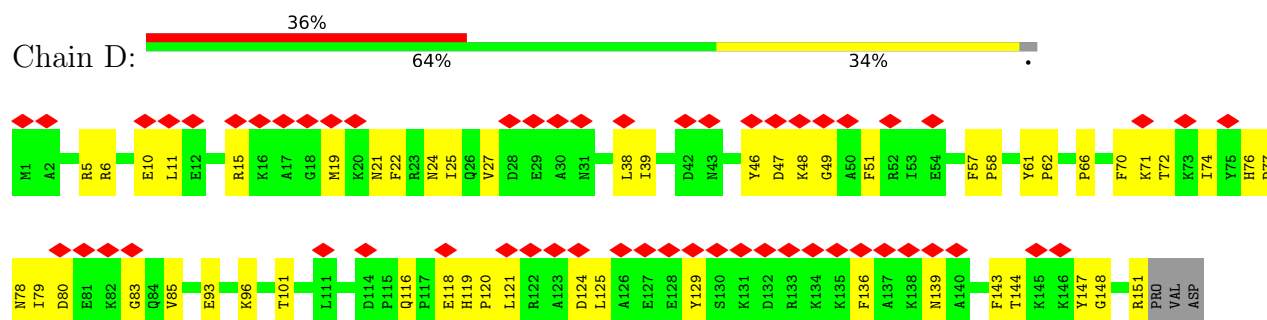
- Molecule 7: NEDD8



- Molecule 8: E3 ubiquitin-protein ligase RBX1



- Molecule 9: Ubiquitin-conjugating enzyme E2 L3



- Molecule 10: Cyclin-dependent kinase 2

Chain L:

- Molecule 11: Cyclin-A2

- Molecule 12: Cyclin-dependent kinase inhibitor 1B

Chain P:

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	623409	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	43.280	Depositor
Minimum map value	-20.065	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.862	Depositor
Recommended contour level	7.42	Depositor
Map size (Å)	348.80002, 348.80002, 348.80002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, ZN, SY8

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	C	0.39	0/5847	0.51	0/7875
2	H	0.39	0/3555	0.49	0/4800
3	T	0.28	0/2585	0.46	0/3509
4	K	0.32	0/618	0.51	0/837
5	S	0.28	0/1114	0.47	1/1507 (0.1%)
6	U	0.28	0/600	0.48	0/808
7	N	0.25	0/604	0.45	0/808
8	R	0.48	0/698	0.54	0/947
9	D	0.29	0/1239	0.45	0/1680
10	L	0.29	0/2325	0.49	0/3154
11	Y	0.27	0/2093	0.46	0/2836
12	P	0.30	0/660	0.50	0/883
All	All	0.34	0/21938	0.49	1/29644 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	2	PRO	N-CA-CB	5.42	109.81	103.30

There are no chirality outliers.

There are no planarity outliers.

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	C	5752	0	5776	165	0
2	H	3472	0	3316	72	0
3	T	2536	0	2560	84	0
4	K	598	0	574	26	0
5	S	1097	0	1087	32	0
6	U	594	0	619	20	0
7	N	599	0	638	28	0
8	R	677	0	627	29	0
9	D	1209	0	1190	39	0
10	L	2279	0	2321	86	0
11	Y	2046	0	2074	79	0
12	P	654	0	605	46	0
13	H	6	0	0	0	0
13	R	3	0	0	0	0
14	U	7	0	0	0	0
All	All	21529	0	21387	639	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 15.

All (639) 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)
3:T:325:ASN:O	3:T:328:PHE:HB2	1.57	1.03
8:R:90:THR:HG22	8:R:91:ARG:HG3	1.52	0.91
2:H:441:LYS:HG2	2:H:513:ILE:HD13	1.55	0.86
11:Y:250:ARG:HH11	12:P:33:PHE:HB3	1.41	0.86
1:C:555:LEU:HD12	1:C:556:PRO:HD2	1.60	0.83
10:L:70:ILE:HB	10:L:77:TYR:HB2	1.62	0.81
10:L:284:PRO:HA	10:L:287:GLN:HG3	1.62	0.80
1:C:168:ARG:NH1	1:C:169:ASP:OD1	2.14	0.80
1:C:651:LEU:HD11	1:C:663:LEU:HD21	1.64	0.79
1:C:591:VAL:H	8:R:23:GLU:HA	1.48	0.78
4:K:52:GLN:HE21	12:P:185:GLU:HB2	1.48	0.77
3:T:364:THR:HG22	3:T:387:GLN:HB2	1.66	0.77
3:T:223:VAL:HG21	3:T:247:ALA:HB1	1.67	0.76
2:H:281:CYS:SG	2:H:283:HIS:ND1	2.54	0.75
10:L:127:ASP:HA	10:L:164:VAL:HG23	1.69	0.74
1:C:607:GLN:HG3	1:C:643:LEU:HD21	1.69	0.74
2:H:535:ARG:HD2	8:R:54:ILE:HD11	1.69	0.74
9:D:80:ASP:HB2	9:D:121:LEU:HD11	1.70	0.72
4:K:27:ASP:OD1	4:K:28:ILE:N	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:509:LEU:O	2:H:513:ILE:HG13	1.90	0.72
10:L:29:VAL:HB	10:L:82:PHE:HB3	1.72	0.71
3:T:283:GLU:OE1	3:T:308:ARG:NH2	2.23	0.71
10:L:22:ARG:NH1	10:L:30:VAL:O	2.25	0.70
3:T:299:LYS:HZ2	3:T:326:ASP:HB2	1.56	0.70
10:L:23:ASN:ND2	12:P:73:LYS:O	2.24	0.70
10:L:164:VAL:HG22	10:L:165:THR:HG22	1.73	0.69
1:C:30:GLN:NE2	1:C:37:MET:SD	2.66	0.69
1:C:352:ILE:HD11	1:C:406:ASN:HB2	1.74	0.69
11:Y:249:LEU:HD23	11:Y:251:GLY:H	1.57	0.69
1:C:308:GLN:NE2	1:C:312:ASP:OD2	2.25	0.69
10:L:283:HIS:O	10:L:287:GLN:N	2.26	0.68
4:K:12:TYR:OH	4:K:21:HIS:ND1	2.25	0.68
3:T:299:LYS:NZ	3:T:327:CYS:SG	2.62	0.68
4:K:71:ARG:NH1	12:P:187:TPO:O3P	2.27	0.68
5:S:143:ASN:ND2	5:S:146:THR:OG1	2.26	0.68
1:C:148:GLU:OE2	1:C:148:GLU:N	2.25	0.68
11:Y:249:LEU:HD22	11:Y:252:LYS:HZ2	1.59	0.68
3:T:329:GLN:HA	3:T:332:PHE:HD2	1.59	0.67
5:S:95:VAL:HG12	5:S:96:ASP:H	1.60	0.67
4:K:51:SER:OG	4:K:52:GLN:N	2.27	0.67
10:L:157:ARG:NH1	11:Y:268:GLU:OE2	2.27	0.67
2:H:408:ARG:HH12	2:H:412:GLN:HB2	1.57	0.67
5:S:91:GLU:HA	5:S:94:LYS:HG2	1.76	0.67
7:N:31:GLU:HB3	7:N:41:GLN:HE22	1.60	0.67
2:H:451:SER:OG	2:H:452:TRP:N	2.27	0.67
3:T:329:GLN:NE2	3:T:330:GLU:OE2	2.28	0.66
9:D:11:LEU:HD21	9:D:27:VAL:HG11	1.78	0.66
1:C:420:GLU:OE1	1:C:424:ARG:NH2	2.28	0.66
2:H:523:GLN:NE2	2:H:527:ASP:OD2	2.28	0.65
10:L:81:GLU:OE2	10:L:142:LYS:NZ	2.30	0.65
3:T:236:ASN:ND2	3:T:397:ALA:O	2.26	0.65
5:S:97:GLN:NE2	5:S:138:THR:O	2.22	0.65
2:H:444:GLU:O	2:H:447:GLN:NE2	2.26	0.65
11:Y:395:HIS:NE2	11:Y:427:PRO:O	2.28	0.65
2:H:201:LEU:HD11	2:H:240:VAL:HG22	1.79	0.64
10:L:169:ARG:O	10:L:187:TRP:NE1	2.30	0.64
2:H:121:ASN:ND2	2:H:126:ASN:O	2.29	0.64
8:R:97:ASP:O	8:R:99:ARG:N	2.31	0.64
9:D:129:TYR:HD1	9:D:136:PHE:HD2	1.42	0.64
3:T:350:PRO:O	3:T:353:LEU:HB2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:U:39:ASP:O	6:U:72:ARG:NH1	2.31	0.64
7:N:6:LYS:HE3	7:N:10:GLY:HA2	1.80	0.64
5:S:20:ILE:HD13	5:S:57:THR:HG22	1.79	0.64
12:P:84:LEU:HD13	12:P:88:TYR:HB2	1.80	0.64
1:C:342:THR:O	1:C:346:ASN:ND2	2.32	0.63
1:C:234:SER:OG	1:C:235:GLN:OE1	2.15	0.63
7:N:36:ILE:O	7:N:41:GLN:NE2	2.31	0.63
11:Y:380:THR:HG23	11:Y:382:TYR:H	1.63	0.63
1:C:172:PHE:O	1:C:173:ARG:NE	2.27	0.63
5:S:55:TRP:NE1	5:S:89:ASP:OD2	2.30	0.63
10:L:136:ASN:OD1	10:L:140:ALA:N	2.29	0.63
1:C:710:LEU:HD22	7:N:36:ILE:HD11	1.81	0.63
1:C:765:VAL:HG12	1:C:773:SER:HB3	1.81	0.63
11:Y:187:ARG:NH1	11:Y:380:THR:OG1	2.32	0.63
2:H:203:CYS:HB3	2:H:238:ILE:HD12	1.81	0.63
1:C:19:GLN:OE1	1:C:19:GLN:N	2.32	0.63
9:D:15:ARG:NH2	9:D:25:ILE:O	2.28	0.63
5:S:12:GLU:N	5:S:12:GLU:OE1	2.32	0.62
1:C:168:ARG:HG3	1:C:213:LEU:HD11	1.80	0.62
2:H:513:ILE:O	2:H:513:ILE:HG22	1.99	0.62
1:C:17:LEU:HB2	1:C:20:ILE:HD12	1.80	0.62
2:H:353:LYS:NZ	2:H:358:ASN:OD1	2.32	0.62
3:T:277:ALA:O	3:T:281:VAL:HG23	1.98	0.62
10:L:109:PHE:HA	10:L:286:PHE:CZ	2.35	0.62
7:N:2:LEU:HD11	7:N:14:GLU:HG3	1.81	0.62
10:L:131:GLN:N	10:L:131:GLN:OE1	2.33	0.62
5:S:136:ARG:NE	5:S:143:ASN:OD1	2.32	0.62
9:D:124:ASP:OD1	9:D:125:LEU:N	2.32	0.62
3:T:326:ASP:O	3:T:329:GLN:HG3	2.00	0.61
11:Y:252:LYS:HG2	12:P:41:LEU:HD21	1.82	0.61
1:C:717:ARG:HG2	1:C:721:MET:HE1	1.82	0.61
3:T:258:LEU:HD21	3:T:261:LEU:HD13	1.82	0.61
2:H:441:LYS:CG	2:H:513:ILE:HG21	2.30	0.61
6:U:24:GLU:HG2	6:U:52:ASP:HB2	1.83	0.61
10:L:164:VAL:HG13	10:L:165:THR:H	1.66	0.61
3:T:100:LEU:O	3:T:126:ARG:NH2	2.28	0.61
9:D:143:PHE:O	9:D:147:TYR:HB2	2.00	0.60
6:U:39:ASP:OD1	6:U:72:ARG:NH1	2.35	0.60
8:R:97:ASP:OD1	8:R:97:ASP:N	2.33	0.60
11:Y:374:GLU:HA	11:Y:377:ILE:HD12	1.82	0.60
10:L:105:LYS:NZ	10:L:285:PHE:O	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:560:GLU:OE2	1:C:564:GLN:NE2	2.35	0.60
1:C:735:LEU:O	1:C:743:LYS:NZ	2.34	0.59
10:L:71:HIS:HA	10:L:76:LEU:HD23	1.84	0.59
10:L:150:ARG:NH1	10:L:160:TPO:O2P	2.35	0.59
11:Y:399:LEU:HD22	11:Y:426:PRO:HB2	1.84	0.59
3:T:332:PHE:HA	3:T:359:ILE:HD13	1.83	0.59
10:L:109:PHE:HA	10:L:286:PHE:HZ	1.67	0.59
3:T:298:GLN:NE2	3:T:322:MET:SD	2.75	0.59
7:N:16:ASP:O	7:N:29:ARG:NH1	2.35	0.59
9:D:49:GLY:H	9:D:151:ARG:HD2	1.66	0.59
1:C:246:ARG:NH1	1:C:250:GLU:OE1	2.36	0.59
12:P:46:GLU:O	12:P:50:ARG:HG2	2.03	0.59
1:C:590:LEU:HB3	8:R:23:GLU:HB3	1.85	0.59
2:H:333:THR:HG22	6:U:47:GLY:H	1.67	0.59
2:H:337:ILE:O	2:H:341:THR:OG1	2.20	0.59
10:L:183:ALA:O	10:L:274:ARG:NH1	2.32	0.59
1:C:577:ARG:NH2	8:R:108:HIS:O	2.36	0.59
4:K:40:GLU:HA	4:K:43:TRP:CE2	2.38	0.59
1:C:718:ILE:HD13	1:C:733:GLU:HB3	1.84	0.58
9:D:10:GLU:OE2	9:D:101:THR:N	2.32	0.58
11:Y:262:LEU:HD11	11:Y:275:VAL:HG12	1.86	0.58
1:C:177:LYS:O	1:C:181:ASN:ND2	2.29	0.58
12:P:75:GLU:N	12:P:75:GLU:OE1	2.36	0.58
3:T:101:PRO:HG2	3:T:104:LEU:HD23	1.86	0.58
3:T:265:TRP:NE1	4:K:41:SER:OG	2.35	0.58
10:L:281:LEU:HD13	10:L:286:PHE:HE2	1.69	0.58
11:Y:186:LEU:HD22	11:Y:309:PRO:HB3	1.85	0.58
1:C:585:LEU:HD12	1:C:585:LEU:O	2.04	0.58
11:Y:351:LEU:HB2	11:Y:354:VAL:HG23	1.85	0.58
3:T:265:TRP:HE1	4:K:41:SER:HG	1.51	0.58
10:L:18:VAL:HG13	12:P:81:LYS:HE3	1.86	0.57
11:Y:250:ARG:NH1	12:P:33:PHE:HB3	2.15	0.57
11:Y:335:PHE:O	11:Y:339:LEU:HG	2.04	0.57
1:C:531:LEU:HB3	1:C:561:ARG:HD3	1.87	0.57
11:Y:385:GLU:HA	11:Y:388:LYS:HG2	1.86	0.57
1:C:603:ALA:HB2	1:C:684:ILE:HG13	1.85	0.57
2:H:326:LYS:O	2:H:414:TYR:OH	2.22	0.57
6:U:54:ARG:NH2	6:U:59:TYR:OH	2.38	0.57
9:D:6:ARG:NH1	9:D:61:TYR:OH	2.38	0.56
1:C:763:GLU:OE2	1:C:773:SER:OG	2.23	0.56
3:T:103:GLU:OE1	3:T:103:GLU:N	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:24:SER:HA	5:S:112:ILE:HG12	1.87	0.56
1:C:755:ILE:HG12	2:H:289:TYR:CE1	2.40	0.56
9:D:51:PHE:HB2	9:D:72:THR:OG1	2.06	0.56
1:C:167:TRP:HD1	1:C:211:LEU:HD21	1.71	0.56
6:U:48:LYS:HZ2	6:U:59:TYR:HD1	1.51	0.56
1:C:575:SER:OG	8:R:108:HIS:N	2.35	0.56
5:S:143:ASN:HD22	5:S:144:ASP:N	2.04	0.56
6:U:60:ASN:OD1	6:U:62:GLN:NE2	2.39	0.56
12:P:31:ASN:OD1	12:P:34:GLY:N	2.36	0.56
1:C:726:LYS:NZ	1:C:770:ASP:O	2.40	0.55
9:D:47:ASP:O	9:D:151:ARG:NH1	2.39	0.55
5:S:133:GLU:OE1	5:S:133:GLU:N	2.38	0.55
7:N:62:LEU:O	7:N:65:SER:OG	2.22	0.55
1:C:157:TYR:N	1:C:215:GLU:OE2	2.39	0.55
9:D:93:GLU:OE1	9:D:93:GLU:N	2.39	0.55
5:S:150:GLU:HA	5:S:153:VAL:HG22	1.88	0.55
11:Y:337:GLY:O	11:Y:340:SER:OG	2.21	0.55
1:C:577:ARG:CG	8:R:33:TRP:HE1	2.20	0.55
4:K:44:ARG:NH2	4:K:50:GLN:O	2.28	0.55
9:D:136:PHE:HA	9:D:139:ASN:HB2	1.89	0.55
1:C:257:VAL:O	1:C:261:MET:HG3	2.07	0.55
1:C:574:HIS:HB3	1:C:577:ARG:HD2	1.89	0.55
3:T:262:ASN:HB2	3:T:396:ILE:HG22	1.88	0.55
11:Y:410:ARG:O	11:Y:414:LYS:HG2	2.07	0.55
10:L:32:LEU:HD21	10:L:77:TYR:HD1	1.70	0.54
1:C:725:LEU:HD22	1:C:730:LEU:CD2	2.37	0.54
1:C:575:SER:HG	8:R:108:HIS:H	1.56	0.54
3:T:98:ASP:O	3:T:126:ARG:NH1	2.39	0.54
3:T:270:THR:OG1	3:T:273:HIS:ND1	2.38	0.54
3:T:289:ASN:HB2	3:T:396:ILE:HD12	1.89	0.54
2:H:408:ARG:O	2:H:408:ARG:NH1	2.33	0.54
3:T:116:GLU:OE2	5:S:128:LYS:HG3	2.08	0.54
10:L:21:ALA:H	10:L:22:ARG:HH11	1.55	0.54
10:L:130:PRO:HG3	10:L:192:ILE:HG23	1.89	0.54
11:Y:250:ARG:HA	11:Y:253:LEU:HD23	1.88	0.54
11:Y:347:TYR:HA	11:Y:350:TYR:HD2	1.72	0.54
3:T:312:LEU:HD13	3:T:315:LEU:HD13	1.88	0.54
3:T:362:LEU:HB3	3:T:386:LEU:HD21	1.89	0.54
10:L:164:VAL:HG13	10:L:165:THR:N	2.23	0.54
11:Y:279:VAL:HG12	11:Y:291:VAL:HG21	1.89	0.54
1:C:86:LEU:HD12	1:C:144:TRP:HZ2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:761:TYR:CE2	7:N:73:LEU:HD12	2.43	0.54
10:L:121:HIS:O	10:L:122:ARG:HG2	2.08	0.54
1:C:285:ASP:OD1	1:C:286:GLU:N	2.40	0.53
7:N:15:ILE:HD13	7:N:29:ARG:HB3	1.91	0.53
3:T:139:THR:OG1	3:T:415:ARG:N	2.33	0.53
10:L:216:PHE:O	10:L:220:GLY:N	2.41	0.53
11:Y:194:LYS:HZ2	11:Y:351:LEU:HD23	1.70	0.53
1:C:536:SER:O	8:R:28:ASN:HA	2.08	0.53
2:H:312:HIS:HA	2:H:474:TYR:CD2	2.44	0.53
2:H:545:GLU:OE1	8:R:46:ARG:NH2	2.34	0.53
3:T:168:SER:O	3:T:191:SER:OG	2.23	0.53
9:D:22:PHE:HD1	9:D:39:ILE:HG22	1.74	0.53
5:S:123:VAL:O	5:S:126:MET:HG3	2.09	0.53
6:U:19:PRO:O	6:U:57:SER:OG	2.22	0.53
8:R:104:GLN:O	8:R:105:LYS:HG3	2.09	0.53
10:L:87:LEU:HD21	10:L:135:ILE:HG23	1.90	0.53
3:T:356:LEU:O	3:T:359:ILE:HG22	2.09	0.53
3:T:279:ALA:O	3:T:308:ARG:NH1	2.42	0.53
5:S:136:ARG:HD3	5:S:143:ASN:HB2	1.91	0.53
8:R:84:ILE:HG13	8:R:88:LEU:HD23	1.91	0.53
2:H:251:ASP:OD1	2:H:253:LYS:N	2.42	0.53
3:T:339:HIS:ND1	3:T:364:THR:OG1	2.31	0.53
4:K:27:ASP:OD1	4:K:28:ILE:HG13	2.09	0.53
4:K:50:GLN:HA	12:P:187:TPO:HG22	1.91	0.53
11:Y:239:ILE:HD11	11:Y:257:GLY:HA2	1.90	0.53
1:C:761:TYR:HE2	7:N:73:LEU:HD12	1.75	0.52
3:T:218:LEU:HD22	3:T:222:ILE:HG21	1.91	0.52
5:S:95:VAL:HG12	5:S:96:ASP:N	2.21	0.52
11:Y:189:MET:SD	11:Y:192:LYS:NZ	2.81	0.52
3:T:314:HIS:HD2	3:T:339:HIS:HB2	1.75	0.52
10:L:34:LYS:HD2	10:L:75:LYS:HD2	1.91	0.52
5:S:82:THR:OG1	5:S:83:ASP:N	2.43	0.52
3:T:232:LEU:HD13	3:T:235:LEU:HD13	1.90	0.52
10:L:23:ASN:OD1	10:L:24:LYS:N	2.41	0.52
11:Y:403:GLN:N	11:Y:403:GLN:OE1	2.41	0.52
3:T:327:CYS:O	3:T:330:GLU:HB2	2.09	0.52
9:D:24:ASN:HB3	9:D:38:LEU:HB3	1.91	0.52
10:L:23:ASN:C	10:L:24:LYS:HD3	2.30	0.52
1:C:550:SER:OG	1:C:551:CYS:N	2.43	0.52
2:H:513:ILE:O	2:H:513:ILE:CG2	2.58	0.52
10:L:35:ILE:HD11	10:L:76:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:18:GLU:OE2	4:K:71:ARG:NE	2.43	0.52
1:C:225:LEU:HD23	1:C:225:LEU:H	1.75	0.52
11:Y:176:PRO:HA	11:Y:179:HIS:CD2	2.45	0.52
11:Y:250:ARG:NH1	12:P:33:PHE:O	2.43	0.52
1:C:360:LEU:HD13	1:C:408:VAL:HG13	1.91	0.52
1:C:525:LEU:HD21	1:C:530:PRO:HG3	1.92	0.52
1:C:597:ASN:HB2	1:C:599:TYR:CE2	2.44	0.52
2:H:232:PRO:O	9:D:96:LYS:HB3	2.10	0.51
3:T:302:LEU:HD11	3:T:331:PHE:HE1	1.75	0.51
1:C:739:SER:OG	1:C:743:LYS:NZ	2.42	0.51
11:Y:273:PRO:HB2	11:Y:278:PHE:HE1	1.75	0.51
11:Y:385:GLU:OE1	11:Y:385:GLU:N	2.35	0.51
1:C:577:ARG:HG2	8:R:33:TRP:HE1	1.75	0.51
3:T:355:GLU:O	3:T:358:GLU:HB2	2.10	0.51
1:C:112:ASP:C	1:C:114:SER:H	2.13	0.51
11:Y:287:THR:N	11:Y:290:GLN:OE1	2.32	0.51
10:L:21:ALA:HB1	12:P:74:TYR:HB3	1.91	0.51
11:Y:175:VAL:HG12	11:Y:177:ASP:H	1.76	0.51
8:R:87:TRP:CZ2	8:R:95:PRO:HB3	2.46	0.51
4:K:54:TRP:CE3	4:K:71:ARG:HB3	2.45	0.51
1:C:592:THR:HG21	1:C:601:LEU:HG	1.91	0.51
1:C:720:LYS:NZ	7:N:74:ARG:O	2.44	0.51
1:C:745:ARG:HB3	1:C:747:PRO:HD2	1.93	0.51
4:K:20:ARG:HH22	12:P:189:LYS:NZ	2.09	0.51
1:C:725:LEU:HD22	1:C:730:LEU:HD23	1.92	0.51
1:C:775:LEU:HD22	7:N:74:ARG:HH22	1.75	0.51
2:H:205:HIS:CE1	2:H:236:CYS:HB2	2.46	0.50
2:H:207:PHE:HZ	2:H:233:ALA:HB2	1.76	0.50
3:T:337:LEU:HD11	3:T:340:LEU:HB2	1.93	0.50
9:D:78:ASN:HD22	9:D:120:PRO:HB3	1.76	0.50
11:Y:332:LEU:O	11:Y:336:LEU:HG	2.10	0.50
2:H:205:HIS:HE1	2:H:236:CYS:HB2	1.75	0.50
3:T:136:LEU:O	3:T:415:ARG:NH2	2.40	0.50
11:Y:214:LEU:HD11	11:Y:253:LEU:HB3	1.91	0.50
3:T:255:CYS:SG	3:T:258:LEU:HB2	2.52	0.50
1:C:446:LEU:HD12	1:C:488:MET:SD	2.51	0.50
1:C:171:LEU:O	1:C:173:ARG:N	2.44	0.50
2:H:442:MET:CG	2:H:455:VAL:HB	2.42	0.50
12:P:186:GLN:O	12:P:188:PRO:HD3	2.11	0.50
1:C:33:THR:O	1:C:35:GLN:NE2	2.45	0.50
4:K:5:GLN:HB3	4:K:25:PRO:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:19:MET:HG3	9:D:21:ASN:H	1.77	0.50
1:C:116:LEU:O	1:C:120:THR:HG23	2.12	0.50
3:T:223:VAL:CG2	3:T:247:ALA:HB1	2.41	0.50
7:N:4:LYS:HB2	7:N:66:VAL:HG22	1.94	0.50
1:C:577:ARG:CD	8:R:33:TRP:HE1	2.25	0.50
4:K:60:HIS:CD2	4:K:62:PRO:HD2	2.47	0.50
3:T:167:ARG:HG3	3:T:190:ASN:HB2	1.94	0.49
7:N:42:ARG:HD3	7:N:49:GLN:NE2	2.26	0.49
9:D:15:ARG:HE	9:D:25:ILE:HB	1.77	0.49
3:T:274:VAL:O	3:T:278:VAL:HG22	2.11	0.49
5:S:113:LYS:NZ	5:S:117:ASP:HB2	2.27	0.49
10:L:137:THR:HG22	10:L:298:LEU:HB2	1.95	0.49
2:H:441:LYS:HG2	2:H:513:ILE:HG21	1.94	0.49
3:T:354:LEU:HD13	3:T:382:ALA:HB1	1.94	0.49
10:L:23:ASN:O	10:L:24:LYS:HD3	2.12	0.49
3:T:132:SER:HA	3:T:137:TRP:HE1	1.78	0.49
8:R:40:ASP:OD2	8:R:48:HIS:NE2	2.45	0.49
2:H:441:LYS:HG3	2:H:513:ILE:HG21	1.93	0.49
11:Y:362:LEU:HD13	11:Y:394:LEU:HD22	1.95	0.49
1:C:473:ARG:HD2	1:C:485:GLU:OE2	2.13	0.49
2:H:453:ILE:O	2:H:456:GLN:HB2	2.12	0.49
3:T:329:GLN:HA	3:T:332:PHE:CD2	2.45	0.49
12:P:57:GLN:OE1	12:P:70:LEU:HD11	2.12	0.49
1:C:735:LEU:O	1:C:739:SER:OG	2.20	0.49
6:U:1:MET:HA	6:U:63:LYS:HD2	1.94	0.49
10:L:20:LYS:HB3	10:L:22:ARG:NH1	2.28	0.49
4:K:6:ILE:HD11	4:K:28:ILE:HD12	1.95	0.49
10:L:181:SER:O	10:L:183:ALA:N	2.41	0.49
1:C:427:ASP:HA	1:C:473:ARG:HH22	1.78	0.49
1:C:114:SER:O	1:C:118:PHE:N	2.38	0.48
1:C:257:VAL:HG11	1:C:302:ILE:HG12	1.95	0.48
3:T:146:ASN:OD1	3:T:147:LEU:N	2.47	0.48
11:Y:242:PHE:HD2	11:Y:243:LEU:HD22	1.78	0.48
1:C:540:LEU:O	8:R:33:TRP:HB3	2.13	0.48
7:N:42:ARG:HB2	7:N:70:VAL:HG13	1.94	0.48
9:D:70:PHE:HB3	9:D:83:GLY:HA2	1.95	0.48
3:T:219:SER:OG	3:T:220:ASP:N	2.46	0.48
11:Y:211:ARG:NH2	11:Y:341:LEU:O	2.46	0.48
1:C:592:THR:HA	8:R:23:GLU:HG2	1.96	0.48
1:C:725:LEU:HD21	1:C:729:GLN:HB2	1.96	0.48
2:H:294:PRO:HB3	2:H:311:TRP:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:207:SER:OG	10:L:208:GLU:N	2.47	0.48
10:L:281:LEU:HA	10:L:286:PHE:CE2	2.48	0.48
1:C:28:ILE:O	1:C:31:VAL:HG12	2.14	0.48
1:C:352:ILE:HD11	1:C:406:ASN:CB	2.41	0.48
1:C:653:ASP:OD1	1:C:656:ALA:N	2.45	0.48
1:C:754:ASP:HA	1:C:757:ILE:HD12	1.94	0.48
2:H:312:HIS:O	2:H:312:HIS:ND1	2.46	0.48
6:U:14:THR:O	6:U:33:LYS:NZ	2.43	0.48
10:L:258:ASP:O	10:L:261:SER:OG	2.29	0.48
12:P:72:GLY:C	12:P:74:TYR:H	2.17	0.48
4:K:17:PHE:CD2	4:K:70:ARG:HD2	2.48	0.48
6:U:22:THR:HG23	6:U:25:ASN:H	1.79	0.48
3:T:380:LYS:NZ	3:T:388:ILE:H	2.12	0.48
4:K:58:MET:SD	10:L:239:SER:OG	2.71	0.48
6:U:4:PHE:HB2	6:U:66:THR:HG22	1.94	0.48
1:C:168:ARG:HE	1:C:213:LEU:HD21	1.79	0.48
2:H:380:GLU:O	2:H:384:SER:OG	2.23	0.48
9:D:119:HIS:N	9:D:120:PRO:HD3	2.28	0.48
1:C:406:ASN:N	1:C:409:THR:OG1	2.40	0.47
12:P:57:GLN:HE22	12:P:63:ASP:HA	1.79	0.47
3:T:284:THR:O	3:T:284:THR:HG22	2.14	0.47
10:L:106:SER:O	10:L:110:GLN:HG3	2.14	0.47
10:L:283:HIS:CG	10:L:284:PRO:HD2	2.49	0.47
1:C:475:VAL:HG11	1:C:585:LEU:HD13	1.95	0.47
2:H:413:ARG:NH2	2:H:480:PHE:O	2.48	0.47
9:D:46:TYR:HD1	9:D:74:ILE:HD11	1.77	0.47
9:D:116:GLN:NE2	9:D:118:GLU:OE2	2.47	0.47
1:C:142:ARG:NH2	5:S:111:ASP:OD1	2.46	0.47
2:H:535:ARG:HH21	2:H:538:VAL:HG21	1.79	0.47
6:U:16:GLU:OE1	6:U:16:GLU:N	2.43	0.47
8:R:80:HIS:HB2	8:R:83:CYS:SG	2.54	0.47
12:P:61:ASN:C	12:P:70:LEU:HD12	2.34	0.47
3:T:141:ASP:OD1	3:T:164:ARG:NH1	2.47	0.47
3:T:316:ASP:OD1	3:T:318:SER:OG	2.31	0.47
10:L:198:THR:HG23	10:L:200:ARG:H	1.79	0.47
1:C:483:ASP:OD1	1:C:483:ASP:N	2.45	0.47
1:C:728:GLN:OE1	1:C:728:GLN:N	2.46	0.47
8:R:36:ASP:O	8:R:72:TRP:HH2	1.98	0.47
10:L:20:LYS:HB2	12:P:77:GLN:OE1	2.15	0.47
11:Y:210:MET:HE3	11:Y:210:MET:HA	1.95	0.47
12:P:60:TRP:HA	12:P:74:TYR:HE2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:CYS:HA	1:C:402:PHE:CE1	2.49	0.47
2:H:230:SER:HA	2:H:239:LEU:HA	1.96	0.47
2:H:251:ASP:OD1	2:H:252:SER:N	2.48	0.47
6:U:7:THR:HG22	6:U:8:LEU:N	2.30	0.47
1:C:634:ASP:N	1:C:634:ASP:OD1	2.47	0.47
5:S:95:VAL:CG1	5:S:96:ASP:H	2.25	0.47
7:N:3:ILE:HG22	7:N:63:GLY:HA2	1.97	0.47
7:N:43:LEU:HB2	7:N:50:MET:HB2	1.97	0.47
10:L:156:VAL:HG11	10:L:181:SER:HB2	1.96	0.46
11:Y:338:GLU:O	11:Y:342:ILE:HG12	2.15	0.46
11:Y:404:HIS:CD2	11:Y:406:GLN:H	2.33	0.46
5:S:12:GLU:HB3	5:S:14:PHE:CE1	2.50	0.46
9:D:79:ILE:HG12	9:D:85:VAL:HG12	1.96	0.46
10:L:272:ASN:HB2	10:L:273:LYS:HZ2	1.79	0.46
11:Y:217:TRP:O	11:Y:221:VAL:HG23	2.15	0.46
11:Y:223:GLU:HG2	11:Y:412:LYS:HG3	1.98	0.46
11:Y:255:LEU:HG	11:Y:294:MET:HG3	1.96	0.46
1:C:214:ASN:OD1	1:C:224:THR:HG21	2.15	0.46
1:C:525:LEU:HD11	1:C:530:PRO:HB3	1.97	0.46
3:T:365:LEU:HB3	3:T:388:ILE:HD13	1.96	0.46
11:Y:339:LEU:HD23	11:Y:409:ILE:HD13	1.96	0.46
1:C:168:ARG:NE	1:C:213:LEU:HD21	2.30	0.46
10:L:135:ILE:HG22	10:L:141:ILE:HB	1.98	0.46
1:C:589:GLU:OE2	1:C:602:GLN:HB2	2.14	0.46
1:C:712:GLN:HB3	1:C:756:LEU:HD11	1.97	0.46
1:C:592:THR:H	8:R:23:GLU:HG2	1.81	0.46
1:C:618:ASP:N	1:C:618:ASP:OD1	2.48	0.46
2:H:190:TYR:CD2	9:D:6:ARG:HG3	2.51	0.46
7:N:2:LEU:HG	7:N:14:GLU:OE2	2.15	0.46
7:N:39:GLN:OE1	7:N:39:GLN:N	2.41	0.46
10:L:281:LEU:HD13	10:L:286:PHE:CE2	2.49	0.46
11:Y:329:VAL:HG22	11:Y:367:VAL:HG21	1.97	0.46
1:C:100:LEU:HD21	1:C:167:TRP:HA	1.97	0.46
1:C:590:LEU:HD23	8:R:23:GLU:HB3	1.96	0.46
3:T:380:LYS:HE2	3:T:388:ILE:HB	1.96	0.46
11:Y:404:HIS:O	11:Y:407:GLN:NE2	2.37	0.46
3:T:288:LEU:HD21	3:T:290:LEU:HG	1.98	0.46
5:S:48:ILE:O	5:S:52:VAL:HG23	2.16	0.46
7:N:22:LYS:O	7:N:26:ILE:HG12	2.16	0.46
12:P:61:ASN:OD1	12:P:74:TYR:HB2	2.15	0.46
1:C:645:LYS:HD3	1:C:659:ASP:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:210:MET:SD	12:P:33:PHE:HZ	2.39	0.46
1:C:719:MET:HG3	1:C:774:TYR:HB2	1.97	0.45
9:D:121:LEU:HD23	9:D:121:LEU:H	1.81	0.45
11:Y:252:LYS:HE2	12:P:41:LEU:HD21	1.97	0.45
1:C:577:ARG:HD3	8:R:33:TRP:HE1	1.82	0.45
2:H:136:SER:HB2	2:H:227:GLN:HE22	1.81	0.45
2:H:420:ARG:HA	2:H:420:ARG:HD3	1.72	0.45
3:T:325:ASN:HA	3:T:328:PHE:CD2	2.51	0.45
3:T:393:PHE:HA	4:K:42:GLU:OE2	2.16	0.45
4:K:51:SER:HA	12:P:186:GLN:HA	1.97	0.45
12:P:54:GLU:O	12:P:58:ARG:HG2	2.16	0.45
1:C:751:LYS:O	1:C:755:ILE:HG13	2.17	0.45
3:T:148:HIS:CG	3:T:149:PRO:HD2	2.51	0.45
10:L:94:SER:O	10:L:94:SER:OG	2.29	0.45
10:L:247:ASP:OD1	10:L:249:SER:OG	2.32	0.45
1:C:664:LYS:H	1:C:667:THR:HG21	1.80	0.45
2:H:190:TYR:HD2	9:D:6:ARG:HG3	1.81	0.45
2:H:324:ILE:HD12	2:H:327:CYS:HB2	1.97	0.45
10:L:122:ARG:HH22	11:Y:307:ALA:HB1	1.81	0.45
11:Y:399:LEU:HD21	11:Y:427:PRO:O	2.17	0.45
11:Y:419:HIS:HB2	11:Y:421:VAL:HG13	1.99	0.45
1:C:717:ARG:HD3	7:N:37:PRO:HG2	1.98	0.45
7:N:3:ILE:HA	7:N:64:GLY:H	1.82	0.45
9:D:118:GLU:C	9:D:120:PRO:HD3	2.37	0.45
1:C:577:ARG:HD3	8:R:33:TRP:NE1	2.32	0.45
1:C:564:GLN:HA	1:C:567:THR:HG22	1.98	0.45
2:H:472:LEU:HD13	2:H:499:GLU:OE1	2.17	0.45
2:H:526:GLN:HA	2:H:529:TYR:CE1	2.52	0.45
5:S:85:ILE:HD12	5:S:85:ILE:H	1.82	0.45
10:L:19:TYR:CE1	12:P:78:GLU:HG3	2.52	0.45
10:L:20:LYS:O	12:P:76:TRP:HA	2.16	0.45
2:H:216:LEU:O	2:H:220:ILE:HG12	2.17	0.45
2:H:520:ASP:OD1	2:H:521:ILE:N	2.50	0.45
3:T:337:LEU:HD21	3:T:340:LEU:HB2	1.99	0.45
5:S:146:THR:HG22	5:S:147:GLU:N	2.32	0.45
10:L:249:SER:HA	10:L:260:ARG:HD3	1.99	0.45
12:P:59:LYS:HE2	12:P:60:TRP:CD1	2.51	0.45
1:C:541:SER:HA	8:R:33:TRP:HE3	1.82	0.44
1:C:716:VAL:HG11	7:N:73:LEU:HB3	2.00	0.44
2:H:535:ARG:HE	2:H:535:ARG:HA	1.83	0.44
9:D:144:THR:O	9:D:148:GLY:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:52:MET:HG2	12:P:52:MET:O	2.18	0.44
5:S:8:SER:OG	5:S:9:SER:N	2.49	0.44
1:C:37:MET:HB2	1:C:42:TYR:OH	2.17	0.44
3:T:108:ILE:HA	5:S:120:CYS:SG	2.56	0.44
11:Y:372:TRP:HB3	11:Y:384:LEU:HD11	2.00	0.44
1:C:41:ARG:HA	1:C:44:GLU:OE1	2.18	0.44
1:C:376:LYS:HE3	1:C:377:TYR:CE2	2.52	0.44
1:C:525:LEU:HD12	1:C:528:SER:OG	2.17	0.44
2:H:207:PHE:CE2	2:H:232:PRO:HB2	2.52	0.44
2:H:442:MET:HG2	2:H:455:VAL:HB	1.98	0.44
3:T:139:THR:HB	3:T:414:CYS:HA	1.98	0.44
10:L:233:MET:HE2	10:L:233:MET:HB3	1.82	0.44
11:Y:376:LEU:O	11:Y:380:THR:HG22	2.17	0.44
1:C:705:GLU:HB3	1:C:708:LYS:HG3	1.99	0.44
3:T:316:ASP:OD1	3:T:317:LEU:N	2.50	0.44
3:T:370:ILE:HG13	3:T:371:VAL:N	2.33	0.44
11:Y:187:ARG:NE	11:Y:190:GLU:OE2	2.47	0.44
11:Y:336:LEU:HA	11:Y:339:LEU:HD12	1.99	0.44
12:P:62:PHE:HB2	12:P:76:TRP:CZ2	2.52	0.44
1:C:406:ASN:H	1:C:409:THR:HG1	1.62	0.44
3:T:104:LEU:HD21	5:S:108:ASN:ND2	2.32	0.44
1:C:164:LEU:HD23	1:C:164:LEU:HA	1.77	0.44
1:C:717:ARG:HG2	1:C:721:MET:CE	2.47	0.44
3:T:328:PHE:CD1	3:T:356:LEU:HD21	2.53	0.44
4:K:55:VAL:O	4:K:69:PHE:HA	2.18	0.44
1:C:399:CYS:HA	1:C:402:PHE:CD1	2.53	0.44
1:C:508:PHE:O	1:C:511:ILE:HG22	2.17	0.44
3:T:416:LEU:HD23	3:T:416:LEU:HA	1.83	0.44
12:P:86:GLU:OE2	12:P:90:ARG:NH2	2.48	0.44
10:L:172:GLU:OE2	10:L:274:ARG:NH2	2.51	0.44
11:Y:315:LEU:HB3	11:Y:319:PHE:CZ	2.53	0.44
1:C:371:LEU:HD23	1:C:371:LEU:HA	1.73	0.43
1:C:453:PHE:CZ	1:C:459:LYS:HD3	2.53	0.43
1:C:746:VAL:HG12	1:C:750:LYS:NZ	2.32	0.43
2:H:215:TYR:CE2	2:H:232:PRO:HG3	2.53	0.43
2:H:336:TRP:CH2	6:U:49:GLN:HB2	2.52	0.43
9:D:22:PHE:CD1	9:D:39:ILE:HG22	2.52	0.43
9:D:76:HIS:CG	9:D:77:PRO:HD2	2.52	0.43
10:L:70:ILE:HA	12:P:52:MET:HE3	1.98	0.43
1:C:197:ASN:HB3	1:C:200:LEU:HD12	2.00	0.43
1:C:457:GLU:OE1	1:C:457:GLU:N	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:331:PHE:HA	3:T:334:LEU:HG	2.00	0.43
10:L:110:GLN:OE1	10:L:141:ILE:N	2.37	0.43
11:Y:279:VAL:HG11	11:Y:288:LYS:HD3	1.99	0.43
1:C:112:ASP:O	1:C:114:SER:N	2.47	0.43
1:C:712:GLN:HG2	1:C:756:LEU:HG	2.01	0.43
6:U:63:LYS:HA	6:U:63:LYS:HD3	1.77	0.43
10:L:50:ARG:NH2	10:L:160:TPO:O2P	2.51	0.43
12:P:55:ALA:O	12:P:59:LYS:HG2	2.18	0.43
1:C:277:VAL:HG23	1:C:278:TYR:CD1	2.52	0.43
2:H:99:TYR:CZ	2:H:287:VAL:HG21	2.53	0.43
9:D:71:LYS:HA	9:D:71:LYS:HD3	1.68	0.43
11:Y:251:GLY:HA3	12:P:36:VAL:HG21	2.00	0.43
3:T:366:GLN:HE22	3:T:391:SER:H	1.65	0.43
10:L:126:ARG:NH1	10:L:160:TPO:O3P	2.48	0.43
10:L:190:GLY:HA3	10:L:267:LEU:HD21	2.01	0.43
12:P:41:LEU:HD23	12:P:41:LEU:HA	1.81	0.43
3:T:302:LEU:HD21	3:T:331:PHE:CE1	2.54	0.43
7:N:11:LYS:HE3	7:N:13:ILE:HD11	2.01	0.43
10:L:85:GLN:HG3	10:L:86:ASP:O	2.18	0.43
10:L:262:LEU:O	10:L:266:MET:HB2	2.18	0.43
1:C:521:PHE:O	1:C:525:LEU:HB2	2.19	0.43
3:T:359:ILE:HG23	3:T:362:LEU:HB2	2.01	0.43
4:K:6:ILE:HD13	4:K:25:PRO:HD2	2.00	0.43
12:P:51:ASP:OD1	12:P:52:MET:N	2.52	0.43
1:C:180:THR:HG23	1:C:232:PHE:HD1	1.84	0.43
1:C:487:SER:O	1:C:491:LYS:HG2	2.19	0.43
1:C:574:HIS:CB	1:C:577:ARG:HD2	2.49	0.43
2:H:207:PHE:HE2	2:H:232:PRO:HB2	1.83	0.43
3:T:332:PHE:CZ	3:T:355:GLU:HG2	2.53	0.43
5:S:55:TRP:HB2	5:S:92:PHE:HE2	1.84	0.43
12:P:59:LYS:HE2	12:P:60:TRP:NE1	2.33	0.43
1:C:582:LEU:HD12	1:C:582:LEU:O	2.19	0.43
1:C:707:ARG:O	1:C:711:ILE:HG13	2.19	0.43
2:H:267:VAL:HG11	2:H:275:TRP:NE1	2.34	0.43
11:Y:350:TYR:OH	11:Y:393:ASP:OD2	2.26	0.43
1:C:525:LEU:HG	1:C:530:PRO:HD3	2.01	0.43
1:C:603:ALA:HB1	1:C:607:GLN:HE21	1.82	0.43
1:C:675:TYR:OH	1:C:677:ASN:HB2	2.19	0.43
5:S:105:LEU:HD23	5:S:105:LEU:HA	1.85	0.43
10:L:272:ASN:HB2	10:L:273:LYS:NZ	2.34	0.43
11:Y:194:LYS:NZ	11:Y:351:LEU:HD23	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:197:VAL:HG11	11:Y:349:LYS:HD2	2.00	0.43
1:C:429:LEU:HD11	1:C:445:THR:CG2	2.49	0.42
2:H:307:CYS:HB3	2:H:317:CYS:SG	2.59	0.42
10:L:258:ASP:HB3	10:L:285:PHE:HB2	2.01	0.42
1:C:355:CYS:HB3	1:C:359:ALA:HB2	2.00	0.42
1:C:219:PHE:HB3	1:C:221:LYS:HZ1	1.84	0.42
2:H:270:ASN:OD1	2:H:271:ARG:N	2.51	0.42
3:T:261:LEU:O	3:T:288:LEU:HA	2.19	0.42
3:T:319:ASP:OD2	3:T:344:ARG:NH2	2.36	0.42
3:T:351:GLU:OE1	3:T:351:GLU:N	2.51	0.42
5:S:146:THR:HG23	5:S:150:GLU:CD	2.40	0.42
12:P:42:THR:O	12:P:45:LEU:HG	2.20	0.42
12:P:183:SER:O	12:P:183:SER:OG	2.35	0.42
5:S:5:LYS:HB3	5:S:13:ILE:HG23	2.00	0.42
6:U:23:ILE:HD13	6:U:50:LEU:HB3	2.02	0.42
9:D:57:PHE:HD1	9:D:66:PRO:HB3	1.85	0.42
11:Y:296:HIS:NE2	12:P:49:CYS:SG	2.90	0.42
1:C:235:GLN:OE1	1:C:235:GLN:N	2.52	0.42
1:C:360:LEU:HD11	1:C:412:ALA:HB2	2.01	0.42
1:C:414:SER:OG	1:C:415:SER:N	2.51	0.42
2:H:417:TYR:CE2	2:H:480:PHE:HA	2.54	0.42
2:H:472:LEU:HA	2:H:472:LEU:HD23	1.74	0.42
10:L:121:HIS:O	10:L:123:VAL:HG23	2.18	0.42
11:Y:295:GLU:HA	11:Y:298:VAL:HG12	2.00	0.42
8:R:54:ILE:HD12	8:R:54:ILE:HA	1.84	0.42
10:L:32:LEU:HD21	10:L:77:TYR:CD1	2.51	0.42
10:L:110:GLN:OE1	10:L:140:ALA:HA	2.20	0.42
11:Y:273:PRO:HB2	11:Y:278:PHE:CE1	2.53	0.42
1:C:393:ALA:O	1:C:397:LYS:HG3	2.19	0.42
1:C:649:LEU:HD12	1:C:669:ILE:HG22	2.02	0.42
2:H:113:MET:O	2:H:117:ILE:HG12	2.20	0.42
2:H:214:GLU:O	2:H:218:THR:HG22	2.19	0.42
2:H:261:LEU:HD23	2:H:261:LEU:HA	1.91	0.42
2:H:452:TRP:O	2:H:455:VAL:HG22	2.19	0.42
3:T:105:LEU:HD23	3:T:105:LEU:HA	1.76	0.42
5:S:143:ASN:ND2	5:S:144:ASP:N	2.66	0.42
9:D:58:PRO:HD3	9:D:66:PRO:HA	2.02	0.42
10:L:136:ASN:ND2	10:L:138:GLU:OE2	2.52	0.42
11:Y:335:PHE:HE1	11:Y:409:ILE:HG12	1.84	0.42
1:C:96:LEU:HD23	1:C:96:LEU:HA	1.79	0.42
1:C:340:LEU:O	1:C:344:ILE:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:609:ALA:O	1:C:613:GLN:HG2	2.19	0.42
1:C:647:LYS:HA	1:C:647:LYS:HD3	1.80	0.42
10:L:262:LEU:HA	10:L:265:GLN:NE2	2.34	0.42
10:L:266:MET:O	10:L:267:LEU:HD23	2.19	0.42
2:H:535:ARG:NH2	2:H:538:VAL:HG11	2.34	0.42
9:D:118:GLU:OE1	9:D:118:GLU:N	2.52	0.42
10:L:88:LYS:HD2	10:L:88:LYS:HA	1.72	0.42
11:Y:200:MET:HE2	11:Y:208:ASN:HA	2.01	0.42
1:C:531:LEU:HG	1:C:532:ASP:OD1	2.20	0.42
1:C:746:VAL:HA	1:C:749:ILE:HD12	2.02	0.42
2:H:295:VAL:O	2:H:302:GLN:HA	2.20	0.41
2:H:333:THR:O	2:H:337:ILE:HG12	2.20	0.41
1:C:131:LYS:HE2	1:C:131:LYS:HB2	1.83	0.41
3:T:236:ASN:O	3:T:237:LEU:HD23	2.20	0.41
1:C:32:TYR:O	1:C:33:THR:OG1	2.38	0.41
10:L:188:SER:O	10:L:192:ILE:HG13	2.20	0.41
10:L:211:GLN:HA	10:L:211:GLN:OE1	2.20	0.41
11:Y:263:LEU:HD23	11:Y:263:LEU:HA	1.82	0.41
11:Y:338:GLU:O	11:Y:341:LEU:HG	2.21	0.41
1:C:171:LEU:O	1:C:176:ASN:HB2	2.20	0.41
10:L:25:LEU:O	10:L:28:GLU:HB2	2.20	0.41
10:L:166:LEU:HD21	10:L:211:GLN:HB2	2.01	0.41
11:Y:396:GLN:HB2	11:Y:400:LYS:NZ	2.34	0.41
4:K:20:ARG:HH22	12:P:189:LYS:HZ2	1.69	0.41
11:Y:180:GLU:O	11:Y:184:THR:HG23	2.20	0.41
11:Y:197:VAL:HG22	11:Y:348:LEU:HG	2.02	0.41
1:C:604:SER:H	1:C:607:GLN:HE21	1.69	0.41
1:C:616:THR:OG1	1:C:617:GLU:N	2.53	0.41
2:H:130:ILE:HG23	2:H:163:VAL:HG11	2.01	0.41
2:H:207:PHE:CZ	2:H:233:ALA:HB2	2.55	0.41
2:H:362:CYS:HA	6:U:73:LEU:HD11	2.02	0.41
10:L:83:LEU:HD23	10:L:134:LEU:HB2	2.03	0.41
10:L:165:THR:O	10:L:169:ARG:HG3	2.19	0.41
11:Y:289:LYS:O	11:Y:293:ARG:HG2	2.21	0.41
11:Y:365:TYR:HD1	11:Y:369:GLY:HA2	1.86	0.41
7:N:36:ILE:HB	7:N:41:GLN:HE21	1.86	0.41
9:D:78:ASN:ND2	9:D:120:PRO:HB3	2.36	0.41
11:Y:186:LEU:HD23	11:Y:186:LEU:HA	1.92	0.41
11:Y:203:GLN:HE22	11:Y:246:MET:C	2.24	0.41
11:Y:242:PHE:CD2	11:Y:243:LEU:HD22	2.56	0.41
1:C:396:ASP:OD1	1:C:455:TYR:OH	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:604:SER:HB3	1:C:607:GLN:HE22	1.85	0.41
3:T:346:TYR:HB3	12:P:181:ALA:N	2.35	0.41
1:C:17:LEU:HB3	1:C:18:ASP:H	1.59	0.41
1:C:732:GLY:O	1:C:736:THR:HG23	2.21	0.41
2:H:109:ILE:HD11	2:H:273:LEU:HD13	2.03	0.41
3:T:257:ARG:HB2	3:T:257:ARG:CZ	2.50	0.41
3:T:295:LYS:HA	3:T:322:MET:CE	2.51	0.41
3:T:302:LEU:HD21	3:T:331:PHE:CZ	2.56	0.41
6:U:72:ARG:HH11	6:U:74:ARG:HH11	1.68	0.41
7:N:5:VAL:HG13	7:N:13:ILE:HB	2.03	0.41
9:D:47:ASP:CG	9:D:48:LYS:HZ2	2.24	0.41
10:L:75:LYS:HE3	10:L:75:LYS:HB2	1.86	0.41
10:L:109:PHE:HD1	10:L:286:PHE:CZ	2.37	0.41
1:C:165:VAL:HG21	1:C:215:GLU:HB2	2.02	0.41
1:C:406:ASN:N	1:C:409:THR:HG1	2.18	0.41
1:C:442:LEU:O	1:C:446:LEU:HD23	2.20	0.41
1:C:723:LYS:HD2	1:C:774:TYR:HB3	2.02	0.41
3:T:303:SER:HA	3:T:306:VAL:HG22	2.01	0.41
7:N:73:LEU:HD23	7:N:73:LEU:HA	1.86	0.41
10:L:19:TYR:HE1	12:P:78:GLU:HG3	1.86	0.41
11:Y:216:ASP:OD1	11:Y:408:SER:OG	2.26	0.41
11:Y:339:LEU:HA	11:Y:342:ILE:HG12	2.03	0.41
1:C:591:VAL:HG12	8:R:23:GLU:H	1.86	0.40
1:C:623:GLN:HB2	1:C:665:PRO:HB3	2.03	0.40
2:H:191:LEU:HD21	9:D:5:ARG:CZ	2.51	0.40
2:H:465:LEU:HD21	2:H:506:SER:HB2	2.02	0.40
3:T:344:ARG:N	3:T:368:PHE:O	2.54	0.40
4:K:43:TRP:HE3	4:K:48:VAL:HB	1.86	0.40
6:U:7:THR:HG22	6:U:8:LEU:H	1.85	0.40
7:N:29:ARG:HA	7:N:32:GLU:CD	2.42	0.40
12:P:42:THR:HA	12:P:45:LEU:CD2	2.51	0.40
1:C:617:GLU:HB2	1:C:620:TYR:CE1	2.56	0.40
9:D:61:TYR:CG	9:D:62:PRO:HA	2.57	0.40
10:L:84:HIS:HB3	10:L:298:LEU:C	2.40	0.40
10:L:115:LEU:HD23	10:L:115:LEU:HA	1.79	0.40
11:Y:347:TYR:HA	11:Y:350:TYR:CD2	2.54	0.40
11:Y:380:THR:HG23	11:Y:382:TYR:HB2	2.03	0.40
1:C:429:LEU:HD11	1:C:445:THR:HG21	2.02	0.40
1:C:614:TYR:OH	1:C:669:ILE:HB	2.22	0.40
1:C:622:VAL:HB	1:C:665:PRO:HA	2.04	0.40
4:K:42:GLU:O	4:K:46:LEU:HD23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:THR:HG23	1:C:224:THR:O	2.22	0.40
1:C:338:LYS:HB2	1:C:338:LYS:HE3	1.84	0.40
1:C:726:LYS:HZ3	1:C:771:THR:HG1	1.68	0.40
3:T:329:GLN:O	3:T:332:PHE:HB2	2.21	0.40
10:L:284:PRO:O	10:L:287:GLN:HG3	2.22	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	C	698/776 (90%)	628 (90%)	70 (10%)	0	100	100
2	H	417/557 (75%)	382 (92%)	35 (8%)	0	100	100
3	T	317/424 (75%)	287 (90%)	30 (10%)	0	100	100
4	K	67/73 (92%)	58 (87%)	9 (13%)	0	100	100
5	S	132/163 (81%)	118 (89%)	14 (11%)	0	100	100
6	U	73/75 (97%)	67 (92%)	6 (8%)	0	100	100
7	N	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
8	R	77/108 (71%)	59 (77%)	18 (23%)	0	100	100
9	D	149/154 (97%)	131 (88%)	18 (12%)	0	100	100
10	L	279/298 (94%)	249 (89%)	30 (11%)	0	100	100
11	Y	247/432 (57%)	235 (95%)	12 (5%)	0	100	100
12	P	72/198 (36%)	60 (83%)	12 (17%)	0	100	100
All	All	2602/3334 (78%)	2347 (90%)	255 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	633/698 (91%)	633 (100%)	0	100	100
2	H	382/488 (78%)	381 (100%)	1 (0%)	91	92
3	T	296/392 (76%)	296 (100%)	0	100	100
4	K	66/70 (94%)	66 (100%)	0	100	100
5	S	124/150 (83%)	123 (99%)	1 (1%)	79	84
6	U	67/68 (98%)	67 (100%)	0	100	100
7	N	66/66 (100%)	66 (100%)	0	100	100
8	R	71/90 (79%)	71 (100%)	0	100	100
9	D	127/136 (93%)	127 (100%)	0	100	100
10	L	247/262 (94%)	247 (100%)	0	100	100
11	Y	228/378 (60%)	227 (100%)	1 (0%)	89	91
12	P	69/170 (41%)	69 (100%)	0	100	100
All	All	2376/2968 (80%)	2373 (100%)	3 (0%)	92	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	511	ARG
5	S	143	ASN
11	Y	201	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	30	GLN
1	C	538	GLN
1	C	607	GLN
2	H	523	GLN
4	K	52	GLN
7	N	41	GLN

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Mol	Chain	Res	Type
11	Y	396	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are 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	$\# Z > 2$
12	TPO	P	187	12	8,10,11	1.60	1 (12%)	10,14,16	1.90	2 (20%)
10	TPO	L	160	10	8,10,11	1.07	0	10,14,16	1.90	1 (10%)

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
12	TPO	P	187	12	-	4/9/11/13	-
10	TPO	L	160	10	-	2/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	P	187	TPO	P-O1P	3.35	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	160	TPO	P-OG1-CB	-5.32	107.12	123.21
12	P	187	TPO	P-OG1-CB	-5.08	107.85	123.21
12	P	187	TPO	CG2-CB-CA	-2.23	108.76	113.16

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	P	187	TPO	N-CA-CB-OG1
12	P	187	TPO	C-CA-CB-CG2
12	P	187	TPO	CB-OG1-P-O3P
10	L	160	TPO	CB-OG1-P-O1P
10	L	160	TPO	CB-OG1-P-O2P
12	P	187	TPO	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	P	187	TPO	2	0
10	L	160	TPO	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	SY8	U	101	9,2,6	6,6,6	0.26	0	6,6,6	0.69	0

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
14	SY8	U	101	9,2,6	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	U	101	SY8	C1-C2-C3-C4
14	U	101	SY8	O-C1-C2-C3
14	U	101	SY8	C-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

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.

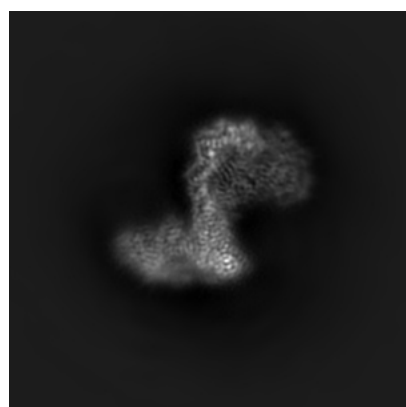
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12037. These allow visual inspection of the internal detail of the map and identification of artifacts.

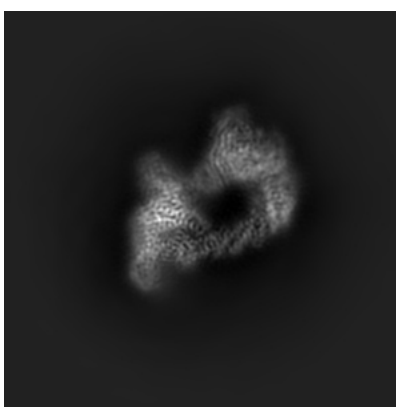
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

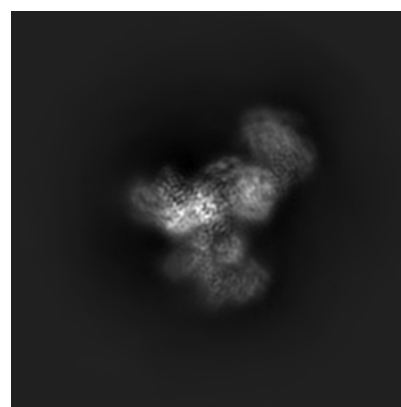
6.1.1 Primary map



X



Y

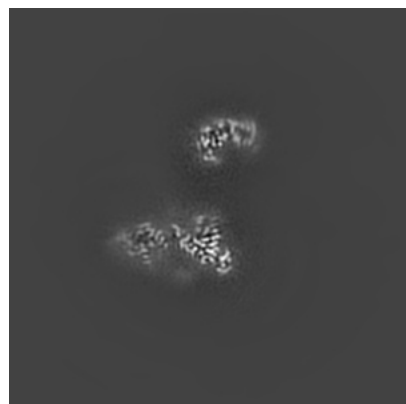


Z

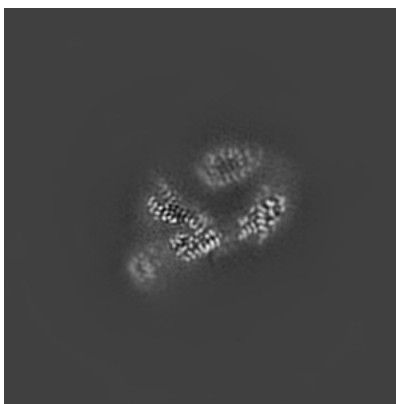
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

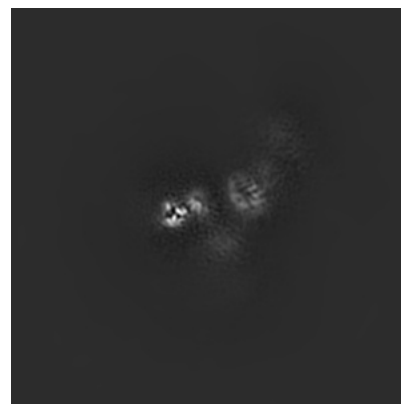
6.2.1 Primary map



X Index: 160



Y Index: 160

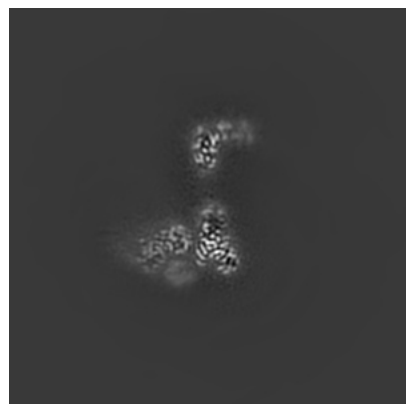


Z Index: 160

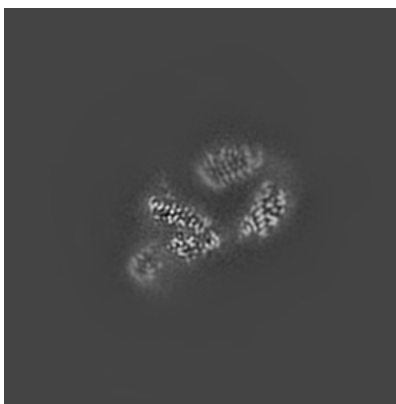
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

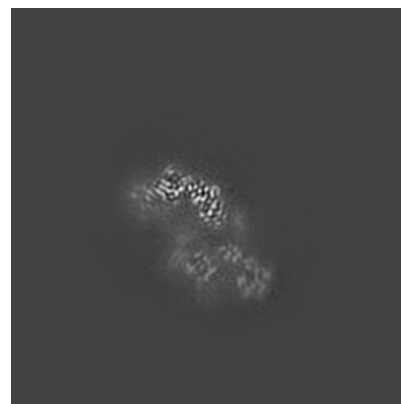
6.3.1 Primary map



X Index: 152



Y Index: 162

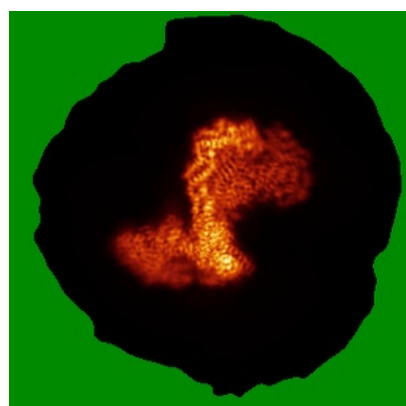


Z Index: 120

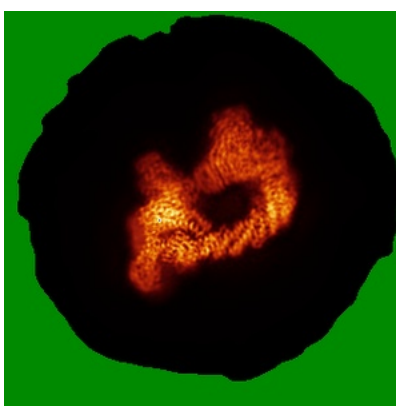
The images above show the largest variance slices of the map in three orthogonal directions.

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

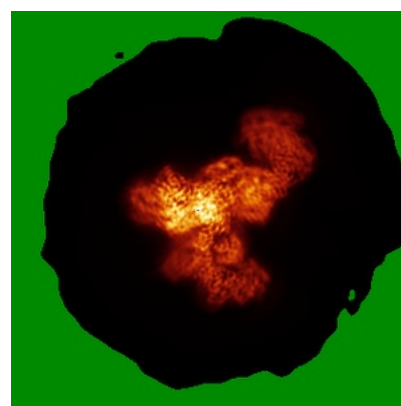
6.4.1 Primary map



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

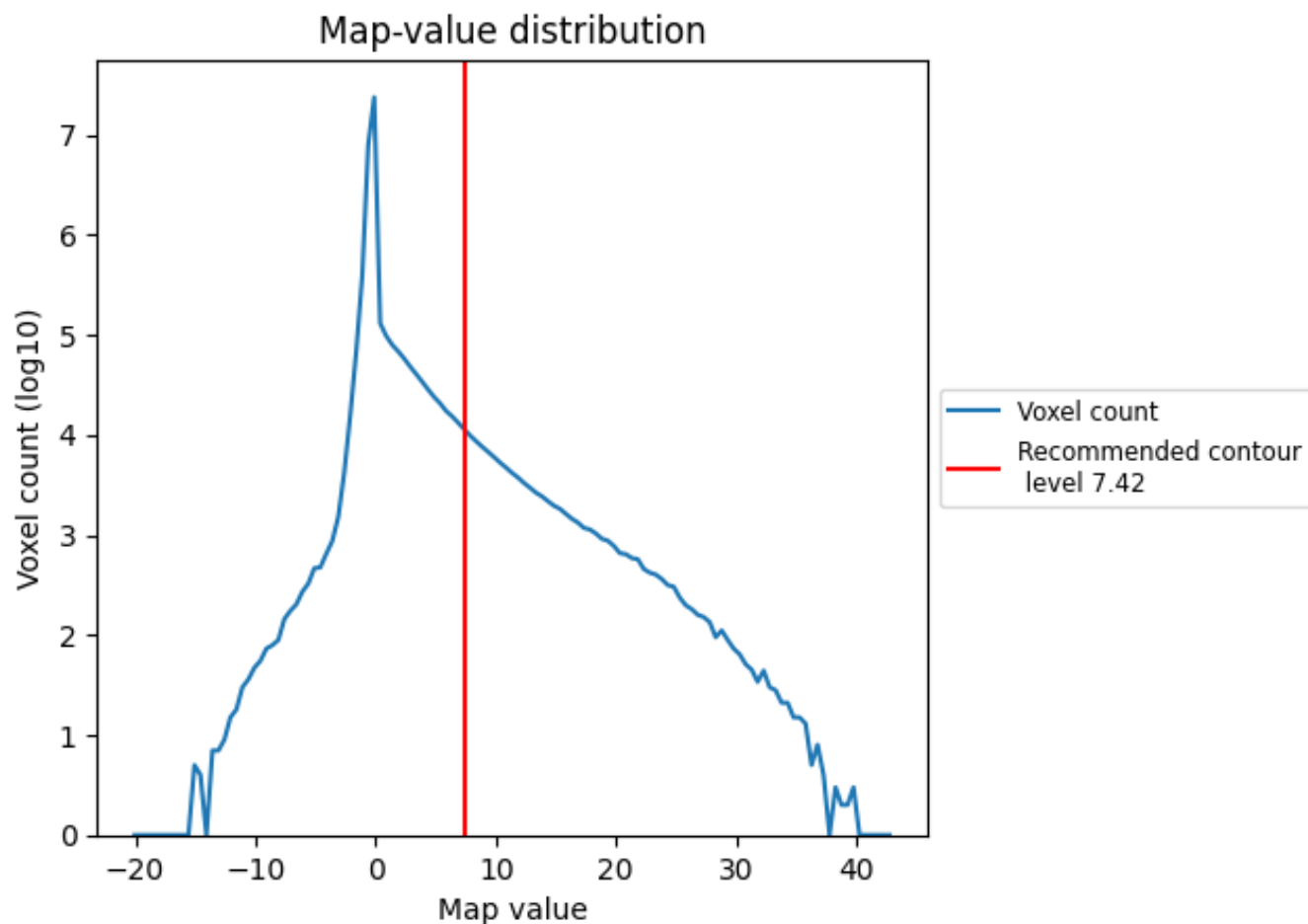
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

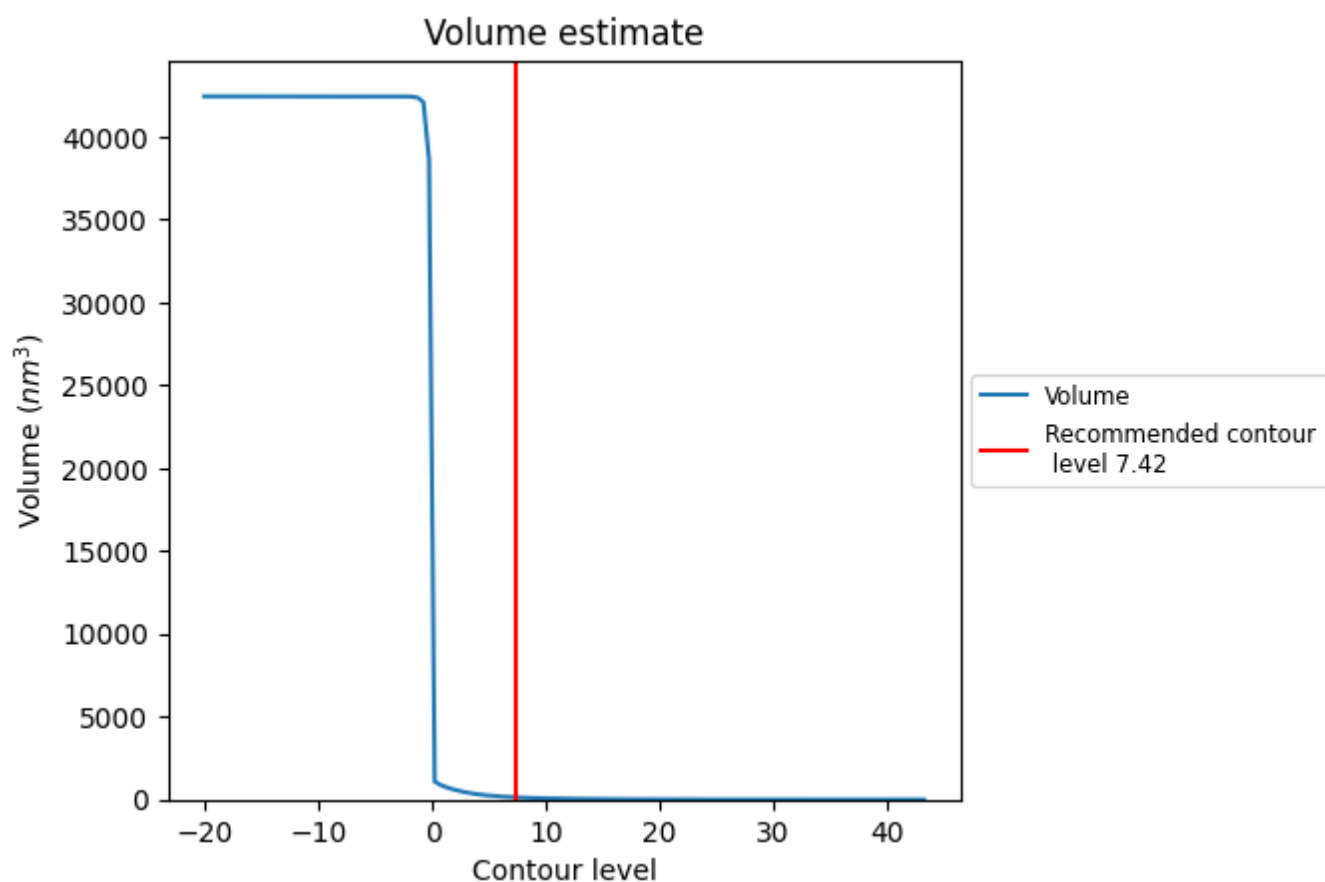
This section contains the results of statistical analysis of the map.

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.

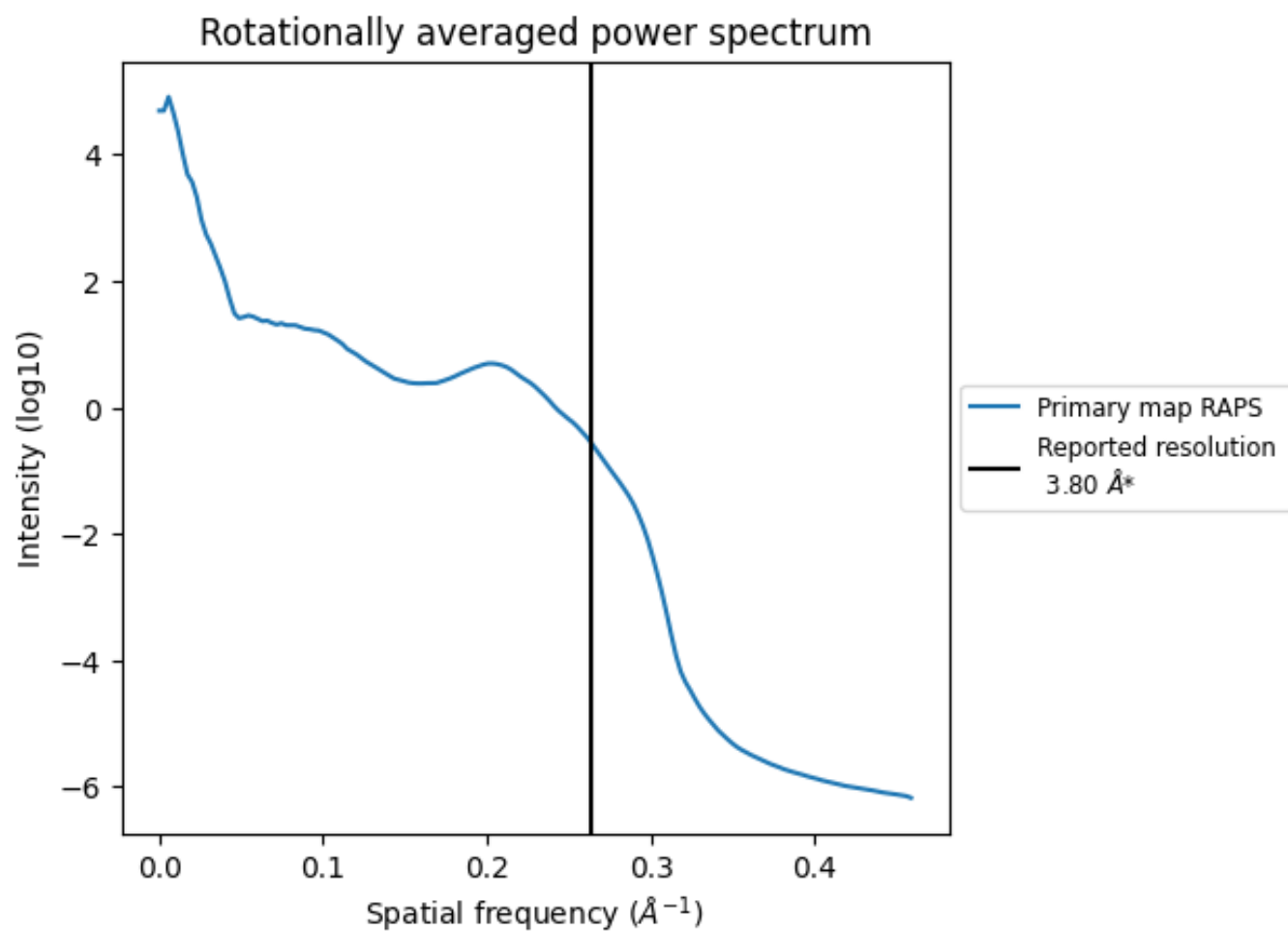
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 131 nm^3 ; this corresponds to an approximate mass of 118 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 0.263 Å⁻¹

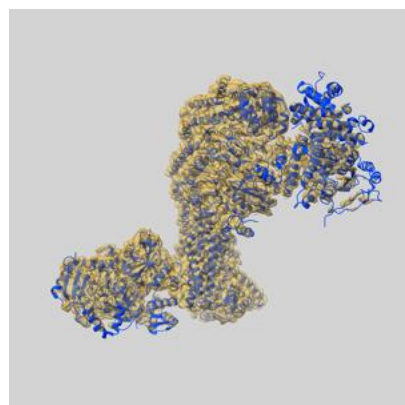
8 Fourier-Shell correlation ⓘ

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

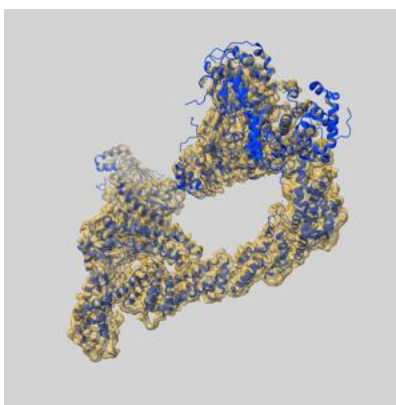
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12037 and PDB model 7B5L. Per-residue inclusion information can be found in section [3](#) on page [7](#).

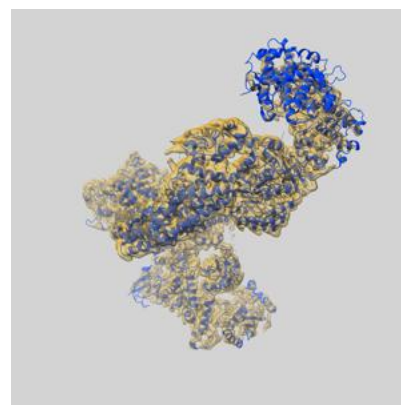
9.1 Map-model overlay [i](#)



X



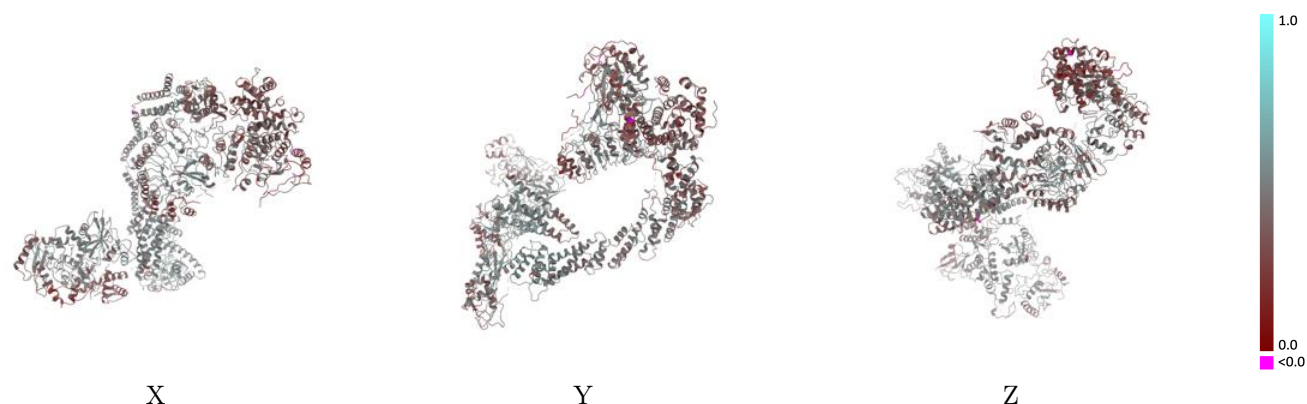
Y



Z

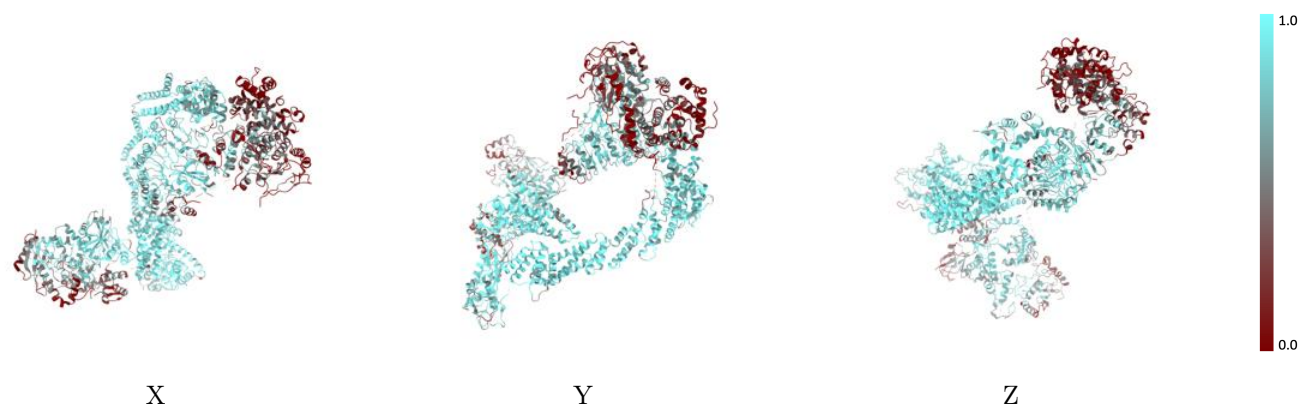
The images above show the 3D surface view of the map at the recommended contour level 7.42 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



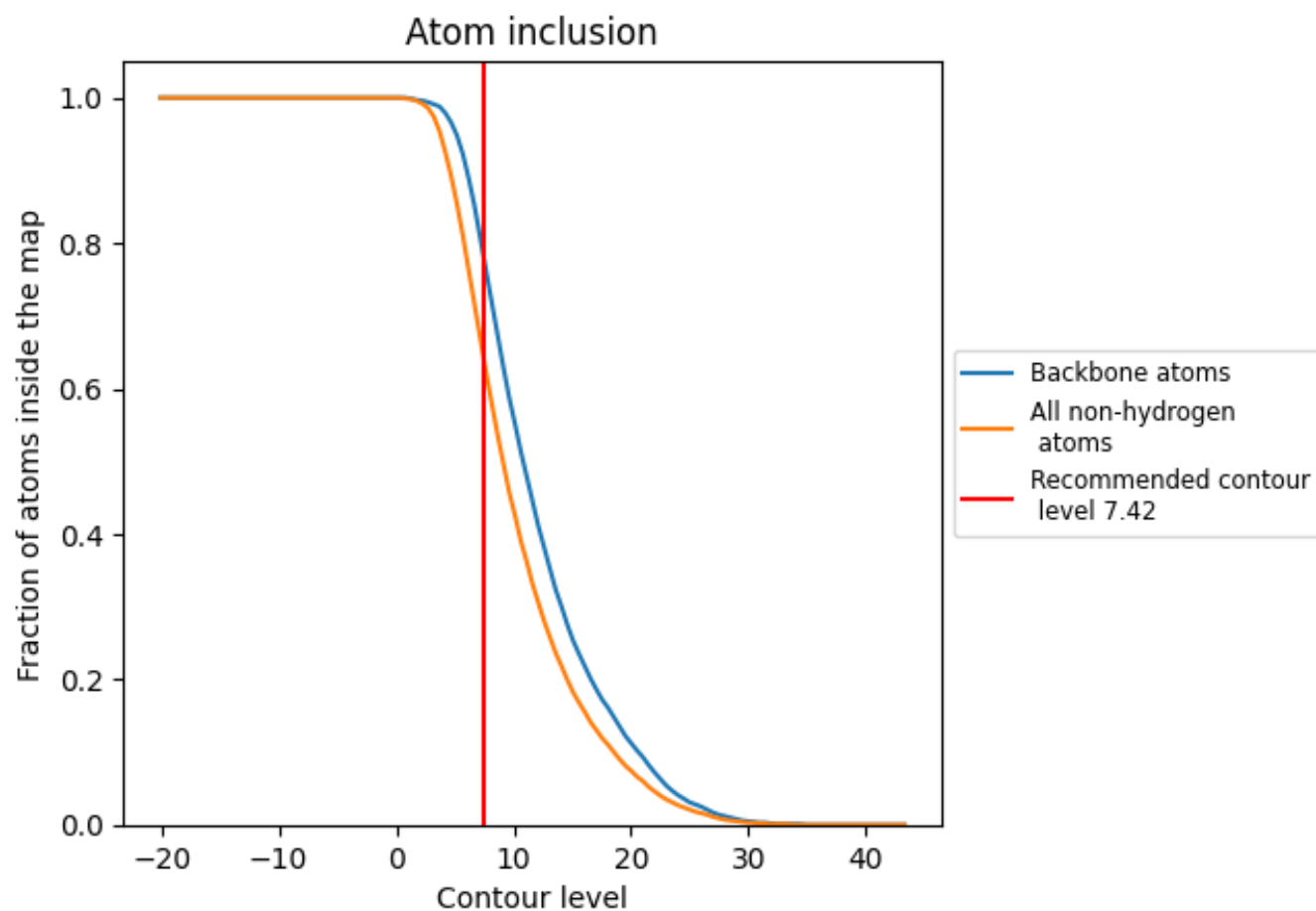
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (7.42).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 64% 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 (7.42) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6430	<div></div> 0.4270
C	<div></div> 0.7970	<div></div> 0.4410
D	<div></div> 0.4600	<div></div> 0.4080
H	<div></div> 0.8010	<div></div> 0.4810
K	<div></div> 0.7860	<div></div> 0.4800
L	<div></div> 0.4500	<div></div> 0.4190
N	<div></div> 0.3020	<div></div> 0.3390
P	<div></div> 0.1010	<div></div> 0.3000
R	<div></div> 0.9260	<div></div> 0.5020
S	<div></div> 0.7170	<div></div> 0.3710
T	<div></div> 0.7340	<div></div> 0.4410
U	<div></div> 0.7330	<div></div> 0.4770
Y	<div></div> 0.2180	<div></div> 0.3390

