



## Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 05:54 AM UTC

PDB ID : 9D2F / pdb\_00009d2f  
EMDB ID : EMD-46494  
Title : 3D structure and atomic model of RS3 of mouse respiratory cilia  
Authors : Yanhe, Z.; Xuewu, Z.; Daniela, N.  
Deposited on : 2024-08-08  
Resolution : 4.70 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

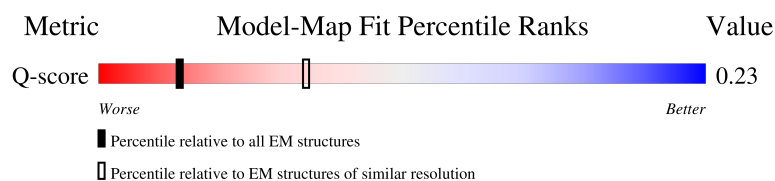
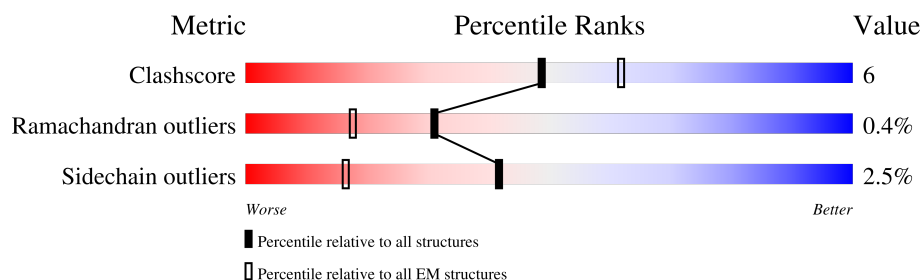
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 4.70 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	1989 ( 4.20 - 5.20 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1894	
2	B	340	
2	C	340	
3	H	321	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	N	783	
5	O	377	
5	R	377	
6	P	258	
6	Q	258	
7	S	172	
8	U	4250	
9	W	1249	
9	X	1249	
10	Y	1682	
11	Z	1843	
12	T	4144	
13	I	170	
14	J	1252	
15	K	1299	
16	L	471	
17	M	363	
18	E	334	
19	F	500	
20	V	93	
21	a	536	
22	b	401	
23	c	520	
24	D	723	
24	G	723	

## 2 Entry composition [i](#)

There are 25 unique types of molecules in this entry. The entry contains 184242 atoms, of which 92030 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 Adenylate kinase 9.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1663	Total	C	H	N	O	S	0	0
			27190	8668	13598	2273	2587	64		

- Molecule 2 is a protein called Leucine-rich repeat-containing protein 23.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	288	Total	C	H	N	O	S	0	0
			4678	1462	2348	408	452	8		
2	C	289	Total	C	H	N	O	S	0	0
			4693	1467	2354	409	455	8		

- Molecule 3 is a protein called Serine/threonine/tyrosine interacting-like 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	H	285	Total	C	H	N	O	S	0	0
			4719	1521	2366	403	415	14		

- Molecule 4 is a protein called Cilia- and flagella-associated protein 91.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	N	292	Total	C	H	N	O	S	0	0
			4857	1508	2433	427	479	10		

- Molecule 5 is a protein called Actin, aortic smooth muscle.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	O	368	Total	C	H	N	O	S	0	0
			5724	1822	2847	486	548	21		
5	R	370	Total	C	H	N	O	S	0	0
			5748	1829	2859	488	551	21		

- Molecule 6 is a protein called Axonemal dynein light intermediate polypeptide 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	P	202	Total	C	H	N	O	S	0	0
			3334	1025	1675	301	325	8		
6	Q	198	Total	C	H	N	O	S	0	0
			3278	1008	1646	297	319	8		

- Molecule 7 is a protein called Centrin-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	S	147	Total	C	H	N	O	S	0	0
			2372	741	1185	192	247	7		

- Molecule 8 is a protein called Dynein axonemal heavy chain 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	U	813	Total	C	H	N	O	S	0	0
			13198	4207	6594	1103	1253	41		

- Molecule 9 is a protein called Cilia- and flagella-associated protein 57.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	W	207	Total	C	H	N	O	S	0	0
			3622	1112	1842	327	335	6		
9	X	227	Total	C	H	N	O	S	0	0
			3937	1205	2005	355	365	7		

- Molecule 10 is a protein called Cilia- and flagella-associated protein 43.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	Y	39	Total	C	H	N	O	S	0	0
			629	192	317	55	63	2		

- Molecule 11 is a protein called Cilia- and flagella-associated protein 44.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	Z	44	Total	C	H	N	O	S	0	0
			751	229	382	70	66	4		

- Molecule 12 is a protein called Dynein, axonemal, heavy chain 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	T	517	Total	C	H	N	O	S	0	0
			8605	2750	4334	728	774	19		

- Molecule 13 is a protein called MORN repeat-containing protein 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	I	165	Total	C	H	N	O	S	0	0
			2663	877	1288	235	253	10		

- Molecule 14 is a protein called Cilia- and flagella-associated protein 61.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	J	1145	Total	C	H	N	O	S	0	0
			18417	5974	9162	1543	1691	47		

- Molecule 15 is a protein called Cilia- and flagella-associated protein 251.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	K	905	Total	C	H	N	O	S	0	0
			14317	4622	7129	1182	1341	43		

- Molecule 16 is a protein called Tetratricopeptide repeat protein 29.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	L	384	Total	C	H	N	O	S	0	0
			6112	1954	3005	532	602	19		

- Molecule 17 is a protein called Zinc finger, MYND domain containing 12.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	M	345	Total	C	H	N	O	S	0	0
			5500	1755	2741	463	525	16		

- Molecule 18 is a protein called Malate dehydrogenase, cytoplasmic.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	E	334	Total	C	H	N	O	S	0	0
			5194	1634	2629	429	490	12		

- Molecule 19 is a protein called Putative malate dehydrogenase 1B.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	F	459	Total	C	H	N	O	S	0	0
			7290	2327	3661	602	678	22		

- Molecule 20 is a protein called UPF0728 protein C10orf53 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	V	92	Total	C	H	N	O	S	0	0
			1433	459	710	121	141	2		

- Molecule 21 is a protein called A kinase (PRKA) anchor protein 14.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	a	124	Total	C	H	N	O	S	0	0
			2133	702	1062	182	186	1		

- Molecule 22 is a protein called cAMP-dependent protein kinase type II-alpha regulatory subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	b	52	Total	C	H	N	O	S	0	0
			837	269	415	71	81	1		

- Molecule 23 is a protein called Ciliogenesis-associated TTC17-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	c	73	Total	C	H	N	O		0	0
			1220	402	607	106	105			

- Molecule 24 is a protein called Adenylate kinase 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	D	678	Total	C	H	N	O	S	0	0
			10879	3476	5413	914	1053	23		
24	G	681	Total	C	H	N	O	S	0	0
			10910	3486	5423	917	1061	23		

- Molecule 25 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
25	M	2	Total	Zn	0
			2	2	







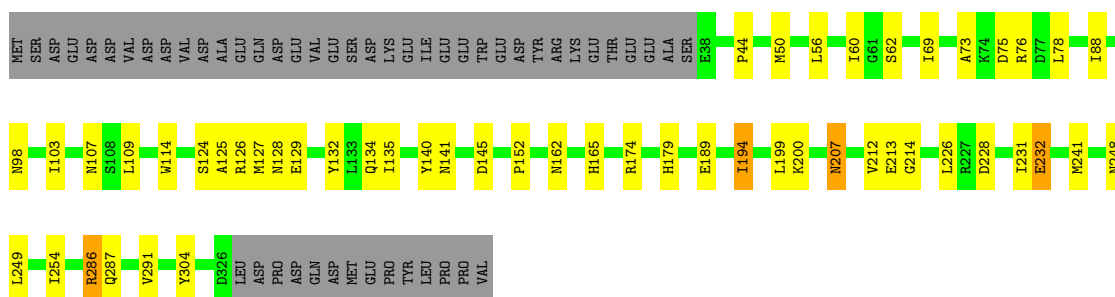
• Molecule 2: Leucine-rich repeat-containing protein 23

Chain B: 75% 9% 15%



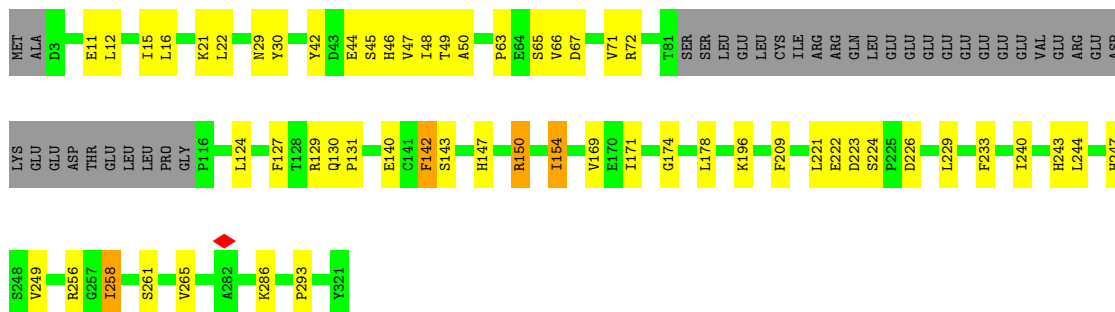
• Molecule 2: Leucine-rich repeat-containing protein 23

Chain C: 69% 14% 15%

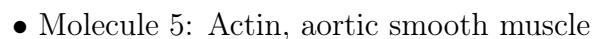
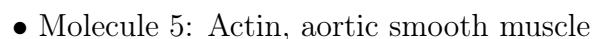


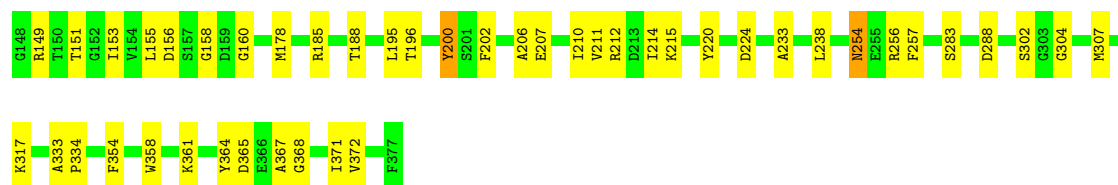
• Molecule 3: Serine/threonine/tyrosine interacting-like 1

Chain H: 71% 17% 11%

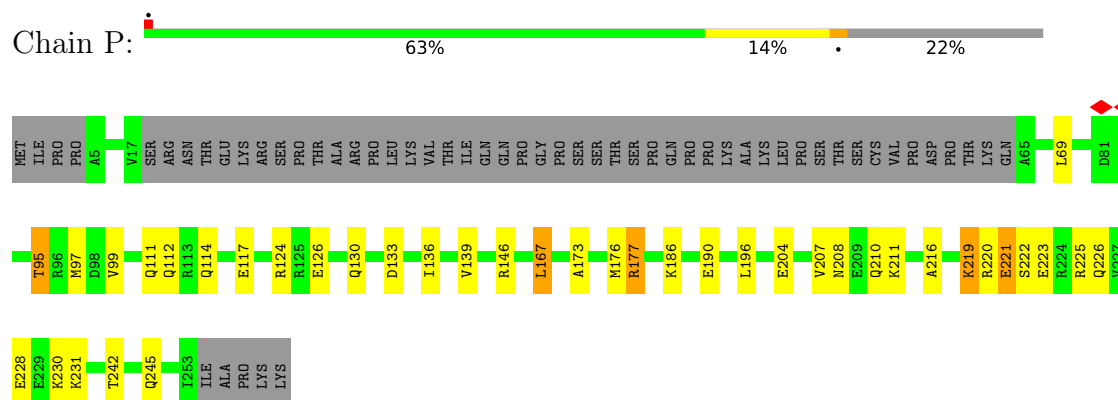


• Molecule 4: Cilia- and flagella-associated protein 91

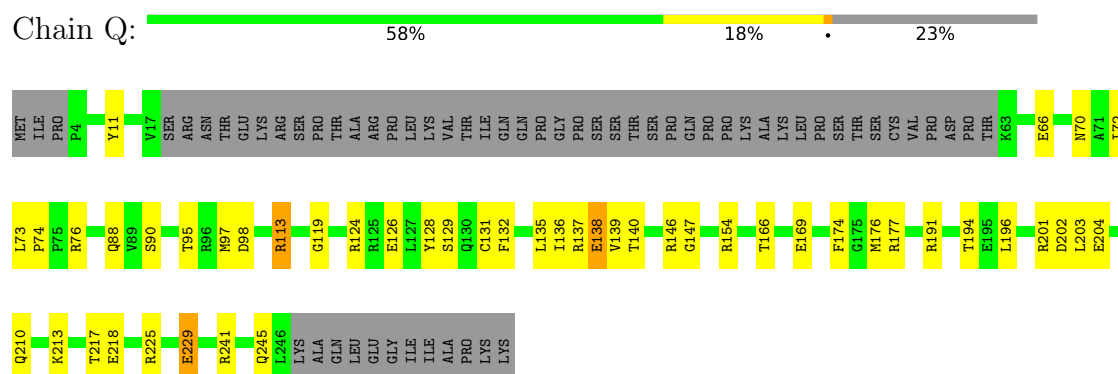




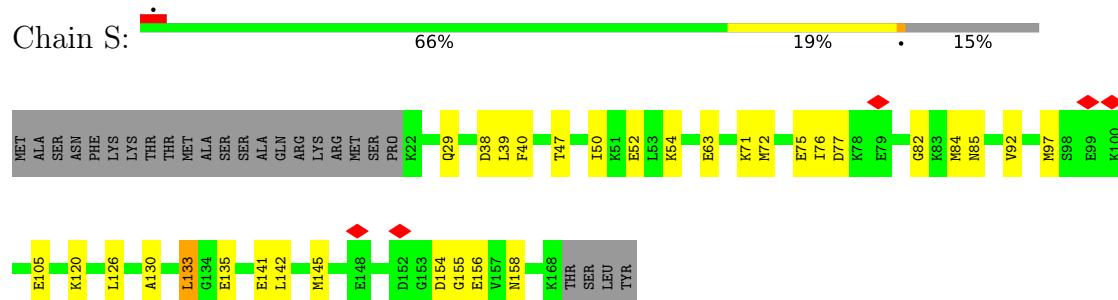
- Molecule 6: Axonemal dynein light intermediate polypeptide 1



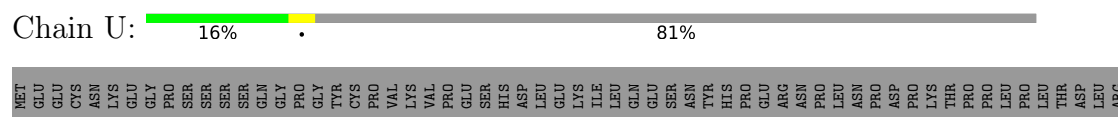
- Molecule 6: Axonemal dynein light intermediate polypeptide 1



- Molecule 7: Centrin-2



- Molecule 8: Dynein axonemal heavy chain 1



WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

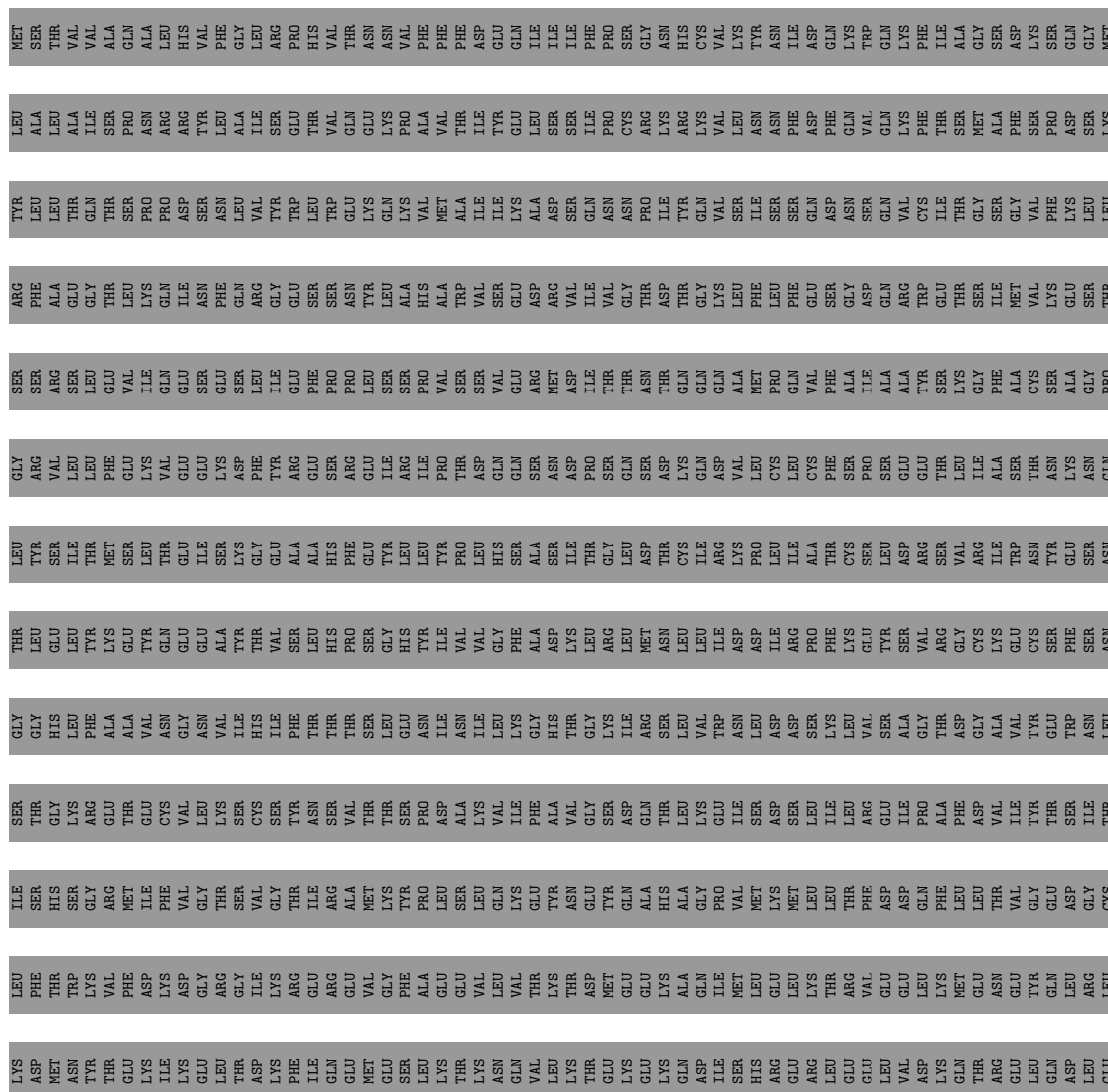




- Molecule 9: Cilia- and flagella-associated protein 57


[illegible]

- Molecule 9: Cilia- and flagella-associated protein 57





- Molecule 10: Cilia- and flagella-associated protein 43

Chain Y: 

[illegible]



WORLDWIDE  
PDB  
PROTEIN DATA BANK





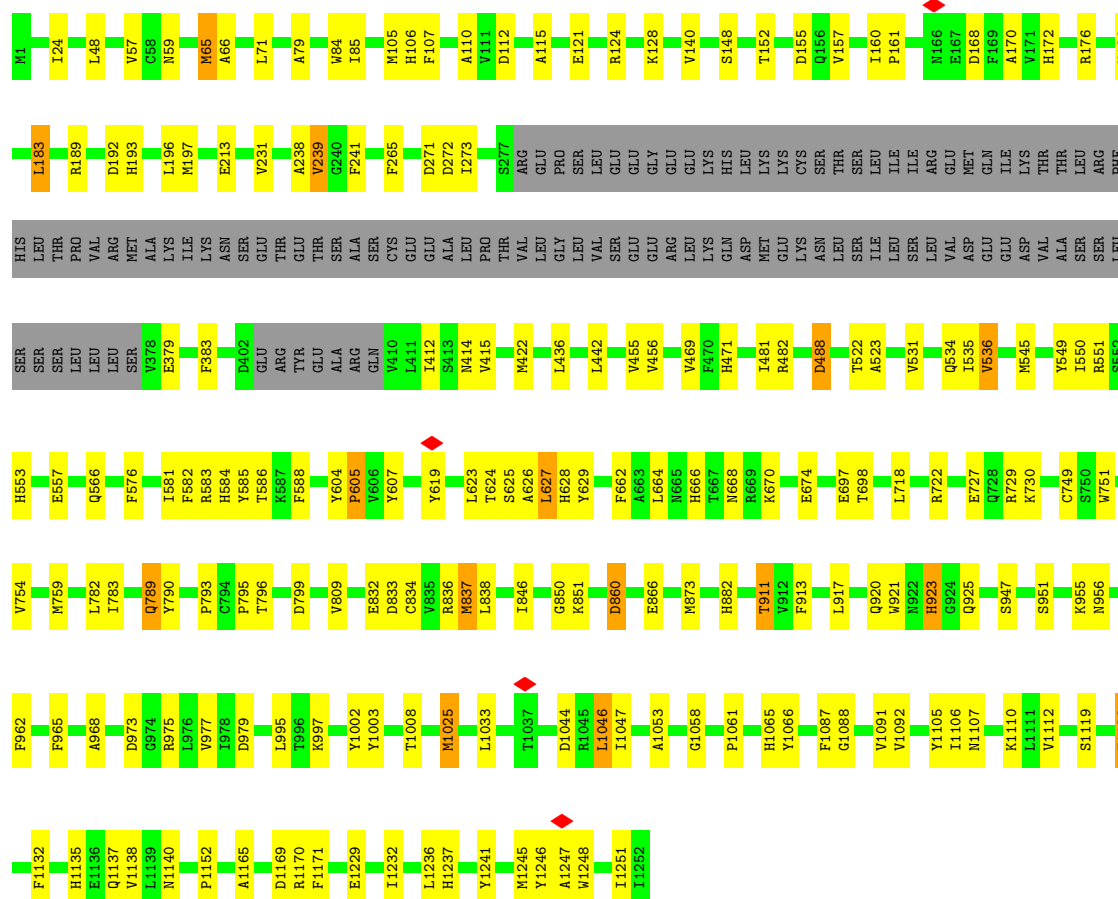






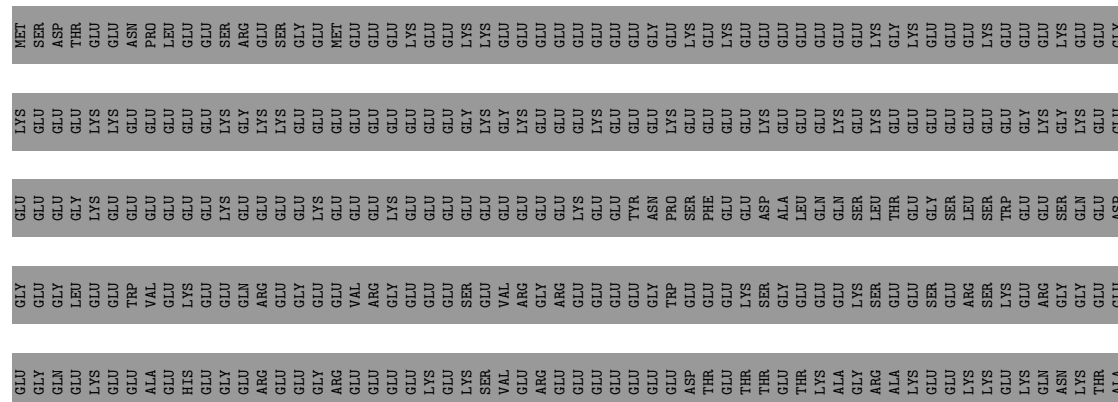
• Molecule 14: Cilia- and flagella-associated protein 61

Chain J: 76% 14% 9%

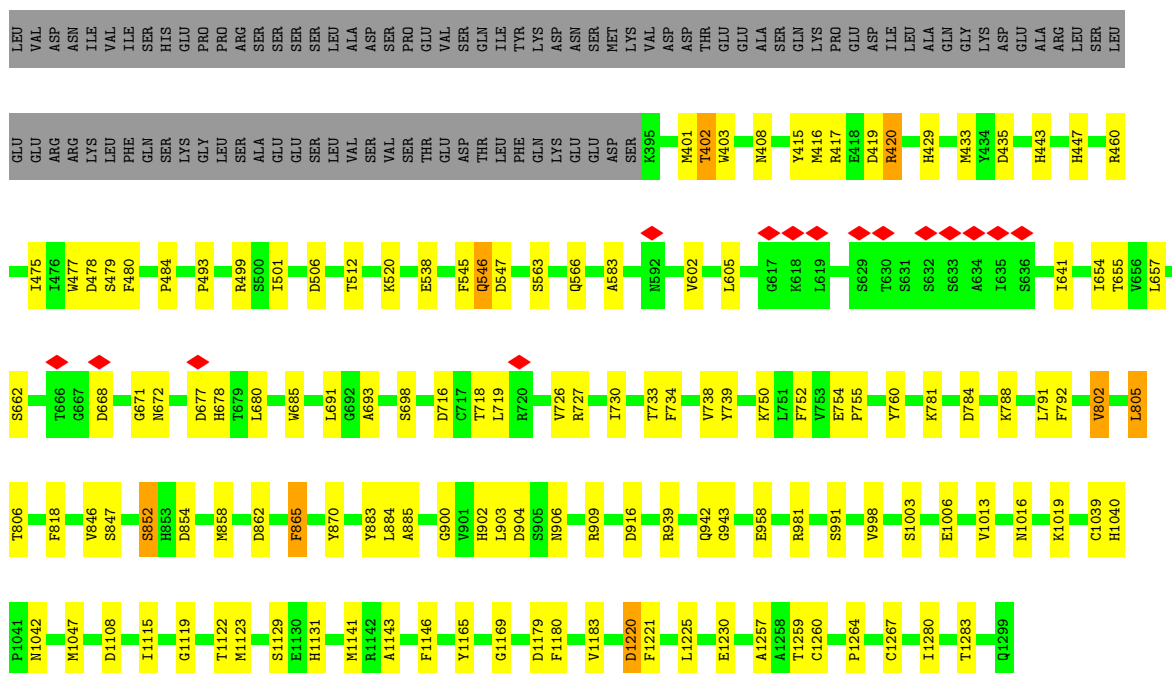


• Molecule 15: Cilia- and flagella-associated protein 251

Chain K: 59% 10% 30%

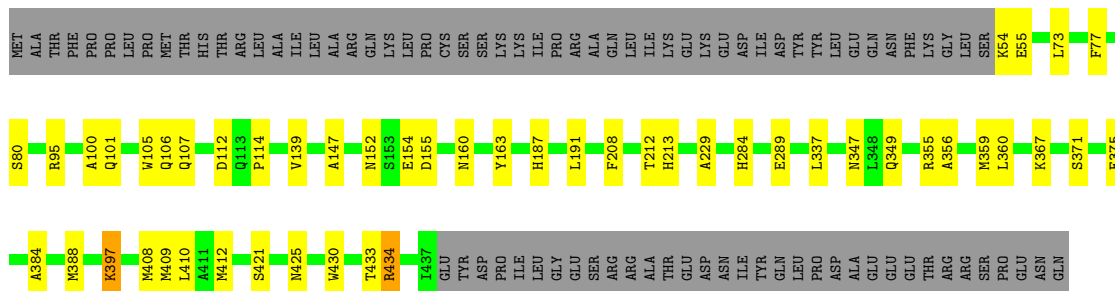






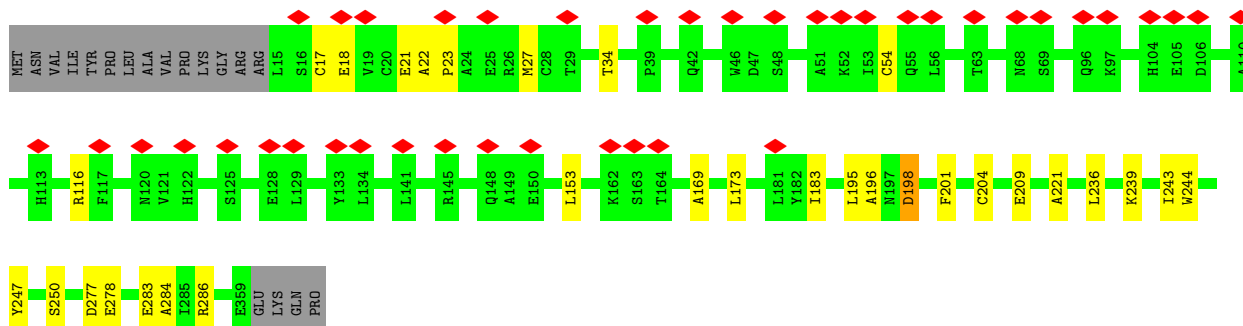
• Molecule 16: Tetratricopeptide repeat protein 29

Chain L: 71% 10% 18%



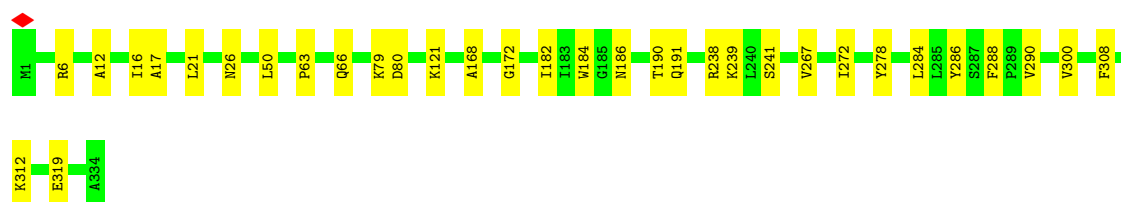
• Molecule 17: Zinc finger, MYND domain containing 12

Chain M: 11% 87% 8% 5%



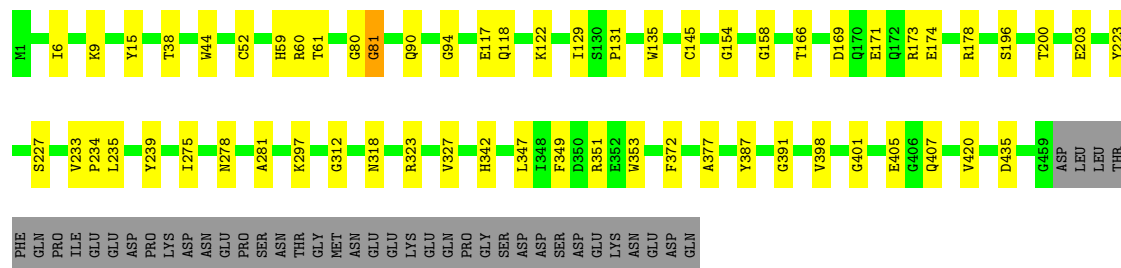
• Molecule 18: Malate dehydrogenase, cytoplasmic

Chain E: 90% 10%



• Molecule 19: Putative malate dehydrogenase 1B

Chain F: 80% 12% 8%



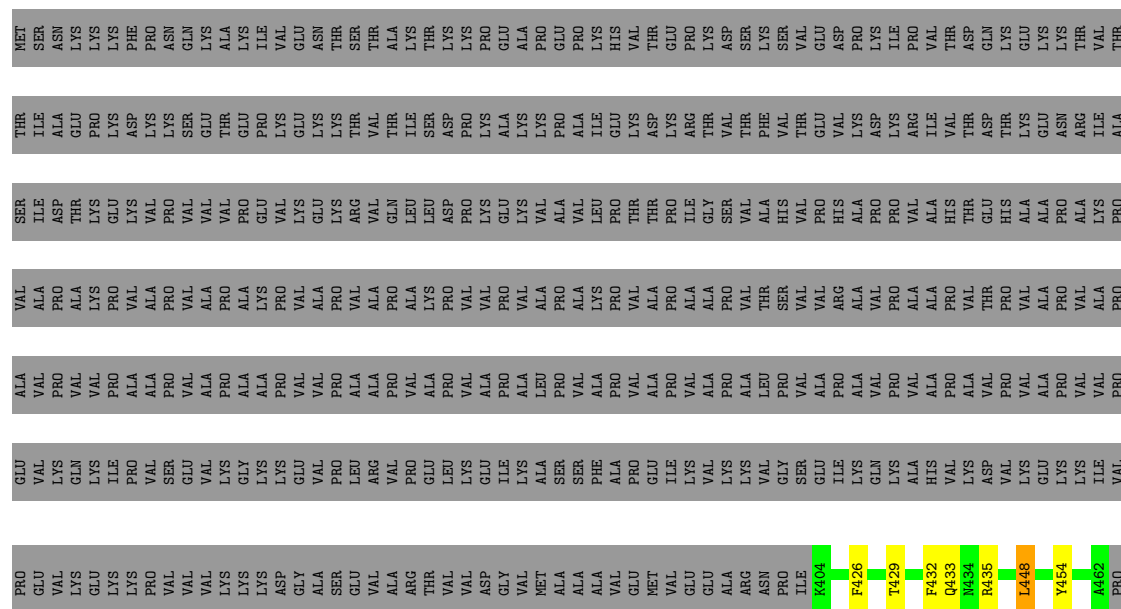
• Molecule 20: UPF0728 protein C10orf53 homolog

Chain V: 80% 18% ..




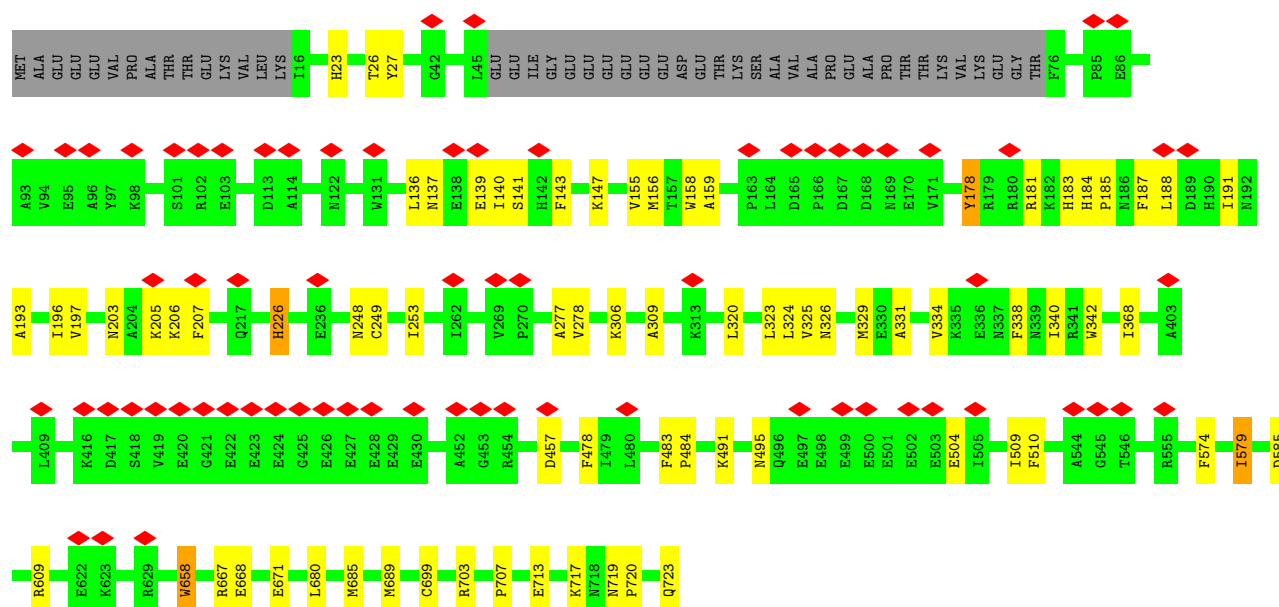
• Molecule 21: A kinase (PRKA) anchor protein 14

Chain a: 20% 77%




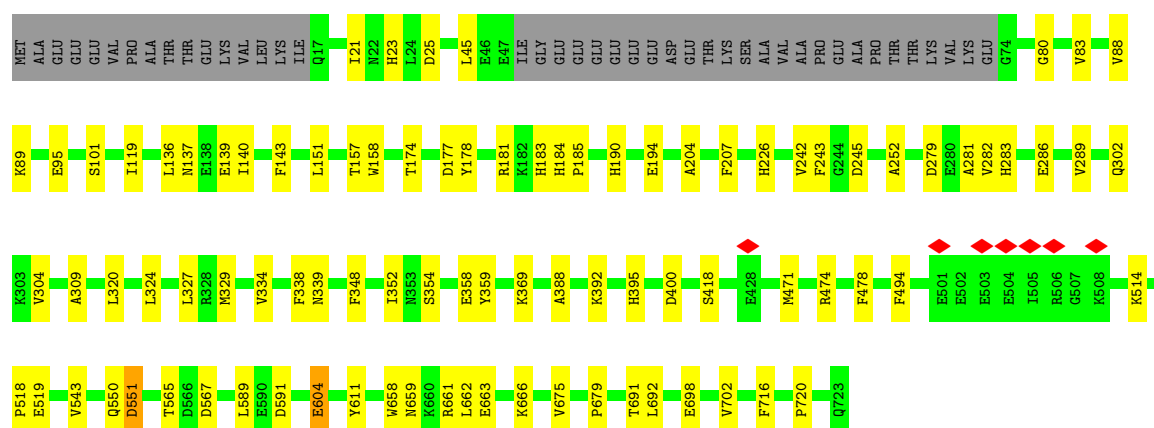


Chain D:  10% 83% 10% 6%



• Molecule 24: Adenylate kinase 7

Chain G:  81% 12% 6%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	63152	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0037	Depositor
Map size (Å)	776.88, 776.88, 776.88	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.158, 2.158, 2.158	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.14	0/13886	0.43	0/18750
2	B	0.11	0/2365	0.40	0/3194
2	C	0.11	0/2374	0.43	0/3206
3	H	0.13	0/2412	0.44	0/3265
4	N	0.19	0/2450	0.49	0/3285
5	O	0.12	0/2940	0.42	0/3980
5	R	0.14	0/2952	0.46	0/3997
6	P	0.18	0/1676	0.44	0/2252
6	Q	0.15	0/1650	0.41	0/2217
7	S	0.15	0/1197	0.43	0/1590
8	U	0.15	0/6745	0.44	0/9131
9	W	0.17	0/1794	0.39	0/2386
9	X	0.19	0/1947	0.44	0/2591
10	Y	0.19	0/313	0.47	0/419
11	Z	0.17	0/373	0.33	0/495
12	T	0.15	0/4362	0.44	0/5889
13	I	0.13	0/1418	0.50	0/1913
14	J	0.12	0/9494	0.43	0/12898
15	K	0.11	0/7367	0.42	0/10000
16	L	0.15	0/3166	0.38	0/4258
17	M	0.15	0/2813	0.42	0/3810
18	E	0.12	0/2608	0.35	0/3524
19	F	0.12	0/3704	0.38	0/5022
20	V	0.13	0/735	0.42	0/997
21	a	0.11	0/1103	0.37	0/1488
22	b	0.15	0/431	0.45	0/586
23	c	0.15	0/632	0.39	0/855
24	D	0.13	0/5573	0.41	0/7525
24	G	0.12	0/5594	0.40	0/7553
All	All	0.14	0/94074	0.42	0/127076

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
2	C	0	1
3	H	0	1
4	N	0	1
5	O	0	1
6	P	0	1
6	Q	0	2
8	U	0	1
12	T	0	1
13	I	0	1
15	K	0	4
23	c	0	1
All	All	0	18

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1838	ARG	Sidechain
1	A	186	ARG	Sidechain
1	A	246	LYS	Mainchain
2	C	286	ARG	Sidechain
3	H	72	ARG	Sidechain
13	I	144	ARG	Sidechain
15	K	402	THR	Peptide
15	K	417	ARG	Sidechain
15	K	420	ARG	Sidechain
15	K	760	TYR	Peptide
4	N	505	ARG	Sidechain
5	O	30	ARG	Sidechain
6	P	177	ARG	Sidechain
6	Q	177	ARG	Sidechain
6	Q	76	ARG	Sidechain
12	T	274	ARG	Sidechain
8	U	359	ARG	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
23	c	298	ARG	Sidechain

## 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	13592	13598	13593	169	0
2	B	2330	2348	2347	15	0
2	C	2339	2354	2353	31	0
3	H	2353	2366	2364	33	0
4	N	2424	2433	2432	55	0
5	O	2877	2847	2846	43	0
5	R	2889	2859	2858	44	0
6	P	1659	1675	1673	31	0
6	Q	1632	1646	1645	32	0
7	S	1187	1185	1184	27	0
8	U	6604	6594	6593	93	0
9	W	1780	1842	1839	18	0
9	X	1932	2005	2003	21	0
10	Y	312	317	316	4	0
11	Z	369	382	381	1	0
12	T	4271	4334	4330	52	0
13	I	1375	1288	1288	32	0
14	J	9255	9162	9160	120	0
15	K	7188	7129	7126	80	0
16	L	3107	3005	3004	31	0
17	M	2759	2741	2736	18	0
18	E	2565	2629	2629	18	0
19	F	3629	3661	3661	34	0
20	V	723	710	710	8	0
21	a	1071	1062	1060	8	0
22	b	422	415	415	5	0
23	c	613	607	607	8	0
24	D	5466	5413	5410	55	0
24	G	5487	5423	5421	52	0
25	M	2	0	0	0	0
All	All	92212	92030	91984	1059	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 6.

All (1059) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LYS:NZ	1:A:150:CYS:O	2.04	0.90
5:O:374:ARG:NE	12:T:318:GLU:OE1	2.13	0.82
14:J:833:ASP:OD1	14:J:836:ARG:NH2	2.13	0.81
14:J:624:THR:HG22	14:J:625:SER:H	1.43	0.81
4:N:654:GLU:OE2	23:c:298:ARG:NH1	2.15	0.80
1:A:1800:ASN:OD1	4:N:686:TYR:OH	2.00	0.79
14:J:1002:TYR:OH	14:J:1044:ASP:OD1	2.00	0.79
1:A:1465:ASP:OD2	1:A:1496:ARG:NH1	2.17	0.78
21:a:426:PHE:O	21:a:429:THR:OG1	2.02	0.77
5:R:361:LYS:NZ	5:R:365:ASP:OD1	2.16	0.77
7:S:120:LYS:NZ	7:S:154:ASP:OD2	2.17	0.77
5:O:133:ALA:HB1	5:O:358:TRP:HB3	1.66	0.76
1:A:330:ARG:NH1	1:A:877:GLU:OE1	2.19	0.75
14:J:583:ARG:O	14:J:629:TYR:OH	2.03	0.75
5:R:367:ALA:HB1	5:R:371:ILE:CG2	2.16	0.75
5:R:367:ALA:HB1	5:R:371:ILE:HG21	1.69	0.74
8:U:726:MET:SD	8:U:730:GLN:NE2	2.60	0.74
4:N:582:LEU:HD11	14:J:1236:LEU:HD11	1.69	0.74
20:V:27:ARG:NH1	20:V:70:LEU:O	2.21	0.72
5:O:80:ASN:ND2	5:O:82:ASP:OD1	2.21	0.72
5:O:72:PRO:O	5:O:79:THR:OG1	2.09	0.70
1:A:988:LYS:NZ	1:A:1108:ASP:OD1	2.25	0.70
3:H:150:ARG:O	3:H:150:ARG:NE	2.25	0.69
6:Q:202:ASP:OD1	6:Q:203:LEU:N	2.25	0.69
6:P:231:LYS:NZ	6:Q:229:GLU:OE1	2.19	0.69
8:U:764:VAL:O	8:U:768:VAL:HG13	1.93	0.69
17:M:18:GLU:OE1	17:M:116:ARG:NH1	2.27	0.67
14:J:722:ARG:NH1	14:J:832:GLU:OE1	2.28	0.67
2:C:165:HIS:O	2:C:189:GLU:N	2.28	0.67
8:U:661:LEU:H	8:U:661:LEU:HD22	1.58	0.67
16:L:107:GLN:NE2	16:L:154:GLU:O	2.28	0.67
5:O:174:PRO:HA	5:O:177:ILE:HD13	1.77	0.66
14:J:1236:LEU:HD13	14:J:1246:TYR:HB3	1.78	0.66
1:A:21:GLU:OE1	1:A:24:ARG:NH1	2.29	0.66
6:P:226:GLN:OE1	6:P:230:LYS:NZ	2.25	0.66
3:H:147:HIS:ND1	13:I:147:ASP:OD1	2.30	0.65
12:T:276:TRP:HA	12:T:279:PHE:CZ	2.30	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:LEU:HD21	1:A:330:ARG:HA	1.79	0.65
8:U:109:ILE:HD11	14:J:628:HIS:ND1	2.12	0.65
6:Q:72:ILE:HD13	6:Q:140:THR:HG21	1.79	0.65
1:A:1157:HIS:ND1	1:A:1161:GLU:OE2	2.27	0.65
9:W:996:MET:HE3	9:X:996:MET:HG3	1.79	0.64
12:T:465:ASP:O	12:T:469:ARG:NH1	2.27	0.64
18:E:238:ARG:NH2	18:E:241:SER:O	2.27	0.64
9:X:999:GLN:NE2	9:X:1003:MET:SD	2.70	0.64
9:W:1211:ARG:NH1	9:W:1215:ASP:OD2	2.30	0.64
15:K:1016:ASN:OD1	15:K:1019:LYS:N	2.31	0.64
18:E:272:ILE:HD12	18:E:284:LEU:O	1.97	0.64
1:A:1830:ASN:O	1:A:1838:ARG:NH1	2.31	0.64
6:P:220:ARG:NH1	6:Q:218:GLU:OE1	2.31	0.63
10:Y:1619:GLU:OE2	10:Y:1620:ARG:NH1	2.32	0.62
24:D:685:MET:HA	24:D:689:MET:HG2	1.81	0.62
1:A:1112:ARG:N	1:A:1116:GLU:OE1	2.32	0.62
4:N:734:GLU:O	4:N:735:THR:HG22	1.99	0.62
20:V:25:THR:O	20:V:29:GLN:N	2.29	0.62
3:H:147:HIS:O	3:H:150:ARG:HG3	2.00	0.62
1:A:19:GLU:OE2	1:A:942:ARG:NH1	2.32	0.62
2:B:179:HIS:O	2:B:200:LYS:N	2.33	0.61
1:A:394:LYS:O	1:A:619:ASP:N	2.33	0.61
1:A:1427:ASP:OD1	1:A:1430:ARG:NH2	2.31	0.61
16:L:384:ALA:O	16:L:388:MET:N	2.31	0.61
4:N:681:GLU:OE1	4:N:684:ARG:NH2	2.32	0.61
18:E:190:THR:OG1	18:E:319:GLU:OE1	2.14	0.61
15:K:858:MET:O	15:K:870:TYR:N	2.32	0.61
1:A:1139:ASP:OD1	1:A:1139:ASP:N	2.34	0.61
13:I:137:ASP:O	13:I:140:ASN:N	2.32	0.61
2:B:290:LEU:HD13	2:B:304:TYR:CE2	2.35	0.61
1:A:1571:SER:HG	1:A:1573:TRP:CD1	2.17	0.60
4:N:578:MET:HE1	13:I:3:TYR:CE2	2.36	0.60
7:S:120:LYS:NZ	7:S:158:ASN:OD1	2.26	0.60
8:U:661:LEU:HD23	8:U:726:MET:HG2	1.81	0.60
15:K:902:HIS:O	15:K:906:ASN:N	2.34	0.60
14:J:57:VAL:HB	14:J:66:ALA:HB3	1.83	0.60
1:A:27:LEU:O	1:A:381:ARG:NH1	2.34	0.60
5:O:368:GLY:HA2	5:O:371:ILE:HG22	1.82	0.60
15:K:1220:ASP:OD1	15:K:1220:ASP:N	2.29	0.60
6:P:177:ARG:NH1	8:U:405:SER:OG	2.35	0.60
2:B:76:ARG:N	2:B:98:ASN:OD1	2.35	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:204:THR:O	5:O:208:ARG:N	2.28	0.60
6:P:146:ARG:NH2	6:Q:138:GLU:OE1	2.32	0.60
8:U:172:PRO:HD2	8:U:175:ILE:HD12	1.84	0.59
8:U:434:MET:O	8:U:438:ASN:ND2	2.34	0.59
21:a:448:LEU:O	21:a:484:LYS:NZ	2.30	0.59
24:G:139:GLU:O	24:G:143:PHE:N	2.34	0.59
15:K:939:ARG:NH2	15:K:942:GLN:OE1	2.35	0.59
14:J:121:GLU:OE2	14:J:124:ARG:NH1	2.33	0.59
16:L:73:LEU:HB3	17:M:196:ALA:HB1	1.85	0.59
1:A:298:LYS:O	1:A:323:LYS:NZ	2.17	0.59
24:D:156:MET:HE1	24:D:325:VAL:HG21	1.85	0.59
1:A:310:ILE:HG22	1:A:311:ASP:N	2.17	0.59
1:A:1137:ASP:OD1	1:A:1138:GLN:N	2.36	0.59
19:F:59:HIS:NE2	19:F:61:THR:O	2.36	0.59
15:K:401:MET:O	15:K:402:THR:HG23	2.03	0.58
8:U:511:MET:HE1	8:U:541:PHE:CZ	2.38	0.58
14:J:1065:HIS:N	14:J:1119:SER:O	2.36	0.58
1:A:1163:LYS:NZ	1:A:1236:GLU:OE2	2.35	0.58
6:Q:119:GLY:O	6:Q:124:ARG:NH2	2.34	0.58
13:I:83:TYR:OH	13:I:92:TYR:N	2.36	0.58
3:H:29:ASN:ND2	14:J:566:GLN:OE1	2.36	0.58
2:B:49:MET:SD	2:B:76:ARG:NH1	2.77	0.58
24:G:691:THR:OG1	24:G:692:LEU:N	2.37	0.58
1:A:1089:SER:O	1:A:1093:GLU:HG2	2.03	0.58
2:B:243:SER:O	2:B:245:GLN:N	2.34	0.58
1:A:422:ASP:OD1	1:A:600:ASN:ND2	2.35	0.58
7:S:120:LYS:HZ2	7:S:158:ASN:CG	2.11	0.58
16:L:430:TRP:O	16:L:434:ARG:N	2.36	0.58
7:S:105:GLU:OE1	12:T:274:ARG:NH1	2.37	0.58
8:U:818:ALA:HB2	8:U:887:LEU:HD22	1.85	0.58
1:A:54:ALA:HB2	1:A:278:PHE:CE2	2.39	0.58
14:J:851:LYS:O	14:J:947:SER:N	2.32	0.58
1:A:1182:ARG:NH2	1:A:1217:GLU:OE1	2.33	0.57
14:J:911:THR:HG22	14:J:913:PHE:CE2	2.39	0.57
16:L:284:HIS:ND1	16:L:289:GLU:OE1	2.37	0.57
14:J:1087:PHE:CG	14:J:1088:GLY:N	2.72	0.57
1:A:280:THR:HG23	1:A:1471:SER:HB3	1.85	0.57
1:A:402:HIS:O	1:A:404:GLY:N	2.38	0.57
5:O:285:MET:SD	5:O:292:ARG:NH1	2.77	0.57
9:X:1102:ARG:NH1	12:T:236:ASP:OD2	2.32	0.57
14:J:535:ILE:O	14:J:536:VAL:HG13	2.05	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1241:ASP:OD1	1:A:1241:ASP:N	2.30	0.57
23:c:293:ARG:NH1	23:c:296:GLN:OE1	2.35	0.57
15:K:738:VAL:HG21	15:K:752:PHE:CE1	2.40	0.57
5:R:147:SER:O	5:R:149:ARG:NH1	2.35	0.57
8:U:710:LEU:HD22	8:U:710:LEU:H	1.69	0.57
5:O:175:HIS:CG	12:T:582:VAL:HG11	2.40	0.57
4:N:732:ASN:O	4:N:735:THR:N	2.37	0.57
6:Q:129:SER:OG	6:Q:154:ARG:NH2	2.38	0.57
9:X:1043:ARG:NH2	9:X:1046:GLU:OE1	2.37	0.57
24:D:155:VAL:O	24:D:159:ALA:N	2.38	0.57
19:F:297:LYS:HZ3	19:F:353:TRP:CD1	2.23	0.56
16:L:160:ASN:OD1	16:L:191:LEU:HD22	2.06	0.56
5:R:27:ASP:OD1	5:R:27:ASP:N	2.37	0.56
4:N:499:GLN:NE2	15:K:1230:GLU:O	2.37	0.56
1:A:1438:ASP:CG	1:A:1438:ASP:O	2.47	0.56
8:U:661:LEU:HD23	8:U:726:MET:CG	2.35	0.56
4:N:553:ARG:HD3	14:J:1046:LEU:HD22	1.87	0.56
14:J:1107:ASN:O	14:J:1110:LYS:N	2.30	0.56
19:F:171:GLU:HA	19:F:174:GLU:HB2	1.86	0.56
6:P:221:GLU:O	6:P:225:ARG:HD2	2.05	0.56
7:S:142:LEU:O	7:S:145:MET:SD	2.64	0.56
14:J:522:THR:HG22	14:J:523:ALA:H	1.70	0.56
14:J:549:TYR:O	14:J:553:HIS:ND1	2.27	0.56
24:D:667:ARG:NH1	24:D:671:GLU:OE2	2.38	0.56
1:A:1808:LYS:NZ	24:D:671:GLU:OE1	2.35	0.56
6:P:111:GLN:O	6:P:114:GLN:NE2	2.38	0.56
19:F:372:PHE:CE1	19:F:377:ALA:HB2	2.41	0.56
14:J:962:PHE:CG	15:K:1123:MET:HE1	2.41	0.56
15:K:501:ILE:HD12	15:K:512:THR:HG22	1.88	0.56
15:K:677:ASP:O	15:K:680:LEU:N	2.38	0.55
1:A:246:LYS:O	1:A:250:LEU:HB3	2.05	0.55
5:R:155:LEU:O	5:R:302:SER:N	2.39	0.55
14:J:488:ASP:N	14:J:488:ASP:OD1	2.37	0.55
7:S:101:ASP:CG	12:T:277:LYS:HZ1	2.13	0.55
13:I:25:LEU:O	13:I:28:ASP:N	2.39	0.55
15:K:668:ASP:OD1	15:K:671:GLY:N	2.39	0.55
17:M:244:TRP:CH2	17:M:284:ALA:HB2	2.41	0.55
1:A:581:GLU:O	1:A:585:ASN:ND2	2.38	0.55
14:J:1165:ALA:HB2	14:J:1246:TYR:CZ	2.42	0.55
16:L:147:ALA:HB1	16:L:163:TYR:CE1	2.42	0.55
24:G:178:TYR:O	24:G:181:ARG:NH1	2.34	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:71:LYS:NZ	7:S:75:GLU:OE2	2.25	0.55
16:L:163:TYR:CD2	16:L:191:LEU:HD21	2.42	0.55
24:G:25:ASP:OD1	24:G:25:ASP:N	2.40	0.55
17:M:198:ASP:OD1	17:M:198:ASP:C	2.50	0.55
1:A:1345:ILE:HG21	1:A:1418:TYR:CD1	2.42	0.55
7:S:77:ASP:OD2	7:S:82:GLY:N	2.40	0.55
4:N:508:GLN:NE2	15:K:1143:ALA:O	2.40	0.54
1:A:1016:LEU:O	19:F:351:ARG:NH2	2.37	0.54
4:N:565:ASN:O	4:N:569:ASP:OD1	2.25	0.54
21:a:433:GLN:OE1	21:a:435:ARG:NH2	2.41	0.54
1:A:39:LYS:NZ	1:A:152:ASP:OD1	2.39	0.54
13:I:16:ARG:NH2	14:J:1140:ASN:OD1	2.40	0.54
8:U:594:ASP:C	8:U:594:ASP:OD1	2.50	0.54
5:O:61:GLN:O	5:O:64:ARG:NH1	2.38	0.54
24:D:325:VAL:HG12	24:D:326:ASN:H	1.71	0.54
4:N:586:LEU:CD1	14:J:1251:ILE:HG21	2.36	0.54
4:N:759:LEU:H	4:N:759:LEU:HD23	1.73	0.54
24:D:226:HIS:C	24:D:226:HIS:ND1	2.66	0.54
24:D:278:VAL:HG22	24:D:331:ALA:HB2	1.89	0.54
4:N:582:LEU:CD1	14:J:1236:LEU:HD11	2.37	0.54
22:b:36:PHE:CZ	23:c:334:ALA:HB3	2.43	0.54
1:A:1799:MET:SD	4:N:693:VAL:HB	2.48	0.54
6:P:112:GLN:O	6:P:114:GLN:NE2	2.40	0.54
14:J:727:GLU:OE2	14:J:730:LYS:NZ	2.36	0.54
17:M:22:ALA:HB1	17:M:23:PRO:CD	2.38	0.54
24:D:188:LEU:HA	24:D:191:ILE:HG22	1.89	0.54
5:O:82:ASP:OD1	5:O:82:ASP:N	2.42	0.53
19:F:6:ILE:HG22	19:F:15:TYR:CE1	2.43	0.53
24:G:174:THR:N	24:G:177:ASP:OD2	2.38	0.53
5:R:224:ASP:OD1	5:R:317:LYS:NZ	2.39	0.53
14:J:481:ILE:HD12	14:J:481:ILE:N	2.22	0.53
22:b:20:GLU:OE1	22:b:23:GLN:NE2	2.40	0.53
6:Q:113:ARG:NH1	8:U:465:ASN:O	2.41	0.53
5:R:195:LEU:HD12	5:R:200:TYR:O	2.08	0.53
10:Y:1619:GLU:O	10:Y:1623:ILE:HD13	2.09	0.53
14:J:545:MET:SD	14:J:545:MET:N	2.81	0.53
14:J:604:TYR:CE2	14:J:623:LEU:HD22	2.43	0.53
1:A:1783:LEU:HA	1:A:1786:TYR:CZ	2.44	0.53
8:U:377:ASN:OD1	8:U:378:LEU:N	2.42	0.53
14:J:482:ARG:NH2	14:J:488:ASP:OD1	2.39	0.53
1:A:909:LYS:O	1:A:1308:LYS:NZ	2.38	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:793:ILE:N	8:U:793:ILE:HD12	2.24	0.53
18:E:80:ASP:O	18:E:121:LYS:NZ	2.35	0.53
23:c:322:LEU:O	23:c:326:ARG:N	2.39	0.53
5:R:367:ALA:HB1	5:R:371:ILE:HG23	1.89	0.53
9:X:970:LYS:HA	9:X:973:PHE:CE2	2.44	0.53
15:K:477:TRP:HE3	15:K:484:PRO:HG2	1.74	0.53
6:Q:66:GLU:OE2	6:Q:70:ASN:ND2	2.39	0.53
4:N:526:ARG:NH2	15:K:1108:ASP:OD1	2.36	0.52
24:D:136:LEU:O	24:D:140:ILE:N	2.39	0.52
5:O:59:GLU:OE1	5:O:63:LYS:NZ	2.33	0.52
6:P:177:ARG:NH1	8:U:405:SER:HG	2.07	0.52
19:F:405:GLU:OE1	19:F:407:GLN:NE2	2.36	0.52
2:C:249:LEU:HD13	2:C:254:ILE:HD11	1.91	0.52
6:P:97:MET:SD	6:P:97:MET:N	2.83	0.52
8:U:234:ASP:OD1	8:U:359:ARG:NH1	2.38	0.52
5:R:155:LEU:HD23	5:R:156:ASP:N	2.25	0.52
12:T:278:ALA:O	12:T:282:TRP:HD1	1.93	0.52
24:D:203:ASN:O	24:D:205:LYS:N	2.35	0.52
1:A:1508:VAL:HG22	1:A:1568:GLY:HA3	1.91	0.52
5:R:368:GLY:O	5:R:371:ILE:HG12	2.10	0.52
1:A:1523:THR:O	1:A:1527:MET:N	2.32	0.52
3:H:45:SER:OG	3:H:46:HIS:N	2.43	0.52
5:O:150:THR:O	5:O:170:GLY:N	2.36	0.52
8:U:203:LEU:O	8:U:230:LEU:HD11	2.10	0.51
18:E:12:ALA:HB3	18:E:50:LEU:HD11	1.91	0.51
24:D:184:HIS:HB3	24:D:187:PHE:HD2	1.75	0.51
4:N:751:GLU:HB3	4:N:758:SER:HB3	1.91	0.51
9:X:984:LYS:O	9:X:988:PRO:CD	2.58	0.51
15:K:545:PHE:O	15:K:547:ASP:N	2.43	0.51
24:G:242:VAL:O	24:G:304:VAL:N	2.37	0.51
4:N:617:ARG:NH2	13:I:94:GLU:OE1	2.37	0.51
6:P:117:GLU:O	6:P:124:ARG:NH2	2.43	0.51
8:U:828:ILE:HD13	8:U:870:ILE:HB	1.92	0.51
15:K:1141:MET:HE2	15:K:1180:PHE:CE2	2.46	0.51
1:A:236:GLU:CD	1:A:236:GLU:H	2.18	0.51
1:A:283:GLU:OE1	1:A:1471:SER:OG	2.18	0.51
9:W:1052:PHE:CD1	9:W:1052:PHE:C	2.87	0.51
24:G:281:ALA:O	24:G:282:VAL:HG12	2.11	0.51
8:U:105:SER:OG	14:J:754:VAL:O	2.23	0.51
1:A:36:ILE:HD11	1:A:114:ILE:HD11	1.93	0.51
14:J:79:ALA:HB1	14:J:84:TRP:HB3	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:176:ARG:NE	14:J:180:TYR:O	2.41	0.51
24:G:158:TRP:CD2	24:G:329:MET:HE3	2.46	0.51
3:H:15:ILE:HG23	3:H:30:TYR:OH	2.09	0.51
5:O:367:ALA:HB1	5:O:371:ILE:HB	1.92	0.51
5:R:210:ILE:O	5:R:214:ILE:HG12	2.11	0.51
8:U:377:ASN:OD1	8:U:377:ASN:C	2.54	0.51
8:U:381:ASP:OD1	8:U:432:ARG:NH1	2.43	0.51
13:I:127:PHE:O	13:I:136:LYS:N	2.44	0.51
15:K:1003:SER:N	15:K:1006:GLU:OE1	2.44	0.51
1:A:1493:LEU:O	1:A:1497:SER:N	2.44	0.51
4:N:751:GLU:O	4:N:758:SER:OG	2.25	0.51
12:T:556:PHE:O	12:T:560:THR:OG1	2.21	0.51
14:J:531:VAL:N	14:J:534:GLN:O	2.35	0.51
3:H:11:GLU:OE1	3:H:286:LYS:NZ	2.33	0.50
7:S:154:ASP:C	7:S:154:ASP:OD1	2.53	0.50
24:G:140:ILE:HD11	24:G:207:PHE:CD2	2.46	0.50
1:A:421:ILE:N	1:A:597:ILE:O	2.31	0.50
5:R:254:ASN:HA	5:R:257:PHE:CE2	2.46	0.50
14:J:965:PHE:O	14:J:968:ALA:HB3	2.12	0.50
15:K:1013:VAL:C	15:K:1047:MET:HE1	2.36	0.50
1:A:296:ILE:H	1:A:296:ILE:HD12	1.77	0.50
1:A:1769:LEU:C	1:A:1771:PRO:HD2	2.36	0.50
7:S:38:ASP:OD1	7:S:39:LEU:N	2.44	0.50
12:T:665:VAL:HB	12:T:668:LEU:O	2.12	0.50
14:J:531:VAL:O	14:J:534:GLN:N	2.44	0.50
1:A:25:ASN:O	1:A:29:SER:N	2.45	0.50
1:A:1301:ASN:O	1:A:1304:SER:N	2.44	0.50
16:L:433:THR:O	16:L:434:ARG:HD3	2.12	0.50
18:E:286:TYR:HB3	18:E:288:PHE:CE2	2.46	0.50
19:F:169:ASP:HB3	19:F:173:ARG:HB2	1.93	0.50
8:U:221:ASP:OD1	8:U:221:ASP:N	2.39	0.50
14:J:522:THR:HG22	14:J:523:ALA:N	2.27	0.50
15:K:605:LEU:HD12	15:K:678:HIS:HB3	1.93	0.50
24:G:716:PHE:O	24:G:720:PRO:HD2	2.12	0.50
1:A:882:TYR:O	1:A:886:THR:HG23	2.12	0.50
5:O:177:ILE:N	5:O:177:ILE:HD12	2.27	0.50
8:U:743:ASN:OD1	8:U:805:LYS:NZ	2.44	0.50
1:A:1582:ASP:O	1:A:1586:MET:HE2	2.12	0.50
14:J:112:ASP:HA	14:J:115:ALA:HB3	1.94	0.50
14:J:860:ASP:OD1	14:J:860:ASP:N	2.43	0.50
24:D:368:ILE:HD11	24:D:609:ARG:H	1.77	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LYS:O	1:A:250:LEU:CB	2.59	0.50
2:B:114:TRP:HA	2:B:135:ILE:O	2.12	0.50
2:C:212:VAL:HG12	2:C:213:GLU:H	1.76	0.50
4:N:569:ASP:OD1	4:N:569:ASP:N	2.45	0.50
16:L:409:MET:SD	16:L:410:LEU:N	2.85	0.50
24:D:483:PHE:CG	24:D:484:PRO:HA	2.47	0.50
5:O:192:MET:SD	5:O:208:ARG:NH1	2.79	0.50
13:I:135:ILE:O	13:I:143:LEU:N	2.43	0.50
1:A:194:LYS:NZ	1:A:205:GLU:OE1	2.32	0.49
6:P:210:GLN:NE2	6:Q:210:GLN:OE1	2.42	0.49
1:A:1075:SER:HB2	1:A:1082:LEU:HD21	1.93	0.49
1:A:1799:MET:HE3	1:A:1799:MET:O	2.11	0.49
4:N:585:GLU:O	4:N:589:LEU:HG	2.13	0.49
6:P:186:LYS:NZ	6:P:190:GLU:OE2	2.38	0.49
8:U:772:LEU:HA	8:U:775:LYS:HD3	1.94	0.49
12:T:319:MET:HB3	12:T:360:PHE:CZ	2.47	0.49
24:G:252:ALA:O	24:G:279:ASP:N	2.45	0.49
5:O:142:LEU:HD13	5:O:345:GLY:HA2	1.94	0.49
8:U:121:VAL:HA	8:U:124:PHE:CD2	2.46	0.49
13:I:31:TYR:CE2	13:I:33:GLY:HA3	2.48	0.49
1:A:223:ILE:O	1:A:227:LEU:N	2.45	0.49
1:A:348:ASN:OD1	1:A:593:HIS:NE2	2.45	0.49
12:T:646:LEU:HD21	12:T:690:LEU:HB2	1.94	0.49
13:I:146:ALA:HB1	13:I:150:GLU:HB3	1.94	0.49
14:J:1106:ILE:HG13	14:J:1112:VAL:HG22	1.94	0.49
15:K:718:THR:HG22	15:K:719:LEU:N	2.28	0.49
15:K:1165:TYR:O	15:K:1169:GLY:N	2.41	0.49
20:V:58:ASN:C	20:V:60:GLU:H	2.20	0.49
24:D:196:ILE:HD12	24:D:197:VAL:N	2.27	0.49
1:A:1238:GLN:N	1:A:1241:ASP:OD2	2.43	0.49
6:P:173:ALA:HA	6:P:176:MET:HE1	1.94	0.49
6:Q:241:ARG:NH2	6:Q:245:GLN:OE1	2.42	0.49
5:R:238:LEU:O	5:R:256:ARG:NH1	2.37	0.49
8:U:751:LEU:HA	8:U:813:MET:HE1	1.94	0.49
9:X:1077:PHE:CE1	9:X:1081:VAL:HG21	2.48	0.49
13:I:30:ARG:O	13:I:47:PHE:N	2.39	0.49
21:a:432:PHE:O	21:a:435:ARG:NH1	2.45	0.49
1:A:836:VAL:CG1	1:A:837:SER:N	2.75	0.49
1:A:931:GLN:NE2	1:A:932:PRO:O	2.46	0.49
1:A:1016:LEU:O	19:F:351:ARG:NH1	2.44	0.49
14:J:796:THR:HB	14:J:809:VAL:CG1	2.43	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:196:LYS:HA	3:H:209:PHE:CZ	2.48	0.49
1:A:54:ALA:HB2	1:A:278:PHE:CD2	2.47	0.49
14:J:551:ARG:NE	14:J:557:GLU:OE2	2.39	0.49
14:J:1053:ALA:HB2	14:J:1132:PHE:CZ	2.47	0.49
15:K:546:GLN:H	15:K:563:SER:CB	2.26	0.49
6:P:216:ALA:HA	6:P:219:LYS:HE3	1.95	0.48
5:R:123:GLN:HA	5:R:364:TYR:OH	2.13	0.48
24:D:248:ASN:ND2	24:D:323:LEU:O	2.46	0.48
24:G:119:ILE:HG12	24:G:151:LEU:HD11	1.94	0.48
24:G:388:ALA:O	24:G:392:LYS:N	2.45	0.48
5:O:126:PHE:CE2	5:O:361:LYS:HD3	2.48	0.48
6:Q:135:LEU:HD12	6:Q:136:ILE:N	2.27	0.48
5:R:158:GLY:O	5:R:160:GLY:N	2.46	0.48
8:U:589:LYS:O	8:U:592:LEU:HD23	2.13	0.48
9:W:1205:MET:SD	9:W:1205:MET:C	2.96	0.48
13:I:137:ASP:OD2	13:I:141:ARG:NE	2.39	0.48
14:J:379:GLU:O	14:J:383:PHE:N	2.45	0.48
19:F:275:ILE:O	19:F:278:ASN:N	2.47	0.48
24:G:514:LYS:HD2	24:G:514:LYS:H	1.79	0.48
5:O:70:LYS:NZ	5:O:80:ASN:OD1	2.44	0.48
5:O:288:ASP:OD2	12:T:438:ARG:NH2	2.46	0.48
5:O:355:GLN:HA	5:O:358:TRP:CD1	2.48	0.48
5:R:196:THR:HA	5:R:200:TYR:O	2.13	0.48
5:R:333:ALA:O	5:R:334:PRO:C	2.56	0.48
14:J:110:ALA:HB3	14:J:115:ALA:CB	2.43	0.48
1:A:1719:GLY:O	1:A:1722:ARG:HG2	2.13	0.48
4:N:586:LEU:HB2	14:J:1247:ALA:HB2	1.95	0.48
5:O:51:GLN:NE2	8:U:700:LEU:O	2.46	0.48
8:U:668:LEU:HD12	8:U:669:LEU:N	2.28	0.48
9:W:984:LYS:O	9:W:988:PRO:CD	2.62	0.48
15:K:791:LEU:HD12	15:K:792:PHE:N	2.29	0.48
1:A:1770:PRO:N	1:A:1771:PRO:CD	2.77	0.48
2:C:103:ILE:C	2:C:103:ILE:HD12	2.38	0.48
12:T:443:LEU:O	12:T:447:THR:HG23	2.13	0.48
15:K:447:HIS:CE1	15:K:475:ILE:HD12	2.48	0.48
15:K:546:GLN:H	15:K:563:SER:HB3	1.78	0.48
15:K:726:VAL:HG12	15:K:727:ARG:N	2.29	0.48
6:P:221:GLU:HG3	6:P:222:SER:N	2.29	0.48
19:F:327:VAL:HG11	19:F:347:LEU:CD1	2.43	0.48
1:A:632:LYS:O	1:A:636:ASN:HB2	2.14	0.48
1:A:632:LYS:O	1:A:636:ASN:ND2	2.47	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:231:ILE:N	2:C:231:ILE:HD12	2.28	0.48
4:N:758:SER:O	4:N:761:SER:N	2.47	0.48
14:J:846:ILE:HG23	14:J:850:GLY:HA3	1.94	0.48
1:A:179:PRO:HA	1:A:182:ILE:HD12	1.95	0.48
6:Q:95:THR:OG1	6:Q:97:MET:SD	2.71	0.48
12:T:637:PRO:HB3	12:T:641:PHE:CD1	2.48	0.48
14:J:414:ASN:OD1	14:J:415:VAL:N	2.46	0.48
15:K:1040:HIS:O	15:K:1042:ASN:N	2.47	0.48
19:F:281:ALA:HB3	19:F:401:GLY:HA3	1.96	0.48
1:A:1701:ARG:NH2	1:A:1736:GLU:OE1	2.40	0.47
7:S:126:LEU:HD21	7:S:145:MET:SD	2.54	0.47
17:M:283:GLU:OE2	17:M:286:ARG:NH2	2.46	0.47
1:A:220:VAL:O	1:A:224:LEU:N	2.46	0.47
2:C:212:VAL:HG12	2:C:213:GLU:N	2.29	0.47
14:J:604:TYR:CZ	14:J:623:LEU:HB2	2.49	0.47
24:G:471:MET:SD	24:G:474:ARG:NH1	2.87	0.47
4:N:584:LYS:NZ	13:I:37:ASP:O	2.46	0.47
9:X:1127:THR:OG1	9:X:1131:ARG:NH2	2.47	0.47
13:I:106:GLN:C	13:I:108:THR:H	2.22	0.47
14:J:176:ARG:O	14:J:180:TYR:N	2.38	0.47
14:J:238:ALA:O	14:J:239:VAL:HG13	2.14	0.47
15:K:958:GLU:OE2	15:K:981:ARG:NH2	2.43	0.47
3:H:42:TYR:OH	3:H:154:ILE:HG23	2.14	0.47
4:N:671:GLU:HG2	4:N:672:GLU:N	2.28	0.47
5:O:359:ILE:N	5:O:359:ILE:HD12	2.29	0.47
8:U:376:TYR:HA	8:U:379:TYR:CD2	2.49	0.47
9:W:1003:MET:SD	9:X:999:GLN:NE2	2.86	0.47
12:T:172:ARG:HG3	12:T:173:GLU:N	2.30	0.47
14:J:471:HIS:HB3	14:J:581:ILE:HD13	1.97	0.47
14:J:973:ASP:C	14:J:975:ARG:H	2.23	0.47
1:A:1440:GLU:N	1:A:1440:GLU:OE1	2.47	0.47
6:P:97:MET:H	6:P:97:MET:HE2	1.79	0.47
6:Q:90:SER:O	6:Q:137:ARG:NH1	2.45	0.47
8:U:122:ASP:OD1	8:U:122:ASP:N	2.48	0.47
9:X:981:GLU:O	9:X:985:GLN:HG2	2.15	0.47
24:D:334:VAL:HG13	24:D:338:PHE:CD2	2.50	0.47
8:U:762:GLU:HG3	8:U:880:MET:HE1	1.96	0.47
9:W:1132:ILE:HG21	9:X:1132:ILE:HD12	1.97	0.47
14:J:623:LEU:HD11	14:J:626:ALA:HB3	1.95	0.47
1:A:1462:GLN:HA	1:A:1465:ASP:OD2	2.15	0.47
1:A:1862:MET:HG3	24:D:658:TRP:CZ2	2.50	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:760:ASP:O	4:N:764:PRO:HD2	2.15	0.47
5:O:138:ILE:HD12	5:O:138:ILE:N	2.29	0.47
6:P:204:GLU:O	6:P:207:VAL:HG22	2.15	0.47
8:U:511:MET:HE1	8:U:541:PHE:CE1	2.50	0.47
9:W:1157:ILE:HD12	9:W:1157:ILE:H	1.80	0.47
13:I:156:ARG:HE	13:I:157:THR:HA	1.78	0.47
15:K:865:PHE:CD1	15:K:865:PHE:N	2.79	0.47
19:F:135:TRP:CH2	19:F:166:THR:HG21	2.50	0.47
24:G:494:PHE:CE1	24:G:518:PRO:HD3	2.49	0.47
1:A:916:THR:OG1	1:A:919:PHE:O	2.23	0.47
6:Q:140:THR:HG23	6:Q:147:GLY:HA3	1.96	0.47
23:c:319:LEU:HD23	23:c:319:LEU:O	2.14	0.47
24:G:190:HIS:O	24:G:194:GLU:HG3	2.15	0.47
6:Q:95:THR:OG1	6:Q:97:MET:HG3	2.15	0.47
8:U:221:ASP:CG	8:U:222:PRO:HD3	2.39	0.47
14:J:1165:ALA:HB2	14:J:1246:TYR:OH	2.15	0.47
20:V:66:ASP:OD1	20:V:66:ASP:C	2.58	0.47
5:R:73:ILE:O	5:R:73:ILE:HG22	2.16	0.47
8:U:589:LYS:HA	8:U:592:LEU:HD22	1.97	0.47
15:K:605:LEU:HD13	15:K:662:SER:HA	1.97	0.47
15:K:1179:ASP:O	15:K:1183:VAL:HG23	2.14	0.47
24:G:369:LYS:HB2	24:G:519:GLU:H	1.80	0.47
24:G:675:VAL:O	24:G:679:PRO:HD2	2.15	0.47
4:N:598:PHE:CD1	4:N:598:PHE:C	2.93	0.46
5:O:221:VAL:HG21	5:O:311:ILE:HB	1.97	0.46
7:S:133:LEU:HD22	12:T:279:PHE:CE2	2.49	0.46
24:D:478:PHE:CD1	24:D:478:PHE:C	2.94	0.46
8:U:216:ILE:HD12	8:U:452:TYR:CD2	2.50	0.46
15:K:416:MET:HE3	15:K:479:SER:HB2	1.97	0.46
1:A:145:ILE:HD12	1:A:260:HIS:CG	2.51	0.46
2:C:141:ASN:N	2:C:162:ASN:OD1	2.48	0.46
5:O:360:SER:N	5:O:363:GLU:OE2	2.47	0.46
6:Q:176:MET:SD	5:R:51:GLN:O	2.73	0.46
4:N:531:LEU:O	4:N:535:ASP:N	2.38	0.46
9:W:980:LYS:NZ	9:W:981:GLU:OE2	2.30	0.46
14:J:1053:ALA:HB2	14:J:1132:PHE:CE1	2.50	0.46
9:W:1202:ILE:HD11	15:K:792:PHE:CG	2.50	0.46
12:T:56:HIS:O	12:T:57:THR:HG23	2.15	0.46
12:T:319:MET:HB3	12:T:360:PHE:CE2	2.50	0.46
12:T:550:LEU:HB3	12:T:556:PHE:CE2	2.51	0.46
14:J:531:VAL:HG21	14:J:582:PHE:CE2	2.50	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:782:LEU:C	14:J:783:ILE:HD12	2.40	0.46
19:F:154:GLY:O	19:F:158:GLY:N	2.48	0.46
24:G:157:THR:HG1	24:G:158:TRP:CD1	2.34	0.46
1:A:1561:GLN:O	1:A:1561:GLN:HG3	2.16	0.46
3:H:71:VAL:HG13	3:H:71:VAL:O	2.15	0.46
8:U:94:LYS:HD2	8:U:95:LEU:N	2.30	0.46
12:T:56:HIS:CG	12:T:57:THR:H	2.34	0.46
14:J:668:ASN:OD1	14:J:670:LYS:HG2	2.15	0.46
14:J:790:TYR:HA	14:J:955:LYS:HA	1.97	0.46
24:G:242:VAL:N	24:G:302:GLN:O	2.48	0.46
24:G:327:LEU:HD13	24:G:329:MET:HE1	1.97	0.46
5:O:236:SER:O	5:O:239:GLU:HG2	2.15	0.46
8:U:198:ILE:HD12	8:U:198:ILE:N	2.31	0.46
15:K:802:VAL:HG22	15:K:818:PHE:CD2	2.50	0.46
1:A:174:ARG:HA	1:A:177:TRP:CD1	2.51	0.46
1:A:1505:GLU:O	1:A:1566:ILE:N	2.49	0.46
4:N:579:PHE:O	4:N:582:LEU:HD23	2.16	0.46
5:R:74:GLU:OE1	5:R:79:THR:HG21	2.16	0.46
13:I:134:VAL:HG22	13:I:145:ASN:HD22	1.81	0.46
20:V:11:TYR:CZ	20:V:46:GLN:HG2	2.50	0.46
24:D:685:MET:HA	24:D:689:MET:CG	2.45	0.46
24:G:243:PHE:CE1	24:G:309:ALA:HB2	2.50	0.46
1:A:1268:PHE:O	1:A:1272:LEU:N	2.48	0.46
2:C:107:ASN:OD1	2:C:128:ASN:N	2.39	0.46
4:N:584:LYS:O	4:N:588:ARG:HG2	2.16	0.46
4:N:708:ASP:O	4:N:712:GLU:HG3	2.16	0.46
8:U:201:ASN:OD1	8:U:206:ARG:NH2	2.49	0.46
9:X:1042:GLU:OE2	9:X:1043:ARG:NE	2.31	0.46
16:L:355:ARG:O	16:L:359:MET:SD	2.74	0.46
2:C:50:MET:SD	2:C:50:MET:N	2.88	0.46
4:N:578:MET:O	4:N:582:LEU:HD22	2.16	0.46
4:N:699:SER:O	4:N:703:PRO:HD2	2.16	0.46
7:S:97:MET:HG2	12:T:273:PHE:CZ	2.51	0.46
7:S:120:LYS:HZ3	7:S:154:ASP:CG	2.16	0.46
12:T:301:ASN:O	12:T:303:PHE:N	2.48	0.46
24:D:155:VAL:O	24:D:158:TRP:N	2.48	0.46
24:D:178:TYR:CD1	24:D:178:TYR:C	2.94	0.46
1:A:809:GLU:O	1:A:812:PRO:HD2	2.16	0.45
1:A:1451:LYS:HD3	1:A:1451:LYS:N	2.31	0.45
4:N:493:MET:SD	15:K:943:GLY:N	2.88	0.45
5:O:80:ASN:C	5:O:80:ASN:HD22	2.24	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:828:ILE:HG12	8:U:866:LEU:HB3	1.97	0.45
14:J:607:TYR:CZ	14:J:619:TYR:HB3	2.51	0.45
14:J:789:GLN:HE21	14:J:789:GLN:HA	1.82	0.45
18:E:16:ILE:N	18:E:16:ILE:HD12	2.31	0.45
24:D:325:VAL:HG12	24:D:326:ASN:N	2.30	0.45
1:A:58:ILE:HG22	1:A:59:ARG:N	2.32	0.45
9:W:1003:MET:HB2	9:X:1003:MET:HE3	1.98	0.45
14:J:583:ARG:O	14:J:586:THR:HB	2.17	0.45
1:A:861:ARG:HB3	1:A:862:PRO:HD3	1.98	0.45
1:A:883:GLN:O	1:A:886:THR:OG1	2.22	0.45
2:C:179:HIS:HA	2:C:199:LEU:HA	1.98	0.45
4:N:595:ILE:HA	4:N:598:PHE:CD2	2.51	0.45
7:S:47:THR:HA	7:S:84:MET:O	2.17	0.45
8:U:110:ARG:HD2	14:J:456:VAL:HG13	1.98	0.45
8:U:493:GLU:CD	8:U:493:GLU:H	2.23	0.45
13:I:19:GLY:O	13:I:34:GLU:HA	2.17	0.45
14:J:979:ASP:OD1	14:J:979:ASP:C	2.59	0.45
3:H:47:VAL:HG12	3:H:48:ILE:H	1.80	0.45
4:N:533:GLU:C	4:N:533:GLU:CD	2.84	0.45
19:F:129:ILE:CG2	19:F:131:PRO:HD3	2.46	0.45
19:F:387:TYR:O	19:F:391:GLY:N	2.45	0.45
3:H:66:VAL:HG12	3:H:67:ASP:N	2.32	0.45
5:R:46:MET:HG2	5:R:47:VAL:N	2.32	0.45
5:R:185:ARG:O	5:R:188:THR:OG1	2.28	0.45
5:R:202:PHE:HB3	5:R:207:GLU:HB3	1.98	0.45
1:A:55:TRP:CE3	1:A:55:TRP:HA	2.52	0.45
1:A:817:LEU:HA	1:A:820:HIS:CD2	2.52	0.45
1:A:1529:TYR:CD1	1:A:1530:PRO:HD2	2.51	0.45
2:C:226:LEU:N	2:C:248:ASN:O	2.44	0.45
4:N:576:ALA:HB2	14:J:1138:VAL:HA	1.98	0.45
15:K:1280:ILE:O	15:K:1283:THR:OG1	2.29	0.45
24:D:713:GLU:O	24:D:717:LYS:HG2	2.17	0.45
24:G:136:LEU:HA	24:G:139:GLU:HG2	1.99	0.45
1:A:1116:GLU:O	1:A:1120:LEU:HG	2.16	0.45
5:O:323:ALA:CB	5:O:329:ILE:HD11	2.47	0.45
6:P:173:ALA:HA	6:P:176:MET:SD	2.57	0.45
6:P:196:LEU:CD2	6:Q:196:LEU:HB3	2.46	0.45
5:R:106:LEU:HD23	5:R:107:LEU:N	2.32	0.45
5:R:122:THR:OG1	5:R:372:VAL:HG21	2.16	0.45
8:U:94:LYS:HD2	8:U:95:LEU:H	1.82	0.45
15:K:719:LEU:HD12	15:K:719:LEU:H	1.81	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:D:141:SER:O	24:D:206:LYS:NZ	2.38	0.45
24:D:181:ARG:HG2	24:D:181:ARG:HH11	1.82	0.45
1:A:957:PHE:HA	1:A:964:TYR:CE2	2.52	0.45
3:H:142:PHE:CG	3:H:143:SER:N	2.84	0.45
6:P:133:ASP:HA	6:P:136:ILE:HG12	1.98	0.45
5:R:66:ILE:HG22	5:R:66:ILE:O	2.15	0.45
5:R:71:TYR:HB3	5:R:74:GLU:OE2	2.17	0.45
5:R:233:ALA:HB1	12:T:95:ASN:ND2	2.31	0.45
8:U:522:SER:HB3	8:U:527:PHE:CE1	2.51	0.45
9:W:1118:VAL:HG21	9:X:1118:VAL:HG11	1.98	0.45
12:T:205:VAL:HG21	12:T:209:SER:HB2	1.99	0.45
18:E:186:ASN:O	18:E:191:GLN:HB3	2.17	0.45
24:D:147:LYS:HB2	24:D:207:PHE:CE2	2.51	0.45
24:G:281:ALA:HB1	24:G:283:HIS:CD2	2.52	0.45
1:A:983:PRO:O	1:A:985:GLY:N	2.50	0.45
3:H:47:VAL:HB	3:H:50:ALA:HB2	1.99	0.45
4:N:680:MET:O	4:N:684:ARG:N	2.50	0.45
5:O:161:VAL:HG22	5:O:162:THR:H	1.82	0.45
5:R:92:PHE:O	5:R:97:ARG:N	2.50	0.45
7:S:29:GLN:HG3	12:T:269:ILE:HD12	1.99	0.45
14:J:148:SER:O	14:J:152:THR:HG23	2.17	0.45
14:J:189:ARG:N	14:J:192:ASP:OD2	2.44	0.45
15:K:654:ILE:O	15:K:655:THR:HG23	2.17	0.45
18:E:267:VAL:O	18:E:290:VAL:HG22	2.17	0.45
24:D:340:ILE:HG22	24:D:342:TRP:H	1.82	0.45
1:A:1402:PRO:HG3	1:A:1508:VAL:HG21	1.98	0.45
5:R:41:ARG:NH1	8:U:232:VAL:O	2.39	0.45
5:R:206:ALA:O	5:R:210:ILE:HG12	2.17	0.45
8:U:544:ASP:O	8:U:548:SER:OG	2.32	0.45
13:I:18:GLU:OE1	13:I:37:ASP:N	2.47	0.45
13:I:77:GLU:H	13:I:81:TRP:CD1	2.35	0.45
13:I:147:ASP:CG	13:I:148:ASP:N	2.75	0.45
14:J:436:LEU:CD2	14:J:469:VAL:HG22	2.46	0.45
14:J:718:LEU:HD11	14:J:749:CYS:HB3	1.98	0.45
14:J:1232:ILE:O	14:J:1236:LEU:HG	2.17	0.45
15:K:520:LYS:NZ	15:K:538:GLU:OE2	2.39	0.45
17:M:239:LYS:HE3	17:M:243:ILE:HD11	1.98	0.45
20:V:10:ARG:NE	20:V:45:GLU:OE2	2.41	0.45
24:D:491:LYS:O	24:D:495:ASN:HB2	2.17	0.45
1:A:245:TYR:CD1	1:A:245:TYR:C	2.95	0.44
2:B:93:VAL:HG23	2:B:112:LEU:HD11	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:142:PHE:CD1	3:H:142:PHE:C	2.95	0.44
5:O:133:ALA:HB1	5:O:358:TRP:CB	2.43	0.44
12:T:79:LEU:C	12:T:79:LEU:HD23	2.42	0.44
13:I:42:GLY:H	13:I:58:TRP:HB2	1.82	0.44
14:J:729:ARG:HG3	14:J:729:ARG:HH11	1.81	0.44
14:J:1237:HIS:HA	14:J:1248:TRP:CZ2	2.52	0.44
24:G:662:LEU:HD11	24:G:666:LYS:HE3	1.98	0.44
2:C:76:ARG:N	2:C:98:ASN:OD1	2.41	0.44
14:J:1165:ALA:N	14:J:1246:TYR:OH	2.50	0.44
15:K:1221:PHE:CZ	15:K:1225:LEU:HD11	2.52	0.44
19:F:223:TYR:HB3	19:F:227:SER:HB3	1.99	0.44
1:A:54:ALA:CB	1:A:278:PHE:CE2	3.00	0.44
1:A:1429:LEU:O	1:A:1433:LEU:HG	2.18	0.44
4:N:586:LEU:HD23	14:J:1245:MET:C	2.41	0.44
8:U:754:TYR:HE2	8:U:767:VAL:HG21	1.82	0.44
16:L:208:PHE:CD2	16:L:229:ALA:HB2	2.52	0.44
22:b:39:LEU:HD12	22:b:43:ARG:HG3	1.99	0.44
1:A:269:ASP:OD1	1:A:271:ASN:ND2	2.49	0.44
2:C:124:SER:OG	2:C:145:ASP:OD1	2.25	0.44
14:J:105:MET:SD	14:J:107:PHE:N	2.91	0.44
18:E:63:PRO:O	18:E:66:GLN:NE2	2.47	0.44
19:F:174:GLU:OE1	19:F:178:ARG:NH2	2.43	0.44
24:D:309:ALA:HB1	24:D:320:LEU:CD2	2.47	0.44
1:A:1075:SER:HB2	1:A:1082:LEU:HD11	2.00	0.44
1:A:1404:LYS:O	1:A:1408:THR:OG1	2.33	0.44
2:C:129:GLU:CG	2:C:152:PRO:HD3	2.47	0.44
6:Q:132:PHE:CD1	6:Q:135:LEU:HD11	2.53	0.44
7:S:133:LEU:HD11	7:S:135:GLU:HB3	1.99	0.44
14:J:196:LEU:HD13	14:J:241:PHE:HB2	1.99	0.44
14:J:1169:ASP:OD1	14:J:1170:ARG:N	2.49	0.44
1:A:1787:LEU:HD23	4:N:702:ILE:HD13	2.00	0.44
2:B:290:LEU:HD13	2:B:304:TYR:CD2	2.53	0.44
3:H:226:ASP:N	3:H:226:ASP:OD1	2.48	0.44
5:R:82:ASP:HA	5:R:85:GLU:HG2	1.99	0.44
14:J:795:PRO:HG3	14:J:921:TRP:CZ2	2.53	0.44
15:K:416:MET:HE1	15:K:433:MET:HE3	1.99	0.44
15:K:754:GLU:HB3	15:K:755:PRO:HD2	2.00	0.44
1:A:36:ILE:HD11	1:A:114:ILE:CD1	2.47	0.44
1:A:1307:GLU:CD	1:A:1307:GLU:N	2.76	0.44
5:O:214:ILE:HG23	5:O:218:LEU:HD12	2.00	0.44
6:P:228:GLU:OE2	6:Q:225:ARG:NH1	2.49	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:X:1009:ARG:O	9:X:1012:LYS:HG3	2.18	0.44
12:T:279:PHE:O	12:T:283:ARG:HG2	2.18	0.44
17:M:169:ALA:O	17:M:173:LEU:HG	2.18	0.44
22:b:20:GLU:OE1	22:b:20:GLU:HA	2.17	0.44
24:D:184:HIS:HB3	24:D:187:PHE:CD2	2.53	0.44
24:D:184:HIS:CG	24:D:185:PRO:HD2	2.52	0.44
24:D:509:ILE:HG22	24:D:510:PHE:N	2.32	0.44
24:D:719:ASN:ND2	24:D:723:GLN:O	2.51	0.44
3:H:47:VAL:HG12	3:H:48:ILE:N	2.32	0.44
5:O:78:ILE:HG21	5:O:81:TRP:CE3	2.53	0.44
6:Q:191:ARG:O	6:Q:194:THR:HG22	2.17	0.44
7:S:72:MET:O	7:S:76:ILE:HG12	2.18	0.44
16:L:408:MET:HE3	16:L:412:MET:SD	2.58	0.44
24:G:45:LEU:O	24:G:339:ASN:ND2	2.50	0.44
2:C:73:ALA:HB1	2:C:78:LEU:HD11	2.00	0.44
2:C:207:ASN:N	2:C:207:ASN:HD22	2.15	0.44
4:N:535:ASP:HA	4:N:539:LYS:CB	2.48	0.44
8:U:381:ASP:HA	8:U:432:ARG:CZ	2.48	0.44
14:J:623:LEU:HD23	14:J:627:LEU:HD13	2.00	0.44
15:K:784:ASP:OD1	15:K:784:ASP:C	2.61	0.44
16:L:101:GLN:O	16:L:106:GLN:NE2	2.44	0.44
24:G:675:VAL:O	24:G:679:PRO:CD	2.65	0.44
1:A:385:LEU:HB3	1:A:386:PRO:HD2	2.00	0.43
5:R:361:LYS:NZ	8:U:406:THR:O	2.42	0.43
8:U:498:LEU:O	8:U:501:VAL:HG22	2.18	0.43
12:T:522:PHE:CE2	12:T:607:ALA:HB1	2.53	0.43
12:T:574:GLY:N	12:T:575:PRO:HD2	2.33	0.43
24:D:158:TRP:CE2	24:D:329:MET:HE3	2.52	0.43
1:A:807:VAL:HB	1:A:808:PRO:CD	2.47	0.43
1:A:1877:ASP:OD2	1:A:1881:GLN:NE2	2.51	0.43
9:W:996:MET:O	9:W:999:GLN:HG2	2.18	0.43
15:K:900:GLY:O	15:K:909:ARG:N	2.50	0.43
16:L:163:TYR:CE2	16:L:187:HIS:HB3	2.53	0.43
16:L:421:SER:O	16:L:425:ASN:ND2	2.47	0.43
17:M:201:PHE:HA	17:M:204:CYS:SG	2.58	0.43
1:A:424:ALA:HA	1:A:428:GLN:CD	2.44	0.43
4:N:586:LEU:HD13	14:J:1251:ILE:HG21	1.99	0.43
4:N:647:GLU:O	4:N:651:LEU:HG	2.18	0.43
8:U:861:GLU:OE2	8:U:862:LYS:NZ	2.38	0.43
13:I:105:SER:C	13:I:107:LEU:H	2.26	0.43
14:J:796:THR:HB	14:J:809:VAL:HG13	2.00	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:691:LEU:HD12	15:K:733:THR:CG2	2.48	0.43
19:F:80:GLY:O	19:F:81:GLY:O	2.36	0.43
1:A:597:ILE:N	1:A:597:ILE:HD12	2.34	0.43
4:N:569:ASP:HA	14:J:1135:HIS:CD2	2.53	0.43
6:P:136:ILE:HA	6:P:139:VAL:HG12	2.01	0.43
14:J:911:THR:HG22	14:J:913:PHE:CZ	2.53	0.43
14:J:925:GLN:OE1	14:J:925:GLN:N	2.51	0.43
15:K:668:ASP:CG	15:K:672:ASN:H	2.23	0.43
21:a:479:THR:N	21:a:495:SER:O	2.41	0.43
1:A:402:HIS:ND1	1:A:406:THR:OG1	2.52	0.43
1:A:607:LEU:C	1:A:607:LEU:HD23	2.43	0.43
1:A:1812:LEU:HB2	1:A:1817:SER:OG	2.18	0.43
4:N:578:MET:HE2	14:J:1229:GLU:HG2	2.00	0.43
5:R:220:TYR:O	5:R:257:PHE:HA	2.19	0.43
8:U:380:VAL:HG21	8:U:436:LYS:HA	2.00	0.43
9:X:1128:ASP:OD1	9:X:1131:ARG:NH2	2.47	0.43
15:K:862:ASP:C	15:K:862:ASP:OD1	2.61	0.43
16:L:356:ALA:HA	16:L:359:MET:HE2	2.00	0.43
19:F:118:GLN:O	19:F:122:LYS:HG2	2.19	0.43
24:D:667:ARG:NH2	24:D:668:GLU:OE2	2.45	0.43
1:A:995:LEU:HD21	1:A:1291:MET:SD	2.58	0.43
2:C:129:GLU:HG2	2:C:152:PRO:HD3	2.00	0.43
2:C:140:TYR:N	2:C:162:ASN:OD1	2.52	0.43
6:Q:241:ARG:NE	6:Q:245:GLN:OE1	2.49	0.43
8:U:764:VAL:O	8:U:767:VAL:HG22	2.18	0.43
12:T:560:THR:C	12:T:562:PRO:HD3	2.43	0.43
14:J:197:MET:HE3	14:J:213:GLU:O	2.18	0.43
14:J:789:GLN:O	14:J:956:ASN:O	2.37	0.43
15:K:415:TYR:O	15:K:460:ARG:NE	2.47	0.43
16:L:187:HIS:O	16:L:191:LEU:HG	2.18	0.43
19:F:90:GLN:O	19:F:94:GLY:HA2	2.19	0.43
19:F:398:VAL:O	19:F:420:VAL:N	2.51	0.43
24:D:178:TYR:O	24:D:181:ARG:NH1	2.46	0.43
1:A:1722:ARG:HA	1:A:1722:ARG:CZ	2.48	0.43
5:O:242:TYR:N	5:O:250:ILE:O	2.48	0.43
6:Q:213:LYS:O	6:Q:217:THR:HG23	2.17	0.43
5:R:83:ASP:O	5:R:87:ILE:HG13	2.19	0.43
12:T:76:LEU:HD23	12:T:76:LEU:H	1.84	0.43
19:F:323:ARG:NH1	19:F:435:ASP:O	2.51	0.43
1:A:395:VAL:HG22	1:A:620:LEU:HB3	2.00	0.43
3:H:140:GLU:HA	13:I:145:ASN:CG	2.43	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:519:LEU:HD23	4:N:519:LEU:O	2.19	0.43
4:N:529:HIS:HA	4:N:539:LYS:HE2	2.01	0.43
12:T:269:ILE:O	12:T:273:PHE:N	2.51	0.43
14:J:265:PHE:HZ	14:J:469:VAL:HG21	1.83	0.43
15:K:566:GLN:NE2	15:K:583:ALA:O	2.52	0.43
15:K:754:GLU:OE1	15:K:781:LYS:NZ	2.52	0.43
17:M:221:ALA:HB2	17:M:236:LEU:HB2	2.01	0.43
19:F:166:THR:HG23	19:F:196:SER:OG	2.18	0.43
24:D:23:HIS:HB3	24:D:26:THR:HG23	2.01	0.43
24:D:156:MET:HA	24:D:159:ALA:HB3	2.01	0.43
24:D:193:ALA:O	24:D:197:VAL:HG23	2.19	0.43
2:C:114:TRP:HA	2:C:135:ILE:O	2.19	0.43
3:H:229:LEU:HD23	3:H:233:PHE:CE1	2.54	0.43
4:N:741:VAL:O	4:N:745:LEU:HG	2.19	0.43
7:S:54:LYS:HE3	7:S:54:LYS:HA	2.00	0.43
8:U:732:TYR:CE2	8:U:736:TYR:CE1	3.06	0.43
15:K:698:SER:O	15:K:730:ILE:N	2.43	0.43
16:L:77:PHE:HB3	16:L:80:SER:HB2	2.00	0.43
16:L:337:LEU:CB	16:L:360:LEU:HD21	2.48	0.43
17:M:22:ALA:HB1	17:M:23:PRO:HD2	2.01	0.43
1:A:38:GLY:C	1:A:245:TYR:HH	2.26	0.43
1:A:42:ALA:HB3	1:A:44:LYS:HG3	2.01	0.43
1:A:44:LYS:HA	1:A:47:LEU:HB3	2.01	0.43
1:A:359:SER:HA	1:A:363:LYS:O	2.19	0.43
1:A:1128:ASP:OD2	1:A:1302:ARG:NH2	2.48	0.43
7:S:63:GLU:OE1	7:S:63:GLU:HA	2.19	0.43
15:K:401:MET:O	15:K:402:THR:CG2	2.66	0.43
15:K:408:ASN:OD1	15:K:408:ASN:C	2.62	0.43
24:G:348:PHE:CZ	24:G:352:ILE:HD13	2.54	0.43
6:P:222:SER:O	6:P:225:ARG:HD3	2.19	0.42
6:Q:201:ARG:CZ	6:Q:201:ARG:HA	2.49	0.42
12:T:76:LEU:HD23	12:T:76:LEU:N	2.34	0.42
14:J:584:HIS:CE1	14:J:585:TYR:CE2	3.07	0.42
15:K:1115:ILE:O	15:K:1119:GLY:N	2.52	0.42
16:L:112:ASP:O	16:L:114:PRO:HD3	2.18	0.42
24:G:543:VAL:O	24:G:543:VAL:HG12	2.19	0.42
1:A:834:ASN:HB3	1:A:836:VAL:HG23	2.01	0.42
2:B:204:LEU:N	2:B:225:HIS:O	2.47	0.42
5:R:178:MET:HE1	5:R:283:SER:CA	2.49	0.42
8:U:326:ILE:HD12	8:U:326:ILE:H	1.84	0.42
12:T:201:MET:N	12:T:201:MET:SD	2.92	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:654:ILE:O	15:K:655:THR:CG2	2.67	0.42
15:K:1260:CYS:O	15:K:1264:PRO:HD2	2.19	0.42
17:M:27:MET:SD	17:M:27:MET:N	2.91	0.42
17:M:277:ASP:OD1	17:M:278:GLU:N	2.51	0.42
24:D:139:GLU:O	24:D:143:PHE:N	2.47	0.42
1:A:1148:GLN:OE1	1:A:1148:GLN:N	2.52	0.42
6:P:167:LEU:C	6:P:167:LEU:HD23	2.45	0.42
8:U:765:ARG:NH2	8:U:880:MET:O	2.52	0.42
13:I:153:TRP:CD1	13:I:157:THR:HG21	2.54	0.42
24:G:226:HIS:ND1	24:G:359:TYR:OH	2.38	0.42
3:H:44:GLU:O	3:H:45:SER:HB2	2.19	0.42
3:H:261:SER:O	3:H:265:VAL:HG23	2.19	0.42
5:R:212:ARG:NH2	5:R:307:MET:HE1	2.34	0.42
9:X:1060:VAL:O	9:X:1063:ILE:HG22	2.19	0.42
13:I:16:ARG:NH2	13:I:37:ASP:OD1	2.45	0.42
14:J:576:PHE:O	14:J:624:THR:HB	2.19	0.42
15:K:415:TYR:CD2	15:K:730:ILE:HD11	2.54	0.42
15:K:805:LEU:HD23	15:K:806:THR:N	2.34	0.42
21:a:514:GLU:OE1	21:a:514:GLU:N	2.52	0.42
24:G:139:GLU:O	24:G:143:PHE:CD1	2.72	0.42
24:G:320:LEU:O	24:G:324:LEU:HG	2.19	0.42
1:A:1581:LYS:O	1:A:1585:GLN:HG2	2.19	0.42
1:A:1801:ALA:HB1	1:A:1821:TYR:CE2	2.55	0.42
2:C:194:ILE:O	2:C:194:ILE:HG22	2.20	0.42
3:H:256:ARG:HB2	3:H:258:ILE:HG23	2.01	0.42
5:O:215:LYS:NZ	5:O:216:GLU:OE2	2.38	0.42
7:S:141:GLU:O	7:S:145:MET:HG3	2.19	0.42
8:U:432:ARG:CZ	8:U:432:ARG:HB3	2.50	0.42
15:K:739:TYR:HA	15:K:750:LYS:HA	2.01	0.42
15:K:883:TYR:CZ	15:K:885:ALA:HA	2.55	0.42
15:K:1129:SER:O	15:K:1131:HIS:N	2.51	0.42
18:E:308:PHE:O	18:E:312:LYS:HG2	2.19	0.42
24:D:183:HIS:CE1	24:D:188:LEU:HD13	2.55	0.42
1:A:37:PHE:O	1:A:147:ASN:HA	2.19	0.42
3:H:240:ILE:O	3:H:244:LEU:HG	2.19	0.42
8:U:375:MET:SD	8:U:379:TYR:OH	2.75	0.42
9:W:1031:THR:HG22	9:X:1031:THR:HG22	2.00	0.42
14:J:140:VAL:O	14:J:170:ALA:N	2.48	0.42
14:J:793:PRO:HG3	14:J:951:SER:HB2	2.02	0.42
19:F:233:VAL:HB	19:F:234:PRO:HD3	2.02	0.42
19:F:312:GLY:HA3	19:F:318:ASN:HA	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:F:398:VAL:O	19:F:420:VAL:HG22	2.20	0.42
24:G:478:PHE:CD1	24:G:478:PHE:C	2.98	0.42
5:O:47:VAL:HG22	5:O:48:GLY:H	1.85	0.42
6:P:126:GLU:OE2	6:P:130:GLN:NE2	2.44	0.42
12:T:691:ASN:O	12:T:695:PRO:CD	2.68	0.42
13:I:119:GLY:O	13:I:161:GLY:HA3	2.20	0.42
14:J:65:MET:O	14:J:65:MET:SD	2.77	0.42
16:L:347:ASN:HB2	16:L:349:GLN:OE1	2.20	0.42
17:M:283:GLU:HG3	17:M:286:ARG:HE	1.85	0.42
18:E:26:ASN:OD1	18:E:26:ASN:C	2.63	0.42
20:V:12:GLY:HA3	20:V:49:ASP:O	2.19	0.42
24:G:589:LEU:O	24:G:591:ASP:N	2.48	0.42
1:A:278:PHE:O	1:A:282:ILE:HG12	2.20	0.42
1:A:625:SER:O	1:A:842:ASP:HA	2.19	0.42
1:A:914:GLY:N	1:A:945:ILE:O	2.37	0.42
1:A:1268:PHE:HA	1:A:1271:VAL:HG22	2.02	0.42
1:A:1799:MET:HE1	24:D:680:LEU:HD21	2.02	0.42
2:C:249:LEU:HD13	2:C:254:ILE:CD1	2.50	0.42
6:Q:201:ARG:NH1	6:Q:204:GLU:OE1	2.45	0.42
7:S:76:ILE:HD11	7:S:92:VAL:HG11	2.02	0.42
8:U:404:LEU:O	8:U:407:PRO:HD2	2.20	0.42
8:U:537:GLN:O	8:U:540:MET:HG2	2.20	0.42
8:U:751:LEU:O	8:U:755:GLN:HG2	2.20	0.42
12:T:218:LYS:HE3	12:T:220:VAL:HG12	2.02	0.42
14:J:24:ILE:HD11	14:J:48:LEU:CD2	2.50	0.42
14:J:128:LYS:HD3	14:J:412:ILE:HG21	2.01	0.42
14:J:977:VAL:HA	14:J:997:LYS:O	2.19	0.42
24:G:604:GLU:HA	24:G:604:GLU:OE1	2.19	0.42
1:A:335:LYS:HG2	1:A:863:PHE:O	2.20	0.42
1:A:915:ASP:OD1	1:A:944:LYS:NZ	2.42	0.42
1:A:1249:GLU:O	1:A:1253:LYS:HG2	2.20	0.42
1:A:1523:THR:O	1:A:1526:SER:HB3	2.20	0.42
3:H:150:ARG:O	3:H:150:ARG:CZ	2.68	0.42
4:N:553:ARG:CD	14:J:1046:LEU:HD22	2.48	0.42
7:S:120:LYS:HE2	7:S:156:GLU:OE2	2.19	0.42
8:U:197:GLY:C	8:U:198:ILE:HD12	2.45	0.42
12:T:234:SER:N	12:T:237:ALA:O	2.52	0.42
14:J:239:VAL:HG23	14:J:239:VAL:O	2.20	0.42
15:K:478:ASP:H	15:K:484:PRO:CB	2.33	0.42
15:K:693:ALA:HB1	15:K:734:PHE:CG	2.55	0.42
17:M:209:GLU:O	17:M:243:ILE:HG23	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:E:168:ALA:O	18:E:172:GLY:N	2.52	0.42
1:A:328:ARG:NH1	1:A:885:GLU:OE2	2.44	0.42
1:A:386:PRO:HA	1:A:388:MET:N	2.34	0.42
1:A:584:LYS:HG3	1:A:595:GLY:H	1.85	0.42
5:R:13:ASP:OD1	5:R:139:GLN:NE2	2.51	0.42
14:J:161:PRO:HA	14:J:168:ASP:HA	2.01	0.42
15:K:419:ASP:OD1	15:K:420:ARG:N	2.50	0.42
15:K:805:LEU:HD23	15:K:806:THR:H	1.84	0.42
24:D:137:ASN:HA	24:D:140:ILE:HD12	2.02	0.42
24:G:716:PHE:O	24:G:720:PRO:CD	2.67	0.42
1:A:394:LYS:HB3	1:A:596:TRP:CZ2	2.55	0.41
1:A:1422:CYS:HA	1:A:1479:VAL:O	2.20	0.41
3:H:63:PRO:C	3:H:65:SER:H	2.27	0.41
5:O:220:TYR:O	5:O:257:PHE:HA	2.20	0.41
12:T:203:SER:HA	12:T:217:LEU:HA	2.01	0.41
14:J:455:VAL:CG2	14:J:469:VAL:HG23	2.50	0.41
14:J:1025:MET:HE2	14:J:1025:MET:HA	2.01	0.41
23:c:336:GLU:OE1	23:c:339:ARG:NH1	2.50	0.41
1:A:76:THR:HA	1:A:79:MET:HG2	2.02	0.41
1:A:807:VAL:HG22	1:A:810:MET:SD	2.59	0.41
2:C:60:ILE:HG13	2:C:62:SER:H	1.85	0.41
3:H:169:VAL:N	3:H:178:LEU:O	2.45	0.41
4:N:595:ILE:HA	4:N:598:PHE:CE2	2.55	0.41
6:Q:97:MET:SD	6:Q:98:ASP:N	2.93	0.41
5:R:84:MET:HA	5:R:87:ILE:HD12	2.02	0.41
12:T:203:SER:HA	12:T:217:LEU:HD23	2.02	0.41
12:T:536:ALA:O	12:T:540:PHE:CD1	2.73	0.41
21:a:522:GLU:OE1	23:c:325:ARG:NH2	2.47	0.41
21:a:530:SER:O	21:a:531:ILE:C	2.63	0.41
24:D:320:LEU:O	24:D:324:LEU:HG	2.20	0.41
1:A:813:LEU:O	1:A:817:LEU:HG	2.20	0.41
1:A:907:LYS:O	1:A:911:ARG:HG3	2.20	0.41
1:A:1816:ARG:NH2	24:D:720:PRO:HA	2.36	0.41
8:U:76:LEU:HD21	14:J:442:LEU:HD22	2.01	0.41
8:U:221:ASP:CG	8:U:222:PRO:CD	2.93	0.41
8:U:765:ARG:HD3	8:U:765:ARG:C	2.45	0.41
10:Y:1592:LEU:HD12	10:Y:1593:GLY:N	2.35	0.41
12:T:365:LYS:HE3	12:T:553:ASP:HB3	2.02	0.41
14:J:271:ASP:O	14:J:272:ASP:C	2.62	0.41
15:K:902:HIS:CD2	15:K:909:ARG:HG2	2.55	0.41
16:L:367:LYS:HE2	16:L:367:LYS:N	2.35	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:D:574:PHE:O	24:D:579:ILE:N	2.53	0.41
24:G:184:HIS:CE1	24:G:185:PRO:HD2	2.55	0.41
24:G:550:GLN:CD	24:G:551:ASP:N	2.78	0.41
1:A:360:PHE:CD1	1:A:361:LEU:HG	2.56	0.41
5:O:374:ARG:HG2	12:T:317:ASN:ND2	2.36	0.41
6:Q:73:LEU:O	6:Q:74:PRO:C	2.61	0.41
12:T:79:LEU:HD23	12:T:79:LEU:O	2.21	0.41
12:T:438:ARG:HG2	12:T:442:TYR:CE2	2.55	0.41
12:T:540:PHE:CD1	12:T:540:PHE:N	2.85	0.41
16:L:337:LEU:HB2	16:L:360:LEU:HD21	2.01	0.41
17:M:183:ILE:HD11	17:M:195:LEU:HD11	2.02	0.41
19:F:6:ILE:HG22	19:F:15:TYR:HE1	1.83	0.41
24:D:226:HIS:ND1	24:D:226:HIS:O	2.47	0.41
24:D:504:GLU:O	24:D:504:GLU:CG	2.69	0.41
24:G:137:ASN:HA	24:G:140:ILE:HD12	2.02	0.41
24:G:245:ASP:OD1	24:G:245:ASP:N	2.53	0.41
1:A:92:ASP:N	1:A:92:ASP:OD1	2.53	0.41
1:A:1458:GLU:CD	1:A:1458:GLU:H	2.27	0.41
2:B:151:HIS:ND1	2:B:151:HIS:N	2.68	0.41
6:P:228:GLU:HA	6:P:231:LYS:HG2	2.02	0.41
6:Q:128:TYR:HA	6:Q:131:CYS:SG	2.61	0.41
6:Q:174:PHE:CD1	6:Q:174:PHE:C	2.99	0.41
7:S:145:MET:CE	12:T:282:TRP:CE3	3.03	0.41
8:U:335:LEU:O	8:U:336:ALA:C	2.63	0.41
8:U:727:MET:HB3	8:U:728:PRO:HD3	2.01	0.41
13:I:31:TYR:CD1	13:I:46:LEU:HG	2.55	0.41
15:K:602:VAL:HG11	15:K:657:LEU:HG	2.02	0.41
20:V:2:PRO:HD2	20:V:5:ALA:HA	2.02	0.41
23:c:336:GLU:O	23:c:340:PRO:CD	2.69	0.41
24:D:585:ASP:OD1	24:D:585:ASP:C	2.64	0.41
24:D:699:CYS:SG	24:D:707:PRO:HA	2.61	0.41
24:G:184:HIS:CG	24:G:185:PRO:CD	3.03	0.41
1:A:291:ARG:O	1:A:291:ARG:NE	2.49	0.41
1:A:1132:ILE:O	1:A:1277:MET:HA	2.21	0.41
8:U:661:LEU:H	8:U:661:LEU:CD2	2.29	0.41
13:I:135:ILE:HD12	13:I:144:ARG:O	2.21	0.41
14:J:624:THR:CG2	14:J:625:SER:H	2.23	0.41
14:J:1058:GLY:O	14:J:1066:TYR:N	2.54	0.41
19:F:9:LYS:HE3	19:F:44:TRP:CD1	2.55	0.41
24:G:21:ILE:O	24:G:80:GLY:HA2	2.20	0.41
24:G:354:SER:O	24:G:358:GLU:HG3	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ALA:HA	1:A:224:LEU:HG	2.01	0.41
1:A:816:VAL:HG12	1:A:820:HIS:CE1	2.55	0.41
1:A:1288:GLN:O	1:A:1291:MET:SD	2.79	0.41
1:A:1362:HIS:NE2	1:A:1363:TYR:CE2	2.89	0.41
2:B:134:GLN:O	2:B:154:LEU:HA	2.21	0.41
5:O:363:GLU:O	5:O:367:ALA:HB3	2.21	0.41
6:Q:139:VAL:HG13	6:Q:146:ARG:HD2	2.02	0.41
6:Q:166:THR:HA	6:Q:169:GLU:HG3	2.03	0.41
8:U:754:TYR:CE2	8:U:767:VAL:HG21	2.56	0.41
9:W:1031:THR:CG2	9:X:1031:THR:HG22	2.51	0.41
9:W:1056:LEU:C	9:W:1056:LEU:HD13	2.46	0.41
9:W:1105:GLU:OE1	12:T:227:LYS:NZ	2.46	0.41
11:Z:1759:MET:SD	11:Z:1760:ASN:N	2.94	0.41
14:J:834:CYS:HA	14:J:837:MET:HE3	2.02	0.41
14:J:1091:VAL:C	14:J:1092:VAL:HG23	2.46	0.41
14:J:1123:PHE:CD1	14:J:1123:PHE:N	2.89	0.41
15:K:791:LEU:CD1	15:K:792:PHE:H	2.34	0.41
15:K:883:TYR:CE1	15:K:884:LEU:O	2.74	0.41
16:L:152:ASN:ND2	16:L:155:ASP:OD2	2.42	0.41
19:F:129:ILE:HG22	19:F:131:PRO:HD3	2.03	0.41
24:D:306:LYS:O	24:D:309:ALA:HB3	2.21	0.41
1:A:220:VAL:O	1:A:224:LEU:HG	2.20	0.41
1:A:324:LEU:CD2	1:A:330:ARG:HA	2.49	0.41
2:C:125:ALA:C	2:C:127:MET:H	2.28	0.41
3:H:124:LEU:HA	3:H:127:PHE:CD1	2.55	0.41
6:P:242:THR:O	6:P:245:GLN:HB3	2.21	0.41
8:U:404:LEU:O	8:U:407:PRO:CD	2.69	0.41
8:U:443:VAL:HA	8:U:450:PHE:CZ	2.56	0.41
14:J:183:LEU:CD2	14:J:183:LEU:H	2.33	0.41
15:K:791:LEU:HD12	15:K:792:PHE:H	1.85	0.41
16:L:212:THR:O	16:L:213:HIS:C	2.64	0.41
16:L:371:SER:O	16:L:375:GLU:HG2	2.20	0.41
1:A:59:ARG:C	1:A:59:ARG:HD2	2.46	0.41
1:A:623:TYR:HB2	1:A:824:TRP:CZ3	2.55	0.41
1:A:1264:ILE:HG22	1:A:1268:PHE:CZ	2.56	0.41
1:A:1266:ASP:HA	1:A:1269:ASP:OD2	2.21	0.41
1:A:1373:LYS:HE2	1:A:1374:GLU:N	2.35	0.41
2:C:231:ILE:HG22	2:C:232:GLU:N	2.36	0.41
2:C:287:GLN:O	2:C:291:VAL:HG23	2.21	0.41
3:H:222:GLU:C	3:H:224:SER:H	2.28	0.41
3:H:243:HIS:O	3:H:247:HIS:N	2.53	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:120:LYS:HE3	5:O:124:ILE:HD11	2.03	0.41
8:U:131:GLN:CD	8:U:131:GLN:C	2.89	0.41
8:U:378:LEU:HD11	16:L:412:MET:SD	2.61	0.41
8:U:791:PHE:HB2	8:U:793:ILE:HD11	2.01	0.41
10:Y:1612:GLU:O	10:Y:1615:VAL:HG22	2.21	0.41
14:J:550:ILE:HG23	14:J:664:LEU:CD2	2.51	0.41
14:J:605:PRO:CB	14:J:662:PHE:CE2	3.03	0.41
14:J:727:GLU:HA	14:J:730:LYS:HG3	2.03	0.41
14:J:866:GLU:OE1	14:J:1061:PRO:HA	2.21	0.41
15:K:415:TYR:CE2	15:K:730:ILE:HD11	2.55	0.41
15:K:435:ASP:C	15:K:435:ASP:OD1	2.64	0.41
15:K:499:ARG:HE	15:K:547:ASP:CG	2.28	0.41
15:K:1257:ALA:O	15:K:1259:THR:N	2.54	0.41
17:M:247:TYR:O	17:M:250:SER:OG	2.36	0.41
18:E:238:ARG:O	18:E:239:LYS:HB2	2.21	0.41
19:F:52:CYS:SG	19:F:60:ARG:NH2	2.94	0.41
19:F:235:LEU:HD11	19:F:239:TYR:CZ	2.56	0.41
19:F:327:VAL:HG12	19:F:342:HIS:O	2.20	0.41
24:D:249:CYS:N	24:D:326:ASN:OD1	2.38	0.41
24:D:253:ILE:CD1	24:D:277:ALA:HB1	2.51	0.41
24:D:504:GLU:O	24:D:504:GLU:HG3	2.21	0.41
24:G:611:TYR:CD1	24:G:611:TYR:N	2.87	0.41
24:G:698:GLU:O	24:G:702:VAL:HG23	2.21	0.41
1:A:324:LEU:HA	1:A:331:TRP:CZ2	2.55	0.41
1:A:447:THR:HA	1:A:550:LEU:HD21	2.03	0.41
1:A:1105:PHE:CD1	1:A:1105:PHE:C	2.99	0.41
1:A:1714:VAL:HG23	1:A:1744:CYS:SG	2.61	0.41
2:B:264:ARG:NH2	2:B:291:VAL:O	2.54	0.41
2:C:88:ILE:HG22	2:C:109:LEU:HD22	2.02	0.41
3:H:12:LEU:HD11	3:H:16:LEU:HD11	2.03	0.41
3:H:22:LEU:N	3:H:22:LEU:HD12	2.36	0.41
3:H:147:HIS:HB3	13:I:147:ASP:H	1.86	0.41
4:N:575:LEU:HD23	4:N:575:LEU:C	2.46	0.41
5:O:306:THR:O	5:O:337:ARG:NH2	2.46	0.41
6:P:95:THR:O	6:P:99:VAL:HG23	2.21	0.41
5:R:72:PRO:HG2	5:R:73:ILE:HG13	2.03	0.41
8:U:471:VAL:HG13	8:U:471:VAL:O	2.21	0.41
8:U:491:ARG:O	8:U:494:VAL:HG22	2.21	0.41
8:U:554:MET:SD	8:U:554:MET:C	3.04	0.41
9:W:1100:TYR:O	9:W:1104:ARG:HG2	2.21	0.41
9:X:970:LYS:O	9:X:974:VAL:HG23	2.20	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:84:TRP:CE3	14:J:85:ILE:HA	2.56	0.41
14:J:623:LEU:HG	14:J:624:THR:O	2.21	0.41
16:L:54:LYS:HG3	16:L:55:GLU:H	1.86	0.41
18:E:17:ALA:O	18:E:21:LEU:HG	2.21	0.41
1:A:153:TYR:O	1:A:157:GLN:HG2	2.21	0.40
1:A:1371:GLN:CD	1:A:1371:GLN:H	2.29	0.40
2:B:250:ARG:HB2	2:B:273:VAL:HG12	2.03	0.40
2:C:69:ILE:O	2:C:69:ILE:HG22	2.21	0.40
2:C:132:TYR:O	2:C:134:GLN:N	2.54	0.40
2:C:179:HIS:O	2:C:200:LYS:N	2.46	0.40
3:H:143:SER:OG	13:I:145:ASN:HB2	2.21	0.40
4:N:732:ASN:O	4:N:735:THR:HA	2.21	0.40
6:P:208:ASN:O	6:P:211:LYS:HG2	2.21	0.40
5:R:74:GLU:N	5:R:74:GLU:CD	2.79	0.40
7:S:154:ASP:OD1	7:S:155:GLY:N	2.54	0.40
8:U:185:LEU:HD13	8:U:185:LEU:C	2.46	0.40
8:U:432:ARG:O	8:U:436:LYS:HG3	2.21	0.40
12:T:646:LEU:HD21	12:T:690:LEU:CB	2.51	0.40
15:K:403:TRP:CH2	15:K:788:LYS:HB3	2.56	0.40
15:K:691:LEU:HD12	15:K:733:THR:HG22	2.03	0.40
16:L:100:ALA:HA	16:L:105:TRP:CE3	2.56	0.40
17:M:17:CYS:O	17:M:21:GLU:N	2.42	0.40
18:E:6:ARG:NH2	18:E:79:LYS:O	2.52	0.40
18:E:278:TYR:OH	18:E:300:VAL:O	2.37	0.40
24:G:23:HIS:CG	24:G:83:VAL:HG22	2.56	0.40
24:G:334:VAL:HG13	24:G:338:PHE:CD2	2.56	0.40
24:G:658:TRP:N	24:G:658:TRP:CE3	2.89	0.40
1:A:1006:PHE:CZ	1:A:1010:LEU:HD11	2.56	0.40
2:C:286:ARG:HG3	2:C:304:TYR:CE1	2.56	0.40
4:N:680:MET:O	4:N:684:ARG:HB2	2.21	0.40
6:Q:11:TYR:HA	6:Q:88:GLN:O	2.21	0.40
8:U:85:ASP:OD1	8:U:86:ILE:N	2.54	0.40
8:U:230:LEU:H	8:U:230:LEU:HD12	1.87	0.40
8:U:347:LEU:HD12	8:U:347:LEU:C	2.47	0.40
8:U:406:THR:N	8:U:407:PRO:CD	2.85	0.40
8:U:754:TYR:O	8:U:758:CYS:N	2.53	0.40
14:J:71:LEU:HB2	14:J:106:HIS:CE1	2.56	0.40
22:b:39:LEU:HG	22:b:43:ARG:HB2	2.03	0.40
1:A:160:CYS:C	1:A:162:GLN:H	2.29	0.40
1:A:161:GLY:C	1:A:177:TRP:HE1	2.28	0.40
1:A:1483:TYR:HA	1:A:1484:PRO:C	2.46	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:101:ASP:OD2	12:T:277:LYS:NZ	2.49	0.40
7:S:130:ALA:HA	7:S:133:LEU:HD23	2.04	0.40
8:U:206:ARG:NH1	8:U:280:ASN:O	2.46	0.40
13:I:118:LEU:HD23	13:I:120:TYR:CZ	2.56	0.40
14:J:155:ASP:O	14:J:172:HIS:HA	2.21	0.40
19:F:200:THR:HB	19:F:203:GLU:OE1	2.21	0.40
1:A:32:THR:HG22	1:A:34:PHE:CE1	2.56	0.40
1:A:832:MET:HE2	1:A:832:MET:N	2.36	0.40
1:A:981:LEU:O	1:A:1132:ILE:HA	2.22	0.40
1:A:1012:GLU:O	1:A:1016:LEU:HG	2.21	0.40
2:B:115:LEU:O	2:B:136:ALA:HA	2.21	0.40
2:C:129:GLU:OE1	2:C:174:ARG:NH2	2.53	0.40
4:N:506:VAL:O	4:N:510:MET:HG2	2.21	0.40
5:R:207:GLU:O	5:R:211:VAL:HG23	2.21	0.40
5:R:304:GLY:C	5:R:307:MET:HE2	2.46	0.40
8:U:139:ILE:HG22	8:U:140:GLY:N	2.36	0.40
8:U:735:GLU:O	8:U:738:LYS:HG2	2.20	0.40
8:U:758:CYS:N	8:U:759:PRO:HD3	2.37	0.40
15:K:846:VAL:HG22	15:K:847:SER:N	2.36	0.40
15:K:852:SER:OG	15:K:854:ASP:N	2.54	0.40
15:K:1039:CYS:O	15:K:1040:HIS:C	2.64	0.40
24:G:88:VAL:HG12	24:G:89:LYS:N	2.36	0.40
24:G:242:VAL:HG22	24:G:289:VAL:HG11	2.02	0.40
1:A:1481:ASP:OD1	1:A:1481:ASP:C	2.65	0.40
2:B:80:ASP:CG	2:B:81:ILE:N	2.79	0.40
4:N:716:ASN:OD1	4:N:719:ARG:NH1	2.54	0.40
5:O:191:LEU:HD12	5:O:194:ILE:HD11	2.03	0.40
5:O:311:ILE:HG23	5:O:312:ALA:N	2.36	0.40
6:P:223:GLU:O	6:P:226:GLN:HG3	2.22	0.40
8:U:153:LEU:HD13	8:U:153:LEU:C	2.47	0.40
8:U:384:PRO:HG2	16:L:397:LYS:HE2	2.04	0.40
8:U:498:LEU:O	8:U:498:LEU:HD23	2.21	0.40
9:X:1153:THR:HG22	9:X:1157:ILE:HD13	2.03	0.40
12:T:76:LEU:HD21	12:T:79:LEU:HD13	2.03	0.40
12:T:556:PHE:O	12:T:560:THR:HG23	2.22	0.40
14:J:624:THR:HG22	14:J:625:SER:N	2.22	0.40
18:E:182:ILE:HG21	18:E:184:TRP:CE2	2.56	0.40
24:G:659:ASN:O	24:G:663:GLU:HG2	2.20	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	1655/1894 (87%)	1568 (95%)	83 (5%)	4 (0%)	43	78
2	B	286/340 (84%)	235 (82%)	49 (17%)	2 (1%)	18	55
2	C	287/340 (84%)	235 (82%)	46 (16%)	6 (2%)	5	29
3	H	281/321 (88%)	253 (90%)	23 (8%)	5 (2%)	6	33
4	N	290/783 (37%)	287 (99%)	3 (1%)	0	100	100
5	O	366/377 (97%)	348 (95%)	17 (5%)	1 (0%)	36	72
5	R	368/377 (98%)	349 (95%)	16 (4%)	3 (1%)	16	53
6	P	198/258 (77%)	191 (96%)	7 (4%)	0	100	100
6	Q	194/258 (75%)	191 (98%)	3 (2%)	0	100	100
7	S	145/172 (84%)	141 (97%)	4 (3%)	0	100	100
8	U	809/4250 (19%)	771 (95%)	35 (4%)	3 (0%)	30	67
9	W	201/1249 (16%)	200 (100%)	1 (0%)	0	100	100
9	X	223/1249 (18%)	221 (99%)	2 (1%)	0	100	100
10	Y	37/1682 (2%)	37 (100%)	0	0	100	100
11	Z	42/1843 (2%)	42 (100%)	0	0	100	100
12	T	509/4144 (12%)	495 (97%)	12 (2%)	2 (0%)	30	67
13	I	163/170 (96%)	138 (85%)	24 (15%)	1 (1%)	21	59
14	J	1139/1252 (91%)	1042 (92%)	91 (8%)	6 (0%)	24	63
15	K	903/1299 (70%)	827 (92%)	73 (8%)	3 (0%)	36	72
16	L	382/471 (81%)	376 (98%)	6 (2%)	0	100	100
17	M	343/363 (94%)	330 (96%)	12 (4%)	1 (0%)	36	72
18	E	332/334 (99%)	323 (97%)	9 (3%)	0	100	100
19	F	457/500 (91%)	435 (95%)	21 (5%)	1 (0%)	43	78
20	V	90/93 (97%)	84 (93%)	5 (6%)	1 (1%)	11	45
21	a	120/536 (22%)	112 (93%)	8 (7%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	b	50/401 (12%)	47 (94%)	3 (6%)	0	100	100
23	c	71/520 (14%)	71 (100%)	0	0	100	100
24	D	674/723 (93%)	642 (95%)	31 (5%)	1 (0%)	48	83
24	G	677/723 (94%)	632 (93%)	43 (6%)	2 (0%)	36	72
All	All	11292/26922 (42%)	10623 (94%)	627 (6%)	42 (0%)	31	67

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	F	81	GLY
1	A	403	ILE
1	A	917	LYS
2	C	75	ASP
3	H	154	ILE
5	R	16	SER
8	U	225	PRO
2	C	56	LEU
3	H	131	PRO
5	R	254	ASN
13	I	106	GLN
15	K	904	ASP
15	K	916	ASP
17	M	54	CYS
24	G	418	SER
2	B	62	SER
2	B	300	ASP
2	C	214	GLY
3	H	21	LYS
5	O	132	PRO
5	R	72	PRO
8	U	85	ASP
12	T	307	PRO
14	J	923	HIS
2	C	126	ARG
2	C	194	ILE
3	H	293	PRO
14	J	605	PRO
15	K	493	PRO
20	V	59	GLU
24	D	579	ILE
24	G	204	ALA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1394	PRO
14	J	273	ILE
14	J	536	VAL
12	T	561	SER
14	J	239	VAL
1	A	1403	PRO
3	H	174	GLY
8	U	321	ILE
2	C	44	PRO
14	J	1152	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1516/1726 (88%)	1465 (97%)	51 (3%)	32	55
2	B	260/310 (84%)	252 (97%)	8 (3%)	35	56
2	C	261/310 (84%)	257 (98%)	4 (2%)	57	71
3	H	262/296 (88%)	252 (96%)	10 (4%)	29	51
4	N	268/711 (38%)	260 (97%)	8 (3%)	36	57
5	O	312/320 (98%)	308 (99%)	4 (1%)	61	72
5	R	313/320 (98%)	299 (96%)	14 (4%)	24	47
6	P	184/236 (78%)	179 (97%)	5 (3%)	39	60
6	Q	182/236 (77%)	178 (98%)	4 (2%)	45	64
7	S	131/153 (86%)	126 (96%)	5 (4%)	29	51
8	U	753/3820 (20%)	723 (96%)	30 (4%)	28	49
9	W	196/1148 (17%)	193 (98%)	3 (2%)	57	71
9	X	213/1148 (19%)	211 (99%)	2 (1%)	70	77
10	Y	36/1536 (2%)	35 (97%)	1 (3%)	38	59
11	Z	42/1659 (2%)	42 (100%)	0	100	100
12	T	480/3730 (13%)	474 (99%)	6 (1%)	61	72

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	I	144/149 (97%)	137 (95%)	7 (5%)	22	44
14	J	1037/1137 (91%)	997 (96%)	40 (4%)	28	50
15	K	803/1161 (69%)	784 (98%)	19 (2%)	43	63
16	L	322/401 (80%)	318 (99%)	4 (1%)	63	74
17	M	299/315 (95%)	296 (99%)	3 (1%)	68	76
18	E	282/282 (100%)	282 (100%)	0	100	100
19	F	401/440 (91%)	397 (99%)	4 (1%)	68	76
20	V	77/78 (99%)	74 (96%)	3 (4%)	28	50
21	a	116/460 (25%)	112 (97%)	4 (3%)	32	55
22	b	47/356 (13%)	46 (98%)	1 (2%)	47	65
23	c	65/467 (14%)	63 (97%)	2 (3%)	35	56
24	D	596/634 (94%)	590 (99%)	6 (1%)	68	76
24	G	598/634 (94%)	587 (98%)	11 (2%)	51	67
All	All	10196/24173 (42%)	9937 (98%)	259 (2%)	42	62

All (259) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ILE
1	A	102	LYS
1	A	110	HIS
1	A	151	SER
1	A	273	SER
1	A	287	TYR
1	A	291	ARG
1	A	316	PHE
1	A	345	LYS
1	A	373	LEU
1	A	438	LEU
1	A	574	GLU
1	A	587	PHE
1	A	635	LEU
1	A	804	TYR
1	A	810	MET
1	A	824	TRP
1	A	828	GLU
1	A	835	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	836	VAL
1	A	878	GLU
1	A	934	ASN
1	A	969	GLU
1	A	1006	PHE
1	A	1019	GLU
1	A	1123	ARG
1	A	1136	ASP
1	A	1139	ASP
1	A	1148	GLN
1	A	1160	LEU
1	A	1241	ASP
1	A	1291	MET
1	A	1292	ASN
1	A	1307	GLU
1	A	1438	ASP
1	A	1440	GLU
1	A	1521	LYS
1	A	1540	TYR
1	A	1545	TYR
1	A	1553	ARG
1	A	1573	TRP
1	A	1576	TRP
1	A	1611	THR
1	A	1650	GLU
1	A	1654	HIS
1	A	1656	TYR
1	A	1658	MET
1	A	1675	VAL
1	A	1707	GLU
1	A	1750	LEU
1	A	1760	TYR
2	B	59	LYS
2	B	66	HIS
2	B	80	ASP
2	B	89	HIS
2	B	134	GLN
2	B	151	HIS
2	B	226	LEU
2	B	274	LEU
2	C	207	ASN
2	C	228	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	C	232	GLU
2	C	241	MET
3	H	49	THR
3	H	129	ARG
3	H	130	GLN
3	H	142	PHE
3	H	150	ARG
3	H	171	ILE
3	H	221	LEU
3	H	223	ASP
3	H	249	VAL
3	H	258	ILE
4	N	535	ASP
4	N	538	VAL
4	N	553	ARG
4	N	569	ASP
4	N	579	PHE
4	N	593	ARG
4	N	671	GLU
4	N	696	LEU
5	O	119	GLU
5	O	144	LEU
5	O	213	ASP
5	O	336	GLU
6	P	69	LEU
6	P	95	THR
6	P	167	LEU
6	P	219	LYS
6	P	221	GLU
6	Q	113	ARG
6	Q	126	GLU
6	Q	138	GLU
6	Q	229	GLU
5	R	19	CYS
5	R	27	ASP
5	R	49	MET
5	R	67	LEU
5	R	123	GLN
5	R	130	ASN
5	R	143	SER
5	R	151	THR
5	R	153	ILE

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
5	R	200	TYR
5	R	215	LYS
5	R	288	ASP
5	R	354	PHE
5	R	358	TRP
7	S	40	PHE
7	S	50	ILE
7	S	52	GLU
7	S	85	ASN
7	S	133	LEU
8	U	120	LYS
8	U	131	GLN
8	U	133	ARG
8	U	182	GLN
8	U	217	GLU
8	U	221	ASP
8	U	267	LEU
8	U	323	ASN
8	U	340	TRP
8	U	376	TYR
8	U	425	GLU
8	U	450	PHE
8	U	453	VAL
8	U	508	VAL
8	U	520	LYS
8	U	550	LEU
8	U	585	MET
8	U	592	LEU
8	U	594	ASP
8	U	610	PHE
8	U	627	TRP
8	U	661	LEU
8	U	668	LEU
8	U	695	ILE
8	U	766	GLU
8	U	768	VAL
8	U	775	LYS
8	U	806	ARG
8	U	868	GLU
8	U	888	THR
9	W	1052	PHE
9	W	1106	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
9	W	1114	LEU
9	X	1144	ASN
9	X	1157	ILE
10	Y	1592	LEU
12	T	76	LEU
12	T	79	LEU
12	T	174	GLU
12	T	236	ASP
12	T	247	GLU
12	T	318	GLU
13	I	3	TYR
13	I	18	GLU
13	I	60	LYS
13	I	138	TYR
13	I	147	ASP
13	I	156	ARG
13	I	162	TRP
14	J	59	ASN
14	J	65	MET
14	J	157	VAL
14	J	160	ILE
14	J	183	LEU
14	J	193	HIS
14	J	231	VAL
14	J	422	MET
14	J	488	ASP
14	J	588	PHE
14	J	627	LEU
14	J	666	HIS
14	J	674	GLU
14	J	697	GLU
14	J	698	THR
14	J	751	TRP
14	J	759	MET
14	J	789	GLN
14	J	799	ASP
14	J	837	MET
14	J	838	LEU
14	J	860	ASP
14	J	873	MET
14	J	882	HIS
14	J	911	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
14	J	917	LEU
14	J	920	GLN
14	J	923	HIS
14	J	995	LEU
14	J	1003	TYR
14	J	1008	THR
14	J	1025	MET
14	J	1033	LEU
14	J	1046	LEU
14	J	1047	ILE
14	J	1105	TYR
14	J	1123	PHE
14	J	1137	GLN
14	J	1171	PHE
14	J	1241	TYR
15	K	429	HIS
15	K	443	HIS
15	K	480	PHE
15	K	506	ASP
15	K	546	GLN
15	K	641	ILE
15	K	685	TRP
15	K	716	ASP
15	K	802	VAL
15	K	805	LEU
15	K	852	SER
15	K	865	PHE
15	K	903	LEU
15	K	991	SER
15	K	998	VAL
15	K	1122	THR
15	K	1146	PHE
15	K	1220	ASP
15	K	1267	CYS
16	L	95	ARG
16	L	139	VAL
16	L	397	LYS
16	L	434	ARG
17	M	34	THR
17	M	153	LEU
17	M	198	ASP
19	F	38	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
19	F	117	GLU
19	F	145	CYS
19	F	349	PHE
20	V	14	TYR
20	V	37	LYS
20	V	58	ASN
21	a	448	LEU
21	a	454	TYR
21	a	514	GLU
21	a	525	HIS
22	b	21	VAL
23	c	280	TRP
23	c	332	THR
24	D	27	TYR
24	D	178	TYR
24	D	226	HIS
24	D	457	ASP
24	D	658	TRP
24	D	703	ARG
24	G	95	GLU
24	G	101	SER
24	G	183	HIS
24	G	286	GLU
24	G	395	HIS
24	G	400	ASP
24	G	551	ASP
24	G	565	THR
24	G	567	ASP
24	G	604	GLU
24	G	661	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	GLN
1	A	448	ASN
1	A	820	HIS
1	A	845	ASN
1	A	968	ASN
1	A	1350	ASN
1	A	1353	ASN
1	A	1434	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1446	ASN
1	A	1450	HIS
1	A	1462	GLN
1	A	1542	ASN
1	A	1546	HIS
1	A	1654	HIS
1	A	1777	HIS
2	B	107	ASN
2	B	141	ASN
2	B	239	GLN
2	C	141	ASN
2	C	187	GLN
3	H	17	ASN
3	H	198	HIS
3	H	271	HIS
4	N	706	GLN
5	O	175	HIS
5	O	299	ASN
6	P	101	HIS
6	Q	158	HIS
5	R	89	HIS
5	R	94	ASN
5	R	163	HIS
5	R	282	ASN
5	R	299	ASN
5	R	373	HIS
8	U	97	ASN
8	U	131	GLN
8	U	305	GLN
8	U	364	ASN
8	U	900	ASN
9	W	1011	HIS
9	W	1156	GLN
9	X	1103	GLN
11	Z	1782	ASN
12	T	95	ASN
12	T	228	ASN
12	T	243	ASN
12	T	261	HIS
12	T	317	ASN
12	T	428	HIS
12	T	446	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
12	T	674	GLN
13	I	82	HIS
13	I	145	ASN
13	I	151	HIS
14	J	15	HIS
14	J	179	HIS
14	J	184	HIS
14	J	227	HIS
14	J	433	ASN
14	J	513	ASN
14	J	564	HIS
14	J	649	ASN
14	J	789	GLN
14	J	895	ASN
14	J	932	ASN
14	J	1079	ASN
14	J	1168	HIS
14	J	1239	ASN
15	K	429	HIS
15	K	548	ASN
15	K	600	GLN
15	K	678	HIS
15	K	712	ASN
15	K	895	GLN
15	K	902	HIS
15	K	931	HIS
16	L	268	ASN
16	L	365	ASN
17	M	79	GLN
17	M	251	HIS
18	E	131	ASN
18	E	191	GLN
19	F	98	ASN
19	F	115	HIS
19	F	160	HIS
19	F	329	ASN
21	a	411	HIS
24	D	125	GLN
24	D	137	ASN
24	D	183	HIS
24	D	580	HIS
24	G	31	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
24	G	394	HIS
24	G	438	GLN
24	G	496	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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.

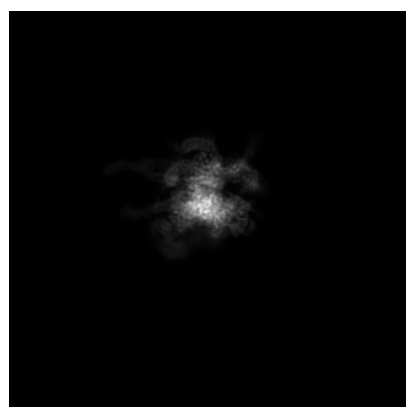
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46494. These allow visual inspection of the internal detail of the map and identification of artifacts.

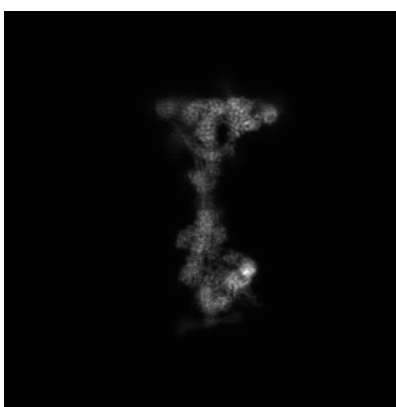
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

#### 6.1.1 Primary map



X



Y

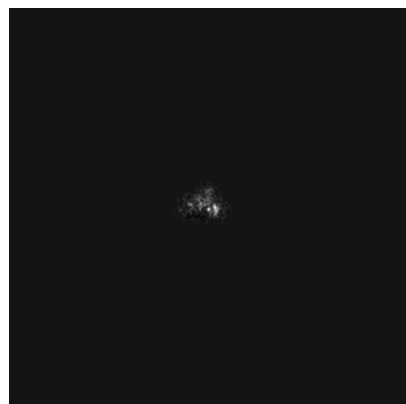


Z

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

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

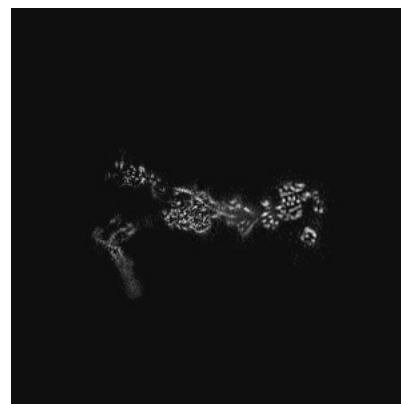
#### 6.2.1 Primary map



X Index: 180



Y Index: 180



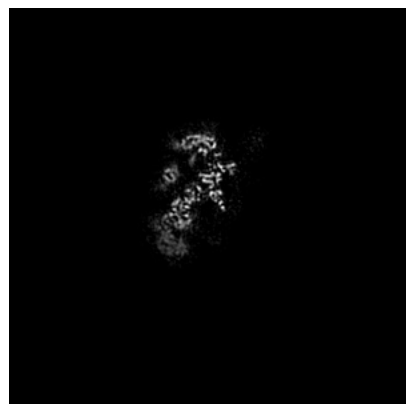
Z Index: 180



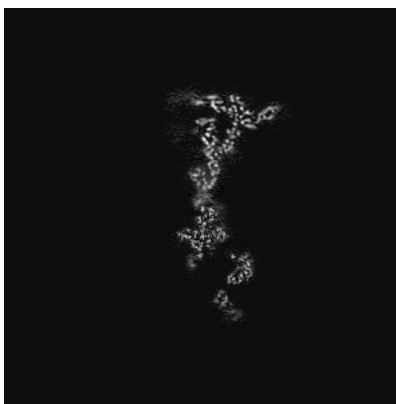
The images above show central slices of the map in three orthogonal directions.

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

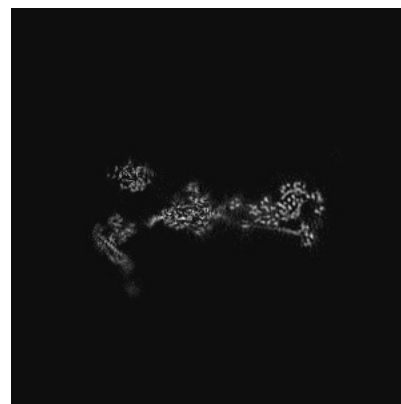
### 6.3.1 Primary map



X Index: 267



Y Index: 180

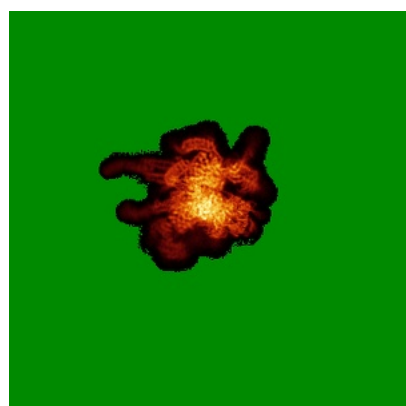


Z Index: 184

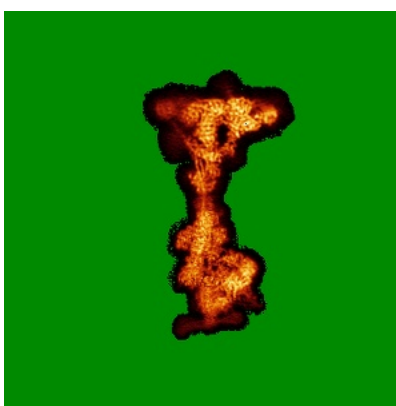
The images above show the largest variance slices of the map in three orthogonal directions.

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

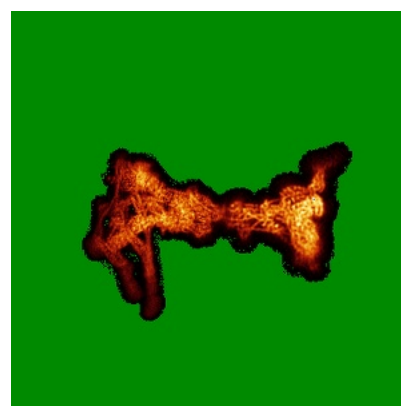
### 6.4.1 Primary map



X



Y

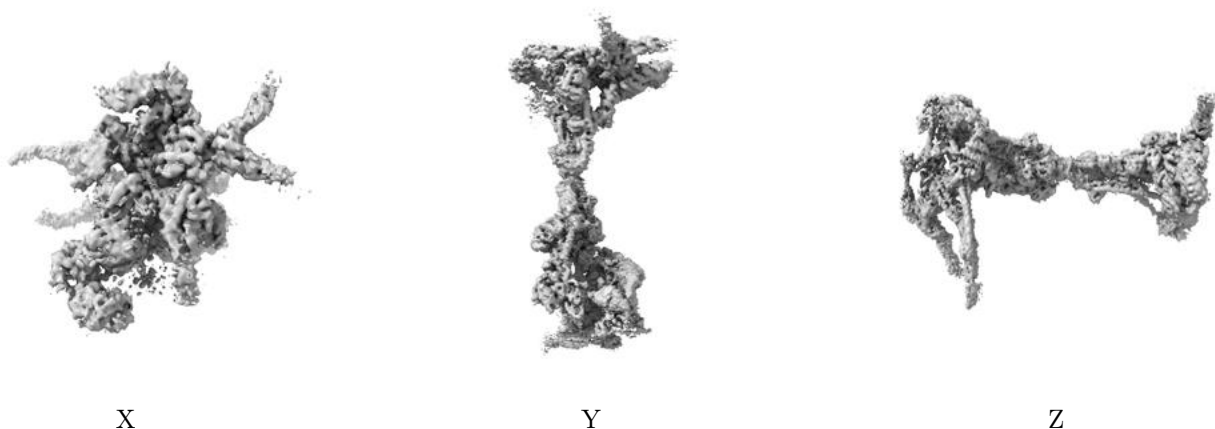


Z

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 0.0037. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

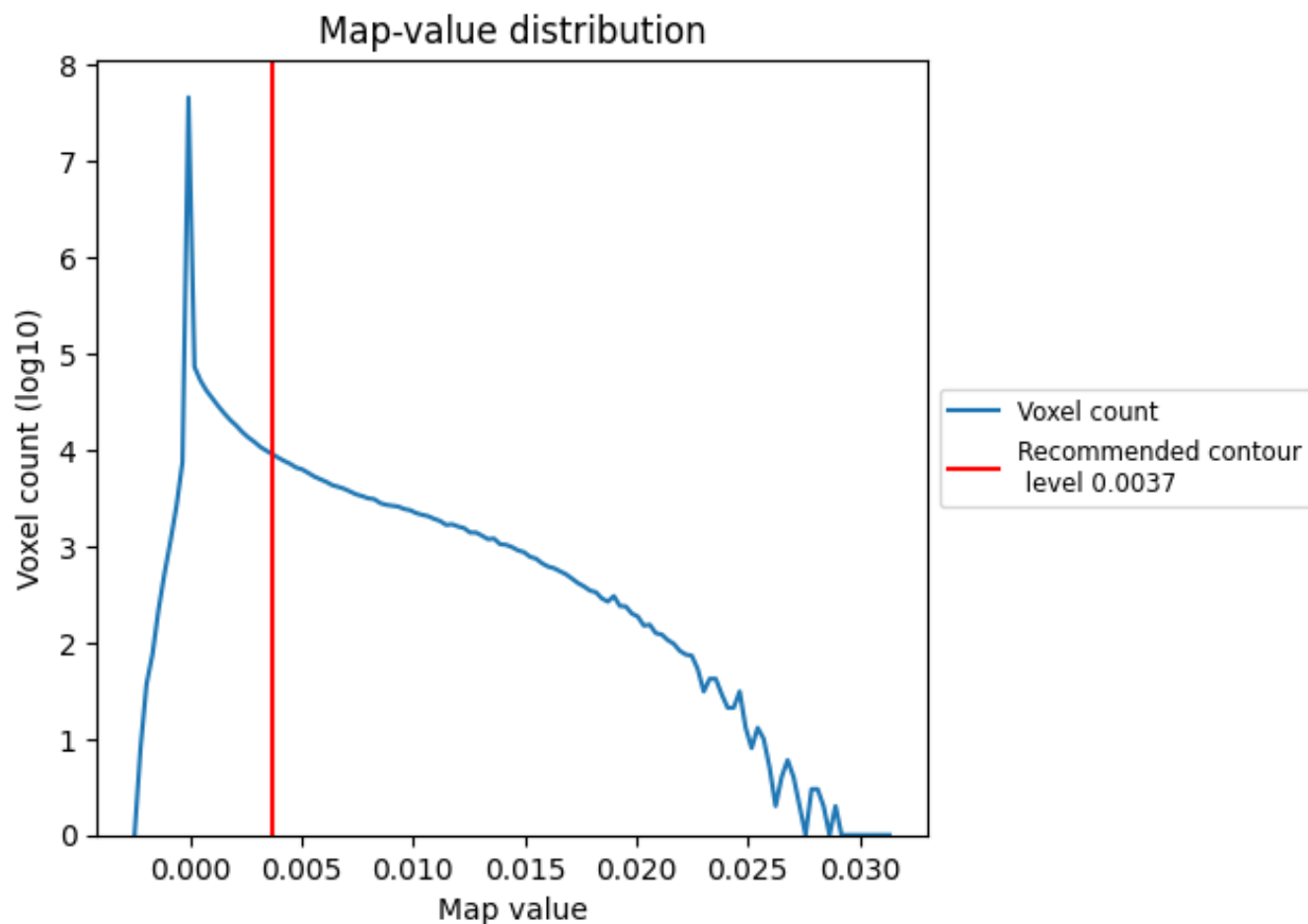
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

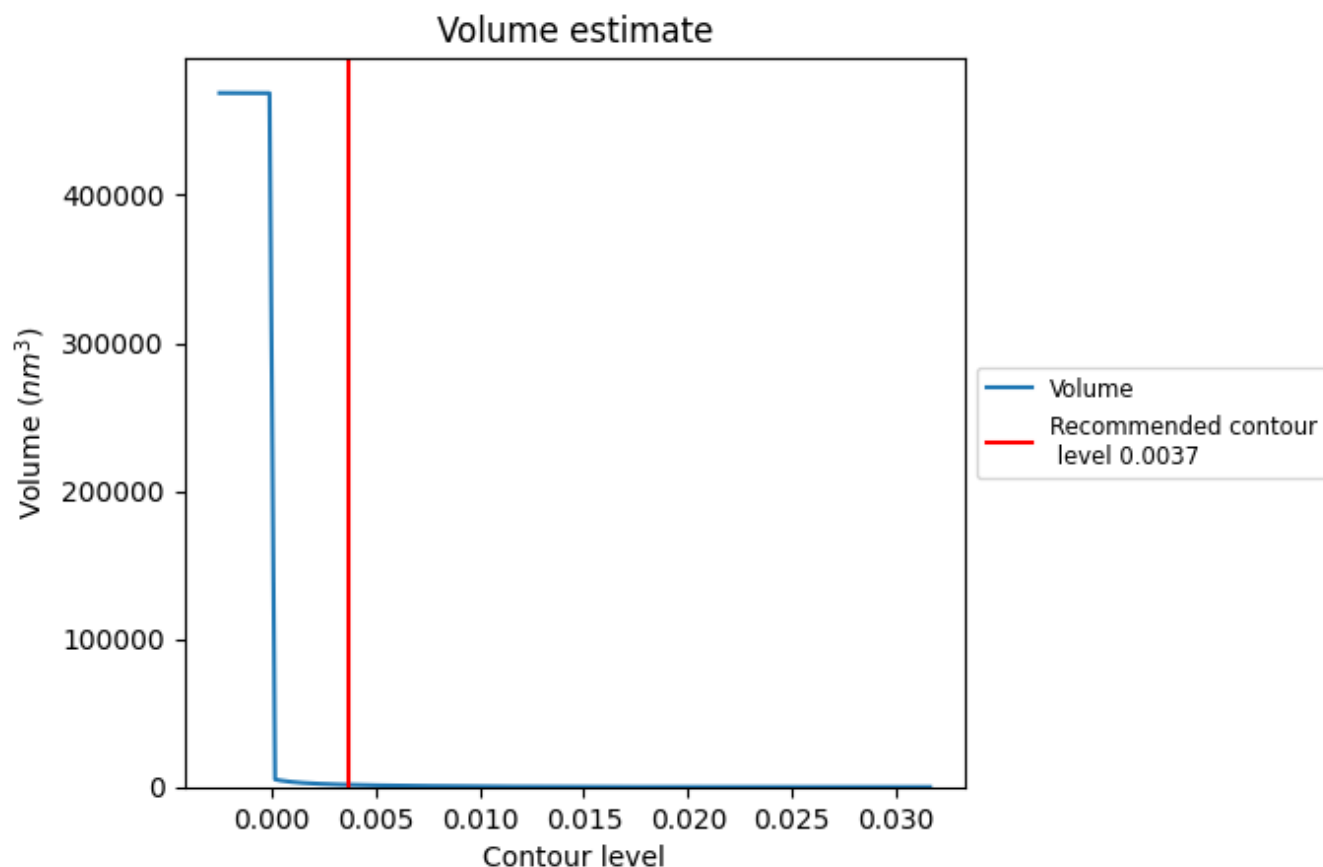
This section contains the results of statistical analysis of the map.

### 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.

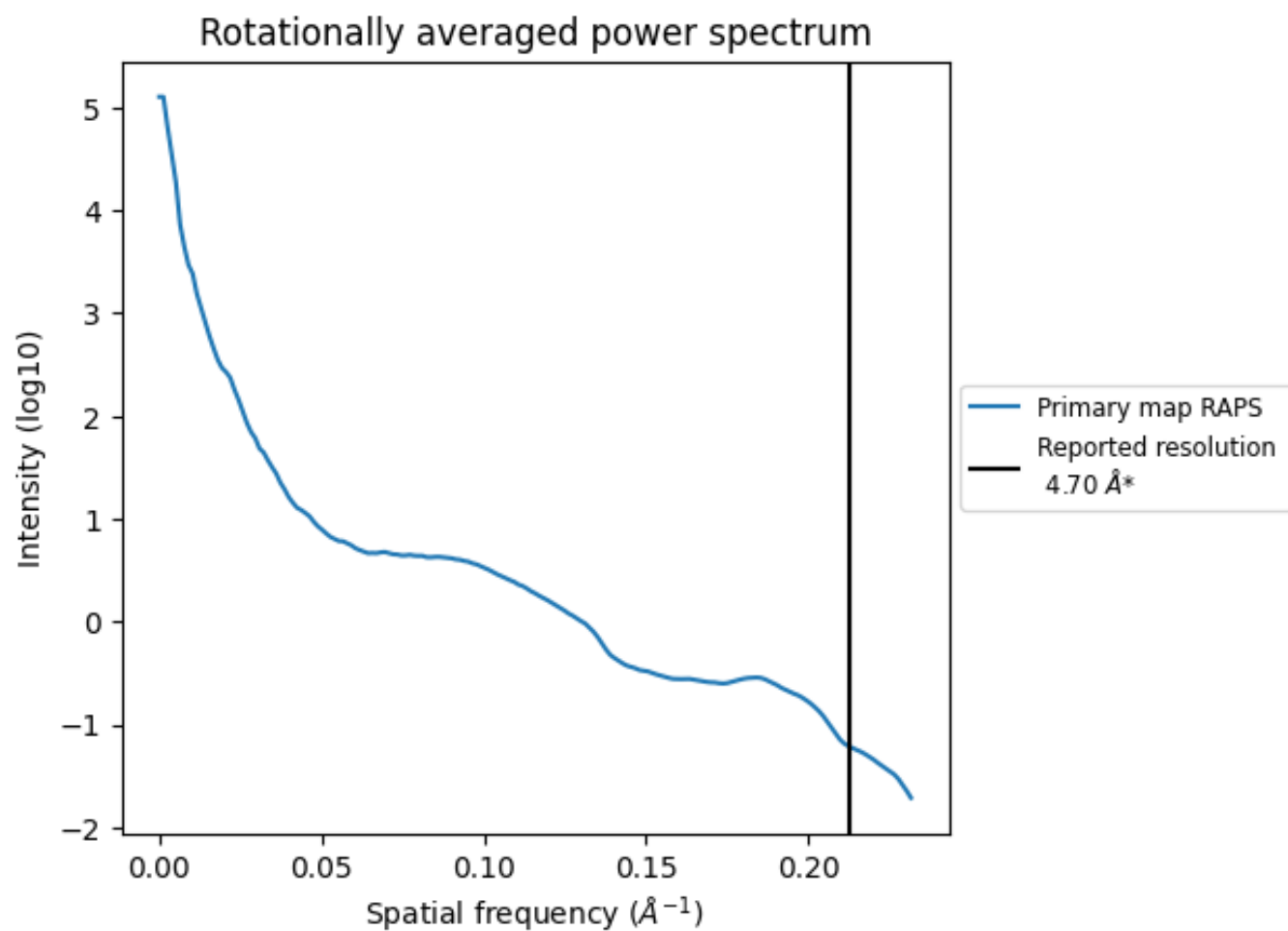
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1486  $\text{nm}^3$ ; this corresponds to an approximate mass of 1342 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 0.213 Å<sup>-1</sup>

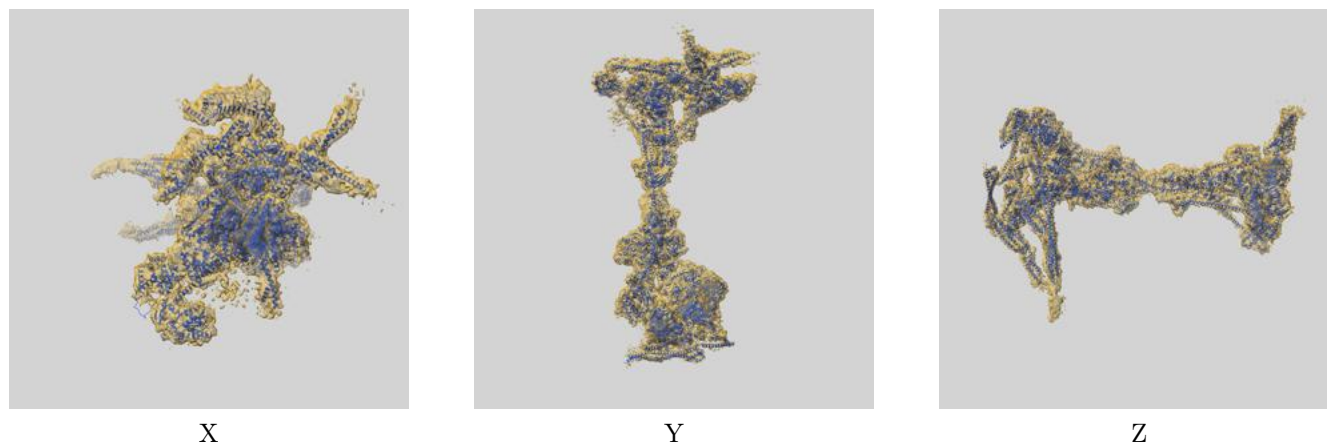
## 8 Fourier-Shell correlation

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

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

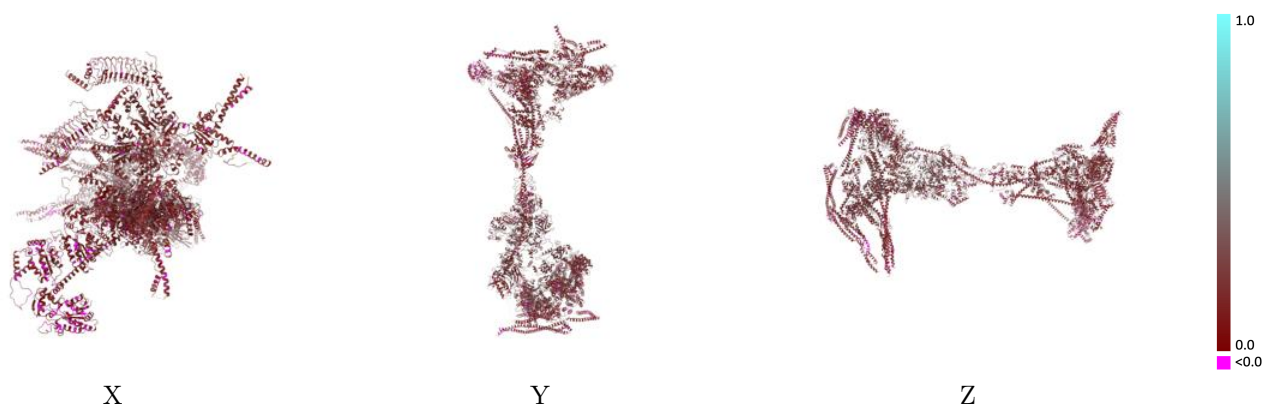
This section contains information regarding the fit between EMDB map EMD-46494 and PDB model 9D2F. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



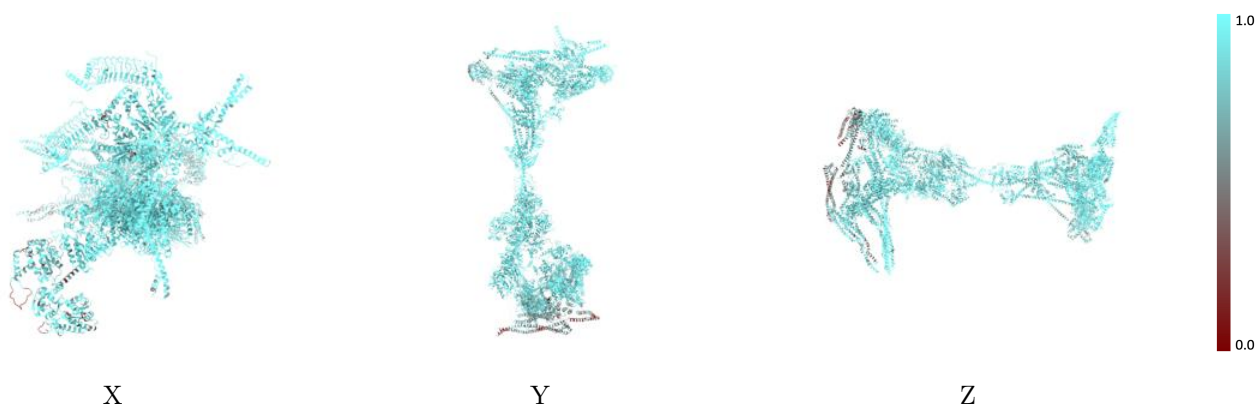
The images above show the 3D surface view of the map at the recommended contour level 0.0037 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

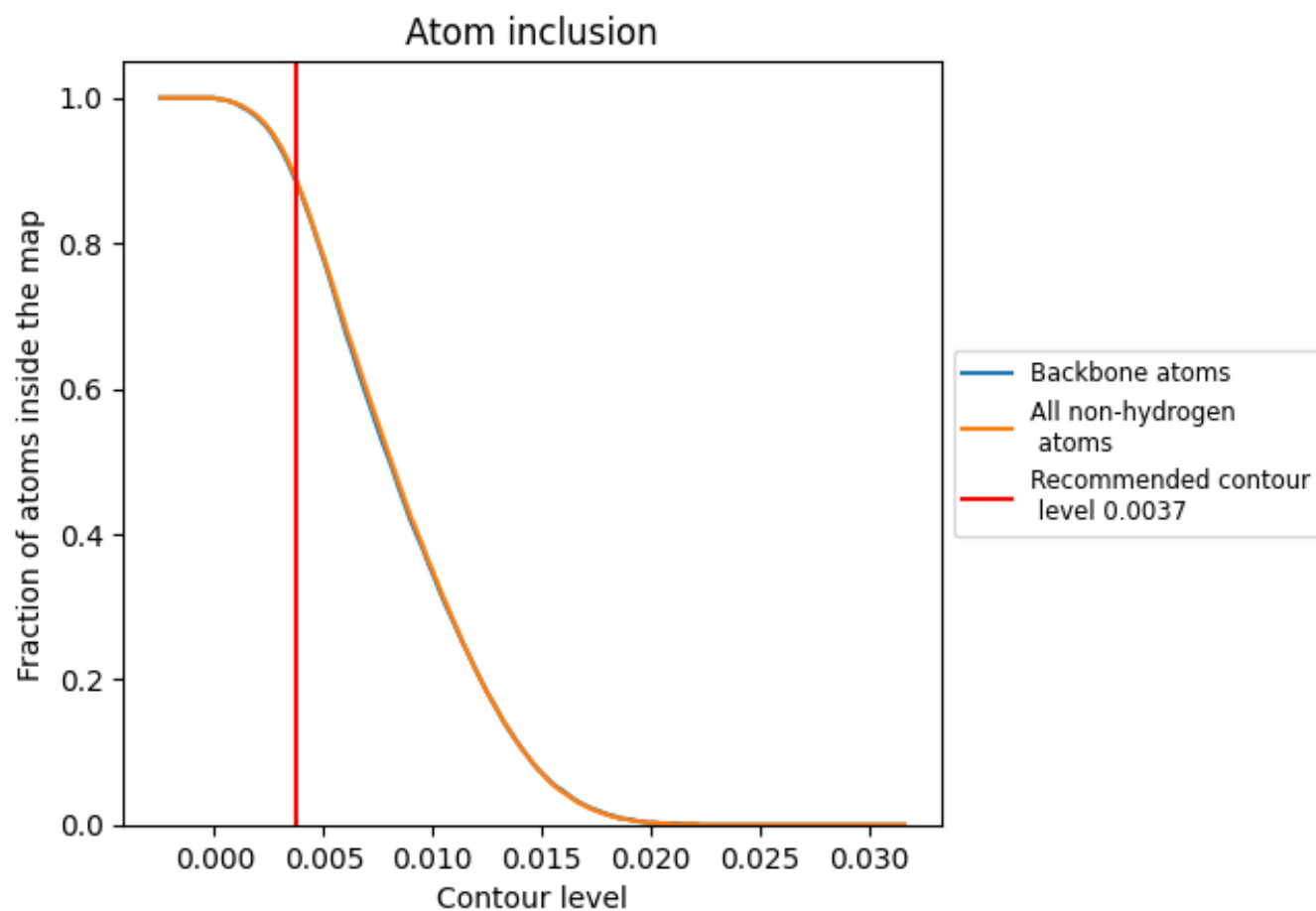
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.0037).































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 89% 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 (0.0037) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8910	 0.2300
A	 0.9380	 0.2190
B	 0.9650	 0.1980
C	 0.9610	 0.1950
D	 0.7990	 0.1570
E	 0.9160	 0.2020
F	 0.9340	 0.2000
G	 0.9210	 0.2100
H	 0.9140	 0.2490
I	 0.9660	 0.2080
J	 0.9510	 0.2870
K	 0.9070	 0.3080
L	 0.9310	 0.2280
M	 0.7470	 0.2070
N	 0.9240	 0.1950
O	 0.9150	 0.2280
P	 0.8950	 0.2350
Q	 0.9020	 0.2380
R	 0.9400	 0.2980
S	 0.7830	 0.2250
T	 0.8270	 0.2070
U	 0.9250	 0.2700
V	 0.9660	 0.2070
W	 0.5750	 0.1870
X	 0.5520	 0.1840
Y	 0.4610	 0.1890
Z	 0.3740	 0.2040
a	 0.9750	 0.1740
b	 0.9930	 0.2120
c	 0.9700	 0.1830

