



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 04:37 AM UTC

PDB ID : 9CF8 / pdb_00009cf8
EMDB ID : EMD-45533
Title : Cryo-EM structure of human kidney V-ATPase state 1
Authors : Zhang, Z.; Lyu, M.
Deposited on : 2024-06-27
Resolution : 3.46 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

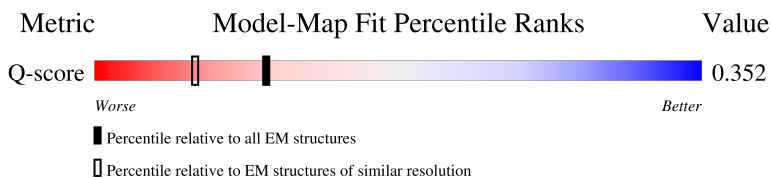
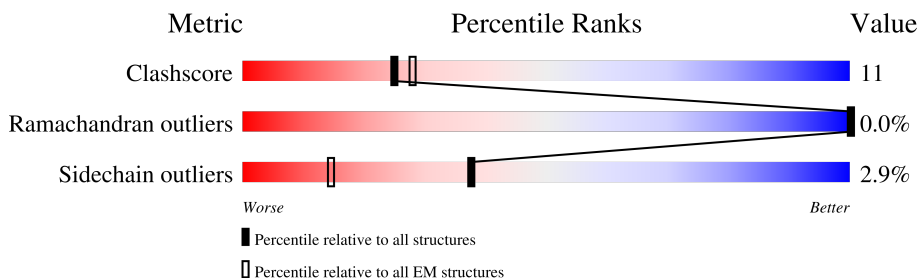
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.46 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.
















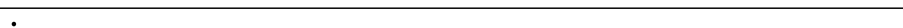











Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13788 (2.96 - 3.96)

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	0	205	80% 18% ..
2	1	155	74% 22% ..
2	2	155	79% 17% .
2	3	155	74% 22% ..

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Mol	Chain	Length	Quality of chain
2	4	155	 74% 23% . .
2	5	155	 76% 21% .
2	6	155	 74% 22% . .
2	7	155	 77% 20% .
2	8	155	 69% 27% . .
2	9	155	 79% 17% .
3	A	617	 66% 25% . 8%
3	B	617	 61% 27% . 10%
3	C	617	 71% 26% .
4	D	511	 66% 23% . 10%
4	E	511	 67% 23% 10%
4	F	511	 66% 23% . 10%
5	G	247	 64% 22% . 12%
6	H	226	 55% 23% . 20%
6	I	226	 75% 21% . .
6	J	226	 68% 25% . 5%
7	K	118	 66% 27% . .
7	L	118	 64% 32% . .
7	M	118	 59% 36% . .
8	N	119	 52% 39% . 8%
9	Q	351	 61% 25% . 13%
10	R	837	 53% 22% . 24%
11	S	81	 79% 16% 5%
12	T	137	 58% . . 38%
13	U	470	 29% 13% . 56%

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Mol	Chain	Length	Quality of chain
14	V	350	<div><div></div><div>10% . 87%</div></div>

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 56307 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 V-type proton ATPase 21 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	202	Total	C	N	O	S	0	0
			1473	975	232	256	10		

- Molecule 2 is a protein called V-type proton ATPase 16 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	150	Total	C	N	O	S	0	0
			1053	692	163	191	7		
2	2	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	3	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	4	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	5	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	6	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	7	150	Total	C	N	O	S	0	0
			1059	695	166	191	7		
2	8	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	9	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		

- Molecule 3 is a protein called V-type proton ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	565	Total	C	N	O	S	0	0
			4318	2745	721	827	25		
3	B	555	Total	C	N	O	S	0	0
			4186	2649	693	817	27		
3	C	601	Total	C	N	O	S	0	0
			4606	2923	773	882	28		

- Molecule 4 is a protein called V-type proton ATPase subunit B, brain isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	459	Total	C	N	O	S	0	0
			3577	2272	606	679	20		
4	E	460	Total	C	N	O	S	0	0
			3589	2278	616	676	19		
4	F	458	Total	C	N	O	S	0	0
			3573	2267	611	675	20		

- Molecule 5 is a protein called V-type proton ATPase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	217	Total	C	N	O	S	0	0
			1720	1091	311	313	5		

- Molecule 6 is a protein called V-type proton ATPase subunit E 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	181	Total	C	N	O	S	0	0
			1470	926	263	273	8		
6	I	219	Total	C	N	O	S	0	0
			1777	1117	315	335	10		
6	J	215	Total	C	N	O	S	0	0
			1748	1100	310	328	10		

- Molecule 7 is a protein called V-type proton ATPase subunit G 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	114	Total	C	N	O	S	0	0
			938	573	179	183	3		
7	L	114	Total	C	N	O	S	0	0
			938	573	179	183	3		
7	M	114	Total	C	N	O	S	0	0
			938	573	179	183	3		

- Molecule 8 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	110	Total	C	N	O	S	0	0
			875	552	157	164	2		

- Molecule 9 is a protein called V-type proton ATPase subunit d 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	307	Total	C	N	O	S	0	0
			2497	1608	408	469	12		

- Molecule 10 is a protein called V-type proton ATPase 116 kDa subunit a isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	R	634	Total	C	N	O	S	0	0
			5166	3397	844	891	34		

- Molecule 11 is a protein called V-type proton ATPase subunit e 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	77	Total	C	N	O	S	0	0
			631	436	97	93	5		

- Molecule 12 is a protein called Ribonuclease kappa.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	85	Total	C	N	O	S	0	0
			654	431	101	115	7		

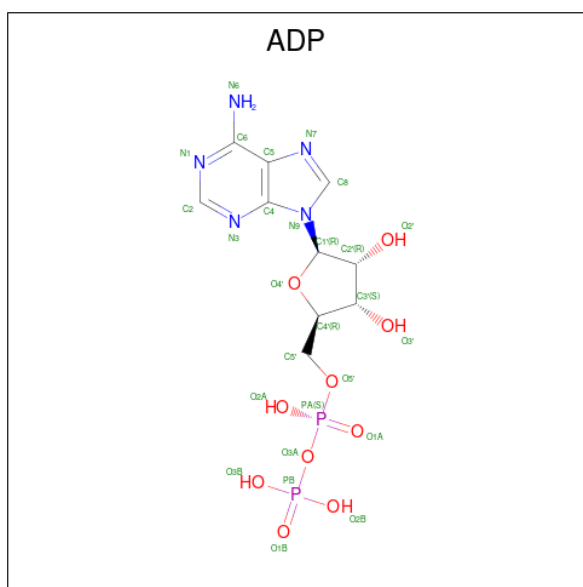
- Molecule 13 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	U	205	Total	C	N	O	S	0	0
			1664	1089	265	300	10		

- Molecule 14 is a protein called Renin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	V	45	Total	C	N	O	S	0	0
			375	255	53	64	3		

- Molecule 15 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

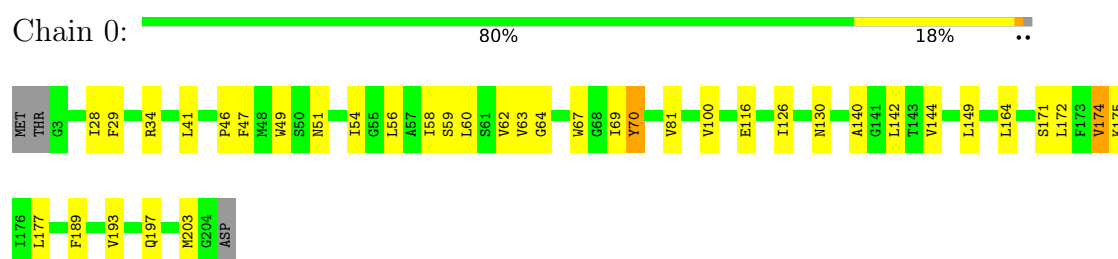


Mol	Chain	Residues	Atoms					AltConf
15	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

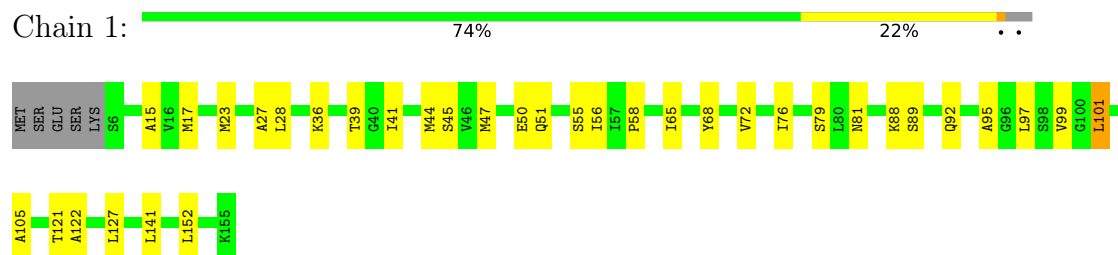
3 Residue-property plots [i](#)

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.

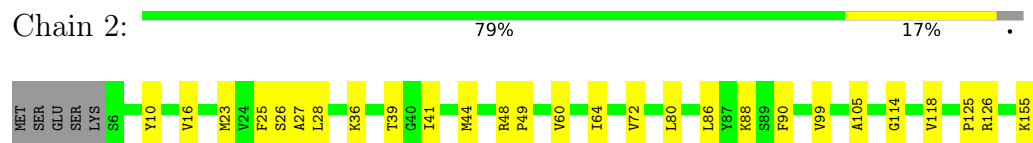
- Molecule 1: V-type proton ATPase 21 kDa proteolipid subunit



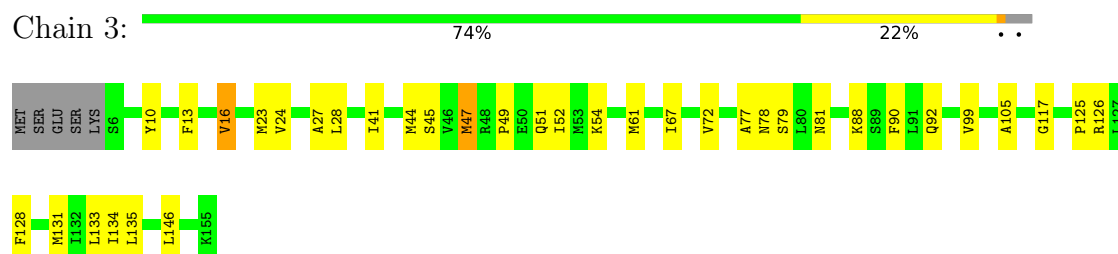
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit



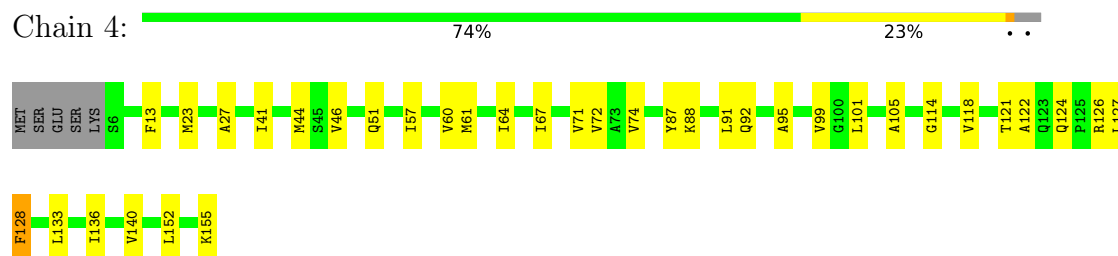
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit



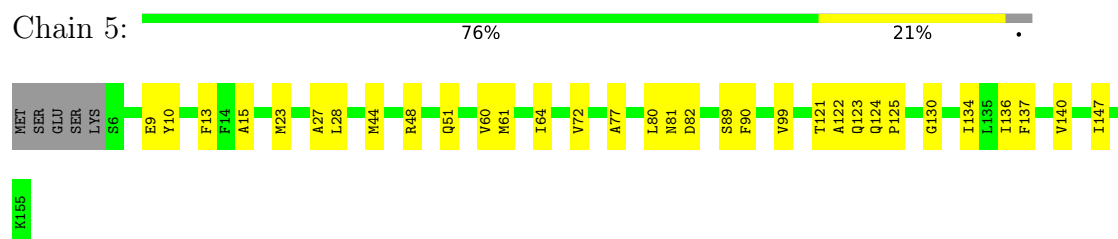
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit



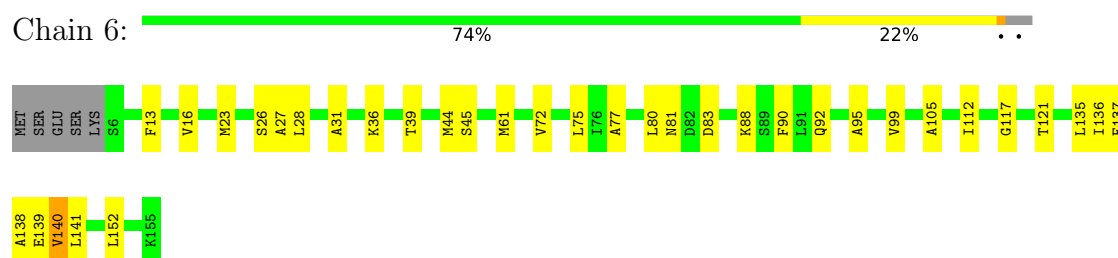
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit



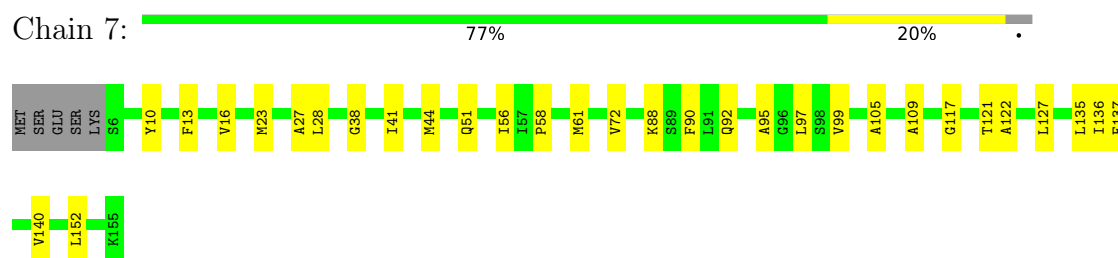
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit



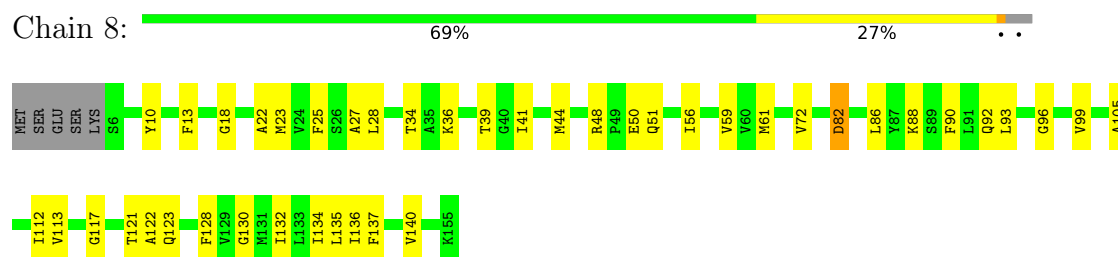
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit



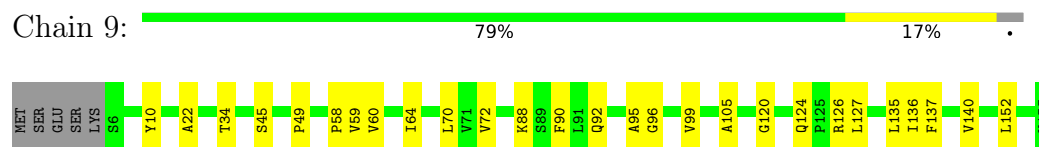
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit



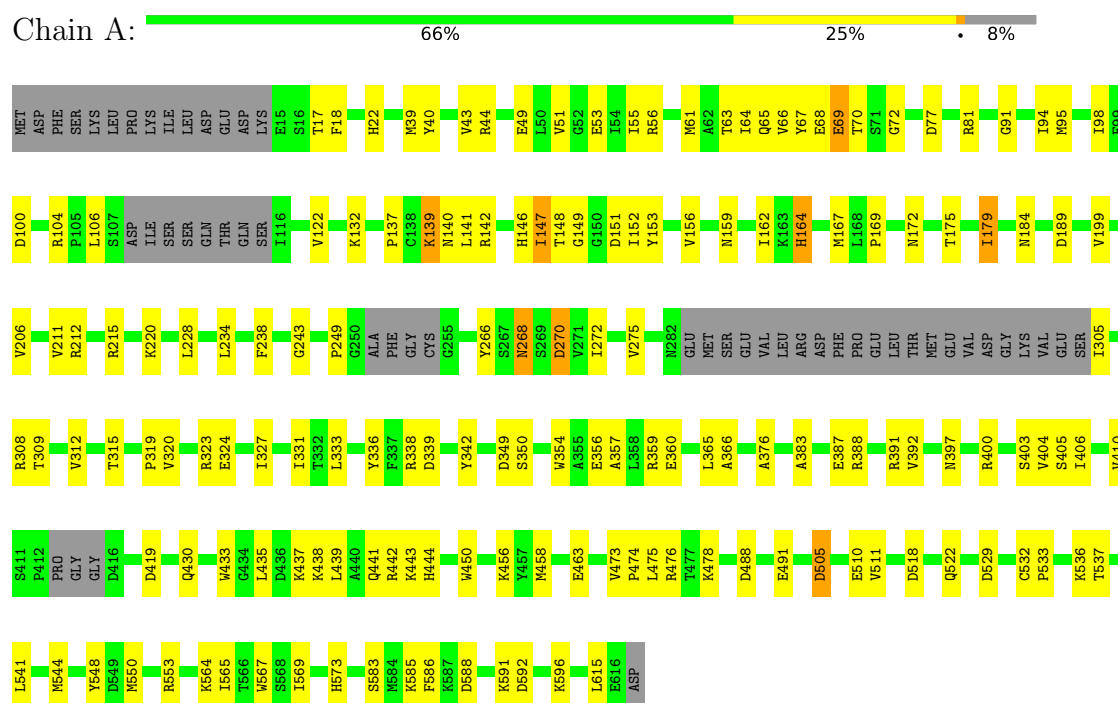
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit



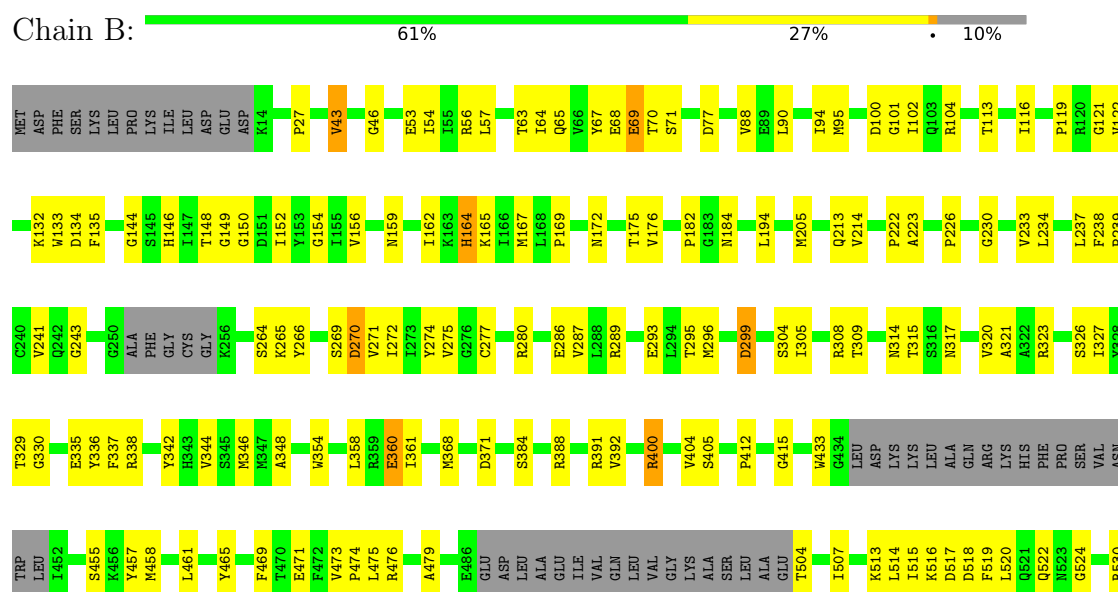
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit



- Molecule 3: V-type proton ATPase catalytic subunit A



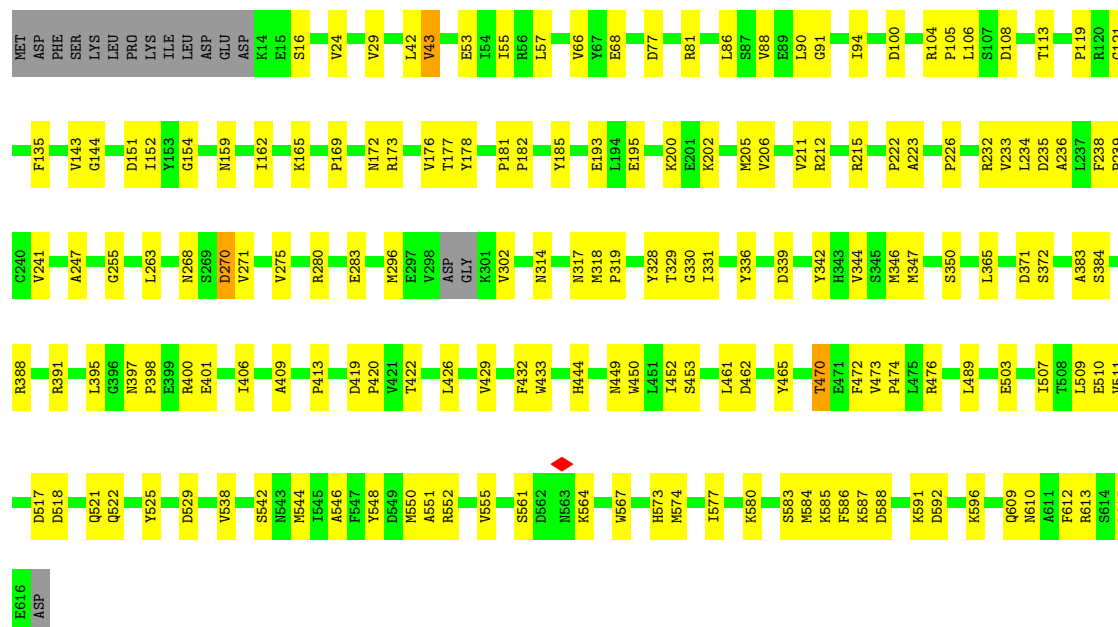
- Molecule 3: V-type proton ATPase catalytic subunit A





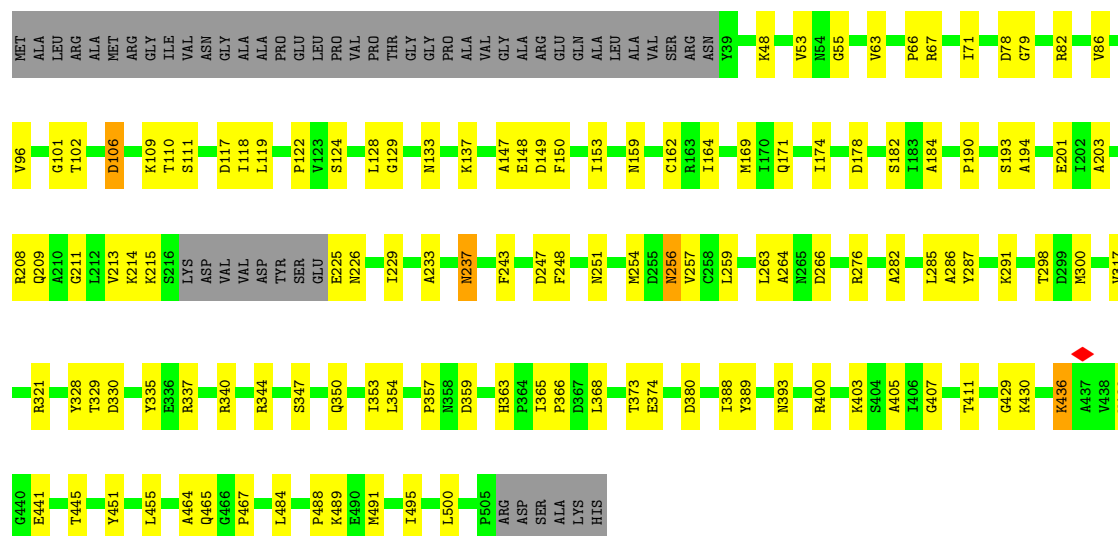
• Molecule 3: V-type proton ATPase catalytic subunit A

Chain C: 71% 26%



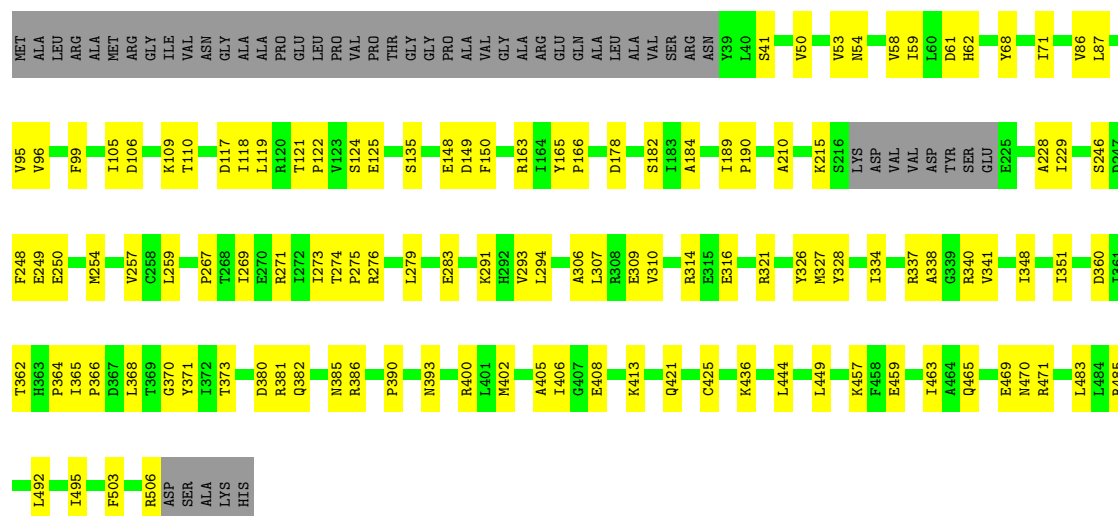
• Molecule 4: V-type proton ATPase subunit B, brain isoform

Chain D: 66% 23% 10%



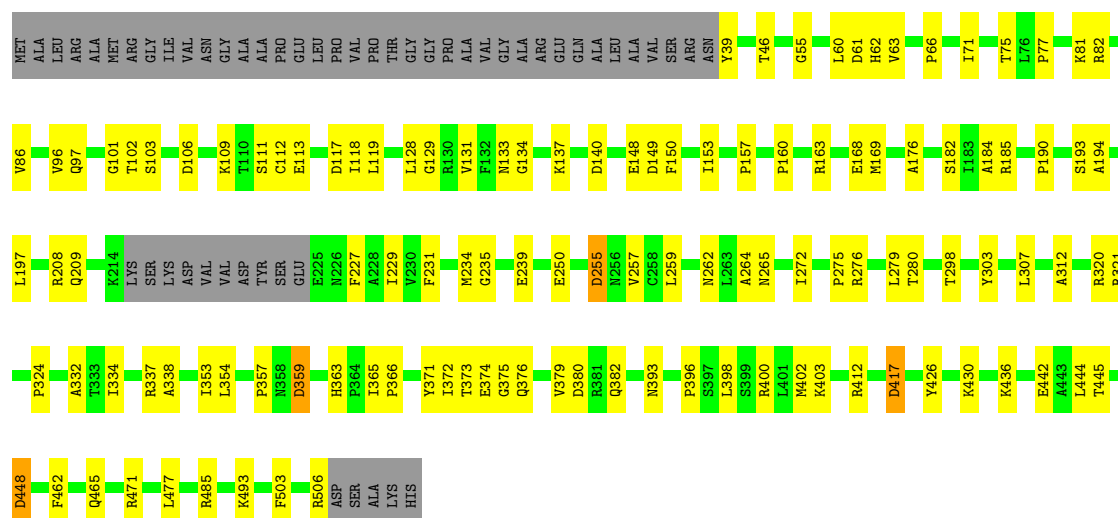
• Molecule 4: V-type proton ATPase subunit B, brain isoform

Chain E: 67% 23% 10%



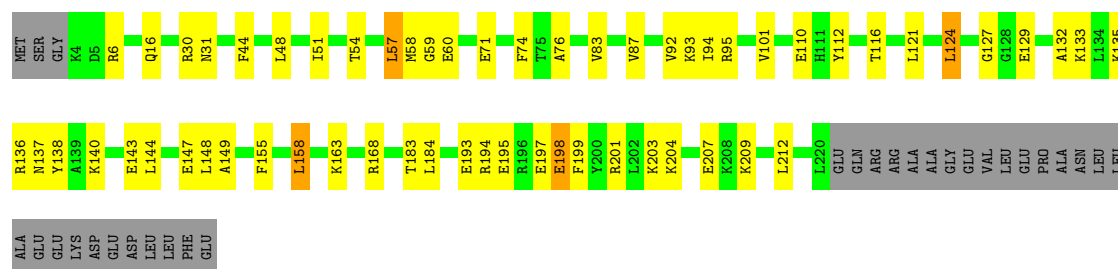
• Molecule 4: V-type proton ATPase subunit B, brain isoform

Chain F: 66% 23% 10%

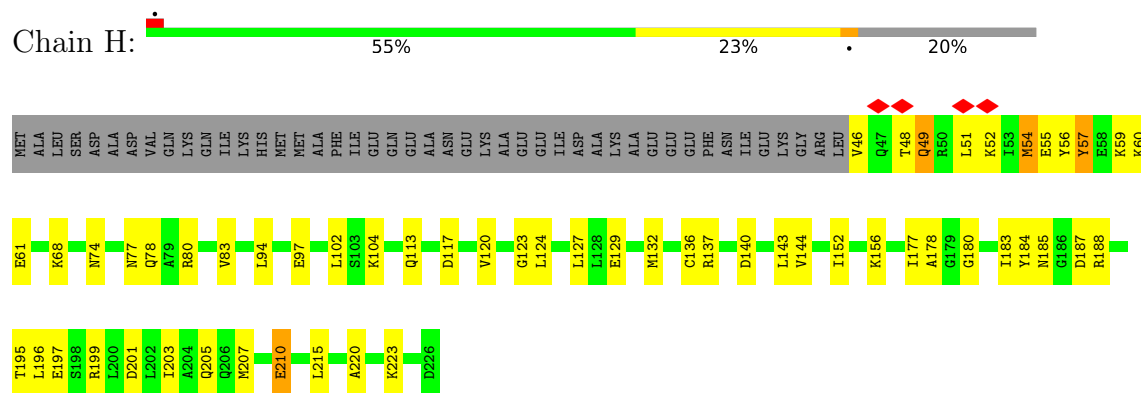


• Molecule 5: V-type proton ATPase subunit D

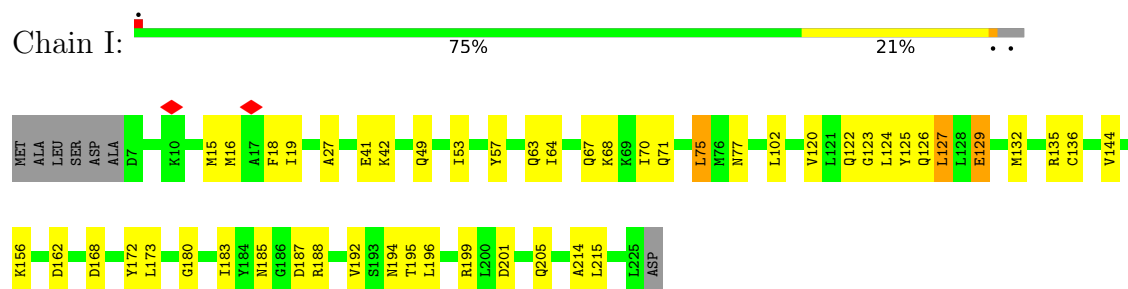
Chain G: 64% 22% 12%



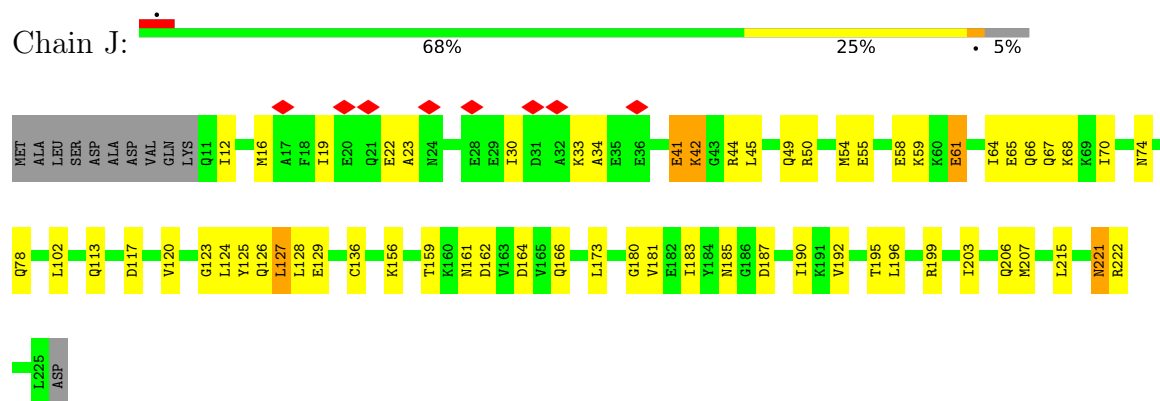
• Molecule 6: V-type proton ATPase subunit E 1



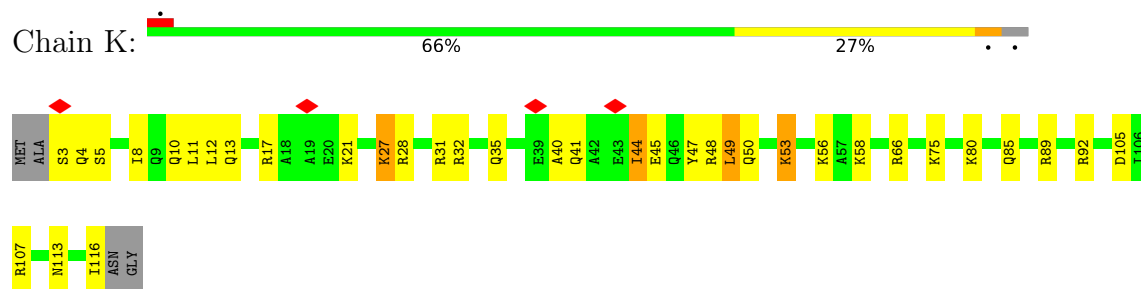
• Molecule 6: V-type proton ATPase subunit E 1



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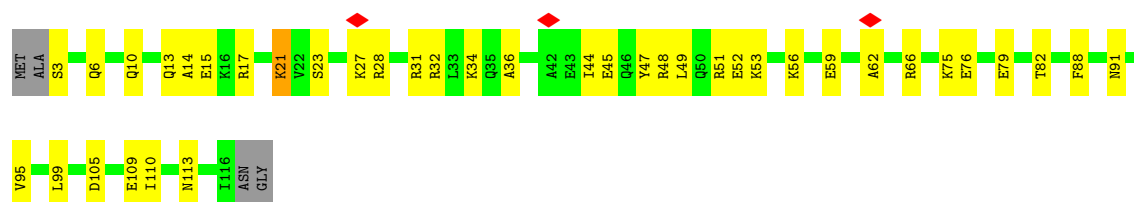


• Molecule 7: V-type proton ATPase subunit G 1



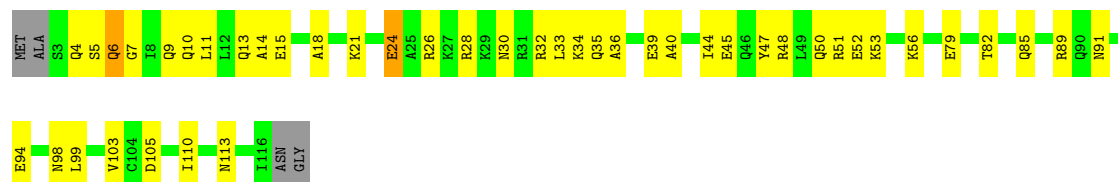
• Molecule 7: V-type proton ATPase subunit G 1





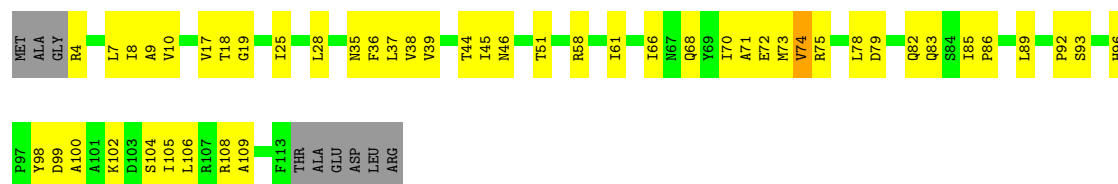
• Molecule 7: V-type proton ATPase subunit G 1

Chain M: 59% 36% . .



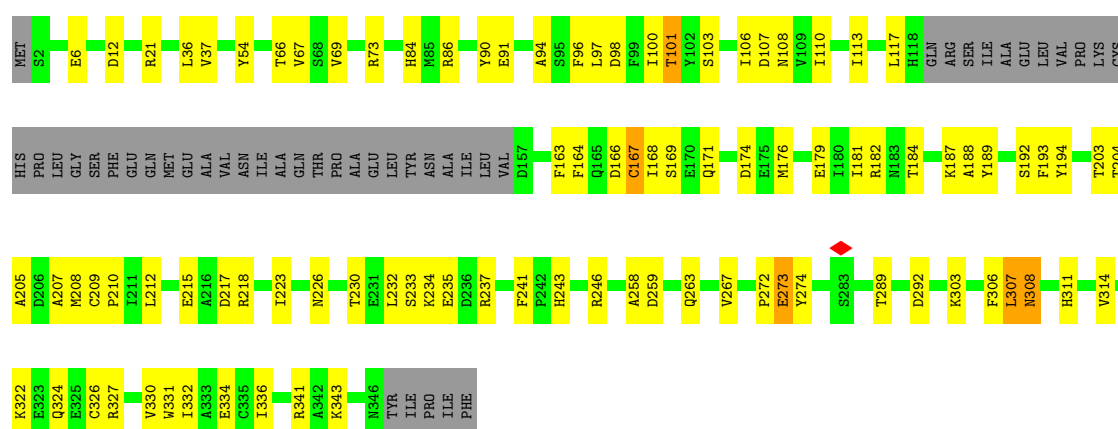
• Molecule 8: V-type proton ATPase subunit F

Chain N: 52% 39% 8%



• Molecule 9: V-type proton ATPase subunit d 1

Chain Q: 61% 25% 13%



• Molecule 10: V-type proton ATPase 116 kDa subunit a isoform 1

Chain R: 53% 22% 24%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35623	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 ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.808	Depositor
Minimum map value	-0.101	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	547.84, 547.84, 547.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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	0	0.16	0/1507	0.29	0/2051
2	1	0.18	0/1068	0.33	0/1447
2	2	0.16	0/1080	0.31	0/1461
2	3	0.36	0/1080	0.52	0/1461
2	4	0.22	0/1080	0.34	0/1461
2	5	0.16	0/1080	0.30	0/1461
2	6	0.17	0/1080	0.31	0/1461
2	7	0.17	0/1074	0.32	0/1454
2	8	0.15	0/1080	0.32	0/1461
2	9	0.15	0/1080	0.29	0/1461
3	A	0.25	0/4405	0.39	0/5977
3	B	0.13	0/4267	0.31	0/5791
3	C	0.17	0/4701	0.33	0/6377
4	D	0.23	0/3648	0.38	0/4945
4	E	0.26	0/3660	0.41	0/4960
4	F	0.37	0/3644	0.51	0/4941
5	G	0.12	0/1738	0.30	0/2330
6	H	0.12	0/1484	0.29	0/1989
6	I	0.10	0/1794	0.27	0/2403
6	J	0.10	0/1765	0.26	0/2363
7	K	0.13	0/945	0.26	0/1258
7	L	0.14	0/945	0.28	0/1258
7	M	0.13	0/945	0.30	0/1258
8	N	0.12	0/889	0.34	0/1200
9	Q	0.11	0/2553	0.27	0/3452
10	R	0.22	0/5303	0.38	0/7183
11	S	0.37	0/657	0.55	0/902
12	T	0.41	0/670	0.62	0/911
13	U	0.15	0/1718	0.35	0/2337
14	V	0.13	0/388	0.23	0/532
All	All	0.21	0/57328	0.36	0/77546

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
3	A	0	1
4	E	0	1
4	F	0	1
10	R	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	212	ARG	Sidechain
4	E	276	ARG	Sidechain
4	F	276	ARG	Sidechain
10	R	339	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	0	1473	0	1503	26	0
2	1	1053	0	1109	25	0
2	2	1065	0	1131	20	0
2	3	1065	0	1131	25	0
2	4	1065	0	1131	30	0
2	5	1065	0	1131	27	0
2	6	1065	0	1131	25	0
2	7	1059	0	1120	26	0
2	8	1065	0	1131	32	0
2	9	1065	0	1131	19	0
3	A	4318	0	4243	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4186	0	4063	118	0
3	C	4606	0	4539	105	0
4	D	3577	0	3570	75	0
4	E	3589	0	3590	73	0
4	F	3573	0	3561	82	0
5	G	1720	0	1797	42	0
6	H	1470	0	1545	36	0
6	I	1777	0	1841	41	0
6	J	1748	0	1818	44	0
7	K	938	0	947	34	0
7	L	938	0	947	30	0
7	M	938	0	947	32	0
8	N	875	0	878	37	0
9	Q	2497	0	2427	61	0
10	R	5166	0	5198	129	0
11	S	631	0	645	8	0
12	T	654	0	641	7	0
13	U	1664	0	1589	47	0
14	V	375	0	365	10	0
15	C	27	0	12	1	0
All	All	56307	0	56812	1191	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 11.

All (1191) 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)
9:Q:67:VAL:HG11	9:Q:334:GLU:HG2	1.51	0.93
5:G:94:ILE:HA	5:G:110:GLU:O	1.81	0.80
3:C:159:ASN:HD21	3:C:162:ILE:HB	1.47	0.79
3:B:27:PRO:HB2	3:B:65:GLN:HE22	1.48	0.77
6:J:42:LYS:HD2	7:M:36:ALA:HB1	1.65	0.77
13:U:401:GLN:HE22	14:V:296:ALA:H	1.31	0.77
3:A:56:ARG:HB3	3:A:63:THR:HB	1.67	0.75
4:E:503:PHE:HA	4:E:506:ARG:HE	1.50	0.75
10:R:341:THR:HB	10:R:350:SER:HB2	1.68	0.75
7:M:18:ALA:HA	7:M:21:LYS:HD3	1.68	0.74
10:R:115:GLN:HE22	10:R:279:ARG:HE	1.36	0.74
4:E:87:LEU:HD21	4:E:314:ARG:HG2	1.70	0.74
8:N:68:GLN:HE22	8:N:99:ASP:H	1.34	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:180:GLY:HA3	6:H:195:THR:HA	1.69	0.73
3:B:56:ARG:HB2	3:B:63:THR:HB	1.70	0.72
8:N:92:PRO:HB3	8:N:98:TYR:HB2	1.70	0.72
3:B:269:SER:O	3:B:308:ARG:NH1	2.23	0.72
7:K:89:ARG:HA	7:K:92:ARG:HD2	1.71	0.72
10:R:335:PHE:HA	10:R:338:ARG:HE	1.53	0.72
6:J:127:LEU:HD12	6:J:183:ILE:HG22	1.72	0.72
4:D:229:ILE:HB	4:D:257:VAL:HG22	1.72	0.71
10:R:25:CYS:HA	10:R:340:GLY:HA3	1.71	0.71
2:1:23:MET:HE3	2:1:27:ALA:HB2	1.73	0.71
10:R:115:GLN:HE21	10:R:276:GLU:HA	1.56	0.71
3:B:223:ALA:HA	3:B:391:ARG:HE	1.55	0.70
7:M:35:GLN:NE2	7:M:39:GLU:OE2	2.24	0.70
10:R:310:CYS:HB2	10:R:321:ALA:HB2	1.72	0.70
4:F:375:GLY:H	4:F:400:ARG:HH11	1.40	0.69
6:I:127:LEU:HD12	6:I:183:ILE:HG22	1.74	0.69
6:I:199:ARG:NH2	7:L:105:ASP:O	2.25	0.69
10:R:41:ASN:HB3	10:R:44:VAL:HB	1.73	0.69
2:1:47:MET:HE1	9:Q:84:HIS:HE1	1.57	0.69
3:B:550:MET:HG2	3:B:553:ARG:HH22	1.58	0.69
5:G:76:ALA:HB2	5:G:127:GLY:HA3	1.73	0.69
6:J:127:LEU:HD22	6:J:129:GLU:HG3	1.75	0.68
4:E:380:ASP:HB2	4:E:393:ASN:HB2	1.74	0.68
13:U:330:ARG:HH22	13:U:341:THR:HB	1.59	0.68
6:J:23:ALA:HA	7:M:21:LYS:HD2	1.76	0.68
9:Q:203:THR:HB	9:Q:311:HIS:HB3	1.76	0.68
3:C:16:SER:O	3:C:81:ARG:NH2	2.28	0.67
3:C:350:SER:H	3:C:409:ALA:HB3	1.59	0.67
9:Q:176:MET:HE3	9:Q:181:ILE:HG13	1.76	0.67
3:A:159:ASN:HD21	3:A:162:ILE:HB	1.59	0.67
3:C:511:VAL:HG21	3:C:548:TYR:HB2	1.75	0.67
6:I:180:GLY:HA3	6:I:195:THR:HA	1.75	0.67
3:B:540:MET:HG2	3:B:584:MET:HB3	1.75	0.67
10:R:364:TYR:HB2	10:R:822:PHE:HB3	1.77	0.67
2:9:120:GLY:O	2:9:124:GLN:N	2.25	0.67
6:I:215:LEU:HD23	7:L:91:ASN:HB2	1.77	0.67
6:J:50:ARG:HB2	7:M:44:ILE:HG12	1.76	0.66
10:R:35:VAL:HG12	10:R:325:CYS:HB3	1.78	0.66
10:R:111:ILE:HG21	10:R:279:ARG:HB2	1.76	0.66
3:C:178:TYR:HB3	3:C:193:GLU:HB3	1.77	0.66
6:J:128:LEU:HD21	7:M:110:ILE:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:386:ARG:NH2	4:E:459:GLU:OE1	2.27	0.66
13:U:329:ASN:HD21	13:U:338:HIS:HB3	1.60	0.66
2:7:23:MET:HE3	2:7:27:ALA:HB2	1.76	0.66
10:R:285:ALA:O	10:R:289:ASN:ND2	2.29	0.66
3:B:320:VAL:HG21	3:B:360:GLU:HG2	1.78	0.66
4:F:376:GLN:NE2	4:F:396:PRO:O	2.28	0.66
6:I:215:LEU:HG	7:L:95:VAL:HG21	1.78	0.66
10:R:69:GLU:HG2	10:R:290:ILE:HG12	1.77	0.66
3:A:132:LYS:HB3	3:A:184:ASN:HB3	1.77	0.65
4:F:148:GLU:O	6:J:222:ARG:NH1	2.29	0.65
10:R:109:LYS:O	10:R:112:ASN:HB2	1.95	0.65
4:D:119:LEU:HD23	4:D:153:ILE:HD13	1.79	0.65
9:Q:246:ARG:NH1	9:Q:273:GLU:OE2	2.30	0.65
10:R:348:VAL:HB	10:R:349:PRO:HD2	1.78	0.65
3:B:265:LYS:NZ	3:B:295:THR:O	2.30	0.65
3:C:247:ALA:HB2	3:C:429:VAL:HG11	1.79	0.65
4:E:314:ARG:NH1	4:E:316:GLU:OE2	2.29	0.65
3:C:574:MET:HB3	3:C:577:ILE:HB	1.79	0.64
3:A:324:GLU:HG3	3:A:354:TRP:HE1	1.60	0.64
5:G:71:GLU:OE2	9:Q:343:LYS:NZ	2.30	0.64
3:C:270:ASP:N	3:C:270:ASP:OD1	2.28	0.64
4:E:71:ILE:HD11	4:E:119:LEU:HB2	1.78	0.64
4:F:503:PHE:HA	4:F:506:ARG:HE	1.62	0.64
12:T:89:ASP:O	12:T:96:ASN:ND2	2.31	0.64
4:D:439:VAL:HG13	5:G:168:ARG:HH12	1.63	0.64
4:F:380:ASP:HB2	4:F:393:ASN:HB2	1.78	0.64
9:Q:237:ARG:NH2	9:Q:258:ALA:O	2.30	0.64
13:U:403:GLN:HE22	13:U:413:SER:H	1.46	0.64
2:4:133:LEU:HA	2:4:136:ILE:HD12	1.79	0.64
3:C:280:ARG:NH1	3:C:283:GLU:OE2	2.30	0.64
3:A:51:VAL:HG23	3:A:67:TYR:HB2	1.79	0.64
10:R:132:LEU:HD23	10:R:133:ARG:HH21	1.63	0.64
4:E:436:LYS:HG3	4:E:444:LEU:HD11	1.80	0.63
7:K:3:SER:N	10:R:353:ASN:OD1	2.31	0.63
10:R:426:ARG:HD3	10:R:429:ARG:HE	1.63	0.63
1:O:47:PHE:O	1:O:51:ASN:ND2	2.28	0.63
4:F:82:ARG:NH1	4:F:101:GLY:O	2.31	0.63
6:H:46:VAL:HG23	7:K:40:ALA:HB1	1.81	0.63
3:B:296:MET:SD	3:B:308:ARG:NE	2.67	0.63
5:G:58:MET:HE3	8:N:92:PRO:HD3	1.80	0.63
4:D:335:TYR:HA	4:D:350:GLN:HE22	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:119:LEU:HD23	4:F:153:ILE:HD13	1.81	0.63
6:H:137:ARG:NH1	6:H:177:ILE:O	2.32	0.63
10:R:521:ILE:HD11	11:S:68:LEU:HD11	1.81	0.63
3:B:88:VAL:HG11	3:B:329:THR:HG23	1.81	0.62
6:J:42:LYS:HE2	7:M:40:ALA:HB2	1.80	0.62
2:3:78:ASN:HD22	10:R:617:LEU:HD12	1.65	0.62
3:B:265:LYS:HA	3:B:296:MET:HG2	1.81	0.62
8:N:45:ILE:HG23	8:N:74:VAL:HG22	1.79	0.62
10:R:406:MET:HE3	10:R:741:LEU:HD23	1.81	0.62
3:C:223:ALA:HA	3:C:391:ARG:HE	1.65	0.62
3:C:226:PRO:HG3	3:C:461:LEU:HD22	1.81	0.62
4:D:86:VAL:HG22	4:D:96:VAL:HG22	1.81	0.62
4:D:208:ARG:HG2	4:D:209:GLN:HG3	1.81	0.62
6:I:168:ASP:OD2	6:I:188:ARG:NH2	2.32	0.62
4:D:247:ASP:OD1	4:D:251:ASN:ND2	2.32	0.62
2:9:72:VAL:HG21	2:9:99:VAL:HG21	1.80	0.62
7:K:50:GLN:HA	7:K:53:LYS:HE2	1.82	0.62
10:R:44:VAL:HG13	10:R:48:GLN:HB2	1.80	0.62
3:B:605:LEU:HA	3:B:608:MET:HE2	1.82	0.62
3:C:53:GLU:OE1	3:C:212:ARG:NH2	2.32	0.62
10:R:399:PHE:HB3	10:R:400:PRO:HD3	1.82	0.62
2:5:140:VAL:HG11	10:R:793:MET:HE2	1.81	0.62
4:D:153:ILE:O	4:D:337:ARG:NH1	2.33	0.62
4:F:153:ILE:O	4:F:337:ARG:NH1	2.31	0.61
3:B:159:ASN:HD21	3:B:162:ILE:HB	1.65	0.61
5:G:124:LEU:HD22	9:Q:223:ILE:HA	1.83	0.61
8:N:75:ARG:NH1	8:N:102:LYS:O	2.33	0.61
4:E:99:PHE:HA	4:E:269:ILE:HD13	1.80	0.61
6:J:185:ASN:ND2	6:J:187:ASP:OD1	2.33	0.61
2:7:117:GLY:O	2:7:121:THR:N	2.31	0.61
3:A:275:VAL:HG22	3:A:312:VAL:HB	1.82	0.61
3:C:222:PRO:O	3:C:391:ARG:NH2	2.23	0.61
3:A:331:ILE:HD13	3:A:406:ILE:HD11	1.82	0.61
3:C:317:ASN:HD22	4:F:157:PRO:HB3	1.66	0.61
4:E:59:ILE:HG13	4:E:95:VAL:HG22	1.82	0.61
6:I:123:GLY:HA3	6:I:183:ILE:HD13	1.82	0.61
3:B:275:VAL:HG21	3:B:330:GLY:HA3	1.82	0.61
3:C:331:ILE:HD13	3:C:406:ILE:HD11	1.81	0.61
3:A:592:ASP:HB3	3:A:596:LYS:HD2	1.83	0.60
6:H:220:ALA:O	6:H:223:LYS:NZ	2.34	0.60
7:L:44:ILE:HA	7:L:47:TYR:CZ	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:88:LYS:NZ	2:2:155:LYS:OXT	2.35	0.60
8:N:17:VAL:HG11	8:N:38:VAL:HG22	1.82	0.60
3:B:518:ASP:HA	3:B:585:LYS:HD3	1.84	0.60
6:I:19:ILE:HG21	7:L:14:ALA:HB1	1.81	0.60
3:A:72:GLY:O	4:D:67:ARG:NH1	2.35	0.60
2:3:23:MET:HE3	2:3:27:ALA:HB2	1.83	0.60
2:8:23:MET:HE3	2:8:27:ALA:HB2	1.83	0.60
6:J:102:LEU:HG	6:J:196:LEU:HD13	1.84	0.60
8:N:72:GLU:HA	8:N:75:ARG:HG2	1.82	0.60
7:M:91:ASN:ND2	7:M:94:GLU:OE2	2.34	0.60
3:A:458:MET:SD	3:A:476:ARG:NH1	2.74	0.60
8:N:37:LEU:HG	8:N:51:THR:HG21	1.83	0.60
3:A:439:LEU:HB3	3:A:444:HIS:HB3	1.82	0.60
3:C:517:ASP:OD2	4:F:493:LYS:NZ	2.34	0.60
6:I:68:LYS:HG3	7:L:66:ARG:HB2	1.84	0.60
13:U:355:TYR:HB2	13:U:387:ARG:HG3	1.83	0.60
2:5:23:MET:HE3	2:5:27:ALA:HB2	1.84	0.60
3:B:222:PRO:O	3:B:391:ARG:NH2	2.30	0.60
9:Q:163:PHE:HB3	9:Q:192:SER:HB2	1.84	0.59
6:H:123:GLY:HA3	6:H:183:ILE:HD13	1.84	0.59
3:C:271:VAL:HB	3:C:344:VAL:HG22	1.85	0.59
9:Q:230:THR:HG22	9:Q:232:LEU:H	1.67	0.59
2:6:117:GLY:O	2:6:121:THR:N	2.26	0.59
5:G:83:VAL:HG21	8:N:18:THR:HG23	1.83	0.59
3:A:511:VAL:HG11	3:A:548:TYR:HB2	1.84	0.59
4:F:365:ILE:HB	4:F:366:PRO:HD3	1.84	0.59
3:A:243:GLY:N	3:A:405:SER:OG	2.35	0.59
10:R:16:PHE:HA	10:R:319:LEU:O	2.03	0.59
4:F:182:SER:HB2	4:F:402:MET:HG3	1.83	0.59
4:F:185:ARG:HH11	4:F:227:PHE:HE1	1.50	0.59
7:K:3:SER:HB2	10:R:353:ASN:HA	1.85	0.59
3:B:77:ASP:OD1	7:L:113:ASN:ND2	2.34	0.58
6:J:70:ILE:O	6:J:74:ASN:ND2	2.36	0.58
7:M:24:GLU:O	7:M:28:ARG:NE	2.36	0.58
14:V:300:ASN:HD21	14:V:302:GLU:HG3	1.68	0.58
2:9:72:VAL:HG11	2:9:99:VAL:HG11	1.84	0.58
3:C:233:VAL:HG13	3:C:234:LEU:HG	1.83	0.58
4:D:365:ILE:HB	4:D:366:PRO:HD3	1.85	0.58
6:I:68:LYS:HD3	7:L:62:ALA:HB1	1.86	0.58
3:A:438:LYS:HB3	3:A:442:ARG:HH12	1.68	0.58
5:G:155:PHE:HZ	8:N:109:ALA:HB2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:48:ARG:HE	7:K:49:LEU:HD22	1.68	0.58
4:F:61:ASP:OD1	4:F:62:HIS:N	2.36	0.58
2:2:28:LEU:HD23	2:3:105:ALA:HB2	1.85	0.58
6:H:113:GLN:NE2	6:H:117:ASP:OD1	2.36	0.58
7:M:26:ARG:O	7:M:30:ASN:ND2	2.32	0.58
3:B:277:CYS:SG	3:B:326:SER:OG	2.56	0.58
4:F:163:ARG:NH2	4:F:338:ALA:O	2.37	0.58
9:Q:86:ARG:NE	9:Q:98:ASP:OD1	2.32	0.58
10:R:648:PRO:HA	10:R:651:LEU:HB3	1.86	0.58
4:D:178:ASP:O	4:D:182:SER:OG	2.21	0.58
2:2:23:MET:HE3	2:2:27:ALA:HB2	1.86	0.58
4:F:380:ASP:OD1	4:F:382:GLN:NE2	2.37	0.58
6:H:199:ARG:NH2	7:K:105:ASP:O	2.37	0.58
10:R:767:LYS:HB2	10:R:770:ALA:HB3	1.86	0.58
2:8:28:LEU:HD23	2:9:105:ALA:HB2	1.86	0.57
2:1:15:ALA:HB2	2:1:89:SER:HA	1.85	0.57
3:B:264:SER:O	3:B:308:ARG:NH2	2.36	0.57
4:F:442:GLU:OE2	5:G:163:LYS:NZ	2.36	0.57
9:Q:336:ILE:HG12	9:Q:341:ARG:HH22	1.69	0.57
4:F:134:GLY:HA3	4:F:262:ASN:HD22	1.68	0.57
5:G:94:ILE:O	8:N:4:ARG:N	2.37	0.57
7:M:45:GLU:HG3	7:M:48:ARG:HH12	1.68	0.57
4:F:168:GLU:HG3	4:F:185:ARG:HB3	1.87	0.57
4:F:375:GLY:H	4:F:400:ARG:NH1	2.03	0.57
6:J:159:THR:O	6:J:161:ASN:ND2	2.38	0.57
3:A:95:MET:HE3	3:A:162:ILE:HG21	1.87	0.57
4:D:184:ALA:HB2	4:D:405:ALA:HB2	1.87	0.57
6:J:19:ILE:O	6:J:23:ALA:N	2.34	0.57
13:U:365:SER:O	13:U:406:ASN:ND2	2.37	0.57
3:A:473:VAL:HG13	3:A:476:ARG:HH21	1.68	0.57
4:D:213:VAL:HB	4:D:215:LYS:HE3	1.86	0.57
3:A:249:PRO:HG2	3:A:435:LEU:HG	1.86	0.57
4:E:250:GLU:HB2	6:I:70:ILE:HG23	1.85	0.57
3:B:135:PHE:O	3:B:182:PRO:HA	2.05	0.57
4:D:276:ARG:NH2	4:D:330:ASP:OD1	2.34	0.57
3:C:518:ASP:HA	3:C:585:LYS:HD3	1.87	0.56
10:R:293:TRP:HA	10:R:296:LYS:HD2	1.87	0.56
13:U:277:ALA:HB2	13:U:282:TRP:CD2	2.40	0.56
3:A:66:VAL:HG12	3:A:68:GLU:H	1.70	0.56
3:C:91:GLY:HA3	3:C:206:VAL:HG22	1.88	0.56
13:U:408:MET:SD	13:U:408:MET:N	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:23:MET:HE3	2:4:27:ALA:HB2	1.86	0.56
2:4:127:LEU:O	2:4:128:PHE:C	2.48	0.56
4:E:61:ASP:OD1	4:E:62:HIS:N	2.36	0.56
5:G:129:GLU:OE1	9:Q:289:THR:OG1	2.23	0.56
6:J:199:ARG:NH2	7:M:105:ASP:O	2.38	0.56
10:R:71:GLU:HA	10:R:74:LYS:HD3	1.86	0.56
10:R:100:ASN:O	10:R:103:LYS:HG3	2.05	0.56
13:U:330:ARG:NH2	13:U:343:GLU:OE2	2.30	0.56
3:A:366:ALA:HA	4:D:317:VAL:HG21	1.88	0.56
3:B:550:MET:HE1	3:B:608:MET:HG3	1.88	0.56
3:C:77:ASP:OD1	7:M:113:ASN:ND2	2.35	0.56
4:F:82:ARG:HH12	4:F:103:SER:H	1.53	0.56
6:I:129:GLU:H	6:I:132:MET:HE2	1.71	0.56
10:R:128:LEU:HD13	10:R:131:ILE:HD12	1.87	0.56
13:U:314:GLU:HA	13:U:320:THR:HA	1.88	0.56
10:R:53:ASN:OD1	10:R:57:ARG:NH2	2.38	0.56
3:A:152:ILE:HG12	3:A:167:MET:HG2	1.88	0.56
3:B:566:THR:OG1	3:B:567:TRP:N	2.39	0.56
3:C:583:SER:HA	3:C:586:PHE:HD2	1.71	0.56
9:Q:326:CYS:O	9:Q:330:VAL:HG23	2.06	0.56
10:R:99:ALA:O	10:R:102:GLU:HB2	2.06	0.56
2:6:28:LEU:HD23	2:7:105:ALA:HB2	1.87	0.56
4:D:484:LEU:HD13	4:D:495:ILE:HD11	1.87	0.56
9:Q:171:GLN:O	9:Q:174:ASP:HB2	2.05	0.56
1:O:59:SER:HB2	2:1:101:LEU:HB3	1.87	0.56
3:B:344:VAL:HB	3:B:404:VAL:HG22	1.88	0.55
4:E:149:ASP:OD1	4:E:150:PHE:N	2.39	0.55
4:E:465:GLN:NE2	4:E:469:GLU:O	2.39	0.55
5:G:137:ASN:O	5:G:140:LYS:HG3	2.06	0.55
3:B:573:HIS:HD2	3:B:574:MET:HE2	1.71	0.55
3:B:587:LYS:HZ3	3:B:597:ILE:HA	1.71	0.55
5:G:59:GLY:HA2	8:N:92:PRO:HG3	1.87	0.55
3:C:280:ARG:NH2	4:F:371:TYR:O	2.39	0.55
3:C:465:TYR:O	3:C:470:THR:N	2.39	0.55
2:2:10:TYR:HB2	14:V:309:MET:HE1	1.87	0.55
3:A:43:VAL:HG21	3:A:64:ILE:HD13	1.87	0.55
7:L:31:ARG:HA	7:L:34:LYS:HZ2	1.70	0.55
8:N:75:ARG:HD2	8:N:78:LEU:HD21	1.88	0.55
10:R:730:GLY:HA2	10:R:733:SER:HB2	1.87	0.55
2:2:48:ARG:HH12	2:2:125:PRO:HG3	1.71	0.55
2:5:81:ASN:OD1	2:5:82:ASP:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:457:TYR:OH	4:F:239:GLU:OE2	2.24	0.55
4:D:159:ASN:HB3	4:D:162:CYS:HB2	1.88	0.55
6:J:113:GLN:NE2	6:J:117:ASP:OD1	2.40	0.55
14:V:304:SER:O	14:V:308:ASN:ND2	2.34	0.55
4:F:448:ASP:N	4:F:448:ASP:OD1	2.37	0.55
6:H:184:TYR:HB3	6:H:188:ARG:HA	1.89	0.55
14:V:323:ILE:O	14:V:327:ASN:ND2	2.31	0.55
2:8:36:LYS:HE2	2:8:112:ILE:HD13	1.89	0.55
2:8:10:TYR:HA	2:9:90:PHE:HE2	1.72	0.55
3:C:280:ARG:HB2	3:C:283:GLU:HG3	1.88	0.55
4:F:55:GLY:O	4:F:102:THR:OG1	2.22	0.55
7:K:8:ILE:HG12	10:R:16:PHE:HB3	1.88	0.55
7:M:94:GLU:O	7:M:98:ASN:ND2	2.32	0.55
2:4:44:MET:HE2	2:4:122:ALA:HB2	1.88	0.54
3:C:165:LYS:NZ	3:C:342:TYR:OH	2.30	0.54
4:D:208:ARG:NH1	4:D:247:ASP:OD2	2.40	0.54
6:H:94:LEU:HD22	6:H:215:LEU:HD11	1.88	0.54
2:2:72:VAL:HG11	2:2:99:VAL:HG11	1.89	0.54
3:B:580:LYS:HE3	3:B:604:LEU:HG	1.89	0.54
12:T:91:GLU:N	12:T:91:GLU:OE1	2.40	0.54
2:5:48:ARG:HD3	2:5:122:ALA:HA	1.90	0.54
2:6:23:MET:HE3	2:6:27:ALA:HB2	1.89	0.54
2:6:81:ASN:ND2	2:6:83:ASP:OD1	2.41	0.54
4:E:365:ILE:HB	4:E:366:PRO:HD3	1.87	0.54
13:U:388:THR:OG1	13:U:391:SER:OG	2.22	0.54
3:B:588:ASP:HB3	3:B:591:LYS:HB2	1.89	0.54
1:0:193:VAL:HG12	1:0:197:GLN:HE21	1.72	0.54
2:1:51:GLN:HE22	2:1:121:THR:HG22	1.73	0.54
3:C:57:LEU:HB2	4:D:53:VAL:HB	1.90	0.54
3:C:106:LEU:HD13	4:F:160:PRO:HD2	1.89	0.54
4:E:184:ALA:HB2	4:E:405:ALA:HB2	1.89	0.54
7:K:32:ARG:HH11	7:K:35:GLN:HE22	1.55	0.54
8:N:68:GLN:NE2	8:N:99:ASP:H	2.05	0.54
4:E:135:SER:HA	4:E:273:ILE:HD11	1.90	0.54
5:G:144:LEU:O	5:G:147:GLU:HG3	2.07	0.54
4:E:41:SER:OG	6:I:199:ARG:NH1	2.38	0.54
6:H:129:GLU:H	6:H:132:MET:HE2	1.73	0.54
6:J:65:GLU:HA	6:J:68:LYS:HE3	1.89	0.54
6:J:164:ASP:OD1	6:J:166:GLN:NE2	2.33	0.54
9:Q:103:SER:HB2	9:Q:189:TYR:CZ	2.43	0.54
9:Q:163:PHE:HB2	9:Q:188:ALA:HB1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:40:TYR:HA	3:A:53:GLU:HG2	1.90	0.54
4:F:321:ARG:N	5:G:193:GLU:OE2	2.41	0.54
3:C:24:VAL:HG22	3:C:29:VAL:HG22	1.89	0.54
3:C:383:ALA:HB1	4:D:264:ALA:HB1	1.90	0.54
7:K:27:LYS:HB3	7:K:31:ARG:HH21	1.73	0.54
9:Q:179:GLU:OE1	9:Q:182:ARG:NH1	2.36	0.54
4:E:408:GLU:HG2	4:E:413:LYS:HB3	1.89	0.53
10:R:482:ARG:NH1	11:S:77:LYS:O	2.41	0.53
1:O:81:VAL:HA	2:1:127:LEU:HD11	1.90	0.53
6:J:64:ILE:HA	6:J:67:GLN:HG2	1.90	0.53
13:U:295:LEU:HD21	13:U:311:LEU:HD22	1.89	0.53
13:U:420:SER:O	14:V:304:SER:OG	2.22	0.53
1:O:172:LEU:HA	1:O:175:LYS:HZ2	1.74	0.53
2:5:136:ILE:O	2:5:140:VAL:HG13	2.09	0.53
3:B:266:TYR:HB3	3:B:531:PHE:HD1	1.73	0.53
3:B:315:THR:OG1	3:B:317:ASN:OD1	2.25	0.53
4:F:75:THR:HG22	4:F:81:LYS:HG2	1.91	0.53
2:8:41:ILE:HD13	2:8:56:ILE:HD13	1.89	0.53
3:B:152:ILE:HG12	3:B:167:MET:HG2	1.90	0.53
3:C:143:VAL:HG13	3:C:177:THR:HA	1.90	0.53
6:J:123:GLY:HA3	6:J:183:ILE:HD13	1.90	0.53
3:B:346:MET:HE2	3:B:348:ALA:HB2	1.90	0.53
4:D:133:ASN:OD1	4:D:137:LYS:N	2.41	0.53
4:D:237:ASN:OD1	4:D:237:ASN:N	2.37	0.53
5:G:194:ARG:NH2	5:G:197:GLU:OE1	2.42	0.53
10:R:60:GLU:O	10:R:63:ARG:HG3	2.07	0.53
3:B:243:GLY:H	3:B:405:SER:HB2	1.74	0.53
3:C:55:ILE:HD12	3:C:365:LEU:HD11	1.90	0.53
3:C:510:GLU:HG3	3:C:567:TRP:CE2	2.43	0.53
6:J:30:ILE:O	6:J:34:ALA:N	2.41	0.53
10:R:53:ASN:HD22	10:R:53:ASN:H	1.56	0.53
3:A:268:ASN:N	3:A:268:ASN:OD1	2.42	0.53
3:B:515:ILE:HG22	3:B:520:LEU:HG	1.89	0.53
2:1:50:GLU:HA	2:2:126:ARG:HH22	1.74	0.53
2:4:71:VAL:HG22	10:R:746:LEU:HD23	1.90	0.53
2:7:28:LEU:HD23	2:8:105:ALA:HB2	1.90	0.53
3:C:181:PRO:O	3:C:185:TYR:OH	2.23	0.53
10:R:291:ARG:HG3	10:R:292:VAL:HG13	1.91	0.53
8:N:39:VAL:HG11	8:N:70:ILE:HD12	1.91	0.53
10:R:16:PHE:CZ	10:R:318:CYS:HB2	2.44	0.53
2:9:120:GLY:HA3	2:9:127:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:583:SER:HA	3:A:586:PHE:HD2	1.74	0.53
7:L:13:GLN:O	7:L:17:ARG:HG2	2.09	0.52
2:7:95:ALA:HB2	2:7:152:LEU:HB2	1.92	0.52
3:A:588:ASP:HB3	3:A:591:LYS:HB2	1.90	0.52
7:K:13:GLN:HB3	7:K:17:ARG:HH22	1.74	0.52
7:K:28:ARG:O	7:K:32:ARG:HG2	2.09	0.52
3:C:238:PHE:HZ	3:C:450:TRP:HA	1.73	0.52
4:F:71:ILE:HD11	4:F:119:LEU:HB2	1.92	0.52
4:F:374:GLU:HA	4:F:400:ARG:HD2	1.91	0.52
2:3:77:ALA:O	2:4:155:LYS:NZ	2.41	0.52
2:7:58:PRO:HG3	2:7:135:LEU:HD11	1.91	0.52
3:B:90:LEU:HD13	3:B:336:TYR:HB2	1.92	0.52
3:C:113:THR:HG21	3:C:119:PRO:HG2	1.91	0.52
4:E:380:ASP:OD1	4:E:382:GLN:NE2	2.42	0.52
13:U:266:ARG:HB3	13:U:302:TRP:CD1	2.44	0.52
3:C:525:TYR:CZ	4:F:403:LYS:HD2	2.45	0.52
8:N:79:ASP:OD1	8:N:104:SER:OG	2.25	0.52
10:R:62:ASP:OD2	10:R:298:ARG:NH2	2.42	0.52
10:R:84:GLU:HA	10:R:87:GLU:HB3	1.91	0.52
10:R:91:PRO:HG2	10:R:94:MET:HB2	1.89	0.52
10:R:768:SER:HA	12:T:107:ASN:HD21	1.74	0.52
2:3:41:ILE:O	2:3:45:SER:HB2	2.10	0.52
2:4:61:MET:O	2:4:64:ILE:HG22	2.10	0.52
4:F:133:ASN:OD1	4:F:137:LYS:N	2.42	0.52
5:G:51:ILE:HG21	8:N:105:ILE:HG12	1.91	0.52
10:R:84:GLU:HG3	10:R:296:LYS:HG3	1.91	0.52
3:C:371:ASP:OD2	4:D:321:ARG:NH2	2.42	0.52
4:F:272:ILE:HA	4:F:303:TYR:HE1	1.74	0.52
4:E:86:VAL:HG22	4:E:96:VAL:HG22	1.92	0.52
4:E:166:PRO:HA	4:E:340:ARG:HD3	1.92	0.52
5:G:121:LEU:HD21	9:Q:230:THR:HG21	1.92	0.52
10:R:717:MET:SD	10:R:720:GLN:NE2	2.77	0.52
13:U:372:GLU:OE1	14:V:301:PHE:N	2.41	0.52
2:9:88:LYS:O	2:9:92:GLN:HG2	2.10	0.52
4:D:149:ASP:OD1	4:D:150:PHE:N	2.43	0.52
4:E:210:ALA:HB3	4:E:229:ILE:HD11	1.91	0.52
3:A:100:ASP:OD1	3:A:104:ARG:N	2.34	0.51
3:A:505:ASP:OD1	3:A:505:ASP:N	2.42	0.51
2:1:55:SER:O	2:1:58:PRO:HD2	2.11	0.51
2:5:44:MET:SD	2:5:44:MET:N	2.83	0.51
8:N:58:ARG:HG3	8:N:61:ILE:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:U:364:PRO:HG2	13:U:367:TYR:HD2	1.75	0.51
4:E:485:ARG:HH21	4:E:506:ARG:HB2	1.74	0.51
6:I:214:ALA:O	7:L:91:ASN:ND2	2.37	0.51
6:J:41:GLU:O	6:J:44:ARG:NH1	2.44	0.51
8:N:8:ILE:HD12	8:N:25:ILE:HG21	1.91	0.51
3:C:317:ASN:ND2	4:F:157:PRO:HB3	2.25	0.51
3:C:584:MET:HA	3:C:587:LYS:HE2	1.93	0.51
2:3:72:VAL:HG21	2:3:99:VAL:HG21	1.91	0.51
2:6:72:VAL:HG21	2:6:99:VAL:HG21	1.92	0.51
2:7:137:PHE:O	2:7:140:VAL:HG22	2.11	0.51
3:A:430:GLN:HB3	3:A:456:LYS:HB2	1.92	0.51
3:C:489:LEU:HB2	3:C:509:LEU:HD21	1.91	0.51
10:R:17:LEU:O	10:R:318:CYS:HB3	2.11	0.51
10:R:402:LEU:HD12	10:R:806:HIS:CE1	2.46	0.51
3:B:473:VAL:HG13	3:B:476:ARG:HH21	1.75	0.51
3:B:515:ILE:O	3:B:520:LEU:N	2.34	0.51
4:E:178:ASP:O	4:E:182:SER:OG	2.27	0.51
2:1:79:SER:O	2:1:81:ASN:ND2	2.43	0.51
4:F:63:VAL:HB	4:F:66:PRO:HG3	1.92	0.51
7:M:5:SER:O	7:M:9:GLN:NE2	2.42	0.51
4:F:444:LEU:HB3	4:F:448:ASP:HB2	1.91	0.51
6:I:27:ALA:HB2	7:L:21:LYS:HB3	1.93	0.51
6:I:185:ASN:ND2	6:I:187:ASP:OD1	2.44	0.51
1:0:172:LEU:HD21	2:9:49:PRO:HB3	1.92	0.51
2:9:137:PHE:O	2:9:140:VAL:HG22	2.11	0.51
3:C:66:VAL:HG12	3:C:68:GLU:H	1.75	0.51
4:D:488:PRO:HD2	4:D:491:MET:HE2	1.92	0.51
4:F:117:ASP:OD1	4:F:118:ILE:N	2.44	0.51
7:K:45:GLU:OE1	7:K:48:ARG:NH2	2.44	0.51
13:U:308:ARG:HD2	13:U:324:LYS:HD3	1.93	0.51
2:8:10:TYR:O	2:8:13:PHE:HB3	2.11	0.50
3:A:238:PHE:HZ	3:A:450:TRP:HA	1.76	0.50
3:B:471:GLU:O	3:B:475:LEU:HG	2.11	0.50
3:C:215:ARG:NH2	3:C:339:ASP:OD2	2.40	0.50
4:D:124:SER:HB3	4:D:148:GLU:H	1.76	0.50
4:E:125:GLU:OE2	4:E:291:LYS:NZ	2.38	0.50
10:R:79:ILE:HB	10:R:291:ARG:HB3	1.93	0.50
2:4:46:VAL:HA	2:5:124:GLN:HB2	1.93	0.50
3:B:272:ILE:HB	3:B:309:THR:HG23	1.91	0.50
10:R:779:PHE:CE1	12:T:61:GLY:HA2	2.46	0.50
3:B:100:ASP:HB2	3:B:314:ASN:HD21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:151:ASP:OD1	3:C:397:ASN:N	2.37	0.50
3:C:449:ASN:HD22	3:C:452:ILE:HG12	1.77	0.50
4:F:354:LEU:HD11	4:F:365:ILE:HG22	1.92	0.50
5:G:30:ARG:NH2	5:G:31:ASN:OD1	2.44	0.50
6:I:53:ILE:HD11	7:L:51:ARG:HH21	1.77	0.50
6:J:136:CYS:O	6:J:173:LEU:N	2.41	0.50
2:8:44:MET:HE1	2:8:51:GLN:HG3	1.93	0.50
7:M:85:GLN:HB3	7:M:89:ARG:HH12	1.76	0.50
13:U:261:ASN:OD1	13:U:261:ASN:N	2.44	0.50
2:3:49:PRO:HG3	2:4:124:GLN:HG2	1.93	0.50
3:B:101:GLY:H	3:B:314:ASN:HD21	1.59	0.50
3:B:338:ARG:HB2	3:B:404:VAL:HG23	1.93	0.50
4:D:380:ASP:HB2	4:D:393:ASN:HB2	1.92	0.50
4:E:470:ASN:HD22	4:E:471:ARG:N	2.09	0.50
2:1:17:MET:HE3	13:U:436:MET:HE2	1.93	0.50
2:5:13:PHE:HB2	2:6:90:PHE:CE2	2.47	0.50
2:8:61:MET:SD	2:8:135:LEU:HB3	2.51	0.50
3:A:44:ARG:HD2	3:A:49:GLU:HB3	1.94	0.50
3:B:270:ASP:OD1	3:B:270:ASP:N	2.43	0.50
3:B:465:TYR:O	3:B:469:PHE:N	2.43	0.50
5:G:93:LYS:O	5:G:112:TYR:N	2.45	0.50
13:U:372:GLU:HB3	14:V:301:PHE:HB2	1.93	0.50
2:1:28:LEU:HD23	2:2:105:ALA:HB2	1.94	0.50
3:A:518:ASP:HA	3:A:585:LYS:HD3	1.93	0.50
3:B:214:VAL:HG21	4:F:265:ASN:HD21	1.77	0.50
4:F:86:VAL:HG22	4:F:96:VAL:HG22	1.93	0.50
2:6:77:ALA:HA	2:6:80:LEU:HD12	1.93	0.50
2:8:18:GLY:HA3	2:8:93:LEU:HA	1.93	0.50
2:8:117:GLY:O	2:8:121:THR:N	2.29	0.50
3:A:272:ILE:HB	3:A:309:THR:HG23	1.94	0.50
4:E:279:LEU:HD11	4:E:334:ILE:HG23	1.94	0.50
4:F:373:THR:O	4:F:400:ARG:NH1	2.45	0.50
6:H:136:CYS:SG	6:H:144:VAL:HG11	2.52	0.50
6:J:12:ILE:HA	7:M:10:GLN:HE22	1.76	0.50
9:Q:289:THR:HG23	9:Q:292:ASP:H	1.76	0.50
10:R:423:MET:HE1	10:R:450:ILE:HD12	1.94	0.50
1:0:126:ILE:O	1:0:130:ASN:ND2	2.45	0.50
2:1:41:ILE:HD13	2:1:56:ILE:HD13	1.94	0.50
3:C:561:SER:O	3:C:564:LYS:NZ	2.39	0.50
4:F:417:ASP:OD1	4:F:417:ASP:N	2.45	0.50
6:J:136:CYS:HB3	6:J:181:VAL:HG12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:S:13:MET:HG3	11:S:52:TRP:CE2	2.46	0.50
3:B:479:ALA:HB2	3:B:541:LEU:HD11	1.93	0.49
3:B:515:ILE:HG23	3:B:519:PHE:HB3	1.94	0.49
3:C:268:ASN:OD1	3:C:268:ASN:N	2.45	0.49
3:C:574:MET:HE1	3:C:612:PHE:CZ	2.47	0.49
4:F:436:LYS:HB3	4:F:444:LEU:HD11	1.93	0.49
9:Q:113:ILE:HG21	9:Q:171:GLN:HE21	1.76	0.49
1:O:69:ILE:HD12	2:1:141:LEU:HD11	1.94	0.49
3:B:280:ARG:NH2	4:E:370:GLY:O	2.42	0.49
4:E:249:GLU:O	6:I:77:ASN:ND2	2.45	0.49
6:J:215:LEU:HD23	7:M:91:ASN:HB2	1.94	0.49
7:L:3:SER:O	7:L:6:GLN:NE2	2.41	0.49
8:N:70:ILE:HA	8:N:73:MET:HE2	1.94	0.49
10:R:125:LEU:HG	10:R:129:LYS:HE3	1.93	0.49
3:B:100:ASP:OD1	3:B:104:ARG:N	2.38	0.49
3:B:270:ASP:HB2	3:B:342:TYR:HB3	1.94	0.49
5:G:57:LEU:O	5:G:60:GLU:HG3	2.12	0.49
9:Q:167:CYS:O	9:Q:171:GLN:HG2	2.13	0.49
10:R:51:PHE:HB2	10:R:308:ASN:ND2	2.27	0.49
2:9:34:THR:HG23	2:9:59:VAL:HG13	1.95	0.49
6:J:74:ASN:O	6:J:78:GLN:HG2	2.12	0.49
10:R:578:PHE:HB2	10:R:646:CYS:HB2	1.94	0.49
2:4:95:ALA:HB2	2:4:152:LEU:HB2	1.94	0.49
4:F:272:ILE:HA	4:F:303:TYR:CE1	2.48	0.49
10:R:409:ASP:HB3	10:R:412:HIS:HB2	1.94	0.49
2:7:44:MET:HE2	2:7:122:ALA:HB2	1.94	0.49
3:B:156:VAL:O	3:B:164:HIS:N	2.45	0.49
3:B:299:ASP:OD1	3:B:299:ASP:N	2.45	0.49
3:B:384:SER:O	3:B:388:ARG:HG3	2.13	0.49
4:D:159:ASN:ND2	4:D:162:CYS:SG	2.82	0.49
4:D:287:TYR:HB3	4:D:344:ARG:HH11	1.78	0.49
4:D:357:PRO:HG2	4:D:363:HIS:CE1	2.47	0.49
1:O:56:LEU:HD22	1:O:60:LEU:HD11	1.95	0.49
3:A:360:GLU:OE1	4:D:329:THR:OG1	2.29	0.49
4:D:106:ASP:OD1	4:D:110:THR:N	2.46	0.49
4:D:256:ASN:OD1	4:D:256:ASN:N	2.46	0.49
6:I:49:GLN:HG3	7:L:44:ILE:HD13	1.94	0.49
1:O:172:LEU:HD13	2:9:45:SER:HB2	1.95	0.49
2:1:39:THR:OG1	13:U:453:MET:SD	2.70	0.49
2:4:87:TYR:CZ	2:4:91:LEU:HD11	2.48	0.49
3:A:100:ASP:OD2	3:A:104:ARG:NE	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:135:PHE:HB2	3:B:205:MET:HE2	1.93	0.49
4:E:492:LEU:HD13	4:E:495:ILE:HD12	1.95	0.49
10:R:61:MET:O	10:R:65:LEU:HD22	2.13	0.49
10:R:481:VAL:HG11	11:S:73:ILE:HG23	1.94	0.49
3:B:320:VAL:HA	3:B:323:ARG:HD3	1.94	0.49
3:C:90:LEU:HD13	3:C:336:TYR:HB2	1.94	0.49
7:K:11:LEU:HB3	10:R:316:GLN:HE21	1.78	0.49
10:R:406:MET:HG2	10:R:741:LEU:HA	1.94	0.49
3:B:150:GLY:O	3:B:400:ARG:NH2	2.46	0.49
7:K:8:ILE:O	7:K:12:LEU:HG	2.13	0.49
2:8:48:ARG:HD3	2:8:122:ALA:HB1	1.94	0.48
3:B:116:ILE:HD12	4:E:341:VAL:HG11	1.95	0.48
4:F:129:GLY:HA3	4:F:255:ASP:HA	1.94	0.48
6:H:55:GLU:O	6:H:59:LYS:HG2	2.13	0.48
3:C:588:ASP:HB3	3:C:591:LYS:HB2	1.96	0.48
4:E:328:TYR:HD1	4:E:368:LEU:HD22	1.78	0.48
4:F:169:MET:HA	4:F:184:ALA:HA	1.95	0.48
6:H:97:GLU:OE1	7:K:92:ARG:NH2	2.46	0.48
2:4:72:VAL:HG11	2:4:99:VAL:HG11	1.96	0.48
3:C:548:TYR:OH	3:C:552:ARG:NH2	2.43	0.48
4:F:60:LEU:HD21	4:F:112:CYS:HB2	1.95	0.48
6:I:126:GLN:NE2	7:L:109:GLU:O	2.46	0.48
6:I:136:CYS:SG	6:I:144:VAL:HG21	2.53	0.48
10:R:362:PRO:HB3	10:R:820:PHE:CE2	2.48	0.48
2:6:61:MET:HE2	2:6:139:GLU:HB2	1.94	0.48
2:6:72:VAL:HG11	2:6:99:VAL:HG11	1.95	0.48
3:A:338:ARG:HD2	3:A:392:VAL:HG22	1.95	0.48
3:B:46:GLY:HA2	3:B:77:ASP:HB3	1.94	0.48
4:F:106:ASP:OD2	4:F:109:LYS:N	2.46	0.48
6:H:127:LEU:HD12	6:H:183:ILE:HG22	1.95	0.48
7:K:4:GLN:NE2	10:R:16:PHE:O	2.46	0.48
9:Q:90:TYR:O	9:Q:94:ALA:N	2.44	0.48
10:R:536:LYS:O	10:R:539:MET:HG3	2.14	0.48
2:4:41:ILE:HD12	2:5:134:ILE:HD11	1.94	0.48
3:C:275:VAL:HG21	3:C:346:MET:HE3	1.94	0.48
8:N:82:GLN:HG3	8:N:108:ARG:HH21	1.77	0.48
3:A:339:ASP:O	3:A:400:ARG:NH2	2.32	0.48
4:D:82:ARG:NH1	4:D:101:GLY:O	2.43	0.48
6:I:102:LEU:HD21	6:I:196:LEU:HB3	1.95	0.48
7:L:76:GLU:O	7:L:79:GLU:HG3	2.13	0.48
10:R:96:ASP:OD1	10:R:97:LEU:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:286:GLU:HB2	4:E:165:TYR:CE1	2.48	0.48
3:C:135:PHE:CE1	3:C:154:GLY:HA3	2.48	0.48
3:C:610:ASN:OD1	3:C:613:ARG:NH1	2.47	0.48
4:E:485:ARG:NH2	4:E:506:ARG:HB2	2.28	0.48
5:G:92:VAL:HG23	8:N:25:ILE:HG23	1.96	0.48
3:A:441:GLN:C	3:A:443:LYS:H	2.21	0.48
4:F:279:LEU:HD11	4:F:334:ILE:HG23	1.94	0.48
5:G:149:ALA:HB2	8:N:89:LEU:HD11	1.96	0.48
6:I:215:LEU:HD22	7:L:88:PHE:HA	1.96	0.48
6:J:180:GLY:HA3	6:J:195:THR:HA	1.95	0.48
10:R:651:LEU:HD12	10:R:724:THR:HB	1.96	0.48
3:B:133:TRP:O	3:B:184:ASN:HA	2.14	0.48
4:D:193:SER:OG	4:D:194:ALA:N	2.47	0.48
6:H:56:TYR:O	6:H:60:LYS:HG2	2.14	0.48
3:C:144:GLY:N	3:C:176:VAL:O	2.44	0.48
4:F:208:ARG:HG3	4:F:209:GLN:HG3	1.96	0.48
10:R:18:GLN:HA	10:R:318:CYS:SG	2.54	0.48
10:R:49:ARG:HB2	10:R:308:ASN:HD22	1.79	0.48
2:5:72:VAL:HG11	2:5:99:VAL:HG11	1.96	0.47
3:A:238:PHE:CZ	3:A:450:TRP:HA	2.49	0.47
3:C:53:GLU:OE2	3:C:212:ARG:NE	2.46	0.47
6:H:102:LEU:HD21	6:H:196:LEU:HB3	1.96	0.47
10:R:768:SER:O	12:T:107:ASN:ND2	2.47	0.47
3:A:376:ALA:HB1	4:E:309:GLU:HA	1.96	0.47
2:4:51:GLN:HE22	2:4:121:THR:HG22	1.79	0.47
2:4:74:VAL:HG13	10:R:529:LEU:HD13	1.96	0.47
3:B:335:GLU:OE1	3:B:388:ARG:NH2	2.46	0.47
3:C:195:GLU:HB2	3:C:200:LYS:HG2	1.96	0.47
5:G:44:PHE:HD1	5:G:158:LEU:HB3	1.79	0.47
9:Q:187:LYS:NZ	9:Q:241:PHE:O	2.34	0.47
13:U:453:MET:HE2	13:U:456:PHE:HE1	1.79	0.47
1:0:64:GLY:HA3	1:0:149:LEU:HA	1.96	0.47
2:6:36:LYS:O	2:6:39:THR:OG1	2.32	0.47
2:6:88:LYS:O	2:6:92:GLN:HG2	2.15	0.47
4:E:99:PHE:O	4:E:267:PRO:HB3	2.14	0.47
8:N:7:LEU:HB2	8:N:61:ILE:HA	1.95	0.47
10:R:56:ARG:O	10:R:60:GLU:HG2	2.15	0.47
2:7:13:PHE:HB2	2:8:90:PHE:CE2	2.49	0.47
3:B:289:ARG:O	3:B:293:GLU:HG2	2.14	0.47
4:F:131:VAL:HG22	4:F:259:LEU:HB2	1.96	0.47
6:J:19:ILE:HG12	7:M:14:ALA:HB1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:53:LYS:HB3	7:M:53:LYS:HE3	1.67	0.47
10:R:310:CYS:SG	10:R:311:ASN:N	2.88	0.47
13:U:357:ASN:OD1	13:U:387:ARG:NE	2.44	0.47
1:0:56:LEU:HD13	1:0:142:LEU:HD13	1.96	0.47
2:7:136:ILE:O	2:7:140:VAL:HG13	2.15	0.47
3:B:514:LEU:HG	3:B:544:MET:HE2	1.96	0.47
3:C:68:GLU:OE1	3:C:121:GLY:N	2.44	0.47
3:C:169:PRO:HB2	3:C:172:ASN:HD22	1.79	0.47
3:C:238:PHE:CZ	3:C:450:TRP:HA	2.48	0.47
3:C:398:PRO:HB2	3:C:400:ARG:HD2	1.96	0.47
4:D:171:GLN:N	4:D:211:GLY:O	2.45	0.47
4:D:429:GLY:HA2	4:D:451:TYR:HB3	1.97	0.47
5:G:48:LEU:HB2	5:G:155:PHE:HE2	1.80	0.47
10:R:618:PHE:HZ	10:R:644:LEU:HD11	1.80	0.47
1:0:46:PRO:HA	1:0:49:TRP:HD1	1.80	0.47
2:2:23:MET:O	2:2:26:SER:OG	2.26	0.47
2:5:15:ALA:HB2	2:5:89:SER:HA	1.97	0.47
3:A:17:THR:H	3:A:81:ARG:NH2	2.12	0.47
3:A:156:VAL:O	3:A:164:HIS:N	2.46	0.47
3:A:522:GLN:HG3	3:A:529:ASP:HB3	1.97	0.47
3:C:372:SER:HB3	3:C:420:PRO:HG2	1.96	0.47
5:G:16:GLN:HG3	5:G:184:LEU:HD11	1.97	0.47
6:H:52:LYS:O	6:H:55:GLU:HG3	2.15	0.47
9:Q:21:ARG:NH2	9:Q:306:PHE:O	2.48	0.47
2:3:72:VAL:HG11	2:3:99:VAL:HG11	1.96	0.47
3:C:193:GLU:HB2	3:C:202:LYS:HD3	1.97	0.47
7:L:79:GLU:O	7:L:82:THR:HG22	2.15	0.47
10:R:764:LEU:HD22	12:T:82:ASP:HB3	1.97	0.47
2:1:97:LEU:HD21	13:U:435:PHE:HE2	1.80	0.47
3:B:513:LYS:O	3:B:517:ASP:N	2.42	0.47
3:C:43:VAL:HG12	3:C:81:ARG:HA	1.96	0.47
7:L:23:SER:O	7:L:27:LYS:HG2	2.15	0.47
9:Q:117:LEU:HG	9:Q:174:ASP:HB3	1.97	0.47
2:1:65:ILE:O	2:1:68:TYR:HB2	2.14	0.47
2:2:41:ILE:HD12	2:3:134:ILE:HD11	1.97	0.47
2:3:125:PRO:O	2:3:128:PHE:HB3	2.14	0.47
3:A:146:HIS:CD2	3:A:175:THR:HG22	2.50	0.47
4:F:465:GLN:HB2	4:F:471:ARG:NH2	2.30	0.47
8:N:85:ILE:HB	8:N:86:PRO:HD3	1.97	0.47
10:R:16:PHE:HD1	10:R:320:ILE:HB	1.80	0.47
10:R:81:ASP:HA	10:R:291:ARG:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:U:444:LEU:HA	13:U:447:ILE:HG22	1.97	0.47
2:3:79:SER:O	2:3:81:ASN:ND2	2.48	0.46
2:9:136:ILE:O	2:9:140:VAL:HG13	2.15	0.46
3:A:91:GLY:HA3	3:A:206:VAL:HG22	1.97	0.46
3:B:295:THR:HG22	3:B:304:SER:HA	1.97	0.46
3:B:296:MET:HG3	3:B:305:ILE:HG22	1.98	0.46
10:R:483:PRO:O	10:R:486:THR:OG1	2.30	0.46
10:R:655:PRO:HA	10:R:658:LEU:HB2	1.97	0.46
2:6:137:PHE:O	2:6:140:VAL:HG22	2.15	0.46
2:8:82:ASP:OD1	2:8:82:ASP:N	2.47	0.46
3:A:349:ASP:OD1	3:A:350:SER:N	2.45	0.46
3:A:488:ASP:O	3:A:491:GLU:HG2	2.15	0.46
3:A:573:HIS:CD2	3:A:615:LEU:HB2	2.50	0.46
3:C:522:GLN:HG3	3:C:529:ASP:HB3	1.97	0.46
6:I:201:ASP:O	6:I:205:GLN:HG2	2.16	0.46
7:M:9:GLN:O	7:M:13:GLN:HG2	2.14	0.46
9:Q:205:ALA:O	9:Q:209:CYS:HB2	2.15	0.46
10:R:50:LYS:O	10:R:53:ASN:ND2	2.49	0.46
2:8:72:VAL:HG21	2:8:99:VAL:HG21	1.96	0.46
4:F:128:LEU:HB3	4:F:255:ASP:O	2.15	0.46
4:F:197:LEU:HD13	4:F:379:VAL:HG12	1.97	0.46
6:H:207:MET:O	6:H:210:GLU:HG2	2.15	0.46
6:J:221:ASN:OD1	6:J:221:ASN:N	2.46	0.46
7:M:7:GLY:O	7:M:10:GLN:HG2	2.15	0.46
10:R:717:MET:O	10:R:720:GLN:HG3	2.14	0.46
1:0:164:LEU:HD22	9:Q:21:ARG:HD2	1.96	0.46
3:A:475:LEU:HB3	3:A:541:LEU:HG	1.98	0.46
3:B:274:TYR:CE1	3:B:287:VAL:HG11	2.50	0.46
4:F:485:ARG:NH2	4:F:506:ARG:HB2	2.30	0.46
6:J:19:ILE:HD12	6:J:22:GLU:HB2	1.98	0.46
6:J:185:ASN:CG	6:J:190:ILE:H	2.22	0.46
2:2:72:VAL:HG21	2:2:99:VAL:HG21	1.97	0.46
2:5:77:ALA:HA	2:5:80:LEU:HD12	1.97	0.46
3:A:147:ILE:HG13	3:A:151:ASP:HB2	1.97	0.46
4:E:381:ARG:HG2	4:E:385:ASN:HD21	1.81	0.46
7:M:52:GLU:O	7:M:56:LYS:HG2	2.15	0.46
13:U:262:ASP:C	13:U:264:ALA:H	2.24	0.46
2:5:140:VAL:HG12	10:R:789:ILE:HD12	1.97	0.46
2:8:130:GLY:O	2:8:134:ILE:HG13	2.16	0.46
3:A:565:ILE:HA	3:A:569:ILE:HD11	1.98	0.46
3:C:68:GLU:HA	3:C:319:PRO:HG2	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:17:ARG:O	7:K:21:LYS:HG2	2.15	0.46
9:Q:194:TYR:HA	9:Q:212:LEU:HD13	1.97	0.46
10:R:51:PHE:HB2	10:R:308:ASN:HD21	1.80	0.46
10:R:342:GLU:HA	10:R:347:THR:HG22	1.97	0.46
10:R:465:ASN:ND2	10:R:471:SER:OG	2.48	0.46
4:D:71:ILE:HD11	4:D:119:LEU:HB2	1.98	0.46
4:F:129:GLY:CA	4:F:255:ASP:HA	2.46	0.46
5:G:93:LYS:HB2	5:G:112:TYR:HD2	1.80	0.46
6:H:49:GLN:HB2	7:K:44:ILE:HD13	1.98	0.46
6:J:156:LYS:HG2	6:J:162:ASP:HA	1.97	0.46
10:R:93:ASP:OD1	10:R:93:ASP:N	2.41	0.46
10:R:115:GLN:HE22	10:R:279:ARG:NE	2.09	0.46
10:R:381:TYR:HB2	10:R:807:TRP:CE2	2.50	0.46
3:A:169:PRO:HB2	3:A:172:ASN:HD22	1.81	0.46
3:B:69:GLU:OE1	3:B:70:THR:N	2.49	0.46
4:D:340:ARG:HG2	4:D:347:SER:HB3	1.98	0.46
4:F:176:ALA:HA	4:F:462:PHE:HE1	1.81	0.46
3:A:139:LYS:NZ	3:A:140:ASN:OD1	2.47	0.46
3:B:119:PRO:HB2	3:B:122:VAL:HB	1.98	0.46
3:B:132:LYS:HB3	3:B:184:ASN:HB3	1.98	0.46
3:B:321:ALA:HA	3:B:361:ILE:HD11	1.98	0.46
3:B:516:LYS:HA	3:B:520:LEU:HB2	1.96	0.46
4:E:421:GLN:NE2	4:E:425:CYS:SG	2.89	0.46
5:G:74:PHE:CE2	9:Q:331:TRP:HA	2.50	0.46
10:R:589:LEU:HD22	10:R:628:LEU:HD12	1.98	0.46
2:7:16:VAL:HG11	2:8:90:PHE:O	2.16	0.46
2:8:50:GLU:HA	2:9:126:ARG:HH22	1.81	0.46
4:E:246:SER:HA	4:E:249:GLU:HG2	1.96	0.46
6:H:54:MET:HA	6:H:57:TYR:HD2	1.81	0.46
7:L:27:LYS:O	7:L:31:ARG:HG2	2.16	0.46
10:R:589:LEU:HB3	10:R:608:LEU:HD22	1.97	0.46
2:4:13:PHE:HB2	2:5:90:PHE:CE2	2.51	0.45
3:A:22:HIS:CG	3:A:61:MET:HE1	2.51	0.45
4:E:269:ILE:HD12	4:E:269:ILE:H	1.80	0.45
5:G:198:GLU:CD	5:G:201:ARG:HH21	2.24	0.45
7:K:44:ILE:HG13	7:K:45:GLU:N	2.30	0.45
10:R:751:LEU:O	10:R:755:LEU:HG	2.16	0.45
3:B:54:ILE:HG12	3:B:64:ILE:HG12	1.99	0.45
3:B:473:VAL:HB	3:B:474:PRO:HD3	1.99	0.45
4:D:78:ASP:OD1	4:D:79:GLY:N	2.47	0.45
4:E:190:PRO:HD3	4:E:373:THR:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:156:LYS:HE3	6:I:156:LYS:HB2	1.82	0.45
2:1:95:ALA:HB2	2:1:152:LEU:HB2	1.98	0.45
2:4:72:VAL:HG21	2:4:99:VAL:HG21	1.99	0.45
2:7:41:ILE:HD12	2:8:134:ILE:HD11	1.97	0.45
2:7:72:VAL:HG11	2:7:99:VAL:HG11	1.99	0.45
2:7:88:LYS:O	2:7:92:GLN:HG2	2.15	0.45
3:C:239:PRO:HB2	3:C:461:LEU:HD12	1.98	0.45
7:K:4:GLN:O	7:K:8:ILE:HG13	2.17	0.45
9:Q:166:ASP:O	9:Q:169:SER:OG	2.25	0.45
1:0:54:ILE:O	1:0:58:ILE:HG22	2.17	0.45
3:B:226:PRO:HG3	3:B:461:LEU:HD22	1.97	0.45
3:C:88:VAL:HG11	3:C:329:THR:HG23	1.98	0.45
4:F:357:PRO:HG2	4:F:363:HIS:CE1	2.51	0.45
2:4:114:GLY:O	2:4:118:VAL:HG22	2.17	0.45
2:5:28:LEU:HD23	2:6:105:ALA:HB2	1.98	0.45
3:A:391:ARG:HA	3:A:403:SER:HA	1.99	0.45
3:B:574:MET:HG2	3:B:577:ILE:HG13	1.97	0.45
8:N:10:VAL:H	8:N:36:PHE:HA	1.81	0.45
2:8:113:VAL:HG21	2:8:134:ILE:HG21	1.99	0.45
3:B:68:GLU:OE1	3:B:121:GLY:N	2.48	0.45
3:C:169:PRO:HB2	3:C:172:ASN:ND2	2.31	0.45
4:E:248:PHE:HD2	4:E:259:LEU:HD22	1.82	0.45
4:E:283:GLU:HA	4:E:348:ILE:HD11	1.97	0.45
4:F:77:PRO:HG3	4:F:109:LYS:HB2	1.98	0.45
4:F:359:ASP:OD1	4:F:359:ASP:N	2.49	0.45
2:7:38:GLY:HA3	2:8:113:VAL:HG23	1.99	0.45
2:9:22:ALA:HB2	2:9:96:GLY:HA2	1.99	0.45
3:A:533:PRO:HD2	3:A:536:LYS:HE2	1.99	0.45
6:H:178:ALA:N	6:H:197:GLU:OE2	2.32	0.45
9:Q:37:VAL:HG13	9:Q:341:ARG:HD3	1.99	0.45
10:R:647:VAL:HB	10:R:648:PRO:HD3	1.99	0.45
11:S:30:LYS:HA	11:S:34:ARG:HD2	1.99	0.45
13:U:430:LEU:HD21	14:V:312:TRP:HE1	1.81	0.45
13:U:436:MET:HE3	13:U:436:MET:HB3	1.84	0.45
1:0:63:VAL:HG22	2:1:105:ALA:HB2	1.98	0.45
2:2:16:VAL:HG11	2:3:90:PHE:O	2.15	0.45
2:3:51:GLN:HG2	2:3:54:LYS:HD3	1.98	0.45
2:5:130:GLY:O	2:5:134:ILE:HG13	2.16	0.45
4:E:106:ASP:CG	4:E:109:LYS:H	2.25	0.45
4:E:321:ARG:N	5:G:195:GLU:OE2	2.30	0.45
8:N:75:ARG:NH2	8:N:104:SER:OG	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:R:72:ILE:HD13	10:R:72:ILE:HA	1.82	0.45
13:U:265:PRO:HG2	13:U:410:GLU:HB3	1.98	0.45
3:A:383:ALA:O	3:A:387:GLU:HG2	2.17	0.45
3:B:230:GLY:O	3:B:522:GLN:NE2	2.35	0.45
3:C:263:LEU:HD22	3:C:347:MET:HE1	1.98	0.45
4:E:283:GLU:OE2	4:E:337:ARG:NE	2.47	0.45
10:R:49:ARG:NH1	10:R:311:ASN:HA	2.32	0.45
1:O:116:GLU:HB2	1:O:203:MET:HB2	1.98	0.44
4:D:388:ILE:HG23	4:D:464:ALA:HB2	1.99	0.44
4:E:228:ALA:HB3	4:E:293:VAL:HG22	1.98	0.44
5:G:95:ARG:HE	8:N:4:ARG:HE	1.63	0.44
7:K:53:LYS:O	7:K:56:LYS:HG3	2.17	0.44
10:R:97:LEU:HB3	10:R:293:TRP:HH2	1.82	0.44
10:R:382:GLY:O	10:R:815:TYR:OH	2.35	0.44
2:3:117:GLY:HA3	2:3:131:MET:SD	2.57	0.44
2:5:10:TYR:O	2:5:13:PHE:HB3	2.17	0.44
2:7:72:VAL:HG21	2:7:99:VAL:HG21	1.99	0.44
3:A:439:LEU:HD23	3:A:442:ARG:HH21	1.82	0.44
3:B:213:GLN:O	3:B:388:ARG:NH2	2.50	0.44
3:C:444:HIS:CE1	3:C:521:GLN:HB2	2.52	0.44
3:C:507:ILE:HD13	3:C:551:ALA:HB1	1.99	0.44
3:C:573:HIS:CD2	3:C:615:LEU:HD23	2.52	0.44
4:D:276:ARG:HH22	4:D:330:ASP:CG	2.23	0.44
4:D:300:MET:HB2	4:D:354:LEU:HG	2.00	0.44
4:F:229:ILE:HB	4:F:257:VAL:HG22	2.00	0.44
6:H:185:ASN:ND2	6:H:187:ASP:OD1	2.50	0.44
9:Q:164:PHE:CD2	9:Q:168:ILE:HG13	2.53	0.44
9:Q:217:ASP:OD2	9:Q:274:TYR:OH	2.31	0.44
10:R:412:HIS:HD2	10:R:748:HIS:CE1	2.35	0.44
13:U:330:ARG:HH11	13:U:330:ARG:HB2	1.82	0.44
2:3:13:PHE:O	2:3:16:VAL:HG22	2.18	0.44
2:3:61:MET:SD	2:3:135:LEU:HB3	2.57	0.44
2:8:72:VAL:HG11	2:8:99:VAL:HG11	1.98	0.44
2:8:88:LYS:O	2:8:92:GLN:HG2	2.18	0.44
3:A:55:ILE:HD13	3:A:65:GLN:HB3	2.00	0.44
3:B:338:ARG:HD2	3:B:392:VAL:HG22	1.99	0.44
7:K:105:ASP:OD2	7:K:107:ARG:NH1	2.50	0.44
10:R:126:THR:HA	10:R:129:LYS:HD2	1.98	0.44
2:1:88:LYS:O	2:1:92:GLN:HG2	2.17	0.44
3:B:226:PRO:HA	3:B:241:VAL:HA	1.99	0.44
3:C:105:PRO:HB2	3:C:108:ASP:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:204:LYS:O	5:G:207:GLU:HG2	2.18	0.44
8:N:44:THR:HG23	8:N:46:ASN:H	1.81	0.44
10:R:53:ASN:O	10:R:57:ARG:HG3	2.18	0.44
13:U:373:TYR:CD1	13:U:396:MET:HE1	2.51	0.44
3:A:39:MET:HG3	4:E:53:VAL:HG11	1.99	0.44
3:A:510:GLU:HG3	3:A:567:TRP:CE2	2.52	0.44
6:H:74:ASN:O	6:H:78:GLN:HG2	2.17	0.44
6:H:113:GLN:HB2	6:H:143:LEU:HD22	1.98	0.44
6:J:54:MET:O	6:J:58:GLU:HG2	2.17	0.44
13:U:327:LEU:HG	13:U:342:MET:HA	1.99	0.44
3:A:55:ILE:HD12	3:A:365:LEU:HD11	1.98	0.44
3:B:238:PHE:HB3	3:B:455:SER:HB2	2.00	0.44
3:B:507:ILE:HG22	3:B:548:TYR:HD1	1.82	0.44
3:B:592:ASP:HB3	3:B:596:LYS:HD2	1.99	0.44
3:C:577:ILE:HD13	3:C:580:LYS:HD2	1.98	0.44
4:F:190:PRO:HD2	4:F:375:GLY:O	2.17	0.44
10:R:15:LEU:O	10:R:320:ILE:HA	2.18	0.44
10:R:830:ILE:HG13	10:R:831:ARG:HG2	2.00	0.44
2:3:88:LYS:O	2:3:92:GLN:HG2	2.17	0.44
2:6:36:LYS:HE2	2:6:112:ILE:HD13	2.00	0.44
2:6:44:MET:HE2	2:6:44:MET:HB2	1.91	0.44
3:B:233:VAL:HG23	3:B:237:LEU:HD12	1.99	0.44
3:C:90:LEU:HA	3:C:94:ILE:HD11	1.99	0.44
4:D:106:ASP:OD1	4:D:110:THR:OG1	2.28	0.44
4:D:436:LYS:HG2	4:D:441:GLU:HG2	1.99	0.44
2:5:10:TYR:HA	2:6:90:PHE:HE2	1.83	0.44
3:C:422:THR:O	3:C:426:LEU:HG	2.17	0.44
4:D:169:MET:HB2	4:D:405:ALA:HB1	2.00	0.44
9:Q:233:SER:OG	9:Q:235:GLU:OE1	2.34	0.44
10:R:101:PHE:CE2	10:R:289:ASN:HB3	2.53	0.44
2:1:47:MET:HB3	2:1:47:MET:HE2	1.88	0.44
2:5:60:VAL:O	2:5:64:ILE:HG13	2.17	0.44
2:8:136:ILE:O	2:8:140:VAL:HG13	2.18	0.44
3:A:137:PRO:HB2	3:A:179:ILE:HD11	1.99	0.44
3:B:169:PRO:HB2	3:B:172:ASN:ND2	2.33	0.44
3:B:516:LYS:HG2	3:B:520:LEU:HD12	2.00	0.44
4:D:225:GLU:HB3	4:D:226:ASN:H	1.53	0.44
4:D:282:ALA:O	4:D:286:ALA:N	2.50	0.44
4:F:106:ASP:CG	4:F:109:LYS:H	2.26	0.44
6:I:136:CYS:O	6:I:173:LEU:N	2.39	0.44
7:K:5:SER:HA	7:K:8:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:137:PHE:O	2:5:140:VAL:HG22	2.18	0.43
2:9:95:ALA:HB2	2:9:152:LEU:HB2	1.99	0.43
3:A:234:LEU:HD22	3:A:433:TRP:CD2	2.53	0.43
3:C:135:PHE:O	3:C:182:PRO:HA	2.18	0.43
4:F:298:THR:HA	4:F:353:ILE:HB	1.99	0.43
6:I:15:MET:HA	6:I:18:PHE:HB3	2.00	0.43
6:J:12:ILE:HG12	7:M:6:GLN:HE22	1.83	0.43
7:K:41:GLN:O	7:K:45:GLU:HG2	2.18	0.43
7:M:11:LEU:O	7:M:15:GLU:HG2	2.18	0.43
10:R:761:HIS:HD2	12:T:82:ASP:HA	1.83	0.43
10:R:763:GLY:HA2	10:R:778:PHE:HD2	1.83	0.43
2:8:137:PHE:HA	2:8:140:VAL:HG22	2.00	0.43
3:C:234:LEU:HD22	3:C:433:TRP:CD2	2.54	0.43
4:D:226:ASN:ND2	4:D:256:ASN:HD22	2.16	0.43
2:4:64:ILE:HD12	2:4:67:ILE:HB	2.01	0.43
2:5:51:GLN:HE22	2:5:121:THR:HG22	1.82	0.43
2:7:61:MET:SD	2:7:135:LEU:HB3	2.59	0.43
3:A:148:THR:OG1	3:A:149:GLY:N	2.52	0.43
3:B:169:PRO:HB2	3:B:172:ASN:HD22	1.83	0.43
3:B:583:SER:HA	3:B:586:PHE:HD2	1.83	0.43
4:E:99:PHE:HD1	4:E:269:ILE:HB	1.83	0.43
6:J:61:GLU:O	6:J:65:GLU:HG2	2.17	0.43
8:N:28:LEU:HD23	8:N:28:LEU:HA	1.91	0.43
13:U:375:SER:OG	13:U:380:LYS:HB3	2.18	0.43
2:5:48:ARG:NH1	2:5:121:THR:O	2.51	0.43
2:6:13:PHE:HB2	2:7:90:PHE:CE2	2.53	0.43
3:B:412:PRO:HG2	3:B:415:GLY:HA2	2.01	0.43
3:C:391:ARG:NH1	3:C:401:GLU:OE2	2.51	0.43
4:F:193:SER:OG	4:F:194:ALA:N	2.51	0.43
4:F:231:PHE:HB3	4:F:259:LEU:HD23	2.00	0.43
7:K:28:ARG:O	7:K:31:ARG:HG2	2.18	0.43
9:Q:97:LEU:O	9:Q:101:THR:OG1	2.35	0.43
9:Q:207:ALA:C	9:Q:210:PRO:HD2	2.44	0.43
13:U:332:TYR:CD1	13:U:339:TRP:HB2	2.54	0.43
13:U:417:ASP:OD1	13:U:418:CYS:N	2.51	0.43
2:4:57:ILE:HG23	10:R:800:LEU:HD11	2.00	0.43
3:A:473:VAL:HB	3:A:474:PRO:HD3	2.00	0.43
3:A:518:ASP:HB2	3:A:544:MET:HE1	2.00	0.43
3:C:177:THR:OG1	3:C:193:GLU:O	2.33	0.43
4:D:63:VAL:HB	4:D:66:PRO:HG3	1.99	0.43
4:F:46:THR:HA	4:F:113:GLU:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:133:LYS:O	5:G:136:ARG:HG2	2.19	0.43
7:M:47:TYR:O	7:M:51:ARG:HG2	2.18	0.43
9:Q:324:GLN:HA	9:Q:327:ARG:HG2	2.01	0.43
2:4:136:ILE:HG23	10:R:804:ARG:HH21	1.84	0.43
4:E:124:SER:HB3	4:E:148:GLU:H	1.83	0.43
6:H:83:VAL:HG21	7:K:80:LYS:HE2	2.01	0.43
6:I:125:TYR:CG	7:L:110:ILE:HG13	2.53	0.43
10:R:737:SER:O	10:R:740:ARG:HG3	2.17	0.43
1:O:171:SER:O	1:O:175:LYS:NZ	2.51	0.43
2:3:67:ILE:HD12	10:R:729:LEU:HD13	2.00	0.43
2:8:34:THR:HG23	2:8:59:VAL:HG13	1.99	0.43
3:A:270:ASP:OD1	3:A:270:ASP:N	2.52	0.43
3:A:338:ARG:HB2	3:A:404:VAL:HG23	2.00	0.43
3:A:438:LYS:HB3	3:A:442:ARG:NH1	2.33	0.43
3:B:53:GLU:OE1	3:B:67:TYR:OH	2.37	0.43
3:B:234:LEU:HD22	3:B:433:TRP:CD1	2.53	0.43
3:C:42:LEU:HD11	3:C:86:LEU:HA	2.01	0.43
3:C:538:VAL:O	3:C:542:SER:OG	2.30	0.43
4:E:274:THR:N	4:E:275:PRO:HD2	2.34	0.43
6:H:57:TYR:O	6:H:61:GLU:HG2	2.18	0.43
6:I:42:LYS:HB2	7:L:36:ALA:HB1	2.00	0.43
10:R:576:ILE:HA	10:R:579:MET:HG2	2.00	0.43
10:R:757:THR:O	10:R:761:HIS:HB3	2.19	0.43
2:2:36:LYS:O	2:2:39:THR:OG1	2.32	0.43
2:6:16:VAL:HG11	2:7:90:PHE:O	2.18	0.43
2:6:45:SER:OG	2:7:127:LEU:HB2	2.18	0.43
2:7:41:ILE:HA	2:7:44:MET:HG3	2.00	0.43
3:A:77:ASP:OD1	7:K:113:ASN:ND2	2.35	0.43
3:B:327:ILE:HD12	3:B:354:TRP:CG	2.54	0.43
3:C:518:ASP:HB2	3:C:544:MET:HE1	2.00	0.43
4:E:248:PHE:O	4:E:254:MET:HB2	2.19	0.43
6:H:68:LYS:HD2	7:K:66:ARG:HB2	2.00	0.43
9:Q:54:TYR:OH	9:Q:322:LYS:NZ	2.49	0.43
9:Q:106:ILE:O	9:Q:110:ILE:HG12	2.19	0.43
13:U:266:ARG:HD2	13:U:302:TRP:CD2	2.54	0.43
13:U:316:LEU:HG	13:U:317:PHE:CD2	2.53	0.43
1:O:41:LEU:HD12	2:9:10:TYR:HD2	1.84	0.43
2:2:41:ILE:HA	2:2:44:MET:HG3	2.00	0.43
2:6:95:ALA:HB2	2:6:152:LEU:HB2	2.01	0.43
2:8:86:LEU:HG	2:8:90:PHE:CE2	2.54	0.43
7:L:53:LYS:HA	7:L:53:LYS:HD3	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:U:367:TYR:CD1	13:U:414:TYR:HB3	2.53	0.43
2:5:147:ILE:HD13	10:R:750:GLN:HB3	2.01	0.43
2:6:23:MET:O	2:6:26:SER:OG	2.24	0.43
3:A:98:ILE:HG22	3:A:106:LEU:HD12	2.00	0.43
3:C:275:VAL:HG21	3:C:330:GLY:HA3	2.01	0.43
6:I:129:GLU:N	6:I:132:MET:HE2	2.34	0.43
3:A:94:ILE:HD13	3:A:333:LEU:HD22	2.01	0.42
3:A:151:ASP:OD1	3:A:397:ASN:N	2.44	0.42
4:D:48:LYS:NZ	4:D:111:SER:OG	2.47	0.42
4:D:285:LEU:O	4:D:291:LYS:HG2	2.19	0.42
4:F:235:GLY:HA2	4:F:264:ALA:HA	2.01	0.42
5:G:158:LEU:HD12	5:G:158:LEU:HA	1.78	0.42
5:G:199:PHE:HE1	5:G:203:LYS:HD2	1.83	0.42
6:J:203:ILE:HD12	7:M:103:VAL:HG22	2.01	0.42
7:L:49:LEU:O	7:L:53:LYS:HG2	2.19	0.42
7:M:28:ARG:HB3	7:M:32:ARG:NH1	2.34	0.42
10:R:751:LEU:O	10:R:754:VAL:HG12	2.19	0.42
2:1:76:ILE:HG23	2:1:92:GLN:HB3	2.01	0.42
2:7:44:MET:HE1	2:7:51:GLN:HG3	2.01	0.42
3:A:215:ARG:HH11	3:A:336:TYR:HA	1.84	0.42
3:A:532:CYS:SG	3:A:537:THR:OG1	2.59	0.42
3:A:550:MET:SD	3:A:553:ARG:NH1	2.93	0.42
3:B:71:SER:HA	4:E:68:TYR:HD2	1.84	0.42
3:B:504:THR:HG22	3:B:552:ARG:HA	2.01	0.42
4:E:294:LEU:HD11	4:E:351:ILE:HG13	2.01	0.42
5:G:124:LEU:HD23	9:Q:226:ASN:HB2	2.00	0.42
7:K:85:GLN:HB3	7:K:89:ARG:HH12	1.83	0.42
9:Q:107:ASP:OD1	9:Q:107:ASP:N	2.52	0.42
2:5:48:ARG:NH1	2:5:125:PRO:HG3	2.35	0.42
3:A:270:ASP:HB2	3:A:342:TYR:HB3	2.01	0.42
3:A:437:LYS:HE2	3:A:437:LYS:HB3	1.92	0.42
4:D:400:ARG:O	4:D:403:LYS:NZ	2.52	0.42
4:D:488:PRO:HG2	4:D:491:MET:HG3	2.00	0.42
4:F:250:GLU:HG3	6:J:66:GLN:HG3	2.02	0.42
10:R:13:ALA:HB1	10:R:352:LEU:HB2	2.02	0.42
10:R:374:PHE:HA	10:R:377:ILE:HG12	2.01	0.42
2:2:49:PRO:O	2:3:126:ARG:NH2	2.53	0.42
3:B:146:HIS:CD2	3:B:175:THR:HG22	2.55	0.42
3:B:371:ASP:OD1	3:B:371:ASP:N	2.52	0.42
3:C:503:GLU:HB2	3:C:555:VAL:HG21	2.02	0.42
4:E:117:ASP:OD1	4:E:118:ILE:N	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:321:ARG:HD3	4:E:364:PRO:HD3	2.02	0.42
4:E:390:PRO:HD2	4:E:463:ILE:O	2.19	0.42
9:Q:113:ILE:HD13	9:Q:171:GLN:HE21	1.83	0.42
10:R:391:PRO:HB3	10:R:814:PHE:CZ	2.55	0.42
1:O:174:VAL:O	1:O:177:LEU:HB3	2.18	0.42
3:A:220:LYS:HG2	3:A:392:VAL:HG12	2.01	0.42
3:C:100:ASP:OD1	3:C:104:ARG:N	2.49	0.42
4:E:421:GLN:HG2	4:E:495:ILE:HD11	2.01	0.42
13:U:401:GLN:NE2	14:V:296:ALA:H	2.07	0.42
2:7:44:MET:HE2	2:7:44:MET:HB2	1.97	0.42
3:A:139:LYS:H	3:A:139:LYS:HG3	1.66	0.42
3:B:239:PRO:HB2	3:B:461:LEU:HD12	2.01	0.42
3:C:211:VAL:HB	3:C:328:TYR:HB3	2.02	0.42
4:E:163:ARG:NH1	4:E:338:ALA:O	2.53	0.42
4:E:229:ILE:O	4:E:257:VAL:HA	2.19	0.42
4:E:310:VAL:O	4:E:314:ARG:HG3	2.19	0.42
6:I:53:ILE:HD13	7:L:48:ARG:HA	2.01	0.42
10:R:52:VAL:HG22	10:R:56:ARG:HE	1.85	0.42
1:O:62:VAL:HG13	2:1:141:LEU:HB3	2.01	0.42
2:6:138:ALA:O	2:6:141:LEU:HB2	2.19	0.42
2:9:58:PRO:HG3	2:9:135:LEU:HD11	2.01	0.42
4:D:201:GLU:OE1	4:D:201:GLU:N	2.48	0.42
4:D:430:LYS:HD3	4:D:455:LEU:HD21	2.00	0.42
6:H:152:ILE:O	6:H:156:LYS:HG3	2.18	0.42
6:J:125:TYR:O	6:J:128:LEU:HG	2.20	0.42
13:U:312:THR:HG22	13:U:322:THR:HG23	2.02	0.42
2:1:44:MET:HB2	2:1:122:ALA:HB2	2.01	0.42
2:3:10:TYR:O	2:3:13:PHE:HB3	2.19	0.42
3:A:162:ILE:HG12	3:A:308:ARG:HG2	2.02	0.42
3:A:323:ARG:HE	3:A:357:ALA:HB2	1.85	0.42
3:B:239:PRO:HD2	3:B:458:MET:HG2	2.01	0.42
3:C:413:PRO:HB2	4:F:320:ARG:CZ	2.49	0.42
4:E:307:LEU:HD11	4:E:326:TYR:HE1	1.85	0.42
6:J:203:ILE:HA	6:J:206:GLN:HG2	2.01	0.42
9:Q:91:GLU:HA	9:Q:94:ALA:HB3	2.01	0.42
9:Q:234:LYS:NZ	9:Q:259:ASP:HB3	2.34	0.42
2:6:31:ALA:HB1	2:7:109:ALA:HB2	2.01	0.42
2:8:25:PHE:HA	2:8:28:LEU:HD12	2.01	0.42
3:B:524:GLY:HA2	3:B:530:ARG:HA	2.02	0.42
3:C:233:VAL:C	3:C:235:ASP:H	2.26	0.42
4:D:106:ASP:OD2	4:D:109:LYS:N	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:140:LYS:O	5:G:143:GLU:HG2	2.19	0.42
9:Q:179:GLU:CD	9:Q:182:ARG:HH12	2.28	0.42
9:Q:204:THR:O	9:Q:208:MET:N	2.47	0.42
10:R:51:PHE:CZ	10:R:319:LEU:HD11	2.54	0.42
11:S:44:CYS:O	11:S:45:SER:C	2.63	0.42
2:3:52:ILE:HD13	2:4:127:LEU:HD12	2.01	0.42
2:4:88:LYS:O	2:4:92:GLN:HG2	2.20	0.42
3:A:140:ASN:O	3:A:142:ARG:NH1	2.53	0.42
4:D:233:ALA:HA	4:D:298:THR:HB	2.02	0.42
4:E:105:ILE:HG23	4:E:110:THR:HG21	2.02	0.42
4:E:457:LYS:HB3	4:E:483:LEU:HD22	2.02	0.42
4:F:75:THR:OG1	4:F:111:SER:HB3	2.19	0.42
6:I:122:GLN:OE1	6:I:194:ASN:ND2	2.50	0.42
7:K:75:LYS:HE2	7:K:75:LYS:HB3	1.85	0.42
2:3:47:MET:HE3	2:3:47:MET:HB3	1.80	0.41
3:A:69:GLU:OE1	3:A:70:THR:N	2.53	0.41
3:A:141:LEU:HD12	3:A:153:TYR:HA	2.02	0.41
3:B:90:LEU:HA	3:B:94:ILE:HD11	2.01	0.41
3:C:384:SER:O	3:C:388:ARG:HG3	2.20	0.41
4:D:129:GLY:HA2	4:D:254:MET:O	2.20	0.41
4:D:214:LYS:HD3	4:D:214:LYS:HA	1.91	0.41
4:D:263:LEU:N	4:D:266:ASP:OD2	2.53	0.41
4:E:402:MET:HG2	4:E:406:ILE:HD13	2.01	0.41
4:F:332:ALA:HA	4:F:372:ILE:HG21	2.01	0.41
6:H:203:ILE:HG22	6:H:207:MET:HE2	2.02	0.41
6:J:120:VAL:O	6:J:124:LEU:HG	2.20	0.41
13:U:257:PRO:HB3	13:U:270:TRP:HB2	2.02	0.41
3:A:68:GLU:HA	3:A:319:PRO:HG2	2.02	0.41
4:F:376:GLN:N	4:F:398:LEU:O	2.51	0.41
5:G:138:TYR:CZ	8:N:19:GLY:HA3	2.54	0.41
6:H:120:VAL:O	6:H:124:LEU:HG	2.21	0.41
7:K:49:LEU:HD13	7:K:49:LEU:HA	1.92	0.41
8:N:83:GLN:HB2	8:N:86:PRO:HD2	2.02	0.41
13:U:368:SER:N	13:U:414:TYR:O	2.46	0.41
2:3:28:LEU:HD23	2:4:105:ALA:HB2	2.02	0.41
3:A:39:MET:HE3	3:A:39:MET:HB3	1.80	0.41
3:A:441:GLN:C	3:A:443:LYS:N	2.78	0.41
3:B:148:THR:OG1	3:B:149:GLY:N	2.53	0.41
4:E:50:VAL:HG13	4:E:58:VAL:HG13	2.01	0.41
4:F:426:TYR:CE2	4:F:430:LYS:HE2	2.54	0.41
5:G:209:LYS:O	5:G:212:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:135:ARG:HH21	6:I:172:TYR:C	2.28	0.41
8:N:66:ILE:HD11	8:N:70:ILE:HG22	2.02	0.41
9:Q:36:LEU:O	9:Q:336:ILE:HD11	2.21	0.41
2:3:49:PRO:HB2	2:4:126:ARG:CZ	2.50	0.41
3:B:43:VAL:HG21	3:B:64:ILE:HD13	2.02	0.41
3:B:271:VAL:HG11	3:B:337:PHE:CD2	2.55	0.41
3:C:314:ASN:HA	3:C:318:MET:SD	2.61	0.41
3:C:462:ASP:OD1	3:C:476:ARG:NH2	2.42	0.41
4:D:55:GLY:O	4:D:102:THR:OG1	2.31	0.41
4:D:407:GLY:N	4:D:411:THR:OG1	2.52	0.41
5:G:6:ARG:HB3	5:G:183:THR:HB	2.03	0.41
6:H:61:GLU:OE1	7:K:58:LYS:HD2	2.19	0.41
6:H:137:ARG:NE	6:H:140:ASP:OD2	2.35	0.41
6:I:120:VAL:O	6:I:124:LEU:HG	2.21	0.41
6:I:127:LEU:HD23	6:I:127:LEU:HA	1.90	0.41
7:M:47:TYR:O	7:M:50:GLN:HG2	2.19	0.41
10:R:54:GLU:HG2	10:R:304:TYR:CZ	2.54	0.41
2:2:25:PHE:HA	2:2:28:LEU:HD12	2.02	0.41
2:7:97:LEU:HD23	2:7:97:LEU:HA	1.90	0.41
3:B:134:ASP:OD1	3:B:134:ASP:N	2.54	0.41
3:B:280:ARG:NH1	4:E:400:ARG:HH12	2.18	0.41
3:C:609:GLN:O	3:C:613:ARG:HG3	2.21	0.41
4:D:359:ASP:OD1	4:D:359:ASP:N	2.52	0.41
4:E:271:ARG:HD2	4:E:306:ALA:HB2	2.02	0.41
4:E:360:ASP:OD1	4:E:362:THR:HG22	2.20	0.41
9:Q:96:PHE:CE2	9:Q:100:ILE:HD11	2.56	0.41
10:R:383:ILE:H	10:R:383:ILE:HG12	1.67	0.41
13:U:403:GLN:NE2	13:U:413:SER:H	2.15	0.41
2:4:64:ILE:HD12	2:4:64:ILE:HA	1.86	0.41
2:5:147:ILE:HD11	10:R:751:LEU:HD23	2.03	0.41
3:B:113:THR:HG21	3:B:119:PRO:HG2	2.03	0.41
3:C:546:ALA:HB1	3:C:550:MET:HE3	2.00	0.41
4:D:389:TYR:HE2	4:D:467:PRO:HA	1.85	0.41
4:E:327:MET:HE3	4:E:368:LEU:HD12	2.01	0.41
4:F:412:ARG:HD3	4:F:477:LEU:HD12	2.01	0.41
5:G:132:ALA:HA	5:G:135:LYS:HG2	2.02	0.41
7:M:85:GLN:HB3	7:M:89:ARG:NH1	2.36	0.41
8:N:66:ILE:HG23	8:N:71:ALA:HB2	2.02	0.41
10:R:549:LEU:O	10:R:552:VAL:HG12	2.20	0.41
13:U:389:GLN:HB2	13:U:390:PRO:HD3	2.03	0.41
2:2:86:LEU:HG	2:2:90:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:46:VAL:HG11	2:5:123:GLN:HE21	1.86	0.41
2:8:22:ALA:HB2	2:8:96:GLY:HA2	2.02	0.41
2:8:123:GLN:HG2	9:Q:272:PRO:HD3	2.02	0.41
3:B:280:ARG:NE	4:E:373:THR:O	2.54	0.41
3:B:507:ILE:HG21	3:B:551:ALA:HB3	2.01	0.41
3:C:255:GLY:HA2	15:C:701:ADP:H5'1	2.02	0.41
4:D:117:ASP:OD1	4:D:118:ILE:N	2.54	0.41
4:E:122:PRO:HB3	4:E:150:PHE:HE1	1.86	0.41
6:I:71:GLN:O	6:I:75:LEU:HD22	2.21	0.41
6:I:162:ASP:OD1	6:I:162:ASP:N	2.54	0.41
6:J:49:GLN:HB3	7:M:44:ILE:HD13	2.02	0.41
2:1:72:VAL:HG21	2:1:99:VAL:HG21	2.02	0.41
2:2:60:VAL:O	2:2:64:ILE:HG13	2.21	0.41
2:4:60:VAL:HG11	10:R:800:LEU:HB3	2.03	0.41
2:9:60:VAL:O	2:9:64:ILE:HG13	2.21	0.41
3:C:432:PHE:CD2	3:C:453:SER:HA	2.55	0.41
3:C:592:ASP:HB3	3:C:596:LYS:HD2	2.01	0.41
4:F:149:ASP:OD1	4:F:150:PHE:N	2.52	0.41
9:Q:36:LEU:HB3	9:Q:332:ILE:HG21	2.02	0.41
9:Q:215:GLU:HA	9:Q:218:ARG:HG2	2.02	0.41
10:R:643:ALA:O	10:R:647:VAL:HG23	2.21	0.41
1:0:140:ALA:O	1:0:144:VAL:HG12	2.21	0.41
2:4:13:PHE:HB2	2:5:90:PHE:CD2	2.56	0.41
2:6:61:MET:SD	2:6:135:LEU:HB3	2.61	0.41
2:6:136:ILE:O	2:6:140:VAL:HG13	2.21	0.41
2:7:10:TYR:O	2:7:13:PHE:HB3	2.21	0.41
2:8:128:PHE:O	2:8:132:ILE:HG12	2.21	0.41
3:A:305:ILE:HD12	3:A:305:ILE:HA	1.95	0.41
3:B:144:GLY:N	3:B:176:VAL:O	2.43	0.41
3:B:234:LEU:HD13	3:B:433:TRP:CD2	2.56	0.41
3:B:587:LYS:HB3	3:B:587:LYS:HE2	1.81	0.41
3:C:152:ILE:HD13	3:C:165:LYS:HG2	2.01	0.41
3:C:236:ALA:HA	3:C:472:PHE:CZ	2.56	0.41
4:D:374:GLU:HA	4:D:400:ARG:NH1	2.36	0.41
4:E:41:SER:O	6:I:122:GLN:NE2	2.54	0.41
4:F:82:ARG:HH12	4:F:103:SER:N	2.17	0.41
4:F:131:VAL:HB	4:F:140:ASP:HB3	2.01	0.41
5:G:54:THR:HB	5:G:148:LEU:HD13	2.03	0.41
6:H:129:GLU:N	6:H:132:MET:HE2	2.36	0.41
6:I:64:ILE:HG21	7:L:59:GLU:HA	2.02	0.41
6:J:55:GLU:O	6:J:59:LYS:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:52:GLU:O	7:L:56:LYS:HG2	2.21	0.41
8:N:9:ALA:HA	8:N:35:ASN:O	2.20	0.41
8:N:93:SER:HB2	8:N:96:HIS:HB2	2.02	0.41
9:Q:243:HIS:O	9:Q:243:HIS:ND1	2.53	0.41
10:R:21:ALA:HA	10:R:344:SER:HB2	2.02	0.41
10:R:51:PHE:HZ	10:R:319:LEU:HD11	1.85	0.41
10:R:578:PHE:O	10:R:581:SER:OG	2.31	0.41
10:R:732:ILE:HA	10:R:735:THR:HG22	2.03	0.41
11:S:10:LEU:HA	11:S:52:TRP:HH2	1.84	0.41
2:2:114:GLY:O	2:2:118:VAL:HG22	2.21	0.41
3:A:211:VAL:O	3:A:388:ARG:NH1	2.52	0.41
3:A:323:ARG:NE	3:A:357:ALA:HB2	2.36	0.41
3:C:135:PHE:HB2	3:C:205:MET:HE2	2.02	0.41
3:C:232:ARG:NH1	3:C:522:GLN:HB2	2.36	0.41
6:H:104:LYS:HE3	6:H:104:LYS:HB3	1.74	0.41
7:K:4:GLN:H	10:R:353:ASN:HB2	1.86	0.41
9:Q:12:ASP:HB2	9:Q:90:TYR:CD2	2.56	0.41
9:Q:108:ASN:OD1	9:Q:108:ASN:N	2.54	0.41
9:Q:263:GLN:O	9:Q:267:VAL:HG23	2.21	0.41
10:R:21:ALA:HB1	10:R:341:THR:HA	2.03	0.41
2:1:41:ILE:O	2:1:45:SER:N	2.53	0.40
2:2:44:MET:HE2	2:2:44:MET:HB2	1.97	0.40
3:B:135:PHE:CE1	3:B:154:GLY:HA3	2.56	0.40
6:I:63:GLN:O	6:I:67:GLN:HG2	2.21	0.40
8:N:100:ALA:HB1	8:N:106:LEU:HD11	2.04	0.40
10:R:823:LEU:H	10:R:823:LEU:HG	1.78	0.40
3:A:356:GLU:HG2	3:A:359:ARG:HH21	1.86	0.40
3:C:241:VAL:HG12	3:C:461:LEU:HD21	2.03	0.40
4:D:122:PRO:CB	4:D:147:ALA:HB2	2.52	0.40
4:D:248:PHE:CE2	4:D:259:LEU:HD21	2.56	0.40
4:F:234:MET:SD	4:F:275:PRO:HD3	2.62	0.40
6:J:59:LYS:HA	6:J:59:LYS:HD3	1.83	0.40
6:J:203:ILE:HG22	6:J:207:MET:HE2	2.02	0.40
9:Q:311:HIS:NE2	9:Q:314:VAL:HG23	2.36	0.40
11:S:25:PRO:HA	11:S:28:ILE:HG12	2.02	0.40
13:U:364:PRO:C	13:U:366:ILE:H	2.29	0.40
2:3:24:VAL:HG22	2:4:101:LEU:HB2	2.03	0.40
3:A:249:PRO:HG2	3:A:435:LEU:H	1.87	0.40
3:B:368:MET:HB2	4:F:312:ALA:HB1	2.03	0.40
3:C:473:VAL:HB	3:C:474:PRO:HD3	2.03	0.40
4:D:174:ILE:HA	4:D:465:GLN:OE1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:203:ALA:HB2	4:D:353:ILE:HD11	2.03	0.40
4:D:489:LYS:HE3	4:D:500:LEU:HB3	2.02	0.40
6:H:201:ASP:O	6:H:205:GLN:HG2	2.20	0.40
6:I:16:MET:HG3	7:L:13:GLN:HE22	1.86	0.40
9:Q:303:LYS:O	9:Q:307:LEU:HD22	2.21	0.40
9:Q:308:ASN:HB2	9:Q:311:HIS:NE2	2.37	0.40
10:R:385:THR:OG1	10:R:388:GLU:HB2	2.21	0.40
13:U:266:ARG:HD2	13:U:302:TRP:CE2	2.56	0.40
1:O:67:TRP:HA	1:O:70:TYR:CD2	2.57	0.40
2:8:36:LYS:O	2:8:39:THR:OG1	2.36	0.40
3:B:95:MET:HE1	3:B:271:VAL:HG13	2.02	0.40
3:B:574:MET:HB3	3:B:577:ILE:HB	2.02	0.40
3:C:234:LEU:HD22	3:C:433:TRP:CG	2.56	0.40
4:D:128:LEU:HD23	4:D:128:LEU:HA	1.95	0.40
4:D:190:PRO:HD3	4:D:373:THR:HB	2.03	0.40
4:D:328:TYR:HB2	4:D:368:LEU:HD13	2.04	0.40
4:F:234:MET:HE3	4:F:234:MET:HB2	1.74	0.40
4:F:307:LEU:HG	4:F:324:PRO:HG3	2.03	0.40
6:H:77:ASN:OD1	6:H:80:ARG:NH2	2.55	0.40
7:L:28:ARG:HB3	7:L:32:ARG:HH21	1.86	0.40
7:M:79:GLU:O	7:M:82:THR:HG22	2.21	0.40
1:O:28:ILE:HG13	1:O:29:PHE:CD1	2.56	0.40
1:O:34:ARG:NH2	13:U:420:SER:OG	2.55	0.40
1:O:189:PHE:CD1	2:9:70:LEU:HD22	2.57	0.40
3:A:463:GLU:H	3:A:463:GLU:HG3	1.69	0.40
3:A:564:LYS:H	3:A:564:LYS:HG2	1.68	0.40
3:B:152:ILE:HD13	3:B:165:LYS:HB3	2.03	0.40
3:B:358:LEU:HD23	3:B:358:LEU:HA	1.97	0.40
9:Q:69:VAL:O	9:Q:73:ARG:HG2	2.21	0.40
9:Q:113:ILE:HD13	9:Q:171:GLN:NE2	2.36	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	0	200/205 (98%)	199 (100%)	1 (0%)	0	100	100
2	1	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
2	2	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
2	3	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
2	4	148/155 (96%)	145 (98%)	2 (1%)	1 (1%)	18	51
2	5	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
2	6	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
2	7	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
2	8	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
2	9	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
3	A	555/617 (90%)	545 (98%)	10 (2%)	0	100	100
3	B	545/617 (88%)	537 (98%)	8 (2%)	0	100	100
3	C	597/617 (97%)	579 (97%)	18 (3%)	0	100	100
4	D	455/511 (89%)	440 (97%)	15 (3%)	0	100	100
4	E	456/511 (89%)	441 (97%)	15 (3%)	0	100	100
4	F	454/511 (89%)	443 (98%)	11 (2%)	0	100	100
5	G	215/247 (87%)	213 (99%)	2 (1%)	0	100	100
6	H	179/226 (79%)	177 (99%)	2 (1%)	0	100	100
6	I	217/226 (96%)	215 (99%)	2 (1%)	0	100	100
6	J	213/226 (94%)	213 (100%)	0	0	100	100
7	K	112/118 (95%)	112 (100%)	0	0	100	100
7	L	112/118 (95%)	111 (99%)	1 (1%)	0	100	100
7	M	112/118 (95%)	109 (97%)	3 (3%)	0	100	100
8	N	108/119 (91%)	101 (94%)	7 (6%)	0	100	100
9	Q	303/351 (86%)	299 (99%)	4 (1%)	0	100	100
10	R	626/837 (75%)	606 (97%)	20 (3%)	0	100	100
11	S	75/81 (93%)	73 (97%)	2 (3%)	0	100	100
12	T	83/137 (61%)	82 (99%)	1 (1%)	0	100	100
13	U	203/470 (43%)	196 (97%)	7 (3%)	0	100	100
14	V	43/350 (12%)	42 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	7195/8608 (84%)	7046 (98%)	148 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	4	128	PHE

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	0	150/155 (97%)	147 (98%)	3 (2%)	48	67
2	1	105/112 (94%)	103 (98%)	2 (2%)	50	68
2	2	107/112 (96%)	106 (99%)	1 (1%)	70	76
2	3	107/112 (96%)	102 (95%)	5 (5%)	23	51
2	4	107/112 (96%)	106 (99%)	1 (1%)	70	76
2	5	107/112 (96%)	105 (98%)	2 (2%)	50	68
2	6	107/112 (96%)	105 (98%)	2 (2%)	50	68
2	7	106/112 (95%)	105 (99%)	1 (1%)	70	76
2	8	107/112 (96%)	106 (99%)	1 (1%)	70	76
2	9	107/112 (96%)	107 (100%)	0	100	100
3	A	462/525 (88%)	442 (96%)	20 (4%)	26	52
3	B	447/525 (85%)	437 (98%)	10 (2%)	45	66
3	C	496/525 (94%)	488 (98%)	8 (2%)	55	71
4	D	390/430 (91%)	383 (98%)	7 (2%)	51	70
4	E	390/430 (91%)	384 (98%)	6 (2%)	57	72
4	F	388/430 (90%)	380 (98%)	8 (2%)	47	66
5	G	179/212 (84%)	172 (96%)	7 (4%)	28	56
6	H	162/199 (81%)	156 (96%)	6 (4%)	30	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	I	193/199 (97%)	187 (97%)	6 (3%)	35	61
6	J	190/199 (96%)	180 (95%)	10 (5%)	20	48
7	K	99/101 (98%)	92 (93%)	7 (7%)	13	40
7	L	99/101 (98%)	93 (94%)	6 (6%)	17	44
7	M	99/101 (98%)	93 (94%)	6 (6%)	17	44
8	N	94/100 (94%)	93 (99%)	1 (1%)	65	75
9	Q	268/306 (88%)	259 (97%)	9 (3%)	32	59
10	R	567/746 (76%)	537 (95%)	30 (5%)	20	48
11	S	69/72 (96%)	68 (99%)	1 (1%)	59	72
12	T	70/116 (60%)	69 (99%)	1 (1%)	59	72
13	U	182/397 (46%)	173 (95%)	9 (5%)	22	50
14	V	40/308 (13%)	40 (100%)	0	100	100
All	All	5994/7185 (83%)	5818 (97%)	176 (3%)	38	62

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	70	TYR
1	0	100	VAL
1	0	174	VAL
2	1	36	LYS
2	1	101	LEU
2	2	80	LEU
2	3	16	VAL
2	3	44	MET
2	3	47	MET
2	3	133	LEU
2	3	146	LEU
2	4	140	VAL
2	5	9	GLU
2	5	61	MET
2	6	75	LEU
2	6	140	VAL
2	7	56	ILE
2	8	82	ASP
3	A	18	PHE
3	A	69	GLU
3	A	122	VAL

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Mol	Chain	Res	Type
3	A	139	LYS
3	A	147	ILE
3	A	164	HIS
3	A	179	ILE
3	A	189	ASP
3	A	199	VAL
3	A	228	LEU
3	A	266	TYR
3	A	268	ASN
3	A	270	ASP
3	A	315	THR
3	A	320	VAL
3	A	327	ILE
3	A	410	VAL
3	A	419	ASP
3	A	478	LYS
3	A	505	ASP
3	B	43	VAL
3	B	57	LEU
3	B	69	GLU
3	B	102	ILE
3	B	164	HIS
3	B	194	LEU
3	B	270	ASP
3	B	299	ASP
3	B	360	GLU
3	B	400	ARG
3	C	43	VAL
3	C	173	ARG
3	C	270	ASP
3	C	296	MET
3	C	302	VAL
3	C	395	LEU
3	C	419	ASP
3	C	470	THR
4	D	106	ASP
4	D	164	ILE
4	D	237	ASN
4	D	243	PHE
4	D	256	ASN
4	D	436	LYS
4	D	445	THR

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Mol	Chain	Res	Type
4	E	54	ASN
4	E	121	THR
4	E	189	ILE
4	E	215	LYS
4	E	371	TYR
4	E	449	LEU
4	F	39	TYR
4	F	97	GLN
4	F	255	ASP
4	F	280	THR
4	F	359	ASP
4	F	417	ASP
4	F	445	THR
4	F	448	ASP
5	G	57	LEU
5	G	87	VAL
5	G	101	VAL
5	G	116	THR
5	G	124	LEU
5	G	158	LEU
5	G	198	GLU
6	H	48	THR
6	H	49	GLN
6	H	51	LEU
6	H	54	MET
6	H	57	TYR
6	H	210	GLU
6	I	41	GLU
6	I	57	TYR
6	I	75	LEU
6	I	127	LEU
6	I	129	GLU
6	I	192	VAL
6	J	16	MET
6	J	33	LYS
6	J	41	GLU
6	J	42	LYS
6	J	45	LEU
6	J	61	GLU
6	J	126	GLN
6	J	127	LEU
6	J	192	VAL

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Mol	Chain	Res	Type
6	J	221	ASN
7	K	10	GLN
7	K	27	LYS
7	K	44	ILE
7	K	47	TYR
7	K	49	LEU
7	K	53	LYS
7	K	116	ILE
7	L	10	GLN
7	L	15	GLU
7	L	21	LYS
7	L	45	GLU
7	L	75	LYS
7	L	99	LEU
7	M	4	GLN
7	M	6	GLN
7	M	24	GLU
7	M	33	LEU
7	M	34	LYS
7	M	99	LEU
8	N	74	VAL
9	Q	6	GLU
9	Q	66	THR
9	Q	101	THR
9	Q	167	CYS
9	Q	184	THR
9	Q	193	PHE
9	Q	273	GLU
9	Q	307	LEU
9	Q	308	ASN
10	R	28	GLU
10	R	44	VAL
10	R	65	LEU
10	R	72	ILE
10	R	92	ARG
10	R	98	GLU
10	R	100	ASN
10	R	133	ARG
10	R	275	THR
10	R	295	ILE
10	R	310	CYS
10	R	316	GLN

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Mol	Chain	Res	Type
10	R	317	LYS
10	R	320	ILE
10	R	325	CYS
10	R	333	ILE
10	R	357	THR
10	R	363	THR
10	R	383	ILE
10	R	385	THR
10	R	555	SER
10	R	568	ILE
10	R	595	THR
10	R	612	PHE
10	R	744	LEU
10	R	760	ILE
10	R	766	VAL
10	R	769	LEU
10	R	823	LEU
10	R	829	HIS
11	S	57	LEU
12	T	96	ASN
13	U	261	ASN
13	U	284	ASP
13	U	286	THR
13	U	312	THR
13	U	321	VAL
13	U	330	ARG
13	U	353	VAL
13	U	408	MET
13	U	453	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (142) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	90	ASN
1	0	130	ASN
1	0	197	GLN
2	1	51	GLN
2	1	78	ASN
2	1	81	ASN
2	1	123	GLN
2	3	78	ASN
2	3	81	ASN

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Mol	Chain	Res	Type
2	3	124	GLN
2	4	51	GLN
2	5	51	GLN
2	5	78	ASN
2	5	123	GLN
2	6	78	ASN
2	8	123	GLN
2	8	124	GLN
3	A	65	GLN
3	A	146	HIS
3	A	172	ASN
3	A	213	GLN
3	A	231	GLN
3	A	441	GLN
3	A	444	HIS
3	A	563	ASN
3	A	603	GLN
3	B	65	GLN
3	B	146	HIS
3	B	172	ASN
3	B	207	GLN
3	B	261	GLN
3	B	521	GLN
3	B	573	HIS
3	C	146	HIS
3	C	172	ASN
3	C	231	GLN
3	C	261	GLN
3	C	397	ASN
3	C	441	GLN
3	C	444	HIS
4	D	85	GLN
4	D	97	GLN
4	D	156	GLN
4	D	171	GLN
4	D	181	ASN
4	D	209	GLN
4	D	226	ASN
4	D	350	GLN
4	D	358	ASN
4	D	385	ASN
4	E	156	GLN

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Mol	Chain	Res	Type
4	E	209	GLN
4	E	237	ASN
4	E	345	ASN
4	E	350	GLN
4	E	382	GLN
4	E	385	ASN
4	E	470	ASN
4	F	73	HIS
4	F	97	GLN
4	F	156	GLN
4	F	209	GLN
4	F	262	ASN
4	F	265	ASN
4	F	350	GLN
4	F	382	GLN
5	G	85	GLN
5	G	91	GLN
5	G	152	GLN
5	G	206	GLN
6	H	71	GLN
6	H	100	GLN
6	H	122	GLN
6	H	166	GLN
6	H	194	ASN
6	H	221	ASN
6	I	11	GLN
6	I	66	GLN
6	I	71	GLN
6	J	21	GLN
6	J	63	GLN
6	J	66	GLN
6	J	67	GLN
6	J	100	GLN
6	J	126	GLN
6	J	149	GLN
6	J	161	ASN
7	K	35	GLN
7	K	50	GLN
7	K	85	GLN
7	K	98	ASN
7	L	4	GLN
7	L	30	ASN

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Mol	Chain	Res	Type
7	L	35	GLN
7	L	98	ASN
7	M	4	GLN
7	M	6	GLN
7	M	9	GLN
7	M	10	GLN
8	N	46	ASN
8	N	57	ASN
8	N	68	GLN
8	N	82	GLN
9	Q	84	HIS
9	Q	171	GLN
9	Q	284	ASN
9	Q	297	HIS
9	Q	338	GLN
9	Q	340	HIS
10	R	14	GLN
10	R	100	ASN
10	R	115	GLN
10	R	278	HIS
10	R	305	HIS
10	R	316	GLN
10	R	412	HIS
10	R	433	GLN
10	R	465	ASN
10	R	547	HIS
10	R	604	ASN
10	R	734	ASN
10	R	748	HIS
10	R	761	HIS
10	R	829	HIS
11	S	67	GLN
12	T	96	ASN
12	T	99	ASN
12	T	107	ASN
12	T	125	GLN
13	U	272	GLN
13	U	273	ASN
13	U	293	GLN
13	U	296	ASN
13	U	329	ASN
13	U	348	HIS

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Mol	Chain	Res	Type
13	U	370	HIS
13	U	394	GLN
13	U	398	GLN
13	U	401	GLN
13	U	403	GLN
13	U	411	GLN
14	V	300	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	ADP	C	701	-	28,29,29	1.42	5 (17%)	43,45,45	1.82	9 (20%)

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
15	ADP	C	701	-	-	3/16/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	701	ADP	C5-C4	4.67	1.47	1.39
15	C	701	ADP	C5-C6	2.63	1.48	1.41
15	C	701	ADP	C5-N7	-2.42	1.34	1.39
15	C	701	ADP	C8-N7	2.27	1.36	1.31
15	C	701	ADP	PA-O3A	2.08	1.61	1.59

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	701	ADP	C5-C4-N3	-5.78	118.76	126.72
15	C	701	ADP	N3-C4-N9	4.62	135.02	127.17
15	C	701	ADP	C2-N3-C4	3.62	120.68	111.83
15	C	701	ADP	C4-C5-N7	-3.31	106.80	110.58
15	C	701	ADP	N3-C2-N1	-3.16	123.80	128.58
15	C	701	ADP	C2'-C1'-N9	-2.80	106.36	113.30
15	C	701	ADP	C4-N9-C8	2.53	108.39	105.74
15	C	701	ADP	C5-N7-C8	2.39	107.21	103.45
15	C	701	ADP	C3'-C2'-C1'	2.13	105.49	101.46

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	C	701	ADP	PB-O3A-PA-O5'
15	C	701	ADP	C5'-O5'-PA-O2A
15	C	701	ADP	C5'-O5'-PA-O3A

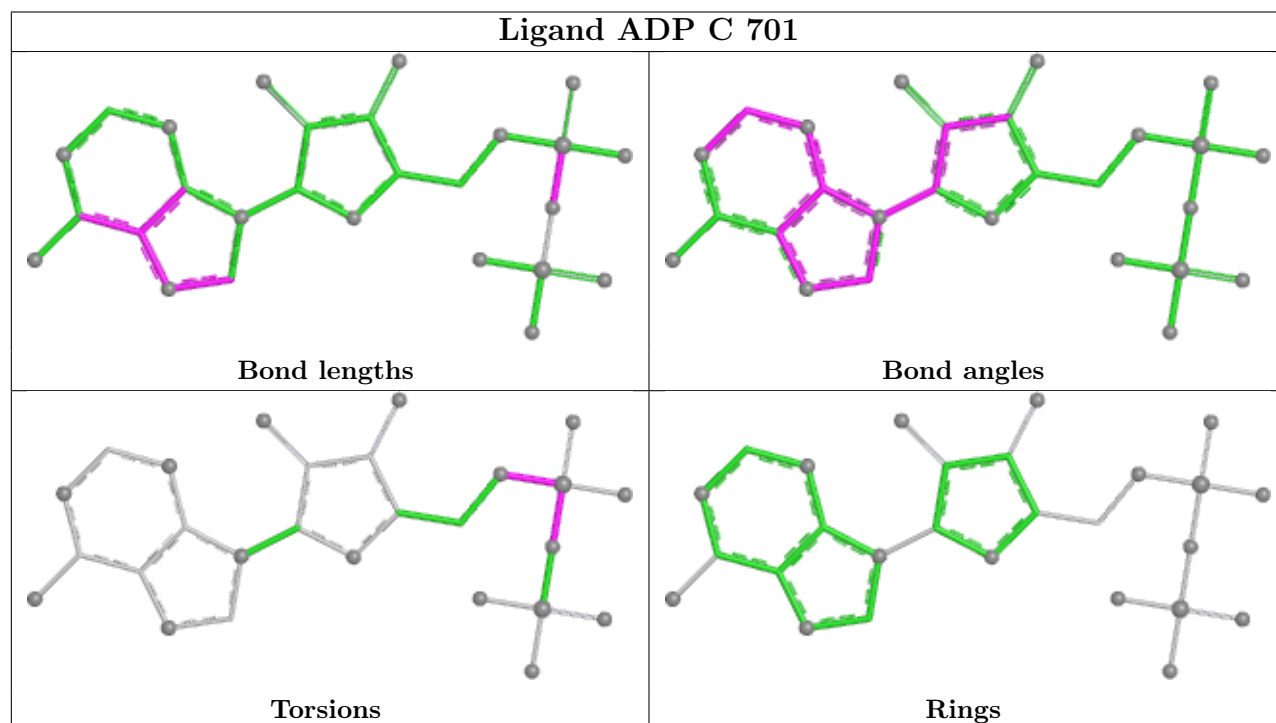
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	701	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

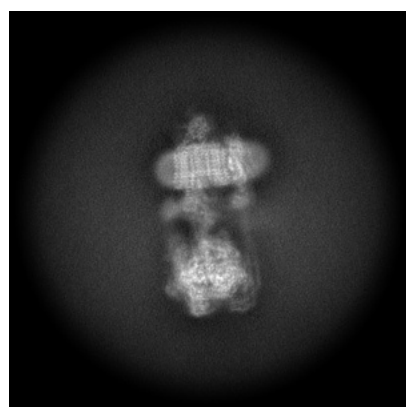
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45533. These allow visual inspection of the internal detail of the map and identification of artifacts.

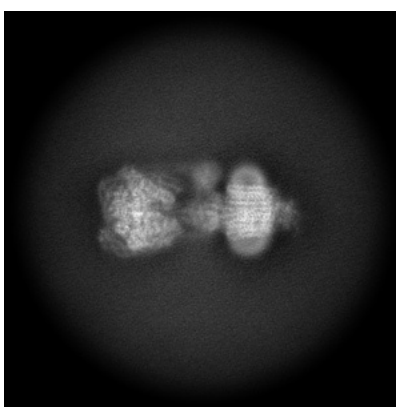
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

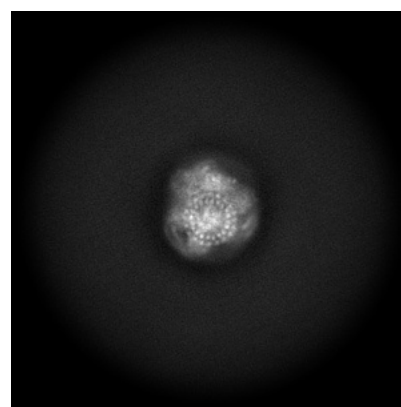
6.1.1 Primary map



X



Y

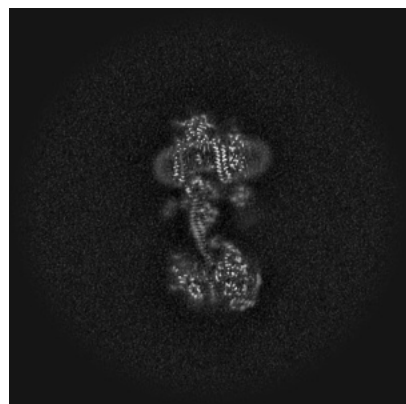


Z

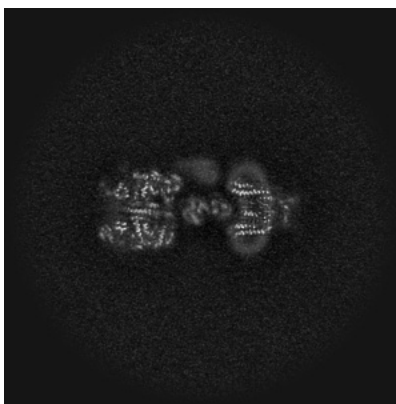
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

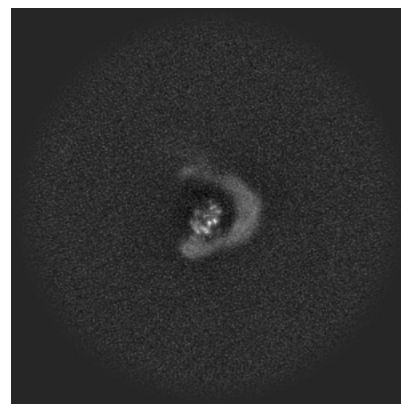
6.2.1 Primary map



X Index: 256



Y Index: 256

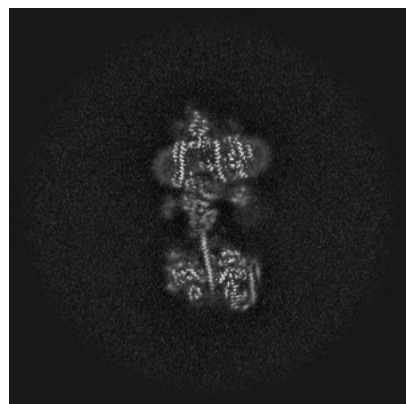


Z Index: 256

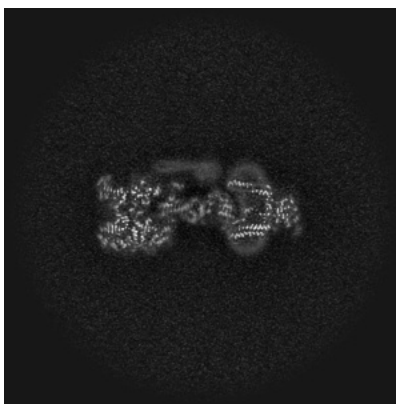
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

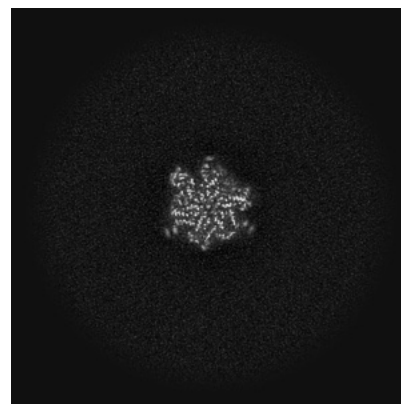
6.3.1 Primary map



X Index: 251



Y Index: 246

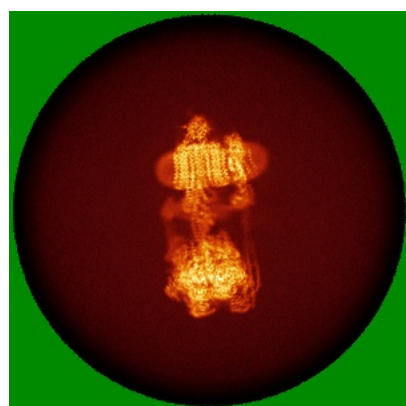


Z Index: 170

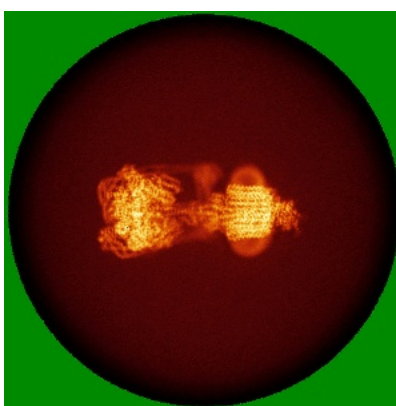
The images above show the largest variance slices of the map in three orthogonal directions.

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

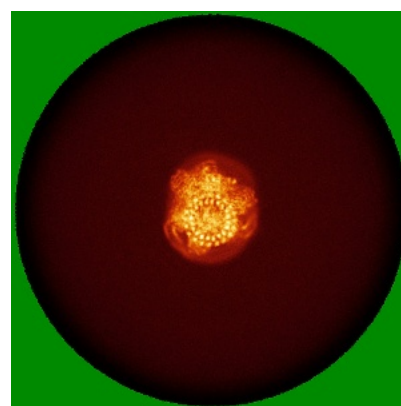
6.4.1 Primary map



X



Y

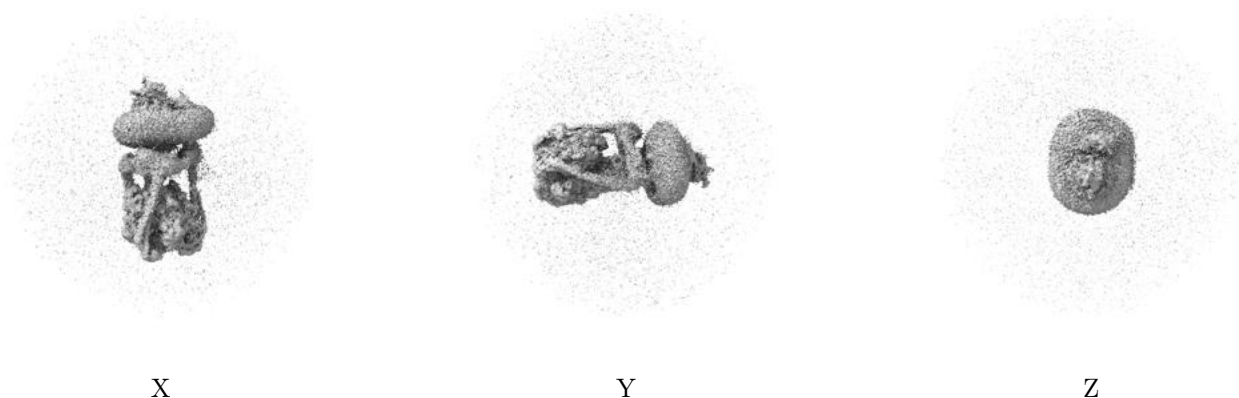


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

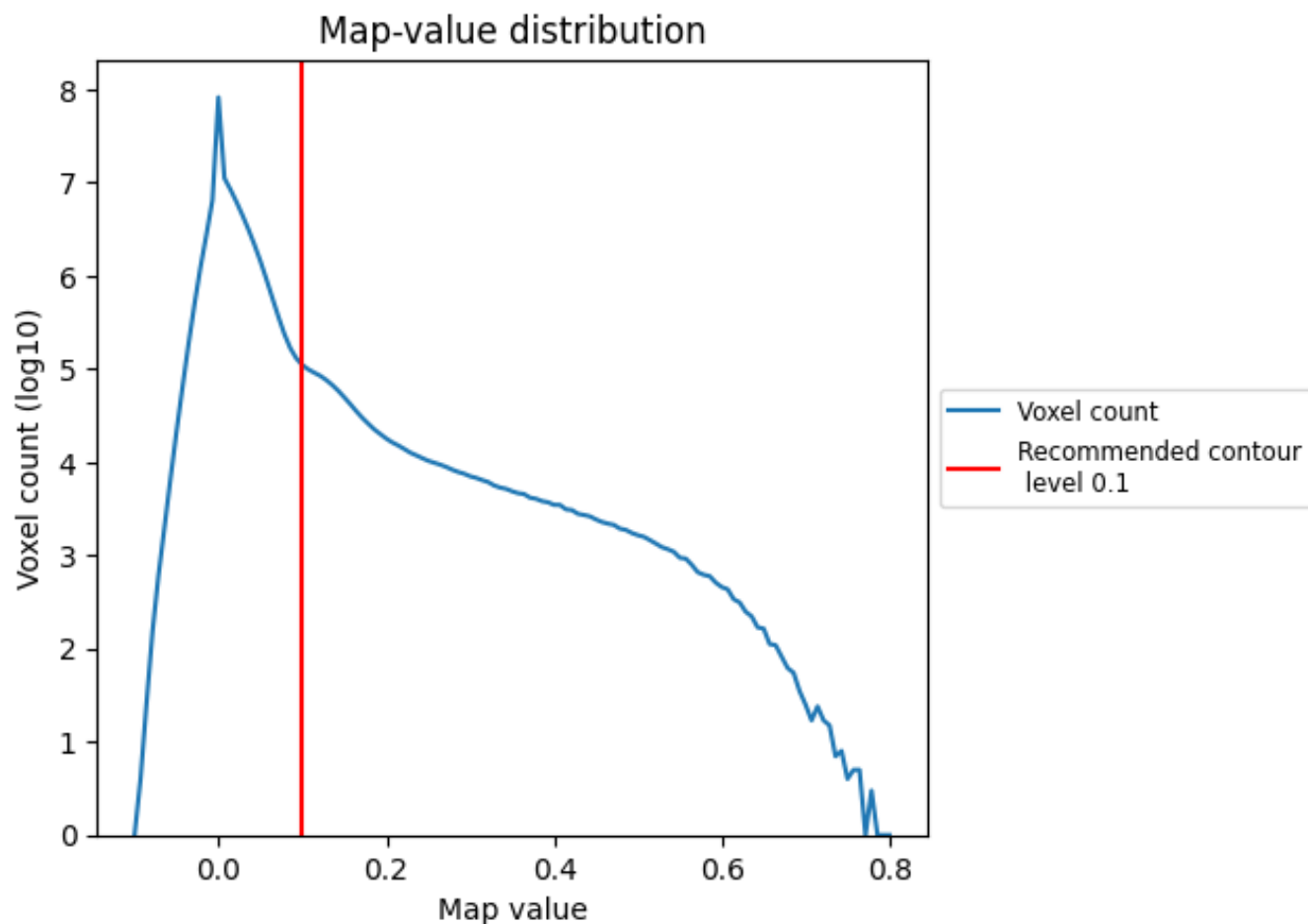
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

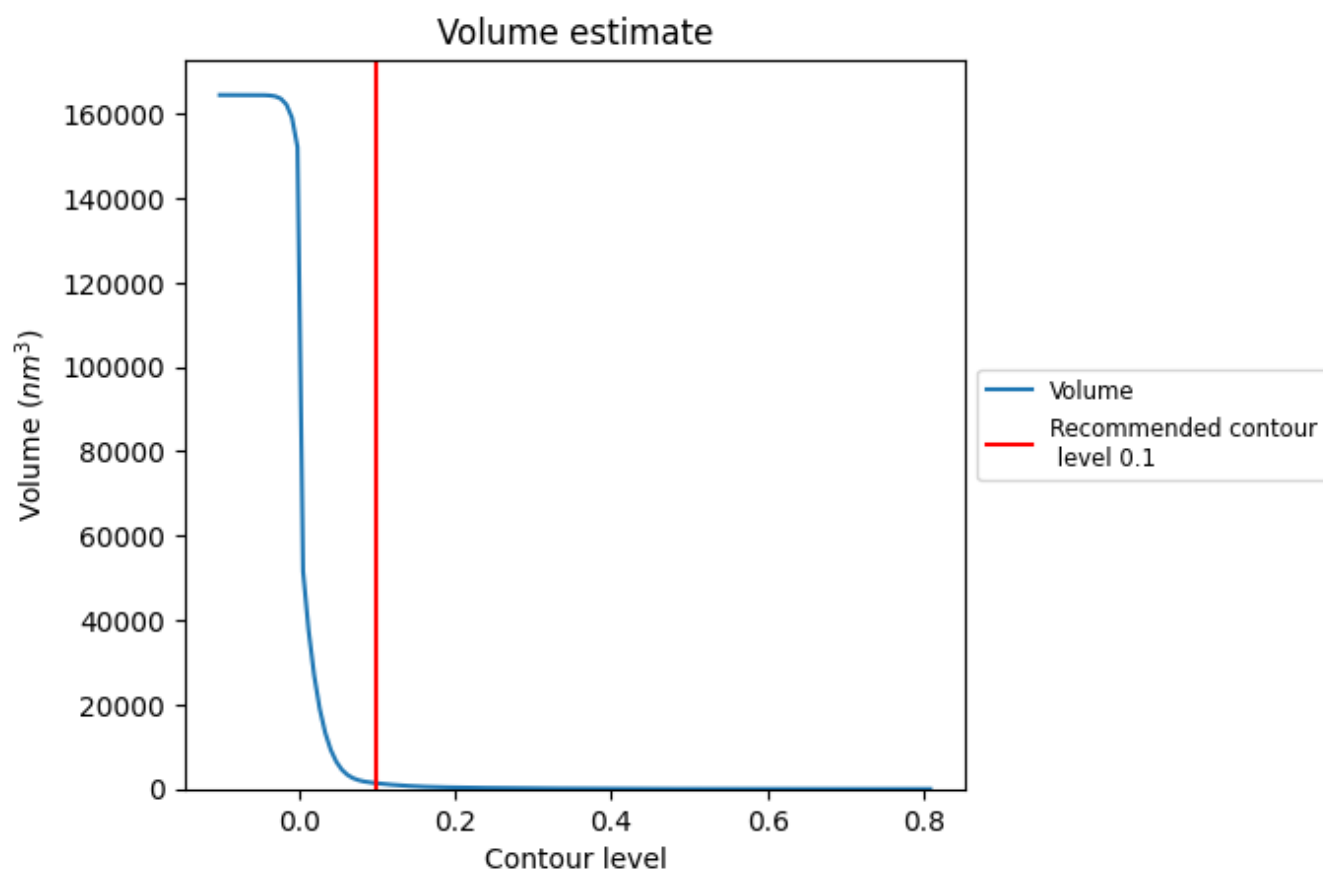
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

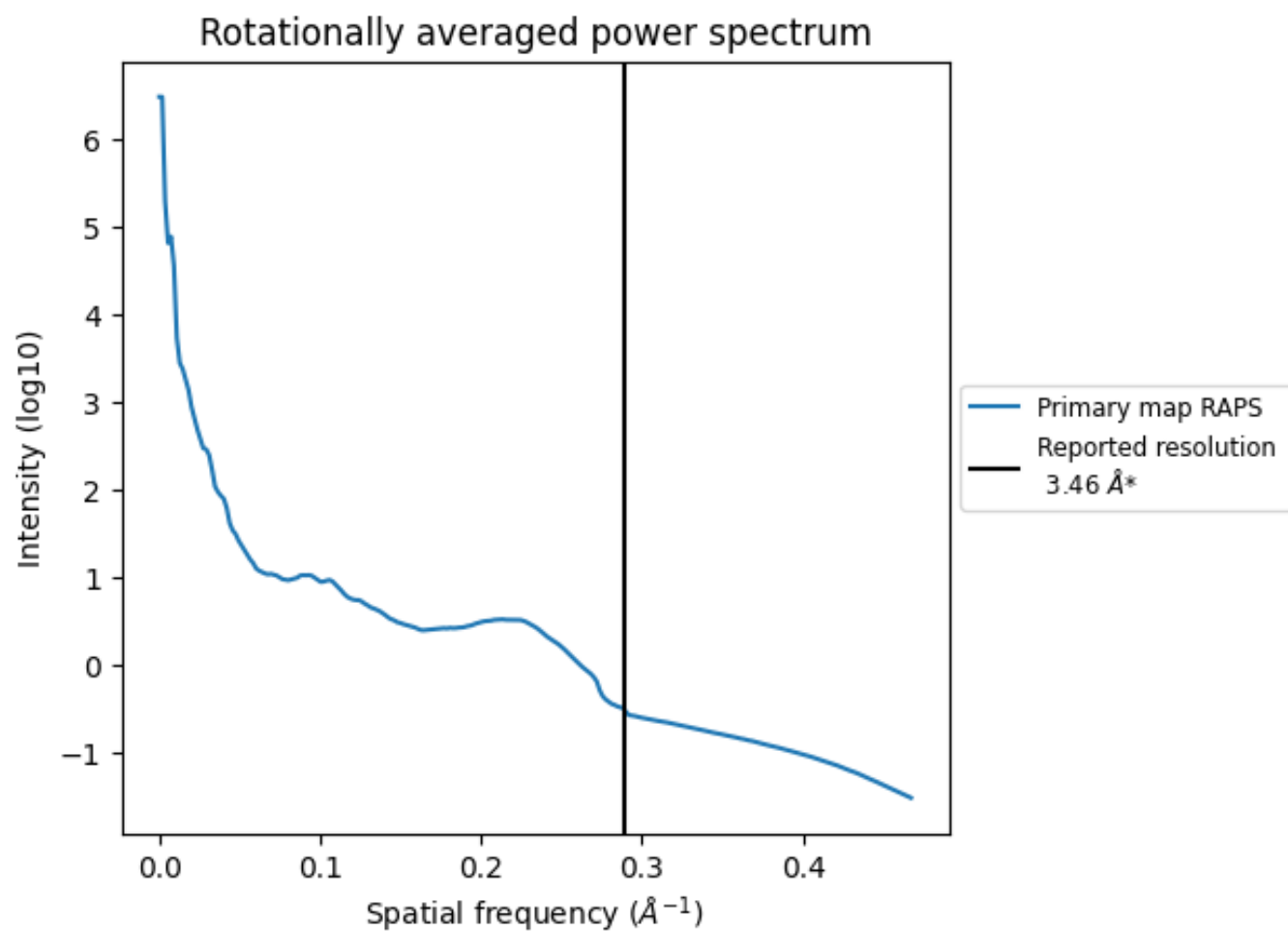
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1344 nm^3 ; this corresponds to an approximate mass of 1214 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 0.289 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

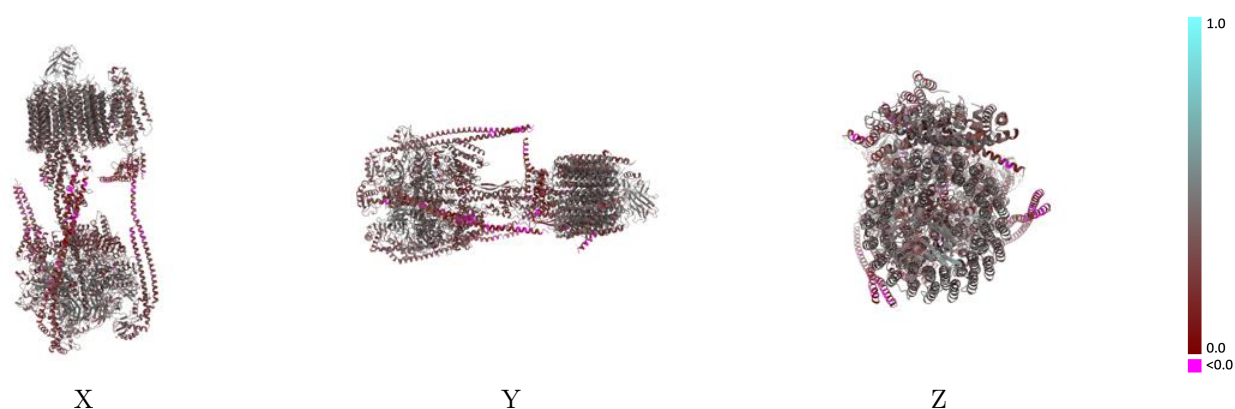
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45533 and PDB model 9CF8. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

This section was not generated.

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

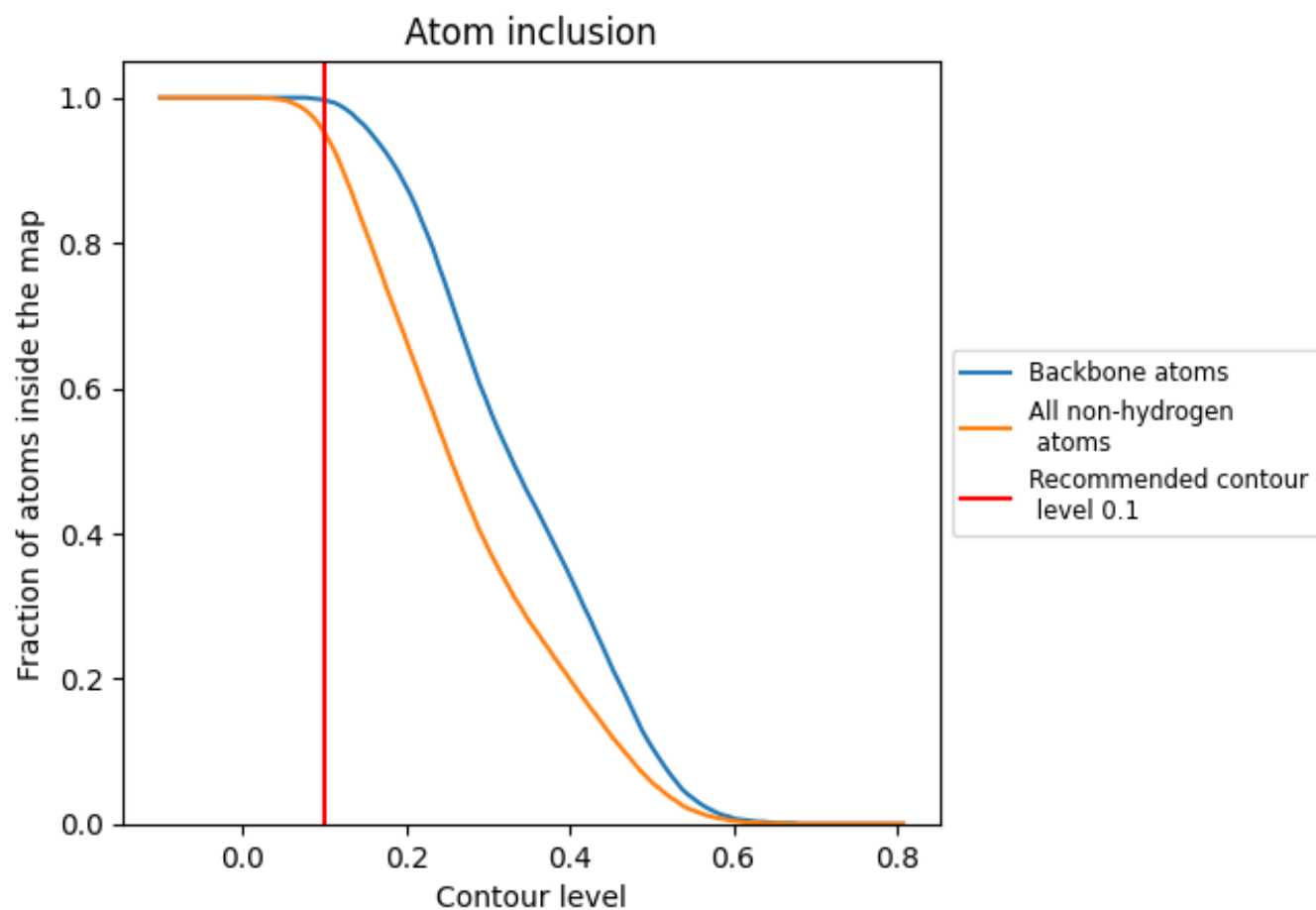


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.































































9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9520	 0.3520
0	 0.9850	 0.4130
1	 0.9800	 0.4100
2	 0.9760	 0.4010
3	 0.9700	 0.3900
4	 0.9750	 0.4080
5	 0.9760	 0.4050
6	 0.9710	 0.4040
7	 0.9730	 0.4080
8	 0.9800	 0.4000
9	 0.9820	 0.4070
A	 0.9630	 0.3740
B	 0.9560	 0.3280
C	 0.9630	 0.3820
D	 0.9570	 0.3620
E	 0.9640	 0.4000
F	 0.9720	 0.3970
G	 0.9390	 0.3180
H	 0.8740	 0.2860
I	 0.8860	 0.2570
J	 0.8880	 0.2590
K	 0.8060	 0.1850
L	 0.8620	 0.1840
M	 0.8840	 0.2030
N	 0.9590	 0.2720
Q	 0.9430	 0.3000
R	 0.9680	 0.3220
S	 0.9650	 0.3990
T	 0.9720	 0.3570
U	 0.9760	 0.4250
V	 0.9670	 0.4390

