



Full wwPDB EM Validation Report ⓘ

May 2, 2026 – 02:16 PM EDT

PDB ID : 9DGR / pdb_00009dgr
EMDB ID : EMD-46845
Title : Composite structure of dynein-dynactin on microtubules
Authors : Rao, Q.; Chai, P.; Zhang, K.
Deposited on : 2024-09-03
Resolution : 15.00 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:

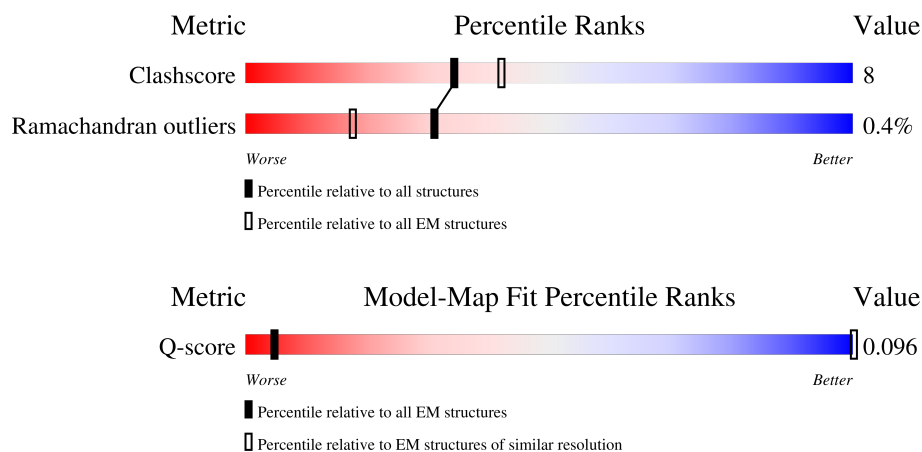
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 15.00 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.



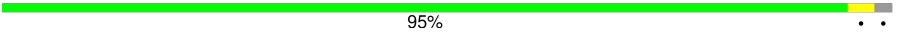
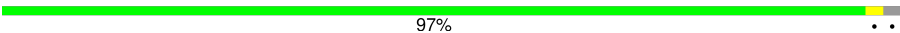
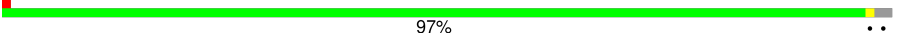
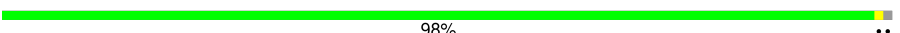











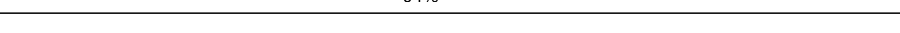





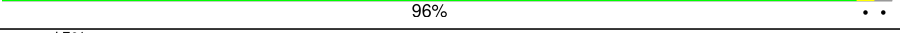
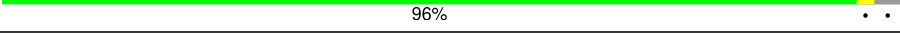


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	37 (14.50 - 15.50)

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

Mol	Chain	Length	Quality of chain
1	A	376	95% ..
1	B	376	96% ..
1	C	376	98% .
1	D	376	95% ..
1	E	376	96% ..


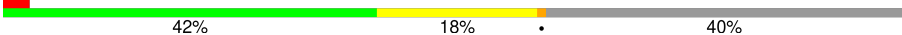
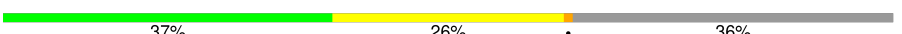



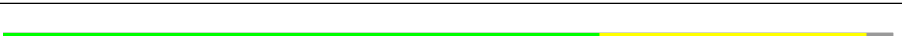
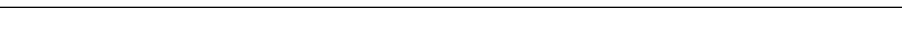
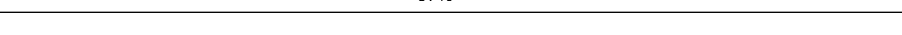
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Mol	Chain	Length	Quality of chain
1	F	376	
1	G	376	
1	I	376	
2	H	375	
3	J	417	
4	K	286	
5	L	272	
6	M	405	
6	N	405	
6	P	405	
6	Q	405	
7	O	186	
7	R	186	
8	U	190	
9	V	182	
10	W	1281	
10	Z	1281	
11	Y	467	
12	e	4646	
12	f	4646	
12	m	4646	
12	n	4646	
13	g	612	
13	h	612	
13	o	612	

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Mol	Chain	Length	Quality of chain
13	p	612	 56%42%
14	i	492	 42%18%40%
14	j	492	 37%26%36%
14	q	492	 60%37%
14	r	492	 57%40%
15	k	96	 66%31%
15	l	96	 67%30%
15	s	96	 97%
15	t	96	 97%

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 131638 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 Alpha-centractin.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	B	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	C	375	Total	C	N	O	0	0
			1847	1097	375	375		
1	D	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	E	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	F	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	G	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	I	370	Total	C	N	O	0	0
			1822	1082	370	370		

- Molecule 2 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	H	370	Total	C	N	O	0	0
			1822	1082	370	370		

- Molecule 3 is a protein called Actin-related protein 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	J	379	Total	C	N	O	0	0
			1868	1110	379	379		

- Molecule 4 is a protein called F-actin-capping protein subunit alpha-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	K	278	Total	C	N	O	0	0
			1378	822	278	278		

- Molecule 5 is a protein called F-actin-capping protein subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	L	269	Total	C	N	O	0	0
			1327	789	269	269		

- Molecule 6 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	M	340	Total	C	N	O	0	0
			1689	1009	340	340		
6	N	280	Total	C	N	O	0	0
			1394	834	280	280		
6	P	325	Total	C	N	O	0	0
			1612	962	325	325		
6	Q	343	Total	C	N	O	0	0
			1707	1021	343	343		

- Molecule 7 is a protein called Dynactin subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	179	Total	C	N	O	0	0
			888	530	179	179		
7	R	170	Total	C	N	O	0	0
			844	504	170	170		

- Molecule 8 is a protein called Dynactin subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	U	167	Total	C	N	O	0	0
			822	488	167	167		

- Molecule 9 is a protein called Dynactin subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	V	179	Total	C	N	O	0	0
			881	523	179	179		

- Molecule 10 is a protein called Dynactin subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	W	152	Total	C	N	O	0	0
			754	450	152	152		
10	Z	192	Total	C	N	O	0	0
			952	568	192	192		

- Molecule 11 is a protein called Dynactin subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	Y	410	Total	C	N	O	0	0
			2038	1218	410	410		

- Molecule 12 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	e	4569	Total	C	N	O	0	0
			22644	13506	4569	4569		
12	f	4565	Total	C	N	O	0	0
			22625	13495	4565	4565		
12	m	4562	Total	C	N	O	0	0
			18883	9759	4562	4562		
12	n	4526	Total	C	N	O	0	0
			18703	9651	4526	4526		

- Molecule 13 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	g	358	Total	C	N	O	0	0
			1767	1051	358	358		
13	h	358	Total	C	N	O	0	0
			1767	1051	358	358		
13	o	358	Total	C	N	O	0	0
			1767	1051	358	358		
13	p	358	Total	C	N	O	0	0
			1767	1051	358	358		

- Molecule 14 is a protein called Dynein light intermediate chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	i	297	Total	C	N	O	0	0
			1472	878	297	297		
14	j	314	Total	C	N	O	0	0
			1555	927	314	314		

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Mol	Chain	Residues	Atoms				AltConf	Trace
14	q	309	Total	C	N	O	0	0
			1241	623	309	309		
14	r	297	Total	C	N	O	0	0
			1193	599	297	297		

- Molecule 15 is a protein called Dynein light chain roadblock.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	k	93	Total	C	N	O	0	0
			462	276	93	93		
15	l	93	Total	C	N	O	0	0
			462	276	93	93		
15	s	93	Total	C	N	O	0	0
			374	188	93	93		
15	t	93	Total	C	N	O	0	0
			374	188	93	93		

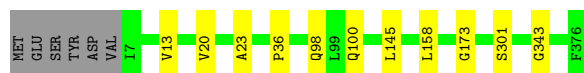
- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
16	Y	3	Total	Zn	0
			3	3	

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
17	m	1	Total	Mg	0
			1	1	
17	n	1	Total	Mg	0
			1	1	

Chain F:  95%



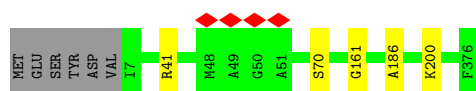
- Molecule 1: Alpha-centractin

Chain G:  97%



- Molecule 1: Alpha-centractin

Chain I:  97%



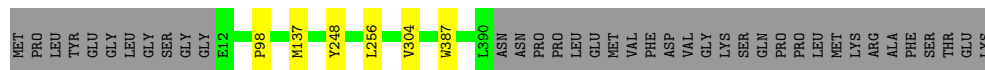
- Molecule 2: Actin, cytoplasmic 1

Chain H:  98%



- Molecule 3: Actin-related protein 10

Chain J:  89%



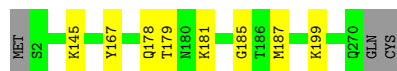
- Molecule 4: F-actin-capping protein subunit alpha-1

Chain K:  92%



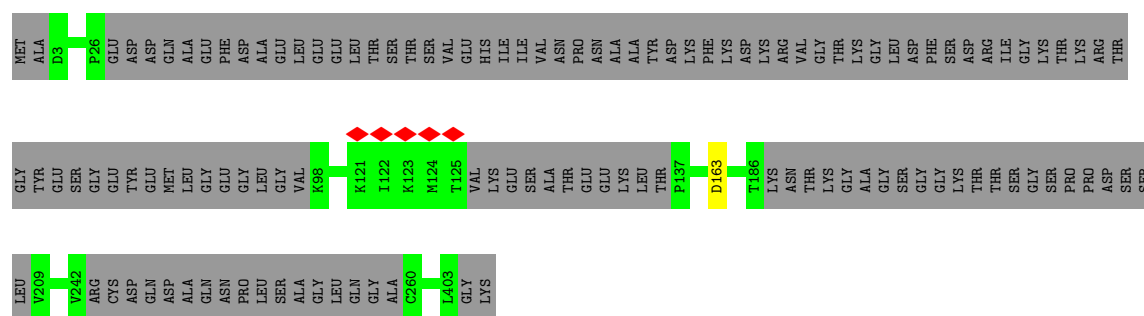
- Molecule 5: F-actin-capping protein subunit beta

Chain L:  96%

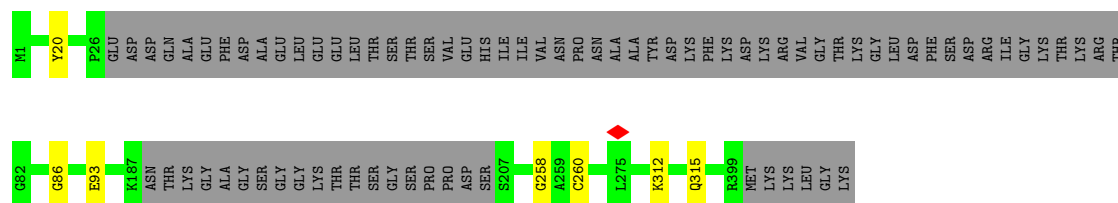


- Molecule 6: Dynactin subunit 2

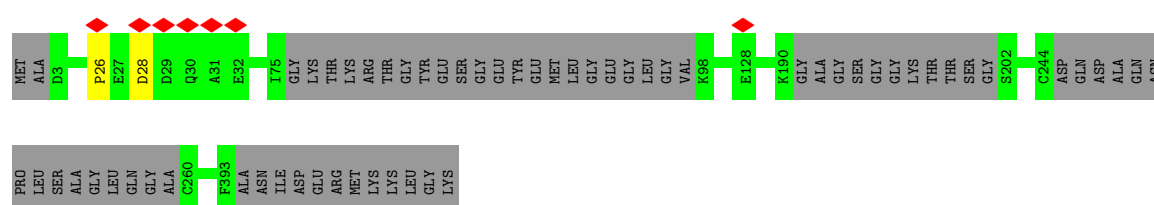
- Molecule 6: Dynactin subunit 2



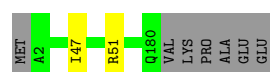
- Molecule 6: Dynactin subunit 2



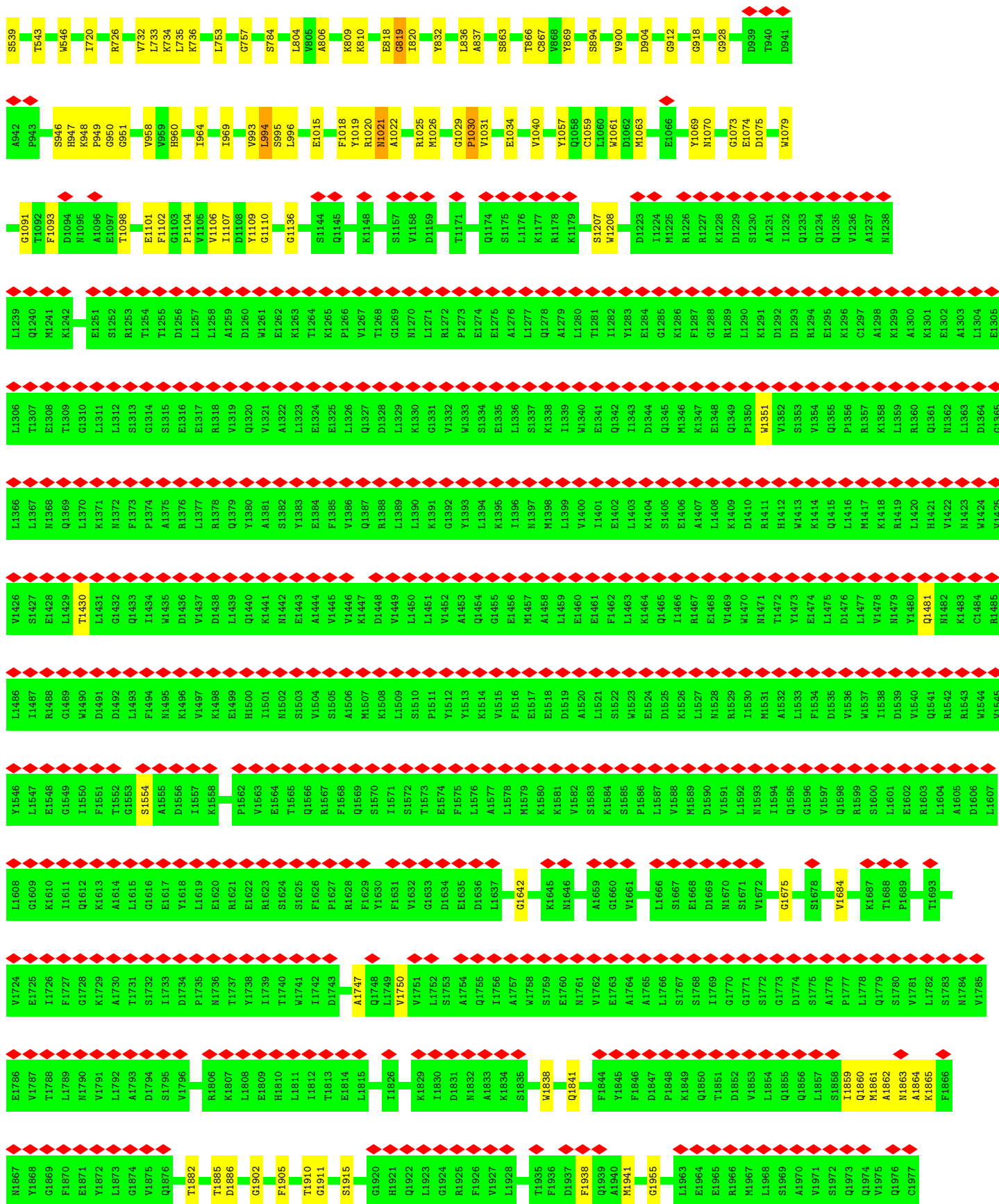
- Molecule 6: Dynactin subunit 2

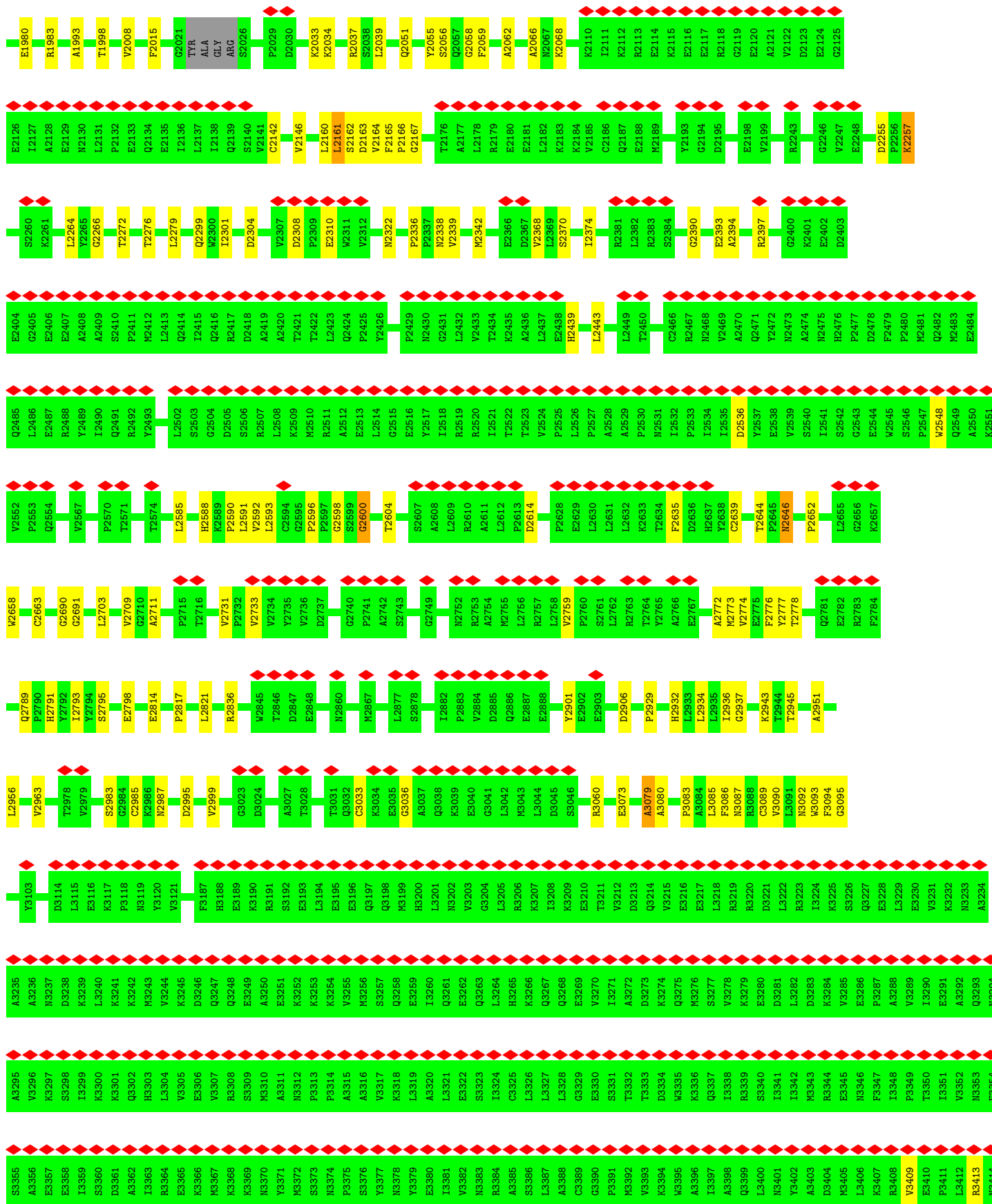


- Molecule 7: Dynactin subunit 3

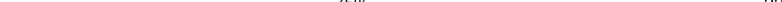






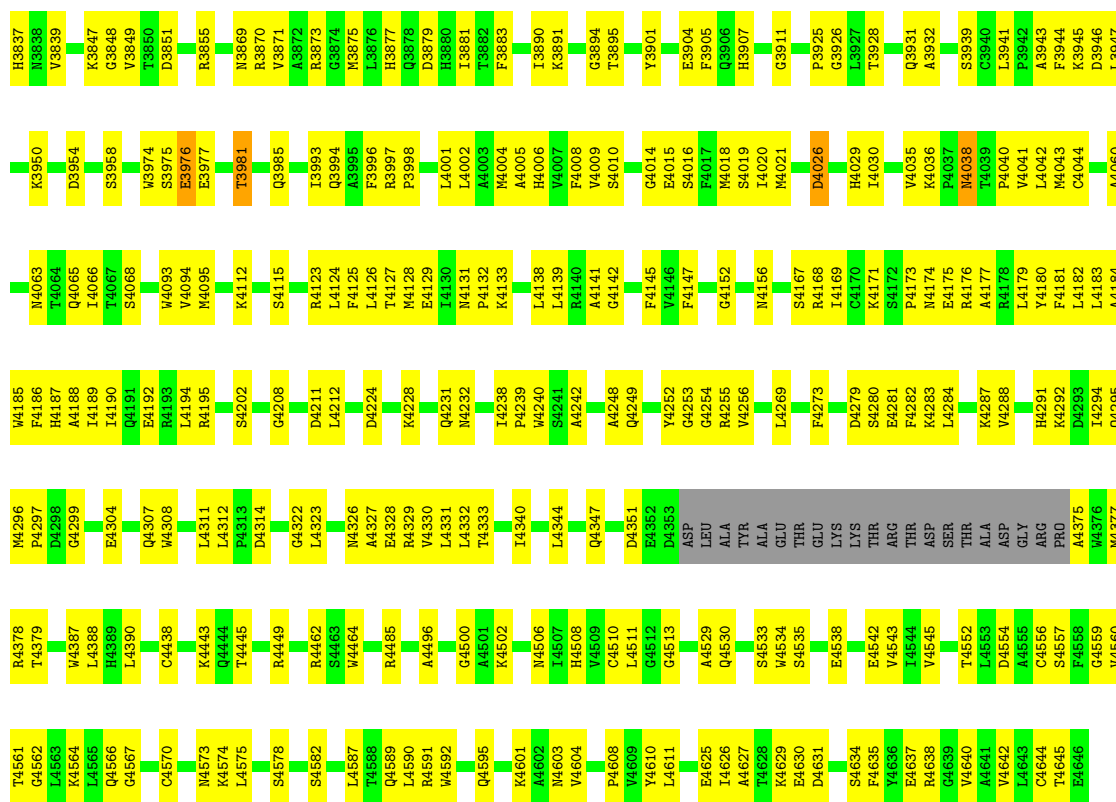


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Q4307	W4308	V4309	E4310	L4311	D4312	P4313	D4314	T4315	Q4316	T4317	P4318	S4319	V4320	L4321	G4322	L4323	P4324	N4325	N4326	A4327	L4331	L4332	T4333	T4334	Q4335	G4336	V4337	D4338	M4339	L4340	N4343	D4353	ASP	LEU	ALA	TYR	GLU	THR	GLU	LYS	THR	ARG	THR	ASP	SER	THR	ALA	ASP	GLY	ARG	PRO	A4375	V4376	N4377																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
F4222	D4225	T4226	A4227	K4228	G4229	R4230	Q4231	N4232	I4233	S4234	P4235	D4236	K4237	L4238	L4246	M4247	A4248	Q4249	S4250	T4251	Y4252	G4253	G4254	D4255	T4274	S4277	F4278	D4279	E4280	S4281	F4282	K4283	L4284	A4285	C4286	K4287	V4288	D4289	Q4290	H4291	K4292	D4293	L4294	Q4295	M4296	P4297	D4298	G4299	R4300	R4301	R4302	E4303	F4304	F4305	V4306																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
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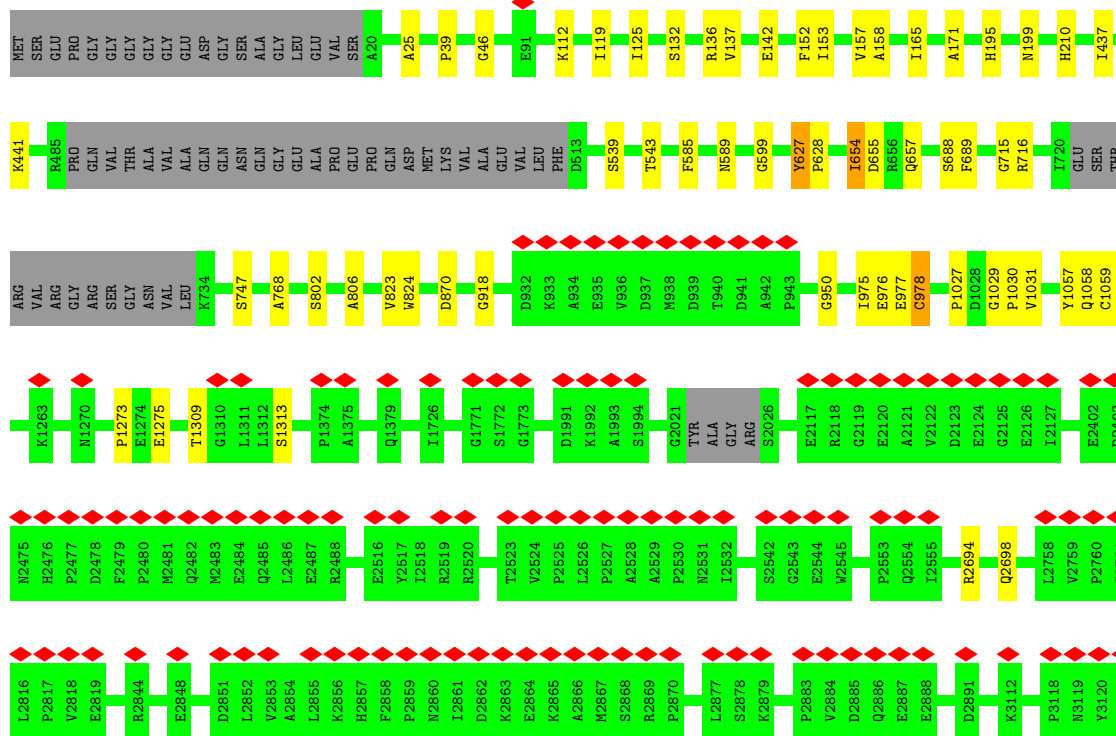
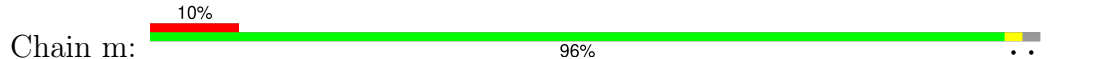
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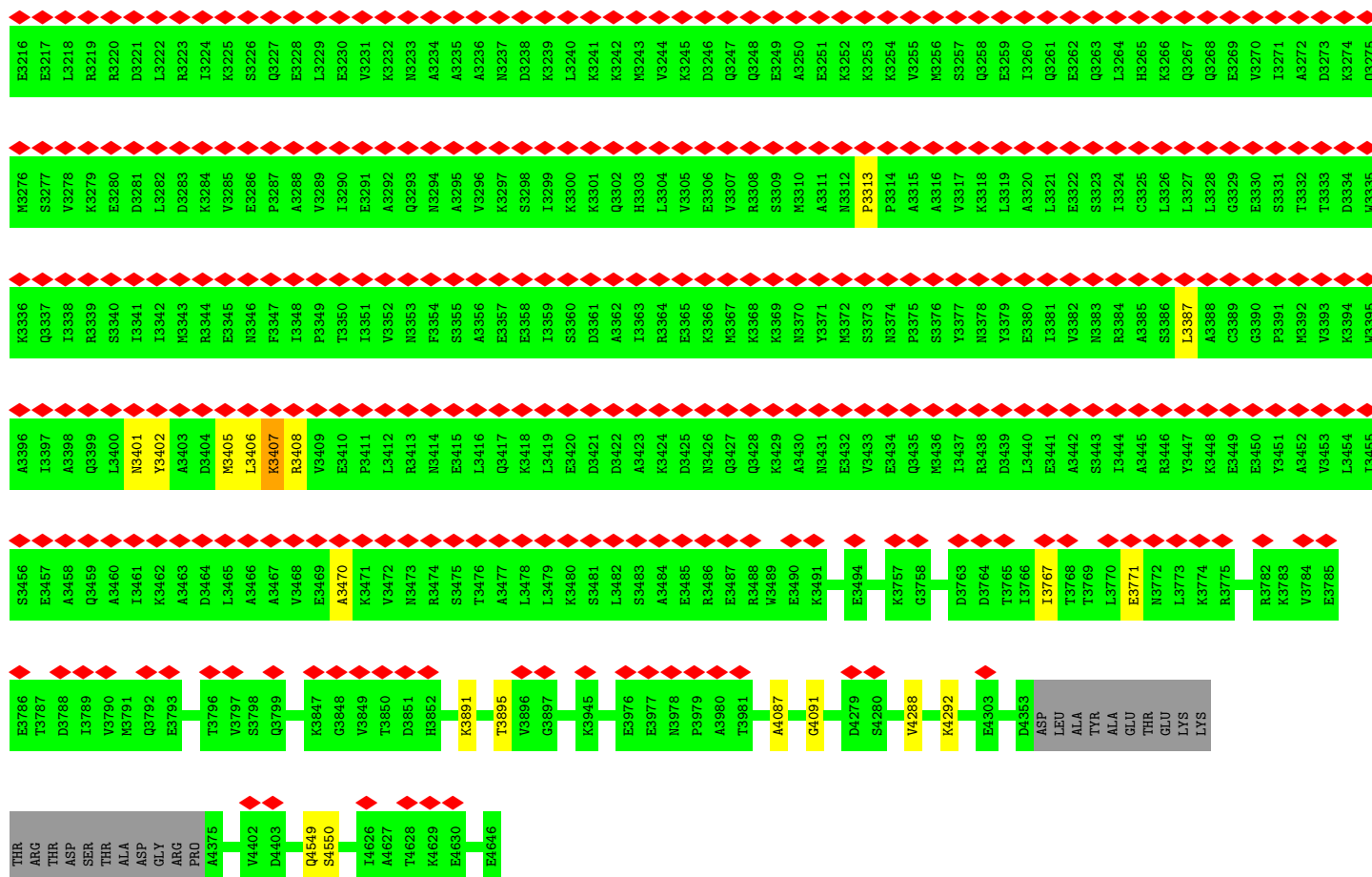


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L3679	L3440		E3380	L3264							P2768	
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T3681	A3442		V3382	K3266								
	S3443		N3383	K3267								
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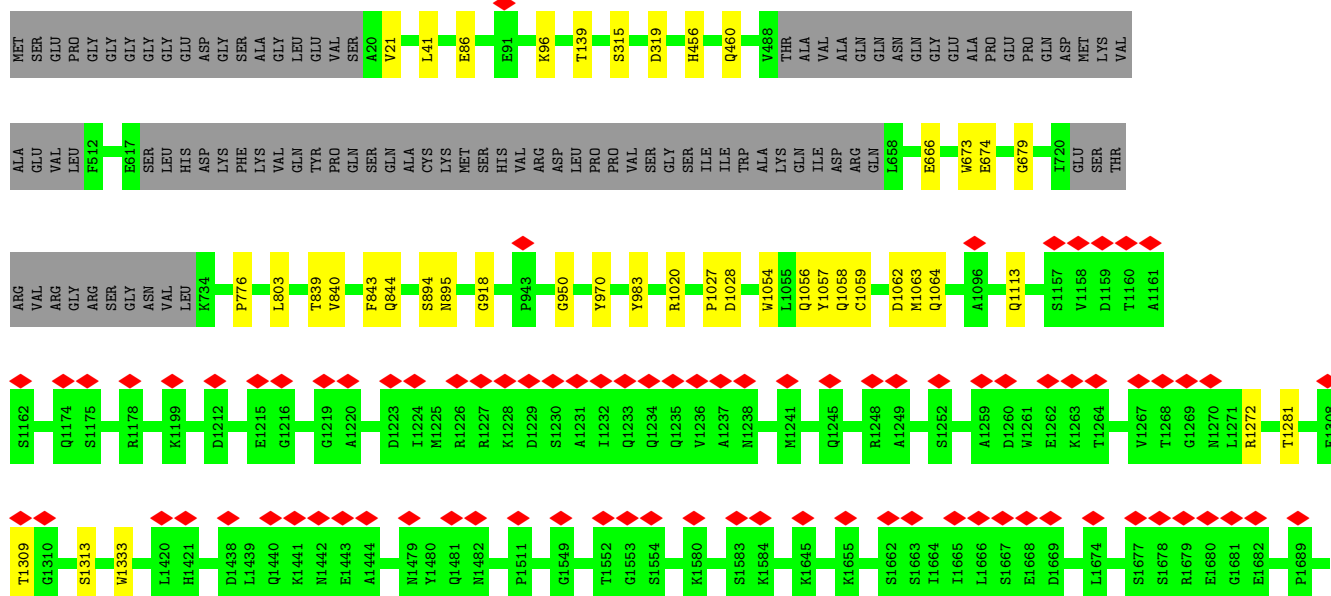


• Molecule 12: Cytoplasmic dynein 1 heavy chain 1





• Molecule 12: Cytoplasmic dynein 1 heavy chain 1

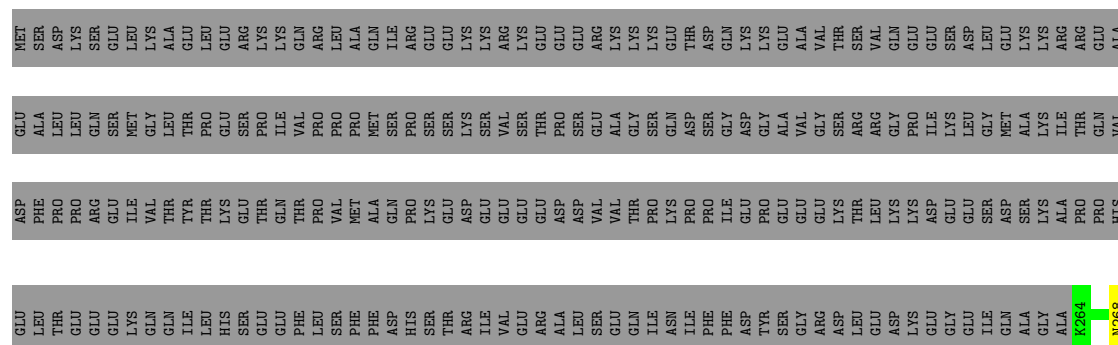






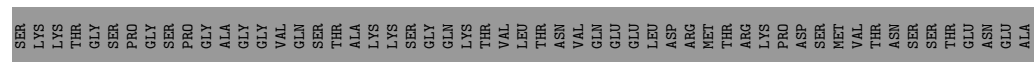
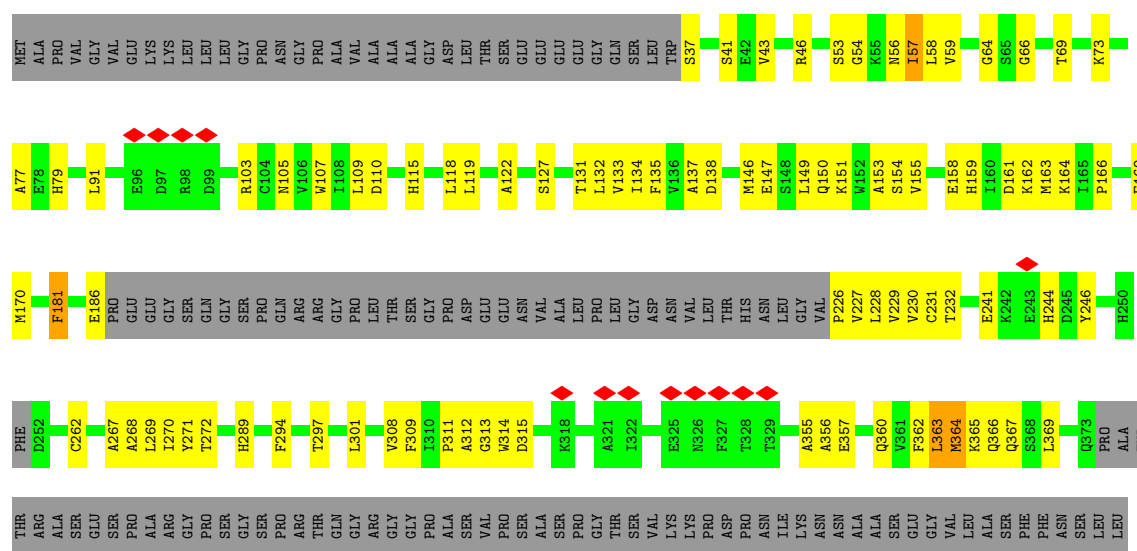
• Molecule 13: Cytoplasmic dynein 1 intermediate chain 2

Chain p: 56% 42%



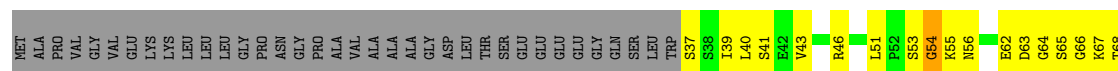
• Molecule 14: Dynein light intermediate chain

Chain i: 42% 18% 40%



• Molecule 14: Dynein light intermediate chain

Chain j: 37% 26% 36%



Chain k:  66% 31% .



- Molecule 15: Dynein light chain roadblock

Chain l:  67% 30% .



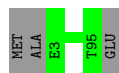
- Molecule 15: Dynein light chain roadblock

Chain s:  97% .



- Molecule 15: Dynein light chain roadblock

Chain t:  97% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16372	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.404	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.05	Depositor
Map size (\AA)	990.0, 990.0, 990.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	3.3, 3.3, 3.3	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.16	0/1821	0.40	0/2531
1	B	0.18	0/1821	0.48	0/2531
1	C	0.18	0/1846	0.46	0/2566
1	D	0.17	0/1821	0.42	0/2531
1	E	0.17	0/1821	0.46	0/2531
1	F	0.18	0/1821	0.46	0/2531
1	G	0.18	0/1821	0.44	0/2531
1	I	0.15	0/1821	0.43	0/2531
2	H	0.17	0/1821	0.40	0/2531
3	J	0.28	0/1867	0.50	0/2596
4	K	0.16	0/1377	0.40	0/1919
5	L	0.16	0/1326	0.37	0/1844
6	M	0.17	0/1684	0.45	0/2343
6	N	0.15	0/1389	0.40	0/1933
6	P	0.17	0/1609	0.42	0/2240
6	Q	0.16	0/1703	0.39	0/2373
7	O	0.15	0/887	0.44	0/1236
7	R	0.17	0/843	0.49	0/1175
8	U	0.21	0/821	0.54	0/1140
9	V	0.15	0/880	0.42	0/1222
10	W	0.16	0/750	0.45	0/1040
10	Z	0.17	0/951	0.48	0/1325
11	Y	0.40	0/2035	0.58	1/2837 (0.0%)
12	e	0.40	1/22639 (0.0%)	0.72	15/31566 (0.0%)
12	f	0.59	3/22620 (0.0%)	0.91	42/31540 (0.1%)
12	m	0.60	1/18878 (0.0%)	0.82	21/24065 (0.1%)
12	n	0.64	6/18697 (0.0%)	0.86	41/23810 (0.2%)
13	g	0.18	0/1766	0.32	0/2457
13	h	0.14	0/1766	0.40	0/2457
13	o	0.13	0/1766	0.37	1/2457 (0.0%)
13	p	0.14	0/1766	0.37	1/2457 (0.0%)
14	i	0.62	1/1469 (0.1%)	1.38	6/2044 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
14	j	0.79	0/1551	1.16	6/2156 (0.3%)
14	q	1.39	2/1237 (0.2%)	1.68	8/1543 (0.5%)
14	r	0.75	2/1190 (0.2%)	1.12	7/1486 (0.5%)
15	k	0.68	1/461 (0.2%)	0.99	1/642 (0.2%)
15	l	0.78	0/461	1.22	2/642 (0.3%)
15	s	1.02	0/373	1.18	0/466
15	t	1.00	0/373	1.16	0/466
All	All	0.50	17/131549 (0.0%)	0.76	152/178291 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	e	0	2
12	f	0	26
14	j	0	2
14	q	0	1
14	r	0	2
15	l	0	1
All	All	0	34

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	i	362	PHE	C-N	-9.03	1.22	1.33
12	n	1063	MET	C-O	8.29	1.33	1.24
12	n	1062	ASP	C-O	-8.15	1.14	1.24
14	r	79	HIS	C-N	7.88	1.38	1.33
12	f	2715	PRO	CA-CB	-7.72	1.42	1.53
12	n	1020	ARG	C-O	-7.27	1.14	1.24
12	n	1027	PRO	C-O	-6.39	1.16	1.24
12	n	3480	LYS	C-O	6.07	1.31	1.24
12	e	1102	PHE	CA-CB	-5.94	1.45	1.53
12	f	1349	GLN	N-CA	-5.88	1.39	1.46
12	m	1273	PRO	C-O	5.86	1.31	1.24
14	q	353	GLU	C-O	5.60	1.30	1.24
12	f	4202	SER	CA-C	-5.38	1.47	1.53
14	r	58	LEU	C-N	-5.33	1.26	1.33
14	q	43	VAL	C-O	-5.32	1.18	1.24
15	k	79	MET	CA-CB	-5.26	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	n	3381	ILE	C-O	-5.15	1.18	1.24

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	i	363	LEU	N-CA-CB	-42.24	48.73	109.98
14	r	79	HIS	CA-C-N	-14.07	108.83	122.20
14	r	79	HIS	C-N-CA	-14.07	108.83	122.20
14	i	362	PHE	CA-C-N	-13.45	102.34	120.63
14	i	362	PHE	C-N-CA	-13.45	102.34	120.63
12	m	1030	PRO	N-CA-C	-12.64	99.88	114.92
12	f	3976	GLU	N-CA-C	-11.95	97.03	112.93
12	n	3407	LYS	N-CA-C	-10.63	99.69	111.07
12	f	3977	GLU	N-CA-C	-10.08	102.05	114.75
12	m	3407	LYS	N-CA-C	-9.94	100.43	111.07
12	e	4038	ASN	N-CA-C	-9.70	99.80	112.41
12	f	889	ASN	N-CA-C	-9.62	100.87	111.36
15	l	82	PRO	CA-C-N	-9.41	103.56	121.54
15	l	82	PRO	C-N-CA	-9.41	103.56	121.54
12	f	1515	VAL	N-CA-C	-9.34	103.58	112.83
14	j	86	LEU	CA-C-N	-9.27	108.84	122.65
14	j	86	LEU	C-N-CA	-9.27	108.84	122.65
12	n	3470	ALA	N-CA-C	-9.15	100.13	111.11
12	n	1062	ASP	CA-C-N	9.01	136.61	122.74
12	n	1062	ASP	C-N-CA	9.01	136.61	122.74
12	m	3470	ALA	N-CA-C	-8.75	100.61	111.11
12	f	4133	LYS	N-CA-C	-8.69	102.69	113.28
14	j	80	GLY	N-CA-C	-8.39	102.58	110.21
12	f	2387	LEU	N-CA-C	-8.23	103.26	113.38
12	n	1027	PRO	CA-C-N	-8.15	109.38	122.66
12	n	1027	PRO	C-N-CA	-8.15	109.38	122.66
12	m	1313	SER	CA-C-O	-8.08	112.99	121.55
12	f	3758	GLY	N-CA-C	-8.01	104.16	115.30
12	f	1986	SER	CA-C-N	-7.88	109.94	120.65
12	f	1986	SER	C-N-CA	-7.88	109.94	120.65
12	m	978	CYS	N-CA-C	-7.79	102.87	111.36
12	e	3618	ALA	N-CA-C	-7.69	104.82	112.97
14	q	217	ASN	N-CA-C	-7.67	101.36	110.41
12	f	1935	THR	N-CA-C	-7.61	104.00	113.28
12	e	1074	GLU	N-CA-C	-7.55	103.52	112.89
12	n	1313	SER	CA-C-O	-7.43	113.68	121.55
14	i	314	TRP	N-CA-C	-7.41	103.97	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	i	363	LEU	CB-CA-C	7.32	122.30	110.95
12	e	2033	LYS	N-CA-C	-7.31	105.53	114.75
12	f	1209	LEU	CA-C-N	-7.00	110.77	120.71
12	f	1209	LEU	C-N-CA	-7.00	110.77	120.71
14	q	215	GLY	CA-C-O	-6.98	115.50	121.57
12	e	2600	GLY	N-CA-C	-6.94	105.64	115.43
15	k	67	THR	N-CA-C	-6.87	104.90	113.28
12	f	1681	GLY	N-CA-C	-6.86	106.29	115.21
12	n	3405	MET	CA-C-O	-6.73	113.41	120.55
12	f	888	LEU	N-CA-C	-6.68	104.14	112.90
12	f	4026	ASP	N-CA-C	-6.68	103.07	113.02
12	f	887	ASP	N-CA-C	-6.61	105.08	113.01
12	n	1058	GLN	N-CA-C	-6.56	105.39	113.19
14	q	47	ALA	CA-C-N	6.55	130.45	120.82
14	q	47	ALA	C-N-CA	6.55	130.45	120.82
12	e	1021	ASN	N-CA-C	-6.51	104.95	114.39
12	f	893	TYR	CB-CA-C	6.39	123.14	110.42
12	n	3346	ASN	N-CA-C	-6.36	105.00	112.89
14	r	48	ARG	N-CA-C	-6.36	99.99	109.15
12	f	2713	ASN	N-CA-C	-6.35	99.70	109.41
12	f	4038	ASN	N-CA-C	-6.27	106.60	114.56
12	m	3405	MET	CA-C-O	-6.27	113.01	120.10
12	e	2322	ASN	N-CA-C	-6.24	105.57	113.43
14	i	363	LEU	CA-C-O	-6.16	114.56	120.90
12	n	3313	PRO	N-CA-C	6.09	118.13	110.70
12	m	1058	GLN	N-CA-C	-6.08	104.98	113.37
14	j	234	CYS	CA-C-N	-6.06	109.96	121.54
14	j	234	CYS	C-N-CA	-6.06	109.96	121.54
12	e	4018	MET	N-CA-C	-6.02	105.89	113.72
12	m	1027	PRO	N-CA-C	6.00	121.87	113.53
12	e	2257	LYS	N-CA-C	-5.99	107.79	114.62
12	e	2646	ASN	N-CA-C	-5.99	107.21	114.75
12	f	891	HIS	N-CA-C	-5.97	105.18	112.88
12	n	3405	MET	O-C-N	5.96	128.43	122.12
12	n	1281	THR	N-CA-C	-5.95	104.18	112.45
12	f	2229	GLY	N-CA-C	-5.92	99.14	113.18
12	f	1932	CYS	N-CA-C	-5.92	98.19	110.80
12	f	1483	LYS	N-CA-C	-5.91	106.11	113.55
12	m	3405	MET	N-CA-C	-5.86	104.97	111.71
12	m	3313	PRO	N-CA-C	5.86	117.85	110.70
12	n	3224	ILE	CA-C-O	-5.85	114.86	120.95
12	f	3129	VAL	N-CA-C	-5.85	106.02	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	m	1069	TYR	CA-C-O	-5.84	114.89	120.90
12	n	3394	LYS	N-CA-C	-5.84	104.92	111.28
14	r	79	HIS	O-C-N	5.84	130.75	123.28
12	m	1275	GLU	CA-C-N	-5.81	110.98	121.14
12	m	1275	GLU	C-N-CA	-5.81	110.98	121.14
14	q	183	ASP	N-CA-C	-5.79	106.55	113.21
12	f	2305	GLY	N-CA-C	-5.75	99.54	113.18
12	e	1030	PRO	N-CA-C	-5.74	106.97	114.03
12	f	2391	GLU	N-CA-C	-5.71	104.99	112.41
12	n	3402	TYR	CA-C-O	-5.69	114.52	120.55
12	m	1273	PRO	CA-C-O	5.68	130.94	120.60
12	e	1910	THR	N-CA-C	-5.61	104.07	112.54
12	n	3431	ASN	CA-C-O	-5.55	114.66	120.55
12	f	2350	TYR	N-CA-C	-5.55	105.11	112.94
12	f	2362	VAL	CA-C-N	-5.53	113.20	120.95
12	f	2362	VAL	C-N-CA	-5.53	113.20	120.95
12	m	3401	ASN	N-CA-C	-5.49	105.29	111.28
12	n	1063	MET	N-CA-C	-5.47	99.51	108.76
12	n	3407	LYS	CA-C-N	-5.47	112.95	120.28
12	n	3407	LYS	C-N-CA	-5.47	112.95	120.28
12	n	3401	ASN	N-CA-C	-5.42	105.37	111.28
12	n	970	TYR	CA-C-N	-5.41	115.47	123.05
12	n	970	TYR	C-N-CA	-5.41	115.47	123.05
12	e	3617	ASP	N-CA-C	-5.41	106.56	112.72
12	f	2089	GLY	CA-C-O	-5.41	118.42	122.37
12	n	3406	LEU	CA-C-N	-5.40	113.42	120.44
12	n	3406	LEU	C-N-CA	-5.40	113.42	120.44
12	m	3405	MET	CA-C-N	5.37	127.92	120.29
12	m	3405	MET	C-N-CA	5.37	127.92	120.29
12	n	1272	ARG	CA-C-O	-5.37	113.94	120.54
12	n	3401	ASN	O-C-N	5.36	127.81	122.12
14	r	72	THR	O-C-N	5.36	127.80	122.12
12	f	928	GLY	N-CA-C	-5.36	107.96	114.92
14	q	47	ALA	CA-C-O	-5.34	115.27	121.15
12	m	3406	LEU	CA-C-N	-5.33	113.51	120.44
12	m	3406	LEU	C-N-CA	-5.33	113.51	120.44
12	n	3224	ILE	O-C-N	5.33	127.04	121.87
14	j	215	GLY	N-CA-C	-5.30	103.04	110.88
12	n	1064	GLN	CA-C-N	5.30	127.64	120.38
12	n	1064	GLN	C-N-CA	5.30	127.64	120.38
12	n	1333	TRP	N-CA-C	-5.28	106.70	112.72
12	f	1019	TYR	CA-C-N	-5.28	114.72	123.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	f	1019	TYR	C-N-CA	-5.28	114.72	123.37
12	n	3461	ILE	CA-C-O	-5.27	115.47	120.95
14	q	50	LYS	CA-C-O	-5.27	115.50	121.72
12	e	2368	VAL	N-CA-C	-5.27	107.69	112.96
12	n	1028	ASP	N-CA-C	-5.25	107.40	112.97
12	f	1349	GLN	N-CA-C	-5.25	97.94	109.11
14	q	217	ASN	CA-C-O	-5.24	116.31	121.02
12	n	983	TYR	N-CA-C	-5.23	105.75	111.82
12	n	1027	PRO	N-CA-C	5.22	120.79	113.53
12	n	3230	GLU	CA-C-O	-5.22	115.34	120.82
14	r	78	GLU	CA-C-N	-5.21	114.69	122.39
14	r	78	GLU	C-N-CA	-5.21	114.69	122.39
12	n	3444	ILE	CA-C-O	-5.19	115.56	120.95
12	m	3402	TYR	CA-C-O	-5.16	115.08	120.55
12	e	1993	ALA	N-CA-C	-5.15	108.02	114.56
12	f	2196	GLY	N-CA-C	-5.15	100.97	113.18
13	o	428	GLN	CB-CA-C	-5.15	110.62	116.54
13	p	428	GLN	CB-CA-C	-5.14	110.63	116.54
12	f	3045	ASP	N-CA-C	-5.13	104.66	112.04
12	n	3401	ASN	CA-C-O	-5.12	115.12	120.55
12	n	1113	GLN	N-CA-C	-5.11	106.74	112.87
12	f	2675	GLY	N-CA-C	-5.09	106.57	113.24
12	f	3639	GLU	N-CA-C	-5.08	107.75	114.31
12	m	3387	LEU	N-CA-C	-5.07	106.87	113.16
12	n	3461	ILE	O-C-N	5.07	126.79	121.87
12	f	3567	LEU	N-CA-C	-5.05	101.48	108.76
12	n	3405	MET	N-CA-C	-5.05	105.78	111.28
12	f	37	LEU	CA-C-N	5.03	131.44	122.13
12	f	37	LEU	C-N-CA	5.03	131.44	122.13
11	Y	51	CYS	CB-CA-C	5.03	116.37	108.63
12	f	2299	GLN	N-CA-C	-5.01	103.86	110.43

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	e	3079	ALA	Peptide
12	e	4316	GLN	Peptide
12	f	1106	VAL	Peptide
12	f	1118	LEU	Peptide
12	f	1207	SER	Peptide
12	f	1312	LEU	Peptide

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Mol	Chain	Res	Type	Group
12	f	1436	ASP	Peptide
12	f	1596	GLY	Peptide
12	f	2165	PHE	Peptide
12	f	2172	ARG	Peptide
12	f	2226	SER	Peptide
12	f	2230	LYS	Peptide
12	f	2427	PHE	Peptide
12	f	2713	ASN	Peptide
12	f	2760	PRO	Peptide
12	f	2874	SER	Peptide
12	f	2876	TRP	Peptide
12	f	3068	MET	Peptide
12	f	3110	THR	Peptide
12	f	3585	ARG	Peptide
12	f	3757	LYS	Peptide
12	f	3761	LEU	Peptide
12	f	3762	ASP	Peptide
12	f	3974	TRP	Peptide
12	f	4094	VAL	Peptide
12	f	4128	MET	Peptide
12	f	4552	THR	Peptide
12	f	934	ALA	Peptide
14	j	234	CYS	Peptide
14	j	331	LYS	Peptide
15	l	53	ALA	Peptide
14	q	44	SER	Mainchain
14	r	37	SER	Mainchain
14	r	80	GLY	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1822	0	820	7	0
1	B	1822	0	820	7	0
1	C	1847	0	830	5	0
1	D	1822	0	820	9	0
1	E	1822	0	820	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1822	0	820	6	0
1	G	1822	0	820	4	0
1	I	1822	0	820	3	0
2	H	1822	0	835	3	0
3	J	1868	0	823	4	0
4	K	1378	0	611	7	0
5	L	1327	0	585	4	0
6	M	1689	0	765	1	0
6	N	1394	0	632	0	0
6	P	1612	0	747	6	0
6	Q	1707	0	769	1	0
7	O	888	0	413	1	0
7	R	844	0	385	1	0
8	U	822	0	370	2	0
9	V	881	0	379	4	0
10	W	754	0	336	1	0
10	Z	952	0	434	3	0
11	Y	2038	0	886	6	0
12	e	22644	0	10062	295	0
12	f	22625	0	10053	725	0
12	m	18883	0	5554	44	0
12	n	18703	0	5475	38	0
13	g	1767	0	796	10	0
13	h	1767	0	796	12	0
13	o	1767	0	796	7	0
13	p	1767	0	796	11	0
14	i	1472	0	645	91	0
14	j	1555	0	681	99	0
14	q	1241	0	329	10	0
14	r	1193	0	315	6	0
15	k	462	0	192	23	0
15	l	462	0	192	24	0
15	s	374	0	95	0	0
15	t	374	0	95	0	0
16	Y	3	0	0	0	0
17	m	1	0	0	0	0
17	n	1	0	0	0	0
All	All	131638	0	52412	1411	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 8.

All (1411) 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)
12:e:733:LEU:CB	14:i:360:GLN:HA	1.53	1.37
12:e:806:ALA:HA	14:i:356:ALA:N	1.45	1.32
12:n:776:PRO:CB	13:p:375:LEU:O	1.81	1.29
12:f:2645:PRO:O	14:q:220:THR:O	1.60	1.18
12:f:2645:PRO:O	14:q:220:THR:C	1.88	1.15
12:n:803:LEU:O	12:n:894:SER:O	1.62	1.15
12:m:806:ALA:HB1	14:q:356:ALA:N	1.60	1.14
12:n:803:LEU:C	12:n:894:SER:O	1.90	1.12
12:f:890:LEU:HA	12:m:689:PHE:HA	1.27	1.11
12:f:963:ARG:O	12:f:969:ILE:HA	1.51	1.08
12:e:4332:LEU:O	12:e:4336:GLY:N	1.87	1.06
12:e:733:LEU:CB	14:i:360:GLN:CA	2.33	1.05
12:f:1660:GLY:HA3	12:f:1873:LEU:HA	1.39	1.04
12:f:2600:GLY:O	12:f:2604:THR:N	1.91	1.03
12:f:2983:SER:HA	12:f:2988:GLU:H	1.25	1.02
12:f:995:SER:HA	12:f:1020:ARG:HA	1.38	1.01
12:e:4180:TYR:O	12:e:4184:ALA:N	1.93	1.01
12:f:2218:HIS:H	12:f:2321:ASP:HA	1.21	1.00
12:f:3801:TYR:O	12:f:3805:SER:N	1.94	1.00
12:f:4564:LYS:O	12:f:4642:VAL:HA	1.59	0.99
12:f:2773:MET:O	12:f:2777:TYR:N	1.95	0.99
12:m:806:ALA:CB	14:q:356:ALA:H	1.74	0.99
12:f:2229:GLY:O	12:f:2233:ALA:N	1.96	0.98
12:f:3981:THR:O	12:f:3985:GLN:N	1.96	0.98
14:j:180:ASP:O	14:j:184:TYR:N	1.97	0.98
12:m:806:ALA:HB1	14:q:356:ALA:H	1.16	0.97
15:l:58:ARG:HA	15:l:62:PRO:HA	1.45	0.97
12:e:1911:GLY:O	12:e:1915:SER:N	1.98	0.97
12:e:4019:SER:O	12:e:4023:GLN:N	1.97	0.97
14:j:152:TRP:O	14:j:156:LEU:N	1.97	0.96
12:e:806:ALA:CB	14:i:355:ALA:C	2.39	0.95
12:n:918:GLY:HA2	12:n:950:GLY:HA2	1.48	0.95
12:e:720:ILE:HA	12:e:735:LEU:HA	1.48	0.95
12:e:806:ALA:HB2	14:i:355:ALA:HA	1.46	0.94
12:e:806:ALA:O	14:i:356:ALA:HA	1.65	0.94
12:f:1474:GLU:HA	12:f:1587:LEU:HA	1.47	0.94
12:f:1964:GLU:O	12:f:1968:LEU:N	1.98	0.94
12:e:4333:THR:O	12:e:4337:VAL:N	2.01	0.94
12:f:2659:LEU:O	12:f:2706:ILE:HA	1.68	0.93
12:f:4183:LEU:O	12:f:4187:HIS:N	2.01	0.93
12:f:1479:ASN:HA	12:f:1485:ARG:HA	1.48	0.93
12:f:4566:GLN:O	12:f:4640:VAL:HA	1.67	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:l:23:VAL:HA	15:l:29:PRO:HA	1.50	0.93
12:e:806:ALA:HB1	14:i:355:ALA:C	1.94	0.93
12:m:918:GLY:HA2	12:m:950:GLY:HA2	1.49	0.93
12:e:806:ALA:HB2	14:i:355:ALA:CA	1.99	0.92
12:f:2089:GLY:O	12:f:2093:LEU:N	2.03	0.92
12:f:4208:GLY:O	12:f:4212:LEU:N	2.02	0.92
14:i:127:SER:O	14:i:131:THR:N	2.02	0.92
12:f:3521:ASP:O	12:f:3525:ARG:N	2.01	0.92
13:g:366:LYS:HA	15:l:3:GLU:HA	1.50	0.92
12:f:1589:MET:O	12:f:1593:ASN:N	2.02	0.92
12:f:4174:ASN:N	12:f:4231:GLN:O	2.03	0.92
12:e:1075:ASP:O	12:e:1079:TRP:N	2.02	0.91
12:f:917:ALA:C	12:f:950:GLY:HA3	1.95	0.91
12:f:4138:LEU:O	12:f:4142:GLY:N	2.03	0.91
12:e:4181:PHE:O	12:e:4185:TRP:N	2.02	0.91
12:f:2740:GLY:O	12:f:2744:LEU:N	2.04	0.91
12:e:1882:THR:O	12:e:1886:ASP:N	2.03	0.91
12:f:2776:PHE:O	12:f:2780:SER:N	2.03	0.91
12:f:3939:SER:HA	12:f:3945:LYS:HA	1.53	0.91
12:e:806:ALA:CB	14:i:355:ALA:CA	2.49	0.91
12:f:3946:ASP:O	12:f:3950:LYS:N	2.03	0.91
12:f:4610:TYR:N	12:f:4642:VAL:O	2.02	0.91
12:f:2263:HIS:O	12:f:2279:LEU:N	2.04	0.90
15:k:68:PHE:HA	15:k:81:ALA:HA	1.53	0.90
12:f:1098:THR:O	12:f:1110:GLY:N	2.04	0.90
14:j:73:LYS:HA	14:j:78:GLU:HA	1.53	0.90
12:f:4575:LEU:O	12:f:4627:ALA:N	2.05	0.90
14:j:273:SER:O	14:j:277:GLU:N	2.05	0.90
12:f:2829:ALA:O	12:f:2834:GLN:N	2.04	0.89
12:f:2370:SER:O	12:f:2374:ILE:N	2.04	0.89
12:e:806:ALA:CA	14:i:356:ALA:N	2.33	0.89
12:f:923:THR:HA	12:f:1036:SER:HA	1.52	0.89
12:f:4004:MET:O	12:f:4008:PHE:N	2.06	0.88
14:j:144:THR:O	14:j:148:SER:N	2.06	0.88
12:e:2164:VAL:HA	12:e:4536:LEU:H	1.39	0.88
12:f:2641:TYR:HA	12:f:2649:VAL:O	1.73	0.88
12:n:803:LEU:O	12:n:894:SER:C	2.15	0.88
14:j:217:ASN:O	14:j:264:GLN:N	2.07	0.87
12:f:2924:ARG:O	12:f:2928:GLN:N	2.07	0.87
12:e:958:VAL:N	12:e:1104:PRO:O	2.07	0.87
12:f:2290:ASN:HA	12:f:2294:GLU:H	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:4190:ILE:O	12:f:4194:LEU:N	2.07	0.87
12:e:3906:GLN:O	12:e:3910:ARG:N	2.06	0.87
14:j:66:GLY:O	14:j:70:LEU:N	2.08	0.87
12:e:4336:GLY:O	12:e:4340:ILE:N	2.08	0.87
12:m:806:ALA:HB1	14:q:356:ALA:CA	2.03	0.87
12:e:918:GLY:CA	12:e:950:GLY:HA2	2.05	0.87
12:e:1030:PRO:O	12:e:1034:GLU:N	2.07	0.86
12:e:1059:CYS:O	12:e:1063:MET:N	2.08	0.86
12:f:2252:HIS:O	12:f:2302:VAL:N	2.08	0.86
14:i:147:GLU:O	14:i:151:LYS:N	2.08	0.86
12:f:82:SER:HA	12:f:113:SER:HA	1.56	0.86
12:f:3086:PHE:O	12:f:3089:CYS:N	2.09	0.86
12:n:803:LEU:CB	12:n:895:ASN:O	2.24	0.85
12:e:4327:ALA:O	12:e:4331:LEU:N	2.09	0.85
12:e:3876:LEU:O	12:e:3880:HIS:N	2.08	0.85
12:f:2367:ASP:HA	12:f:2370:SER:HA	1.57	0.85
12:f:4175:GLU:O	12:f:4179:LEU:N	2.08	0.85
12:f:3879:ASP:O	12:f:3883:PHE:N	2.10	0.85
14:i:115:HIS:O	14:i:119:LEU:N	2.09	0.85
14:j:112:ASP:O	14:j:116:LYS:N	2.08	0.85
12:e:806:ALA:HA	14:i:356:ALA:H	1.42	0.84
12:e:918:GLY:HA2	12:e:950:GLY:HA2	1.56	0.84
12:f:2724:SER:O	12:f:2728:LEU:N	2.09	0.84
14:i:166:PRO:O	14:i:170:MET:N	2.10	0.84
14:j:262:CYS:O	14:j:267:ALA:N	2.10	0.84
15:k:69:LEU:N	15:k:80:VAL:O	2.10	0.84
12:f:4557:SER:HA	12:f:4591:ARG:HA	1.59	0.84
12:n:803:LEU:CB	12:n:895:ASN:C	2.51	0.84
12:e:2929:PRO:HA	12:e:3060:ARG:HA	1.58	0.84
12:f:2299:GLN:O	12:f:2339:VAL:HA	1.77	0.84
14:j:179:LYS:O	14:j:183:ASP:N	2.09	0.84
12:f:3555:ASN:O	12:f:3559:ARG:N	2.09	0.84
12:f:2161:LEU:O	12:f:2165:PHE:N	2.09	0.83
12:e:4335:GLN:O	12:e:4339:MET:N	2.11	0.83
12:f:2830:LEU:O	12:f:2835:ASP:N	2.11	0.83
14:j:158:GLU:O	14:j:162:LYS:N	2.10	0.83
12:e:806:ALA:HA	14:i:355:ALA:C	2.03	0.83
12:e:1101:GLU:HA	12:e:1106:VAL:HA	1.60	0.83
12:f:1349:GLN:O	12:f:1431:LEU:N	2.10	0.82
14:j:127:SER:O	14:j:131:THR:N	2.11	0.82
12:f:4016:SER:O	12:f:4020:ILE:N	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:1801:PRO:O	12:f:1805:ARG:N	2.11	0.82
14:j:146:MET:O	14:j:150:GLN:N	2.11	0.82
12:f:3993:ILE:O	12:f:3997:ARG:N	2.12	0.82
14:j:336:TYR:O	14:j:340:ILE:N	2.12	0.82
12:f:1672:VAL:HA	12:f:1691:SER:HA	1.61	0.81
12:f:2198:GLU:O	12:f:2202:MET:N	2.13	0.81
12:e:1955:GLY:O	12:e:2015:PHE:N	2.11	0.81
12:f:1836:PHE:O	12:f:1840:SER:N	2.14	0.81
12:e:995:SER:HA	12:e:1018:PHE:HA	1.62	0.81
12:f:2198:GLU:H	12:f:2202:MET:N	1.78	0.81
12:e:1069:TYR:O	12:e:1073:GLY:N	2.14	0.81
12:f:2219:GLY:HA3	12:f:2319:LEU:HA	1.63	0.81
12:f:3219:ARG:HA	12:f:3472:VAL:HA	1.62	0.80
12:f:4249:GLN:O	12:f:4254:GLY:N	2.14	0.80
14:j:37:SER:O	14:j:41:SER:N	2.11	0.80
12:f:2218:HIS:H	12:f:2321:ASP:CA	1.94	0.80
12:f:2499:LEU:O	12:f:2503:SER:N	2.14	0.80
12:f:3037:ALA:O	12:f:3042:LEU:N	2.14	0.80
12:f:3612:THR:O	12:f:3636:GLN:N	2.11	0.80
12:f:4282:PHE:O	12:f:4296:MET:N	2.13	0.80
12:e:1481:GLN:HA	12:e:2272:THR:HA	1.62	0.80
12:f:2614:ASP:O	12:f:2658:TRP:N	2.15	0.80
12:e:4549:GLN:O	12:e:4550:SER:CB	2.30	0.79
12:f:1101:GLU:HA	12:f:1106:VAL:HA	1.63	0.79
12:f:3098:SER:O	12:f:3102:LEU:N	2.16	0.79
12:f:1430:THR:O	12:f:1434:ILE:N	2.15	0.79
14:i:146:MET:O	14:i:150:GLN:N	2.12	0.79
12:f:3661:LEU:HA	12:f:3671:LEU:H	1.48	0.79
12:f:85:LYS:HA	12:f:97:GLU:HA	1.65	0.79
12:f:1368:ASN:O	12:f:1372:ASN:N	2.12	0.79
12:f:4611:LEU:O	12:f:4645:THR:N	2.16	0.79
14:j:95:ASP:O	14:j:99:ASP:N	2.15	0.79
12:f:1549:GLY:O	12:f:1553:GLY:N	2.16	0.79
12:f:2250:VAL:N	12:f:2298:ARG:O	2.13	0.79
12:f:2269:ASP:N	12:f:2274:GLU:O	2.15	0.79
12:f:2616:GLU:N	12:f:2658:TRP:O	2.16	0.79
14:j:321:ALA:O	14:j:325:GLU:N	2.14	0.79
12:f:1580:LYS:O	12:f:1584:LYS:N	2.14	0.78
12:f:4065:GLN:O	12:f:4093:TRP:N	2.15	0.78
12:f:4556:CYS:O	12:f:4592:TRP:N	2.16	0.78
12:f:4608:PRO:O	12:f:4642:VAL:N	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:e:733:LEU:CB	14:i:360:GLN:O	2.31	0.78
12:e:806:ALA:O	14:i:356:ALA:CA	2.31	0.78
12:f:1548:GLU:O	12:f:1552:THR:N	2.16	0.78
12:e:4317:THR:O	12:e:4319:SER:N	2.15	0.78
12:f:2220:LEU:O	12:f:2343:PHE:N	2.17	0.78
12:n:918:GLY:HA2	12:n:950:GLY:CA	2.13	0.78
12:m:918:GLY:HA2	12:m:950:GLY:CA	2.13	0.78
12:e:806:ALA:CA	14:i:355:ALA:C	2.56	0.78
12:f:3851:ASP:O	12:f:3855:ARG:N	2.14	0.78
14:i:133:VAL:O	14:i:228:LEU:N	2.14	0.78
12:f:4375:ALA:O	12:f:4379:THR:N	2.13	0.78
14:i:58:LEU:N	14:i:132:LEU:O	2.17	0.78
14:i:270:ILE:HA	14:i:309:PHE:HA	1.65	0.78
12:e:3956:GLN:O	12:e:3960:TRP:N	2.16	0.77
12:e:2773:MET:O	12:e:2777:TYR:N	2.17	0.77
12:e:4001:LEU:O	12:e:4005:ALA:N	2.12	0.77
12:f:3871:VAL:O	12:f:3875:MET:N	2.18	0.77
12:f:4182:LEU:O	12:f:4186:PHE:N	2.16	0.77
12:f:1765:ALA:O	12:f:1769:ILE:CB	2.33	0.77
12:f:3655:ARG:HA	12:f:3660:VAL:HA	1.66	0.77
12:e:2439:HIS:O	12:e:2443:LEU:N	2.16	0.77
12:f:2595:GLY:O	12:f:2713:ASN:HA	1.84	0.77
12:f:2639:CYS:HA	12:f:2652:PRO:HA	1.66	0.77
12:e:2034:LYS:HA	12:e:4208:GLY:HA3	1.66	0.77
12:f:4545:VAL:O	12:f:4573:ASN:N	2.17	0.77
12:f:961:GLU:N	12:f:972:ASN:O	2.18	0.76
12:f:2355:THR:O	12:f:2359:CYS:N	2.19	0.76
12:f:2438:GLU:O	12:f:2442:LYS:CB	2.33	0.76
12:f:3519:TYR:HA	12:f:3698:PHE:O	1.85	0.76
12:f:4288:VAL:N	12:f:4292:LYS:O	2.19	0.76
14:i:363:LEU:O	14:i:366:GLN:N	2.18	0.76
12:e:4559:GLY:HA2	12:e:4588:THR:O	1.86	0.76
12:f:3704:THR:O	12:f:3708:LEU:N	2.16	0.76
12:e:733:LEU:O	14:i:363:LEU:C	2.29	0.76
12:f:2677:GLN:O	12:f:2681:SER:N	2.15	0.76
14:i:151:LYS:O	14:i:155:VAL:N	2.18	0.76
12:f:2482:GLN:O	12:f:2486:LEU:N	2.18	0.75
12:e:1861:MET:O	12:e:1863:ASN:N	2.16	0.75
12:e:3535:HIS:O	12:e:3539:ALA:N	2.19	0.75
12:f:1409:LYS:O	12:f:1413:TRP:N	2.20	0.75
14:j:166:PRO:O	14:j:170:MET:N	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:j:181:PHE:HA	14:j:313:GLY:HA2	1.68	0.75
12:f:3950:LYS:O	12:f:3954:ASP:N	2.19	0.74
14:r:85:GLY:O	14:r:110:ASP:N	2.21	0.74
12:f:997:PRO:HA	12:f:1019:TYR:H	1.51	0.74
12:f:2779:MET:O	12:f:2783:ARG:N	2.20	0.74
12:f:3726:GLU:O	12:f:3730:ASP:N	2.20	0.74
12:f:4066:ILE:HA	12:f:4093:TRP:O	1.87	0.74
12:f:997:PRO:HA	12:f:1019:TYR:N	2.02	0.74
12:f:1380:TYR:O	12:f:1383:TYR:N	2.20	0.74
12:f:4566:GLN:HA	12:f:4582:SER:HA	1.69	0.74
15:l:69:LEU:O	15:l:79:MET:HA	1.88	0.74
12:e:3083:PRO:O	12:e:3086:PHE:N	2.20	0.74
12:f:2267:THR:O	12:f:2276:THR:N	2.14	0.74
12:f:3037:ALA:O	12:f:3041:GLY:N	2.21	0.74
12:f:1416:LEU:O	12:f:1420:LEU:N	2.17	0.74
12:f:4005:ALA:O	12:f:4009:VAL:N	2.17	0.74
9:V:73:PHE:HA	9:V:82:PHE:HA	1.70	0.73
12:f:4347:GLN:O	12:f:4351:ASP:N	2.21	0.73
12:e:4564:LYS:HA	12:e:4585:LEU:H	1.53	0.73
15:k:24:ASN:N	15:k:28:ILE:O	2.20	0.73
12:f:1469:VAL:O	12:f:1473:TYR:N	2.22	0.73
12:f:1766:LEU:O	12:f:1770:GLY:N	2.20	0.73
12:f:4603:ASN:O	12:f:4626:ILE:N	2.20	0.73
12:e:4177:ALA:O	12:e:4181:PHE:N	2.18	0.73
12:f:2218:HIS:N	12:f:2321:ASP:HA	2.00	0.73
12:f:2123:ASP:O	12:f:2127:ILE:N	2.16	0.73
12:f:1587:LEU:O	12:f:1591:VAL:N	2.21	0.73
12:f:4015:GLU:O	12:f:4019:SER:N	2.22	0.73
12:f:890:LEU:HA	12:m:689:PHE:CA	2.13	0.72
12:f:1330:LYS:O	12:f:1334:SER:N	2.20	0.72
12:e:1998:THR:HA	12:e:2008:VAL:H	1.54	0.72
12:e:2160:LEU:O	12:e:2163:ASP:N	2.20	0.72
14:j:236:ALA:O	14:j:240:LEU:N	2.17	0.72
12:f:1775:SER:O	12:f:1779:GLN:N	2.22	0.72
14:j:227:VAL:O	14:j:267:ALA:HA	1.89	0.72
12:f:1557:ILE:O	12:f:1561:LEU:N	2.23	0.72
12:m:1057:TYR:C	12:m:1059:CYS:H	1.97	0.72
12:e:344:LEU:HA	12:e:356:ALA:HB1	1.71	0.72
12:f:2312:VAL:O	12:f:2316:ASN:N	2.20	0.72
12:f:2623:SER:C	12:f:2625:ALA:H	1.96	0.72
14:i:135:PHE:O	14:i:230:VAL:N	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:i:229:VAL:N	14:i:268:ALA:O	2.23	0.72
14:i:363:LEU:O	14:i:364:MET:C	2.28	0.72
12:n:456:HIS:O	12:n:460:GLN:N	2.19	0.72
12:f:994:LEU:HA	12:f:1022:ALA:H	1.55	0.72
12:f:1351:TRP:N	12:f:1430:THR:HA	2.04	0.72
12:f:1374:PRO:O	12:f:1378:ARG:N	2.17	0.72
12:f:2765:TYR:O	12:f:2769:LEU:N	2.17	0.72
12:f:2839:GLU:O	12:f:2843:ARG:N	2.23	0.72
9:V:58:GLY:HA3	9:V:89:ASP:HA	1.70	0.72
12:f:4328:GLU:O	12:f:4332:LEU:N	2.19	0.72
12:f:2937:GLY:N	12:f:3068:MET:O	2.19	0.71
15:l:72:ARG:HA	15:l:77:GLU:HA	1.71	0.71
14:j:69:THR:HA	14:j:78:GLU:O	1.89	0.71
14:j:137:ALA:O	14:j:232:THR:N	2.22	0.71
12:f:4042:LEU:O	12:f:4145:PHE:N	2.19	0.71
14:i:231:CYS:N	14:i:270:ILE:O	2.23	0.71
12:f:1210:TYR:O	12:f:1213:ASN:N	2.24	0.71
12:f:1272:ARG:O	12:f:1276:ALA:N	2.18	0.71
12:f:2248:GLU:O	12:f:2298:ARG:N	2.24	0.71
14:j:75:GLN:HA	14:j:91:LEU:HA	1.72	0.71
12:f:2424:GLN:O	12:f:2428:THR:N	2.18	0.71
12:e:2393:GLU:O	12:e:2397:ARG:N	2.24	0.71
12:f:1660:GLY:HA3	12:f:1873:LEU:CA	2.18	0.71
12:f:2754:ALA:O	12:f:2756:LEU:N	2.23	0.71
15:k:72:ARG:HA	15:k:77:GLU:HA	1.72	0.71
12:n:918:GLY:CA	12:n:950:GLY:HA2	2.20	0.71
12:f:2473:ASN:HA	12:f:2480:PRO:HA	1.72	0.70
12:f:3618:ALA:O	12:f:3622:ASN:N	2.24	0.70
12:f:4340:ILE:O	12:f:4344:LEU:N	2.23	0.70
12:e:2817:PRO:O	12:e:2821:LEU:N	2.24	0.70
12:e:733:LEU:O	14:i:363:LEU:CA	2.39	0.70
12:e:810:LYS:N	14:i:357:GLU:H	1.89	0.70
12:f:4529:ALA:O	12:f:4534:TRP:N	2.18	0.70
14:i:154:SER:O	14:i:158:GLU:N	2.17	0.70
12:f:1930:PHE:O	12:f:1958:ASP:N	2.25	0.70
12:f:4269:LEU:O	12:f:4273:PHE:N	2.25	0.70
14:i:271:TYR:N	14:i:308:VAL:O	2.25	0.70
12:f:4288:VAL:O	12:f:4292:LYS:N	2.25	0.70
12:e:806:ALA:HB1	14:i:355:ALA:O	1.90	0.70
15:l:27:GLY:O	15:l:44:ASN:N	2.25	0.70
12:f:1435:TRP:O	12:f:1438:ASP:HA	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:m:918:GLY:CA	12:m:950:GLY:HA2	2.20	0.69
12:f:4184:ALA:O	12:f:4188:ALA:N	2.26	0.69
12:f:4043:MET:O	12:f:4127:THR:HA	1.93	0.69
12:e:720:ILE:CA	12:e:735:LEU:HA	2.21	0.69
12:e:733:LEU:CB	14:i:360:GLN:C	2.66	0.69
12:e:1021:ASN:O	12:e:1025:ARG:N	2.25	0.69
12:f:1906:GLY:HA3	12:f:2042:THR:HA	1.72	0.69
12:f:2933:LEU:O	12:f:3066:PHE:N	2.18	0.69
12:m:4288:VAL:N	12:m:4292:LYS:O	2.26	0.69
12:n:4288:VAL:N	12:n:4292:LYS:O	2.26	0.69
14:r:262:CYS:O	14:r:266:GLY:N	2.26	0.68
14:i:53:SER:O	14:i:105:ASN:N	2.21	0.68
12:e:486:PRO:HA	12:e:512:PHE:HA	1.75	0.68
12:e:3873:ARG:O	12:e:4146:VAL:N	2.23	0.68
12:f:2686:MET:HA	12:f:2691:GLY:O	1.94	0.68
12:f:4152:GLY:O	12:f:4156:ASN:N	2.25	0.68
12:f:994:LEU:O	12:f:1021:ASN:N	2.26	0.68
12:f:1898:ALA:HA	12:f:1986:SER:HA	1.75	0.68
10:W:1130:ALA:O	10:W:1134:LEU:N	2.25	0.68
12:e:2614:ASP:O	12:e:2658:TRP:N	2.26	0.68
12:e:3926:GLY:O	12:e:3958:SER:HA	1.92	0.68
12:f:2315:LEU:O	12:f:2319:LEU:N	2.17	0.68
15:k:69:LEU:HA	15:l:71:ILE:HA	1.74	0.68
15:l:23:VAL:HA	15:l:29:PRO:CA	2.23	0.68
12:f:2175:MET:O	12:f:2179:ARG:N	2.22	0.68
12:f:2489:TYR:HA	12:f:2543:GLY:HA2	1.76	0.68
12:f:3928:THR:O	12:f:3932:ALA:N	2.25	0.68
12:f:4631:ASP:O	12:f:4635:PHE:N	2.22	0.68
12:f:3637:ASP:N	12:f:3680:SER:O	2.27	0.68
14:j:181:PHE:O	14:j:313:GLY:HA2	1.94	0.68
12:f:4152:GLY:HA3	12:f:4314:ASP:O	1.93	0.67
15:l:27:GLY:HA3	15:l:44:ASN:HA	1.75	0.67
12:f:1057:TYR:O	12:f:1060:LEU:N	2.28	0.67
12:f:1481:GLN:HA	12:f:2272:THR:H	1.58	0.67
12:e:918:GLY:HA2	12:e:950:GLY:CA	2.24	0.67
12:f:2223:VAL:O	12:f:2364:PHE:N	2.21	0.67
12:f:2595:GLY:HA3	12:f:2736:VAL:O	1.94	0.67
12:f:2951:ALA:O	12:f:2956:LEU:N	2.21	0.67
12:e:2142:CYS:O	12:e:2146:VAL:N	2.25	0.67
12:f:3926:GLY:HA3	12:f:3958:SER:CB	2.25	0.67
14:j:233:LYS:N	14:j:273:SER:HA	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:k:23:VAL:HA	15:k:29:PRO:HA	1.76	0.67
15:k:70:ARG:O	15:l:70:ARG:N	2.28	0.67
12:f:3617:ASP:O	12:f:3620:ARG:N	2.25	0.67
15:k:26:GLU:O	15:k:44:ASN:HA	1.94	0.67
12:e:3589:ILE:HA	12:e:3699:VAL:O	1.95	0.66
12:e:2836:ARG:HA	12:e:3093:TRP:H	1.59	0.66
12:f:2068:LYS:O	12:f:2072:PHE:N	2.28	0.66
12:f:4496:ALA:O	12:f:4500:GLY:N	2.25	0.66
14:i:159:HIS:O	14:i:163:MET:N	2.16	0.66
12:f:960:HIS:O	12:f:1108:ASP:N	2.29	0.66
12:f:1512:TYR:O	12:f:1516:PHE:N	2.29	0.66
12:e:2985:CYS:O	12:e:3036:GLY:HA3	1.96	0.66
12:f:3135:GLN:HA	12:f:3136:PRO:C	2.19	0.66
12:f:3828:SER:O	12:f:3832:PHE:N	2.19	0.66
12:f:1903:SER:HA	12:f:2017:THR:HA	1.78	0.66
12:f:3700:ASN:C	12:f:3702:THR:H	2.02	0.66
12:e:4334:THR:O	12:e:4338:ASP:N	2.20	0.66
12:f:117:ALA:N	12:f:138:LEU:O	2.17	0.66
12:f:2268:LEU:HA	12:f:2275:TRP:HA	1.77	0.66
12:f:2862:ASP:O	12:f:2866:ALA:N	2.28	0.66
12:f:4562:GLY:O	12:f:4644:CYS:HA	1.95	0.66
12:m:3767:ILE:O	12:m:3771:GLU:N	2.29	0.66
12:f:1937:ASP:O	12:f:1941:MET:N	2.23	0.66
12:f:2324:LEU:HA	12:f:2334:SER:HA	1.78	0.66
12:f:3637:ASP:H	12:f:3681:THR:HA	1.59	0.66
14:i:155:VAL:O	14:i:159:HIS:N	2.24	0.66
12:n:3767:ILE:O	12:n:3771:GLU:N	2.29	0.66
14:i:133:VAL:N	14:i:226:PRO:O	2.30	0.65
12:f:1854:LEU:HA	12:f:1869:GLY:HA2	1.78	0.65
12:e:2370:SER:O	12:e:2374:ILE:N	2.21	0.65
12:f:1546:TYR:O	12:f:1549:GLY:N	2.29	0.65
12:f:3105:VAL:O	12:f:3109:PHE:N	2.29	0.65
12:e:866:THR:HA	12:e:946:SER:HA	1.78	0.65
12:e:1882:THR:O	12:e:1885:THR:N	2.30	0.65
12:e:1905:PHE:N	12:e:2039:LEU:O	2.22	0.65
12:f:1313:SER:O	12:f:1315:SER:N	2.29	0.65
12:f:3104:GLN:O	12:f:3108:GLU:N	2.18	0.65
14:j:173:LEU:C	14:j:224:GLY:HA3	2.21	0.65
12:e:3537:GLN:HA	12:e:3543:PHE:H	1.61	0.65
12:f:3939:SER:CA	12:f:3945:LYS:HA	2.25	0.65
12:f:4502:LYS:O	12:f:4506:ASN:N	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:g:366:LYS:CA	15:l:3:GLU:HA	2.25	0.65
12:e:810:LYS:CA	14:i:357:GLU:H	2.09	0.65
12:e:1015:GLU:HA	12:e:1018:PHE:O	1.97	0.65
12:f:1911:GLY:O	12:f:1915:SER:N	2.28	0.65
12:f:3086:PHE:C	12:f:3089:CYS:H	2.05	0.65
14:i:137:ALA:N	14:i:230:VAL:O	2.23	0.65
12:f:4044:CYS:N	12:f:4145:PHE:O	2.30	0.64
12:f:2219:GLY:HA2	12:f:2341:ILE:O	1.97	0.64
12:f:3837:HIS:C	12:f:3839:VAL:H	2.03	0.64
2:H:42:GLY:HA3	3:J:387:TRP:HA	1.79	0.64
12:e:4246:LEU:O	12:e:4251:ILE:N	2.31	0.64
14:r:37:SER:C	14:r:39:ILE:N	2.55	0.64
12:e:270:THR:O	12:e:274:GLU:N	2.24	0.64
12:e:283:ARG:HA	12:f:175:GLY:HA3	1.78	0.64
12:e:2936:ILE:O	12:e:3094:PHE:N	2.31	0.64
12:f:948:LYS:O	12:f:951:GLY:N	2.30	0.64
12:f:2242:GLU:HA	12:f:2249:GLY:H	1.63	0.64
12:f:2518:ILE:O	12:f:2522:THR:N	2.27	0.64
12:f:3107:LYS:O	12:f:3111:SER:N	2.25	0.64
12:f:3498:ASN:O	12:f:3500:MET:N	2.31	0.64
12:f:3760:ILE:O	12:f:3764:ASP:HA	1.97	0.64
12:f:3773:LEU:O	12:f:3776:GLU:N	2.30	0.64
12:f:4535:SER:O	12:f:4538:GLU:N	2.30	0.64
14:j:234:CYS:C	14:j:236:ALA:N	2.53	0.64
12:f:3681:THR:O	12:f:3683:ASP:N	2.31	0.64
12:e:1860:GLN:HA	12:e:1864:ALA:O	1.98	0.64
12:f:829:LEU:O	12:f:833:VAL:N	2.30	0.64
12:f:2188:GLU:C	12:f:2190:TYR:H	2.04	0.64
12:f:2423:LEU:O	12:f:2427:PHE:N	2.30	0.64
12:f:3591:ASP:O	12:f:3683:ASP:N	2.32	0.63
12:f:1932:CYS:N	12:f:1958:ASP:O	2.27	0.63
14:j:62:GLU:O	14:j:64:GLY:N	2.31	0.63
4:K:186:ALA:N	4:K:216:VAL:O	2.30	0.63
12:f:2983:SER:O	12:f:2987:ASN:HA	1.99	0.63
14:j:288:VAL:O	14:j:293:GLY:N	2.31	0.63
12:e:2264:LEU:O	12:e:2279:LEU:N	2.28	0.63
12:e:2600:GLY:O	12:e:2604:THR:N	2.27	0.63
12:e:2932:HIS:O	12:e:3090:VAL:N	2.28	0.63
12:f:2638:TYR:O	12:f:2653:VAL:N	2.32	0.63
12:e:2690:GLY:O	12:e:2703:LEU:N	2.32	0.63
12:f:885:VAL:O	12:f:889:ASN:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:e:2691:GLY:HA2	12:e:2703:LEU:H	1.64	0.62
12:f:2062:ALA:O	12:f:2066:ALA:N	2.28	0.62
12:f:2618:VAL:O	12:f:2662:PHE:N	2.32	0.62
12:f:4138:LEU:O	12:f:4141:ALA:N	2.32	0.62
12:f:2039:LEU:HA	12:f:4255:ARG:HA	1.80	0.62
12:f:2635:PHE:O	12:f:2639:CYS:N	2.25	0.62
12:e:4317:THR:C	12:e:4319:SER:H	2.07	0.62
1:C:51:ALA:HB2	1:E:173:GLY:HA3	1.80	0.62
12:e:4249:GLN:O	12:e:4254:GLY:N	2.32	0.62
12:f:1405:SER:HA	12:f:3658:GLY:HA2	1.80	0.62
12:f:2771:ALA:O	12:f:2775:GLU:N	2.22	0.62
12:f:1902:GLY:H	12:f:2015:PHE:HA	1.65	0.62
12:f:2260:SER:O	12:f:2264:LEU:N	2.32	0.62
12:f:2645:PRO:C	14:q:220:THR:O	2.39	0.62
14:i:149:LEU:O	14:i:153:ALA:N	2.18	0.62
8:U:25:GLY:HA3	8:U:43:ALA:HB3	1.81	0.62
12:f:2254:ILE:O	12:f:2304:ASP:N	2.32	0.62
12:f:3006:GLU:O	12:f:3010:THR:N	2.26	0.62
12:e:2163:ASP:HA	12:e:4529:ALA:C	2.25	0.62
12:f:121:ARG:H	12:f:135:LEU:HA	1.64	0.62
14:i:69:THR:HA	14:i:79:HIS:HA	1.80	0.62
14:j:257:HIS:N	14:j:332:PRO:HA	2.14	0.62
9:V:38:GLY:HA3	9:V:59:ARG:HA	1.82	0.61
12:f:1417:MET:O	12:f:1421:HIS:N	2.33	0.61
12:f:2301:ILE:O	12:f:2342:MET:N	2.33	0.61
12:f:1920:GLY:O	12:f:1924:GLY:N	2.34	0.61
7:O:47:ILE:O	7:O:51:ARG:N	2.33	0.61
12:f:2992:PHE:O	12:f:3064:VAL:HA	2.00	0.61
12:e:1022:ALA:O	12:e:1026:MET:N	2.32	0.61
14:i:262:CYS:O	14:i:267:ALA:N	2.33	0.61
12:f:806:ALA:HB2	14:j:354:LEU:O	2.00	0.61
12:f:961:GLU:HA	12:f:1108:ASP:O	2.01	0.61
12:f:4538:GLU:O	12:f:4595:GLN:N	2.29	0.61
12:e:4002:LEU:O	12:e:4006:HIS:N	2.18	0.61
12:f:2557:VAL:O	12:f:2754:ALA:HA	1.99	0.61
12:e:4235:PRO:HA	12:e:4238:ILE:H	1.65	0.61
12:f:1667:SER:N	12:f:1672:VAL:O	2.24	0.61
12:f:2762:LEU:O	12:f:2766:ALA:N	2.34	0.61
12:e:403:HIS:HA	12:e:532:GLU:HA	1.83	0.61
13:p:551:LEU:O	13:p:562:THR:N	2.33	0.61
12:e:2039:LEU:HA	12:e:4255:ARG:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:2663:CYS:O	12:f:2711:ALA:N	2.33	0.60
12:f:4001:LEU:O	12:f:4005:ALA:N	2.21	0.60
12:f:4139:LEU:HA	12:f:4142:GLY:O	2.01	0.60
12:f:1930:PHE:N	12:f:1956:CYS:O	2.35	0.60
14:j:182:GLN:HA	14:j:214:LEU:N	2.16	0.60
15:k:58:ARG:HA	15:k:61:ASP:O	2.00	0.60
13:o:508:LEU:O	13:o:517:LEU:N	2.35	0.60
12:e:2162:SER:O	12:e:4530:GLN:HA	2.02	0.60
12:f:923:THR:HA	12:f:1036:SER:CA	2.28	0.60
12:f:4284:LEU:N	12:f:4294:ILE:O	2.32	0.60
12:f:4323:LEU:HA	12:f:4637:GLU:O	2.01	0.60
13:p:508:LEU:O	13:p:517:LEU:N	2.35	0.60
12:e:2901:TYR:O	12:e:2906:ASP:HA	2.00	0.60
12:f:2040:ALA:N	12:f:4254:GLY:O	2.34	0.60
15:k:27:GLY:HA3	15:k:43:ALA:C	2.27	0.60
12:f:2795:SER:O	12:f:2798:GLU:N	2.30	0.60
14:i:137:ALA:O	14:i:232:THR:N	2.32	0.60
13:o:551:LEU:O	13:o:562:THR:N	2.33	0.60
1:I:41:ARG:O	1:I:70:SER:N	2.34	0.60
12:e:3822:HIS:O	12:e:3824:LEU:N	2.33	0.60
12:f:2598:GLY:O	12:f:2797:ARG:N	2.35	0.60
12:e:152:PHE:O	12:e:157:VAL:N	2.35	0.60
12:f:1370:LEU:O	12:f:1373:PHE:N	2.35	0.60
12:f:1655:LYS:C	12:f:1657:MET:H	2.09	0.60
12:f:1983:ARG:C	12:f:1985:HIS:N	2.59	0.59
12:e:947:HIS:O	12:e:948:LYS:C	2.45	0.59
12:f:2659:LEU:N	12:f:2705:ARG:O	2.36	0.59
13:h:409:SER:N	13:h:420:ASP:O	2.25	0.59
12:f:1956:CYS:O	12:f:1958:ASP:N	2.35	0.59
12:f:2302:VAL:O	12:f:2304:ASP:N	2.35	0.59
12:f:2989:LYS:HA	12:f:3061:ASN:O	2.02	0.59
14:j:149:LEU:O	14:j:153:ALA:N	2.27	0.59
12:f:2245:GLU:C	12:f:2247:VAL:H	2.10	0.59
12:e:3518:GLY:HA3	12:e:3699:VAL:HA	1.84	0.59
12:f:1355:GLN:O	12:f:1359:LEU:N	2.27	0.59
12:f:2297:LYS:O	12:f:2299:GLN:N	2.36	0.59
12:f:4002:LEU:O	12:f:4006:HIS:N	2.31	0.59
11:Y:45:GLU:N	11:Y:281:SER:O	2.35	0.59
12:f:733:LEU:CB	14:j:364:MET:HA	2.33	0.59
12:f:1983:ARG:O	12:f:1986:SER:N	2.33	0.59
12:m:152:PHE:O	12:m:157:VAL:N	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ASP:HA	6:P:93:GLU:H	1.68	0.59
12:f:3106:GLY:O	12:f:3110:THR:N	2.24	0.59
14:j:234:CYS:C	14:j:236:ALA:H	2.11	0.59
12:f:4329:ARG:O	12:f:4333:THR:N	2.32	0.59
12:e:2266:GLY:HA2	12:e:2276:THR:O	2.02	0.58
12:f:1731:THR:HA	12:f:1784:ASN:HA	1.83	0.58
12:f:2760:PRO:HA	12:f:2763:ARG:H	1.67	0.58
12:e:3874:GLY:HA2	12:e:4146:VAL:N	2.18	0.58
12:f:156:ALA:O	12:f:160:PHE:N	2.26	0.58
12:f:2566:ASP:O	12:f:2603:MET:HA	2.03	0.58
12:f:2873:TYR:HA	12:f:2882:ILE:O	2.02	0.58
14:i:363:LEU:C	14:i:365:LYS:N	2.61	0.58
14:j:53:SER:O	14:j:55:LYS:N	2.36	0.58
14:j:181:PHE:CA	14:j:313:GLY:HA2	2.34	0.58
12:m:153:ILE:O	12:m:158:ALA:N	2.34	0.58
12:m:1057:TYR:C	12:m:1059:CYS:N	2.60	0.58
12:e:1554:SER:HA	12:e:1642:GLY:HA3	1.86	0.58
12:e:2951:ALA:O	12:e:2956:LEU:N	2.22	0.58
12:e:2639:CYS:HA	12:e:2652:PRO:HA	1.85	0.58
12:f:2933:LEU:N	12:f:3064:VAL:O	2.37	0.58
12:f:3873:ARG:N	12:f:4021:MET:O	2.36	0.58
14:i:37:SER:O	14:i:41:SER:N	2.29	0.58
12:e:2167:GLY:N	12:e:4533:SER:HA	2.18	0.58
12:e:4039:THR:HA	12:e:4141:ALA:O	2.04	0.58
12:f:888:LEU:C	12:f:891:HIS:H	2.11	0.58
14:i:59:VAL:O	14:i:109:LEU:N	2.29	0.58
14:r:273:SER:O	14:r:277:GLU:N	2.36	0.58
12:e:2166:PRO:C	12:e:4533:SER:HA	2.28	0.58
12:e:3874:GLY:HA2	12:e:4146:VAL:H	1.68	0.58
12:f:220:CYS:O	12:f:225:GLU:N	2.37	0.58
12:f:1015:GLU:HA	12:f:1018:PHE:O	2.04	0.58
12:f:1398:MET:HA	12:f:2903:GLU:HA	1.85	0.58
12:e:733:LEU:O	14:i:364:MET:N	2.36	0.58
12:f:868:VAL:O	12:f:870:ASP:N	2.37	0.58
12:f:2213:ILE:O	12:f:2217:ASN:N	2.35	0.58
12:f:915:LEU:C	12:f:918:GLY:H	2.12	0.58
12:e:3993:ILE:O	12:e:3997:ARG:N	2.37	0.57
12:f:1513:TYR:O	12:f:1517:GLU:N	2.36	0.57
15:l:80:VAL:HA	15:l:88:LEU:O	2.04	0.57
12:e:1554:SER:HA	12:e:1642:GLY:CA	2.33	0.57
12:f:963:ARG:O	12:f:969:ILE:CA	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:4040:PRO:HA	12:f:4124:LEU:O	2.04	0.57
12:f:4041:VAL:N	12:f:4124:LEU:O	2.37	0.57
15:l:57:VAL:O	15:l:61:ASP:N	2.32	0.57
12:f:4249:GLN:HA	12:f:4253:GLY:HA3	1.85	0.57
12:f:4322:GLY:O	12:f:4637:GLU:HA	2.03	0.57
14:r:56:ASN:O	14:r:132:LEU:N	2.27	0.57
12:e:80:GLU:HA	12:e:115:SER:HA	1.87	0.57
12:f:2538:GLU:H	12:f:2547:PRO:HA	1.68	0.57
12:f:3562:TRP:O	12:f:3566:SER:N	2.29	0.57
14:i:73:LYS:HA	14:i:77:ALA:O	2.04	0.57
13:o:391:GLY:HA3	13:o:396:HIS:HA	1.86	0.57
12:e:4192:GLU:C	12:e:4194:LEU:H	2.12	0.57
12:f:1309:THR:C	12:f:1311:LEU:H	2.13	0.57
12:f:1983:ARG:C	12:f:1985:HIS:H	2.13	0.57
14:j:218:VAL:HA	14:j:263:LEU:C	2.29	0.57
12:n:803:LEU:O	12:n:894:SER:CA	2.52	0.57
12:e:4036:LYS:O	12:e:4038:ASN:N	2.33	0.57
12:f:2162:SER:O	12:f:2167:GLY:N	2.23	0.57
14:j:233:LYS:H	14:j:273:SER:HA	1.70	0.57
14:j:355:ALA:O	14:j:356:ALA:C	2.46	0.57
12:e:2590:PRO:O	12:e:2731:VAL:HA	2.04	0.57
12:f:918:GLY:N	12:f:950:GLY:HA3	2.20	0.57
12:f:2728:LEU:O	12:f:2731:VAL:N	2.31	0.57
12:f:3890:ILE:O	12:f:3894:GLY:HA3	2.05	0.57
12:f:3517:ALA:HA	12:f:3525:ARG:HA	1.86	0.56
12:e:165:ILE:O	12:e:171:ALA:N	2.38	0.56
12:e:1019:TYR:C	12:e:1021:ASN:H	2.12	0.56
12:e:2934:LEU:O	12:e:3092:ASN:N	2.35	0.56
12:f:948:LYS:O	12:f:949:PRO:C	2.47	0.56
12:f:962:LEU:HA	12:f:970:TYR:O	2.05	0.56
12:m:39:PRO:O	12:m:46:GLY:N	2.37	0.56
12:e:283:ARG:HA	12:f:176:ASP:H	1.71	0.56
12:e:869:TYR:H	12:e:951:GLY:HA2	1.70	0.56
12:e:918:GLY:N	12:e:950:GLY:HA2	2.20	0.56
12:e:3409:VAL:O	12:e:3413:ARG:N	2.34	0.56
12:f:1261:TRP:O	12:f:1265:LYS:N	2.38	0.56
12:f:1725:GLU:O	12:f:1729:LYS:N	2.38	0.56
12:f:2381:ARG:O	12:f:2385:ILE:N	2.38	0.56
12:f:2618:VAL:N	12:f:2660:VAL:O	2.33	0.56
12:f:2961:ILE:O	12:f:2963:VAL:N	2.38	0.56
12:f:4287:LYS:HA	12:f:4291:HIS:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:i:56:ASN:HA	14:i:105:ASN:O	2.05	0.56
12:f:962:LEU:HA	12:f:971:LEU:HA	1.87	0.56
12:f:4443:LYS:O	12:f:4445:THR:N	2.37	0.56
5:L:181:LYS:O	5:L:185:GLY:N	2.32	0.56
14:i:229:VAL:O	14:i:269:LEU:HA	2.05	0.56
14:j:53:SER:C	14:j:55:LYS:H	2.14	0.56
12:e:2163:ASP:O	12:e:4536:LEU:N	2.38	0.56
12:f:1348:GLU:HA	12:f:1432:GLY:CA	2.36	0.56
12:f:2324:LEU:HA	12:f:2335:LEU:H	1.71	0.56
12:f:2439:HIS:O	12:f:2443:LEU:N	2.29	0.56
12:e:4179:LEU:O	12:e:4183:LEU:N	2.35	0.56
12:f:884:ALA:O	12:f:888:LEU:N	2.38	0.56
12:f:1516:PHE:O	12:f:1520:ALA:N	2.27	0.56
13:p:391:GLY:HA3	13:p:396:HIS:HA	1.86	0.56
12:f:2503:SER:C	12:f:2505:ASP:H	2.13	0.56
12:f:3514:ILE:O	12:f:3518:GLY:HA3	2.06	0.56
12:f:3847:LYS:C	12:f:3849:VAL:H	2.12	0.56
12:f:4043:MET:N	12:f:4126:LEU:O	2.39	0.56
14:j:62:GLU:O	14:j:65:SER:N	2.32	0.56
12:n:776:PRO:CA	13:p:375:LEU:O	2.53	0.56
12:f:924:GLN:O	12:f:929:GLN:N	2.31	0.56
12:f:1902:GLY:HA2	12:f:2037:ARG:O	2.05	0.56
12:f:2220:LEU:N	12:f:2341:ILE:O	2.39	0.56
12:f:3928:THR:O	12:f:3931:GLN:N	2.38	0.56
13:p:573:LEU:HA	13:p:589:ASP:HA	1.88	0.56
12:f:80:GLU:N	12:f:102:ASN:O	2.27	0.55
12:f:912:GLY:O	12:f:1026:MET:HA	2.06	0.55
12:f:2559:THR:HA	12:f:2754:ALA:C	2.31	0.55
12:f:2594:CYS:HA	12:f:2712:CYS:O	2.05	0.55
12:f:2504:GLY:O	12:f:2734:VAL:HA	2.07	0.55
13:h:394:ASN:O	12:m:599:GLY:HA3	2.06	0.55
12:f:2600:GLY:O	12:f:2603:MET:N	2.39	0.55
12:e:2789:GLN:C	12:e:2791:HIS:H	2.13	0.55
12:f:3513:PHE:O	12:f:3518:GLY:N	2.39	0.55
14:i:91:LEU:O	14:i:103:ARG:HA	2.06	0.55
14:i:227:VAL:O	14:i:268:ALA:N	2.39	0.55
3:J:137:MET:O	3:J:304:VAL:N	2.39	0.55
12:f:803:LEU:HA	14:j:355:ALA:HA	1.88	0.55
12:f:2250:VAL:O	12:f:2300:TRP:N	2.39	0.55
13:o:573:LEU:HA	13:o:589:ASP:HA	1.88	0.55
12:e:1861:MET:C	12:e:1863:ASN:H	2.12	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:2952:TRP:O	12:f:2955:GLY:N	2.32	0.55
12:f:4327:ALA:O	12:f:4331:LEU:N	2.34	0.55
12:f:2189:MET:C	12:f:2191:LEU:H	2.15	0.55
14:i:301:LEU:O	14:i:309:PHE:N	2.23	0.55
12:f:917:ALA:O	12:f:950:GLY:HA3	2.06	0.55
12:f:1880:VAL:O	12:f:1882:THR:N	2.39	0.55
12:e:3997:ARG:C	12:e:3999:ASP:H	2.14	0.55
12:f:1026:MET:C	12:f:1028:ASP:H	2.15	0.55
12:f:4167:SER:O	12:f:4171:LYS:N	2.25	0.55
15:k:37:PRO:O	15:k:42:TYR:N	2.34	0.55
12:e:2255:ASP:O	12:e:2257:LYS:N	2.40	0.54
12:f:1906:GLY:HA3	12:f:2042:THR:CA	2.38	0.54
12:f:3944:PHE:HA	12:f:3975:SER:O	2.07	0.54
12:e:2308:ASP:O	12:e:2310:GLU:N	2.36	0.54
12:f:1474:GLU:CA	12:f:1587:LEU:HA	2.28	0.54
12:f:2499:LEU:O	12:f:2502:LEU:N	2.34	0.54
12:f:4326:ASN:O	12:f:4330:VAL:N	2.27	0.54
14:j:75:GLN:HA	14:j:91:LEU:CA	2.38	0.54
12:f:2597:PRO:O	12:f:2599:SER:N	2.41	0.54
12:f:995:SER:HA	12:f:1020:ARG:CA	2.25	0.54
12:f:4543:VAL:HA	12:f:4589:GLN:O	2.08	0.54
13:g:409:SER:O	13:g:419:GLN:N	2.40	0.54
14:i:363:LEU:O	14:i:365:LYS:N	2.40	0.54
12:e:2985:CYS:HA	12:e:3033:CYS:HA	1.88	0.54
12:f:2639:CYS:HA	12:f:2653:VAL:H	1.73	0.54
12:f:4604:VAL:HA	12:f:4625:GLU:HA	1.88	0.54
12:e:435:ARG:HA	12:e:447:LYS:HA	1.90	0.54
12:f:1959:GLU:N	12:f:2017:THR:O	2.41	0.54
12:f:4248:ALA:O	12:f:4253:GLY:N	2.41	0.54
12:m:119:ILE:O	12:m:136:ARG:N	2.40	0.54
1:C:48:MET:CB	1:E:173:GLY:HA2	2.38	0.54
12:e:483:VAL:O	12:e:512:PHE:N	2.40	0.54
12:f:1093:PHE:C	12:f:1095:ASN:H	2.16	0.54
13:h:551:LEU:O	13:h:562:THR:N	2.41	0.54
14:i:181:PHE:O	14:i:313:GLY:HA3	2.07	0.54
14:j:56:ASN:O	14:j:131:THR:HA	2.05	0.54
4:K:94:ILE:HA	4:K:110:PRO:HA	1.90	0.54
12:f:2536:ASP:O	12:f:2548:TRP:N	2.21	0.54
12:f:4167:SER:O	12:f:4169:ILE:N	2.41	0.54
1:B:42:PRO:HA	1:B:69:LEU:HA	1.89	0.54
12:e:753:LEU:O	12:e:757:GLY:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:912:GLY:C	12:f:1026:MET:HA	2.33	0.54
12:f:2227:GLY:C	12:f:2229:GLY:H	2.15	0.54
12:f:2937:GLY:C	12:f:3069:ASN:HA	2.32	0.54
12:e:2162:SER:C	12:e:4530:GLN:HA	2.32	0.54
12:e:2789:GLN:O	12:e:2791:HIS:N	2.39	0.54
12:f:4485:ARG:HA	12:f:4513:GLY:O	2.07	0.54
14:j:257:HIS:CA	14:j:332:PRO:HA	2.38	0.54
12:f:2242:GLU:CA	12:f:2249:GLY:H	2.20	0.53
12:f:2365:SER:O	12:f:2368:VAL:N	2.41	0.53
12:f:3690:PRO:O	12:f:3694:SER:N	2.39	0.53
12:f:4010:SER:O	12:f:4014:GLY:HA2	2.07	0.53
12:f:4378:ARG:HA	12:f:4438:CYS:O	2.08	0.53
13:p:384:VAL:HA	13:p:402:SER:HA	1.90	0.53
12:f:2548:TRP:O	12:f:2552:VAL:N	2.42	0.53
12:f:2740:GLY:O	12:f:2743:SER:N	2.41	0.53
12:e:960:HIS:O	12:e:1107:ILE:HA	2.09	0.53
12:e:4167:SER:O	12:e:4171:LYS:N	2.40	0.53
12:f:2229:GLY:O	12:f:2232:MET:N	2.42	0.53
12:f:4283:LYS:HA	12:f:4295:GLN:HA	1.89	0.53
15:l:16:GLY:HA3	15:l:93:ASN:H	1.74	0.53
12:m:132:SER:H	12:n:41:LEU:C	2.17	0.53
12:n:3891:LYS:O	12:n:3895:THR:N	2.42	0.53
13:o:384:VAL:HA	13:o:402:SER:HA	1.89	0.53
12:f:948:LYS:O	12:f:950:GLY:N	2.41	0.53
12:f:4174:ASN:N	12:f:4232:ASN:HA	2.24	0.53
15:k:65:ASP:O	15:l:74:LYS:N	2.41	0.53
12:e:720:ILE:CB	12:e:735:LEU:HA	2.39	0.53
12:e:3685:THR:O	12:e:4446:ASN:HA	2.09	0.53
12:e:734:LYS:HA	14:i:363:LEU:CA	2.39	0.53
12:f:1210:TYR:C	12:f:1212:ASP:N	2.66	0.53
12:f:1639:GLU:O	12:f:1643:ASN:N	2.36	0.53
12:f:2599:SER:O	12:f:2738:TYR:HA	2.08	0.53
12:f:2926:PHE:O	12:f:3061:ASN:HA	2.08	0.53
12:f:4174:ASN:H	12:f:4232:ASN:HA	1.72	0.53
14:i:43:VAL:O	14:i:46:ARG:N	2.35	0.53
12:f:2227:GLY:C	12:f:2229:GLY:N	2.65	0.53
12:f:4185:TRP:O	12:f:4189:ILE:N	2.30	0.53
12:e:818:GLU:O	12:e:819:GLY:C	2.50	0.53
5:L:145:LYS:O	5:L:178:GLN:N	2.38	0.53
12:e:4631:ASP:O	12:e:4633:ARG:N	2.41	0.53
12:f:2147:PRO:O	12:f:2362:VAL:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:j:239:VAL:O	14:j:243:GLU:N	2.31	0.53
12:f:1313:SER:C	12:f:1315:SER:N	2.67	0.53
12:f:1731:THR:O	12:f:1784:ASN:HA	2.09	0.53
14:j:56:ASN:N	14:j:130:GLU:O	2.42	0.53
14:j:140:SER:HA	14:j:236:ALA:HA	1.91	0.53
14:j:274:VAL:HA	14:j:277:GLU:HA	1.91	0.53
12:f:1344:ASP:O	12:f:1348:GLU:N	2.41	0.52
12:f:1793:ALA:HA	12:f:2058:GLY:HA2	1.91	0.52
12:f:2365:SER:C	12:f:2367:ASP:H	2.17	0.52
12:m:3891:LYS:O	12:m:3895:THR:N	2.41	0.52
12:f:539:SER:O	12:f:543:THR:N	2.37	0.52
12:f:2898:LYS:O	12:f:2902:GLU:N	2.25	0.52
12:e:3926:GLY:HA3	12:e:3958:SER:CB	2.39	0.52
12:n:4087:ALA:O	12:n:4091:GLY:N	2.43	0.52
12:e:2592:VAL:O	12:e:2733:VAL:HA	2.10	0.52
12:f:38:VAL:O	12:f:42:LEU:N	2.35	0.52
12:f:1272:ARG:O	12:f:1275:GLU:N	2.42	0.52
12:f:2302:VAL:HA	12:f:2342:MET:O	2.08	0.52
14:j:289:HIS:HA	14:j:294:PHE:N	2.24	0.52
6:P:312:LYS:O	6:P:315:GLN:N	2.42	0.52
12:f:4631:ASP:O	12:f:4634:SER:N	2.43	0.52
15:k:12:GLN:O	15:k:17:VAL:N	2.42	0.52
12:f:2162:SER:HA	12:f:2168:VAL:H	1.74	0.52
12:f:3133:LEU:O	12:f:3135:GLN:N	2.37	0.52
4:K:163:PHE:HA	4:K:170:ASN:HA	1.91	0.52
12:f:929:GLN:O	12:f:931:GLU:N	2.42	0.52
12:f:2785:THR:C	12:f:2787:ASP:H	2.18	0.52
12:f:3058:VAL:O	12:f:3062:LEU:N	2.43	0.52
12:e:806:ALA:HA	14:i:356:ALA:CA	2.32	0.52
12:f:1405:SER:CA	12:f:3658:GLY:HA2	2.40	0.52
12:f:2301:ILE:O	12:f:2341:ILE:HA	2.09	0.52
12:f:2623:SER:C	12:f:2625:ALA:N	2.67	0.52
12:e:810:LYS:N	14:i:357:GLU:N	2.57	0.52
12:e:3073:GLU:O	12:e:3080:ALA:N	2.43	0.52
12:e:4604:VAL:HA	12:e:4624:PHE:O	2.10	0.52
12:f:1650:LEU:C	12:f:1652:LYS:H	2.17	0.52
12:f:2931:GLY:O	12:f:3063:HIS:HA	2.10	0.52
12:f:3941:LEU:O	12:f:3944:PHE:N	2.43	0.52
12:f:3943:ALA:HA	12:f:3976:GLU:O	2.09	0.52
13:g:359:LEU:N	13:g:371:GLN:O	2.42	0.52
12:m:4087:ALA:O	12:m:4091:GLY:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:e:806:ALA:CB	14:i:355:ALA:HA	2.19	0.52
12:e:2255:ASP:C	12:e:2257:LYS:H	2.17	0.52
12:f:1406:GLU:H	12:f:3658:GLY:CA	2.23	0.52
12:f:3489:TRP:O	12:f:3492:THR:N	2.42	0.52
12:f:3656:THR:O	12:f:3658:GLY:N	2.43	0.52
12:m:975:ILE:C	12:m:977:GLU:N	2.68	0.52
12:f:2145:MET:O	12:f:2149:LEU:N	2.43	0.51
12:f:3517:ALA:CA	12:f:3525:ARG:HA	2.41	0.51
14:j:53:SER:C	14:j:55:LYS:N	2.68	0.51
12:e:806:ALA:HB1	14:i:355:ALA:CA	2.33	0.51
12:f:1112:VAL:O	12:f:1113:GLN:C	2.52	0.51
12:f:2253:ILE:HA	12:f:2302:VAL:O	2.10	0.51
12:f:3555:ASN:O	12:f:3558:GLU:N	2.43	0.51
14:j:320:ILE:O	14:j:323:LEU:N	2.44	0.51
12:e:4248:ALA:O	12:e:4253:GLY:HA3	2.11	0.51
12:f:2778:THR:O	12:f:2782:GLU:N	2.44	0.51
12:f:3516:TYR:O	12:f:3519:TYR:N	2.39	0.51
1:B:325:ASP:HA	6:P:93:GLU:N	2.25	0.51
12:f:891:HIS:C	12:m:688:SER:CB	2.83	0.51
12:f:1908:ALA:O	12:f:1910:THR:N	2.40	0.51
12:f:2128:ALA:O	12:f:2131:LEU:N	2.42	0.51
12:f:2319:LEU:O	12:f:2359:CYS:HA	2.11	0.51
12:f:2548:TRP:O	12:f:2551:LYS:N	2.44	0.51
12:f:2766:ALA:O	12:f:2770:THR:N	2.30	0.51
12:f:3757:LYS:H	12:f:3759:ARG:H	1.59	0.51
12:f:3901:TYR:O	12:f:3904:GLU:N	2.43	0.51
14:q:55:LYS:O	14:q:105:ASN:N	2.42	0.51
12:e:2301:ILE:O	12:e:2342:MET:N	2.34	0.51
12:e:4234:SER:O	12:e:4238:ILE:N	2.44	0.51
12:f:3613:SER:HA	12:f:3636:GLN:O	2.11	0.51
12:f:3670:ASP:O	12:f:3672:SER:N	2.43	0.51
12:f:3692:LEU:O	12:f:3695:ARG:N	2.44	0.51
9:V:60:HIS:O	9:V:90:HIS:HA	2.10	0.51
12:e:3587:PRO:HA	12:e:3697:THR:O	2.11	0.51
12:f:1109:TYR:O	12:f:1113:GLN:N	2.41	0.51
12:f:1363:LEU:O	12:f:1366:LEU:N	2.44	0.51
12:f:4530:GLN:C	12:f:4533:SER:H	2.19	0.51
15:k:18:GLN:H	15:k:92:GLN:HA	1.75	0.51
12:f:1905:PHE:O	12:f:2042:THR:HA	2.10	0.51
12:f:4308:TRP:O	12:f:4312:LEU:N	2.38	0.51
14:j:269:LEU:N	14:j:310:ILE:O	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:GLY:N	1:D:170:ILE:O	2.36	0.51
12:f:3217:GLU:O	12:f:3220:ARG:N	2.44	0.51
14:j:216:ASP:C	14:j:218:VAL:H	2.19	0.51
12:e:1098:THR:HA	12:e:1110:GLY:HA2	1.94	0.50
12:f:948:LYS:C	12:f:950:GLY:N	2.65	0.50
12:f:1135:LEU:O	12:f:1138:ASN:N	2.44	0.50
12:f:2533:PRO:O	12:f:2536:ASP:N	2.44	0.50
12:m:806:ALA:CB	14:q:356:ALA:N	2.43	0.50
12:f:2500:TRP:O	12:f:2504:GLY:HA3	2.11	0.50
12:f:3891:LYS:O	12:f:3895:THR:N	2.44	0.50
12:f:4445:THR:O	12:f:4449:ARG:N	2.36	0.50
12:f:2004:LYS:O	12:f:2006:VAL:N	2.44	0.50
12:f:2620:LEU:HA	12:f:3019:GLY:HA2	1.94	0.50
12:f:2714:PRO:C	12:f:2716:THR:H	2.19	0.50
12:f:4238:ILE:O	12:f:4240:TRP:N	2.44	0.50
14:j:181:PHE:C	14:j:313:GLY:HA2	2.36	0.50
12:m:1029:GLY:C	12:m:1031:VAL:H	2.20	0.50
12:e:2255:ASP:HA	12:e:2304:ASP:O	2.11	0.50
12:f:1351:TRP:H	12:f:1430:THR:HA	1.73	0.50
12:f:2768:PRO:O	12:f:2772:ALA:N	2.39	0.50
12:f:3901:TYR:O	12:f:3905:PHE:N	2.34	0.50
12:f:2667:ASN:O	12:f:2720:ARG:HA	2.12	0.50
12:f:3024:ASP:O	12:f:3027:ALA:N	2.45	0.50
12:f:4176:ARG:O	12:f:4180:TYR:N	2.22	0.50
14:j:356:ALA:O	14:j:357:GLU:C	2.54	0.50
12:f:2686:MET:HA	12:f:2691:GLY:C	2.36	0.50
12:f:3627:LEU:O	12:f:3671:LEU:HA	2.12	0.50
12:f:3637:ASP:N	12:f:3681:THR:HA	2.25	0.50
13:o:315:VAL:O	13:o:326:GLU:N	2.45	0.50
10:Z:1141:LEU:O	10:Z:1145:GLU:N	2.45	0.50
12:e:2759:VAL:HA	12:e:2814:GLU:O	2.12	0.50
12:f:1895:ALA:O	12:f:1900:LEU:N	2.45	0.50
12:f:3198:GLN:HA	12:f:3493:SER:HA	1.92	0.50
12:f:4093:TRP:HA	12:f:4123:ARG:H	1.77	0.50
14:j:37:SER:O	14:j:40:LEU:N	2.45	0.50
1:E:41:ARG:O	1:E:70:SER:N	2.33	0.50
12:e:818:GLU:O	12:e:820:ILE:N	2.45	0.50
12:e:4538:GLU:O	12:e:4595:GLN:N	2.37	0.50
12:f:4462:ARG:C	12:f:4464:TRP:N	2.70	0.50
14:i:137:ALA:O	14:i:231:CYS:HA	2.12	0.50
15:k:25:THR:C	15:k:27:GLY:H	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:98:GLN:O	1:G:100:GLN:N	2.45	0.50
12:f:2597:PRO:C	12:f:2599:SER:N	2.70	0.50
12:f:2686:MET:O	12:f:2691:GLY:N	2.44	0.50
12:f:3837:HIS:C	12:f:3839:VAL:N	2.66	0.50
12:m:437:ILE:O	12:m:441:LYS:N	2.42	0.50
14:j:257:HIS:HA	14:j:332:PRO:HA	1.94	0.49
14:j:369:LEU:O	14:j:373:GLN:N	2.19	0.49
12:f:3489:TRP:O	12:f:3490:GLU:C	2.55	0.49
14:i:57:ILE:O	14:i:59:VAL:N	2.45	0.49
6:M:155:HIS:O	6:M:160:LEU:N	2.33	0.49
12:f:1590:ASP:O	12:f:1594:ILE:N	2.44	0.49
12:f:2983:SER:C	12:f:2987:ASN:HA	2.38	0.49
12:f:3506:ASP:N	12:f:3543:PHE:HA	2.28	0.49
12:f:4560:VAL:O	12:f:4587:LEU:HA	2.12	0.49
1:E:20:VAL:HA	1:E:36:PRO:HA	1.94	0.49
12:f:33:HIS:O	12:f:37:LEU:N	2.36	0.49
12:f:957:ASN:HA	12:f:1104:PRO:O	2.12	0.49
12:f:1758:TRP:O	12:f:1761:ASN:N	2.45	0.49
12:f:3751:GLN:C	12:f:3753:LEU:H	2.21	0.49
12:f:4169:ILE:O	12:f:4177:ALA:N	2.45	0.49
14:i:119:LEU:C	14:i:122:ALA:H	2.20	0.49
15:k:17:VAL:HA	15:k:92:GLN:HA	1.93	0.49
12:f:1479:ASN:HA	12:f:1484:CYS:O	2.12	0.49
12:f:2306:ASP:O	12:f:2308:ASP:N	2.45	0.49
12:m:195:HIS:O	12:m:199:ASN:N	2.45	0.49
5:L:167:TYR:N	5:L:199:LYS:O	2.31	0.49
12:e:995:SER:HA	12:e:1018:PHE:CA	2.38	0.49
12:f:1726:ILE:C	12:f:1733:ILE:HA	2.37	0.49
14:j:232:THR:O	14:j:233:LYS:C	2.55	0.49
12:n:1054:TRP:C	12:n:1056:GLN:H	2.20	0.49
12:e:2774:VAL:O	12:e:2778:THR:N	2.38	0.49
12:f:925:VAL:HA	12:f:930:ALA:N	2.28	0.49
12:f:1380:TYR:C	12:f:1382:SER:N	2.71	0.49
12:f:2981:ARG:O	12:f:2986:LYS:N	2.34	0.49
12:n:315:SER:O	12:n:319:ASP:N	2.45	0.49
13:p:315:VAL:O	13:p:326:GLU:N	2.45	0.49
12:e:2635:PHE:O	12:e:2639:CYS:N	2.45	0.49
12:e:2995:ASP:O	12:e:2999:VAL:N	2.46	0.49
12:f:888:LEU:O	12:f:893:TYR:N	2.28	0.49
12:f:2300:TRP:HA	12:f:2340:ARG:O	2.12	0.49
13:h:266:SER:O	13:h:598:ASP:N	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:h:436:SER:O	13:h:450:GLY:N	2.40	0.49
12:f:1420:LEU:C	12:f:1422:VAL:H	2.21	0.49
12:f:2163:ASP:O	12:f:4535:SER:HA	2.12	0.49
12:f:3626:ALA:O	12:f:3630:GLY:N	2.46	0.49
12:f:3700:ASN:C	12:f:3702:THR:N	2.70	0.49
1:E:42:PRO:HA	1:E:69:LEU:HA	1.95	0.49
12:f:4462:ARG:C	12:f:4464:TRP:H	2.21	0.49
12:n:776:PRO:C	13:p:375:LEU:O	2.56	0.49
12:f:1846:PHE:HA	12:f:1857:LEU:HA	1.95	0.48
12:f:4634:SER:O	12:f:4638:ARG:N	2.44	0.48
12:e:3999:ASP:C	12:e:4001:LEU:H	2.21	0.48
12:e:4335:GLN:O	12:e:4338:ASP:C	2.56	0.48
12:f:4060:ALA:C	12:f:4063:ASN:H	2.21	0.48
14:j:231:CYS:O	14:j:272:THR:O	2.31	0.48
12:n:840:VAL:O	12:n:844:GLN:N	2.37	0.48
12:f:1655:LYS:C	12:f:1657:MET:N	2.71	0.48
12:f:2089:GLY:O	12:f:2092:ALA:N	2.47	0.48
3:J:248:TYR:O	3:J:256:LEU:N	2.40	0.48
12:f:1542:ARG:O	12:f:1545:VAL:N	2.45	0.48
12:f:4252:TYR:O	12:f:4256:VAL:N	2.39	0.48
8:U:82:MET:HA	8:U:99:MET:O	2.14	0.48
12:e:4234:SER:O	12:e:4237:LYS:N	2.46	0.48
12:f:846:LYS:O	12:f:850:LEU:N	2.26	0.48
12:f:1964:GLU:O	12:f:1967:MET:N	2.46	0.48
12:f:4375:ALA:O	12:f:4378:ARG:N	2.46	0.48
12:f:4570:CYS:HA	12:f:4574:LYS:O	2.13	0.48
13:g:551:LEU:O	13:g:562:THR:N	2.47	0.48
12:f:2245:GLU:C	12:f:2247:VAL:N	2.72	0.48
12:f:4044:CYS:O	12:f:4147:PHE:N	2.40	0.48
14:j:289:HIS:HA	14:j:294:PHE:O	2.14	0.48
1:G:41:ARG:O	1:G:70:SER:N	2.38	0.48
12:f:892:SER:O	12:f:893:TYR:C	2.56	0.48
12:f:1758:TRP:O	12:f:1760:GLU:N	2.47	0.48
12:f:2958:VAL:HA	12:f:2991:ALA:O	2.14	0.48
14:i:186:GLU:HA	14:i:297:THR:HA	1.96	0.48
14:j:257:HIS:HA	14:j:332:PRO:O	2.13	0.48
12:m:585:PHE:O	12:m:589:ASN:N	2.47	0.48
12:m:747:SER:HA	12:m:768:ALA:HB1	1.95	0.48
12:e:539:SER:O	12:e:543:THR:N	2.43	0.48
12:e:2160:LEU:O	12:e:2161:LEU:C	2.56	0.48
12:f:209:ILE:O	12:f:210:HIS:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:2365:SER:O	12:f:2367:ASP:N	2.47	0.48
14:i:289:HIS:HA	14:i:294:PHE:N	2.29	0.48
12:f:918:GLY:HA2	12:f:950:GLY:CA	2.44	0.48
12:f:2936:ILE:O	12:f:3095:GLY:N	2.37	0.48
12:f:3907:HIS:O	12:f:3911:GLY:N	2.47	0.48
13:h:435:THR:H	13:h:451:SER:HA	1.77	0.48
14:j:273:SER:O	14:j:276:GLU:N	2.47	0.48
12:e:2585:LEU:C	12:e:2588:HIS:H	2.22	0.47
12:f:1028:ASP:O	12:f:1031:VAL:N	2.47	0.47
12:f:2085:HIS:HA	12:f:2357:SER:HA	1.96	0.47
12:f:2426:TYR:HA	12:f:2431:GLY:HA3	1.95	0.47
12:f:4510:CYS:HA	12:f:4561:THR:O	2.13	0.47
14:i:59:VAL:N	14:i:107:TRP:O	2.47	0.47
14:j:159:HIS:O	14:j:163:MET:N	2.29	0.47
12:e:3588:LEU:O	12:e:3698:PHE:HA	2.13	0.47
12:e:4458:GLY:C	12:e:4474:THR:HA	2.38	0.47
12:f:1057:TYR:C	12:f:1059:CYS:N	2.72	0.47
12:f:2772:ALA:O	12:f:2776:PHE:N	2.40	0.47
12:f:3759:ARG:C	12:f:3762:ASP:H	2.22	0.47
1:A:98:GLN:O	1:A:100:GLN:N	2.48	0.47
12:f:2199:VAL:C	12:f:2201:GLY:H	2.22	0.47
12:f:2482:GLN:O	12:f:2485:GLN:N	2.47	0.47
12:f:3891:LYS:C	12:f:3894:GLY:H	2.22	0.47
12:e:4182:LEU:O	12:e:4186:PHE:N	2.31	0.47
12:e:4192:GLU:C	12:e:4194:LEU:N	2.71	0.47
12:f:887:ASP:O	12:f:891:HIS:N	2.47	0.47
12:f:2356:VAL:O	12:f:2359:CYS:N	2.48	0.47
12:f:2397:ARG:HA	12:f:2403:ASP:H	1.79	0.47
12:f:3699:VAL:O	12:f:3701:PHE:N	2.42	0.47
12:f:4030:ILE:O	12:f:4035:VAL:N	2.46	0.47
14:j:323:LEU:O	14:j:326:ASN:N	2.47	0.47
12:n:2694:ARG:O	12:n:2698:GLN:N	2.48	0.47
1:A:200:LYS:O	1:B:117:PRO:HA	2.15	0.47
1:D:156:VAL:HA	1:D:169:PRO:HA	1.97	0.47
12:e:4529:ALA:O	12:e:4534:TRP:O	2.31	0.47
12:f:2644:THR:C	12:f:2646:ASN:N	2.72	0.47
12:e:1902:GLY:HA2	12:e:2037:ARG:O	2.14	0.47
12:e:4150:PRO:O	12:e:4152:GLY:N	2.47	0.47
12:e:4152:GLY:N	12:e:4314:ASP:O	2.46	0.47
12:f:479:VAL:O	12:f:483:VAL:N	2.42	0.47
12:f:2930:GLN:O	12:f:2932:HIS:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:j:64:GLY:C	14:j:66:GLY:H	2.22	0.47
12:m:2694:ARG:O	12:m:2698:GLN:N	2.47	0.47
12:n:86:GLU:O	12:n:96:LYS:N	2.42	0.47
1:F:145:LEU:O	1:F:343:GLY:HA3	2.14	0.47
1:I:161:GLY:O	1:I:186:ALA:HB1	2.15	0.47
11:Y:427:LYS:HA	11:Y:457:HIS:HA	1.96	0.47
12:e:900:VAL:O	12:e:904:ASP:N	2.36	0.47
12:e:2663:CYS:O	12:e:2711:ALA:N	2.45	0.47
12:e:3601:MET:O	12:e:3605:LYS:N	2.48	0.47
12:f:1995:ALA:C	12:f:1997:ILE:H	2.23	0.47
12:f:2191:LEU:O	12:f:2192:THR:C	2.57	0.47
12:f:3482:LEU:O	12:f:3483:SER:C	2.57	0.47
12:f:3773:LEU:O	12:f:3775:ARG:N	2.47	0.47
12:f:4542:GLU:O	12:f:4590:LEU:HA	2.13	0.47
14:i:43:VAL:C	14:i:46:ARG:H	2.23	0.47
14:j:66:GLY:O	14:j:69:THR:N	2.48	0.47
14:j:137:ALA:O	14:j:139:MET:N	2.48	0.47
14:j:272:THR:HA	14:j:278:LYS:O	2.14	0.47
15:l:58:ARG:HA	15:l:62:PRO:CA	2.30	0.47
1:A:20:VAL:HA	1:A:36:PRO:HA	1.97	0.47
12:f:1527:LEU:O	12:f:1528:ASN:C	2.56	0.47
12:f:2677:GLN:O	12:f:2680:ILE:N	2.48	0.47
12:f:4068:SER:HA	12:f:4095:MET:O	2.15	0.47
12:f:4567:GLY:O	12:f:4578:SER:N	2.30	0.47
14:j:218:VAL:HA	14:j:263:LEU:O	2.14	0.47
12:e:535:GLY:HA2	12:e:546:TRP:HA	1.97	0.47
12:e:4606:THR:HA	12:e:4622:VAL:O	2.14	0.47
12:f:1486:LEU:O	12:f:1488:ARG:N	2.48	0.47
12:f:1902:GLY:N	12:f:2015:PHE:HA	2.29	0.47
15:k:27:GLY:HA3	15:k:44:ASN:N	2.30	0.47
12:m:4549:GLN:O	12:m:4550:SER:CB	2.63	0.47
4:K:160:SER:O	4:K:173:TRP:N	2.35	0.47
12:e:435:ARG:O	12:e:447:LYS:N	2.48	0.47
12:e:1018:PHE:O	12:e:1020:ARG:N	2.47	0.47
12:f:1731:THR:CA	12:f:1784:ASN:HA	2.45	0.47
12:f:2499:LEU:C	12:f:2502:LEU:H	2.18	0.47
12:f:2777:TYR:O	12:f:2781:GLN:N	2.32	0.47
12:f:3869:ASN:C	12:f:3871:VAL:N	2.71	0.47
14:i:119:LEU:O	14:i:122:ALA:N	2.47	0.47
14:i:232:THR:HA	14:i:272:THR:O	2.15	0.47
12:n:1054:TRP:C	12:n:1056:GLN:N	2.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:e:819:GLY:O	12:e:820:ILE:C	2.57	0.46
12:e:1351:TRP:H	12:e:1430:THR:HA	1.79	0.46
12:f:2257:LYS:O	12:f:2678:ARG:HA	2.15	0.46
12:f:888:LEU:O	12:f:892:SER:N	2.48	0.46
12:e:120:LYS:HA	12:e:135:LEU:HA	1.96	0.46
12:e:810:LYS:HA	14:i:357:GLU:H	1.80	0.46
12:e:4249:GLN:HA	12:e:4253:GLY:HA3	1.97	0.46
12:f:4387:TRP:O	12:f:4388:LEU:C	2.59	0.46
14:i:64:GLY:C	14:i:66:GLY:H	2.24	0.46
12:f:1380:TYR:O	12:f:1382:SER:N	2.48	0.46
12:f:4015:GLU:HA	12:f:4018:MET:H	1.81	0.46
14:i:367:GLN:C	14:i:369:LEU:H	2.22	0.46
1:C:145:LEU:O	1:C:343:GLY:HA3	2.15	0.46
12:e:1098:THR:O	12:e:1109:TYR:N	2.44	0.46
12:f:1475:LEU:H	12:f:1586:PRO:C	2.24	0.46
12:f:2660:VAL:HA	12:f:2707:GLN:O	2.16	0.46
12:f:3588:LEU:HA	12:f:3679:LEU:O	2.16	0.46
14:j:269:LEU:O	14:j:309:PHE:HA	2.15	0.46
12:f:960:HIS:N	12:f:1106:VAL:O	2.48	0.46
12:f:2754:ALA:C	12:f:2756:LEU:H	2.24	0.46
13:g:315:VAL:O	13:g:326:GLU:N	2.48	0.46
1:D:51:ALA:HB2	1:F:173:GLY:HA3	1.98	0.46
1:E:145:LEU:O	1:E:343:GLY:HA3	2.15	0.46
11:Y:50:TYR:HA	11:Y:56:GLU:O	2.16	0.46
12:e:119:ILE:O	12:e:136:ARG:N	2.49	0.46
12:f:1309:THR:C	12:f:1311:LEU:N	2.74	0.46
12:f:1896:LEU:C	12:f:1899:ARG:H	2.24	0.46
12:f:2597:PRO:O	12:f:2598:GLY:C	2.58	0.46
12:f:2937:GLY:HA3	12:f:3095:GLY:C	2.41	0.46
12:f:3945:LYS:C	12:f:3947:LEU:H	2.23	0.46
12:m:716:ARG:HA	12:m:823:VAL:HA	1.97	0.46
12:m:3407:LYS:O	12:m:3408:ARG:C	2.58	0.46
12:e:1675:GLY:HA3	12:e:1684:VAL:O	2.16	0.46
12:e:3997:ARG:C	12:e:3999:ASP:N	2.73	0.46
12:f:1371:LYS:C	12:f:1373:PHE:H	2.24	0.46
1:G:200:LYS:O	2:H:112:PRO:HA	2.16	0.46
12:f:1926:PHE:O	12:f:1953:ALA:HA	2.16	0.46
14:j:186:GLU:HA	14:j:297:THR:O	2.16	0.46
13:o:268:ASN:N	13:o:596:ILE:O	2.49	0.46
12:f:333:ASN:O	12:f:336:MET:N	2.49	0.46
12:f:972:ASN:HA	12:f:973:PRO:C	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:4026:ASP:O	12:f:4029:HIS:N	2.48	0.46
12:m:715:GLY:O	12:m:824:TRP:N	2.46	0.46
12:n:1057:TYR:C	12:n:1059:CYS:H	2.23	0.46
12:e:1136:GLY:HA3	12:e:1208:TRP:HA	1.98	0.45
12:f:1585:SER:O	12:f:1587:LEU:N	2.50	0.45
15:l:26:GLU:C	15:l:28:ILE:H	2.25	0.45
12:e:1351:TRP:N	12:e:1430:THR:HA	2.31	0.45
12:e:4537:GLU:C	12:e:4539:LEU:H	2.23	0.45
12:f:113:SER:O	12:f:141:SER:HA	2.17	0.45
12:f:116:LEU:HA	12:f:139:THR:HA	1.98	0.45
12:f:1758:TRP:O	12:f:1759:SER:C	2.57	0.45
12:f:4387:TRP:O	12:f:4390:LEU:N	2.48	0.45
14:j:182:GLN:HA	14:j:214:LEU:H	1.79	0.45
12:e:4184:ALA:O	12:e:4188:ALA:N	2.49	0.45
12:f:3577:ALA:O	12:f:3580:LEU:N	2.45	0.45
12:m:654:ILE:O	12:m:657:GLN:N	2.50	0.45
12:n:4549:GLN:O	12:n:4550:SER:CB	2.63	0.45
12:e:4402:VAL:C	12:e:4404:ASN:H	2.25	0.45
12:f:2255:ASP:HA	12:f:2304:ASP:O	2.16	0.45
12:f:2667:ASN:C	12:f:2720:ARG:HA	2.41	0.45
12:f:4545:VAL:HA	12:f:4587:LEU:O	2.16	0.45
13:p:268:ASN:N	13:p:596:ILE:O	2.49	0.45
12:f:929:GLN:O	12:f:930:ALA:C	2.58	0.45
12:f:2365:SER:C	12:f:2367:ASP:N	2.75	0.45
12:f:3773:LEU:C	12:f:3775:ARG:N	2.74	0.45
14:j:185:ILE:O	14:j:297:THR:HA	2.16	0.45
12:e:2066:ALA:C	12:e:2068:LYS:N	2.74	0.45
12:f:1841:GLN:O	12:f:1843:ARG:N	2.50	0.45
1:A:145:LEU:O	1:A:343:GLY:HA3	2.17	0.45
12:f:1283:TYR:O	12:f:1284:GLU:C	2.60	0.45
12:f:2489:TYR:CA	12:f:2543:GLY:HA2	2.46	0.45
12:f:2503:SER:C	12:f:2505:ASP:N	2.72	0.45
12:f:3130:TYR:C	12:f:3132:LYS:H	2.24	0.45
12:n:3407:LYS:O	12:n:3408:ARG:C	2.59	0.45
1:D:161:GLY:O	1:D:186:ALA:HB1	2.17	0.45
1:G:161:GLY:O	1:G:186:ALA:HB1	2.16	0.45
12:e:3612:THR:O	12:e:3635:VAL:HA	2.16	0.45
12:f:82:SER:O	12:f:84:LEU:N	2.50	0.45
12:f:948:LYS:C	12:f:951:GLY:H	2.23	0.45
12:f:1395:LYS:C	12:f:1397:ASN:N	2.73	0.45
12:f:2968:THR:O	12:f:2972:PHE:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:3869:ASN:HA	12:f:4020:ILE:O	2.17	0.45
12:f:4224:ASP:O	12:f:4228:LYS:N	2.33	0.45
14:j:117:GLY:C	14:j:119:LEU:H	2.24	0.45
12:n:776:PRO:CB	13:p:375:LEU:C	2.80	0.45
12:e:2162:SER:O	12:e:2165:PHE:O	2.35	0.45
12:e:2644:THR:C	12:e:2646:ASN:H	2.25	0.45
12:e:4527:TYR:O	12:e:4530:GLN:N	2.46	0.45
12:f:995:SER:C	12:f:1019:TYR:O	2.60	0.45
12:f:1272:ARG:C	12:f:1274:GLU:N	2.75	0.45
12:f:2593:LEU:O	12:f:2712:CYS:O	2.35	0.45
12:f:3645:LEU:O	12:f:3649:LEU:N	2.34	0.45
12:f:4060:ALA:HA	12:f:4063:ASN:HA	1.98	0.45
12:f:4208:GLY:O	12:f:4211:ASP:N	2.50	0.45
12:m:802:SER:O	12:m:806:ALA:HB2	2.17	0.45
12:n:803:LEU:CA	12:n:894:SER:O	2.63	0.45
12:e:2596:PRO:O	12:e:2598:GLY:N	2.49	0.45
12:f:1983:ARG:O	12:f:1985:HIS:N	2.50	0.45
12:f:2162:SER:HA	12:f:2168:VAL:N	2.31	0.45
12:f:2189:MET:C	12:f:2191:LEU:N	2.74	0.45
15:l:67:THR:O	15:l:81:ALA:HA	2.17	0.45
12:n:839:THR:O	12:n:843:PHE:N	2.38	0.45
12:e:1070:ASN:O	12:e:1073:GLY:N	2.51	0.44
12:e:1747:ALA:O	12:e:1750:VAL:N	2.50	0.44
12:f:1475:LEU:H	12:f:1587:LEU:HA	1.82	0.44
15:k:25:THR:O	15:k:27:GLY:N	2.50	0.44
4:K:62:PHE:HA	4:K:76:ILE:O	2.17	0.44
12:f:2406:GLU:O	12:f:2410:SER:N	2.51	0.44
12:f:3637:ASP:HA	12:f:3681:THR:HA	2.00	0.44
14:i:367:GLN:C	14:i:369:LEU:N	2.74	0.44
12:e:2051:GLN:HA	12:e:2062:ALA:O	2.17	0.44
12:e:2056:SER:C	12:e:2058:GLY:H	2.24	0.44
12:f:1030:PRO:O	12:f:1034:GLU:N	2.49	0.44
12:f:2621:ASN:H	12:f:3019:GLY:N	2.16	0.44
15:l:69:LEU:C	15:l:71:ILE:H	2.25	0.44
1:B:332:ALA:H	6:P:86:GLY:HA3	1.82	0.44
12:e:720:ILE:HA	12:e:735:LEU:CA	2.34	0.44
12:e:912:GLY:CA	12:e:1026:MET:HA	2.48	0.44
12:f:1348:GLU:HA	12:f:1432:GLY:N	2.32	0.44
12:f:2388:ASP:O	12:f:2390:GLY:N	2.50	0.44
12:f:3505:GLY:N	12:f:3542:GLN:O	2.40	0.44
12:f:4279:ASP:C	12:f:4281:GLU:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:h:527:VAL:HA	13:h:544:ASP:HA	1.99	0.44
12:e:2772:ALA:O	12:e:2776:PHE:N	2.39	0.44
12:f:1313:SER:O	12:f:1316:GLU:N	2.47	0.44
12:f:1692:ILE:C	12:f:1695:HIS:H	2.24	0.44
12:f:2855:LEU:O	12:f:2859:PRO:HA	2.17	0.44
12:f:3069:ASN:O	12:f:3070:PRO:C	2.61	0.44
12:f:3700:ASN:O	12:f:3702:THR:N	2.49	0.44
12:f:4508:HIS:HA	12:f:4559:GLY:O	2.18	0.44
14:i:311:PRO:O	14:i:315:ASP:N	2.51	0.44
14:j:151:LYS:O	14:j:155:VAL:N	2.35	0.44
12:f:961:GLU:HA	12:f:1108:ASP:C	2.43	0.44
12:f:2249:GLY:HA2	12:f:2298:ARG:O	2.17	0.44
12:f:3602:ASN:C	12:f:3605:LYS:H	2.26	0.44
12:f:4129:GLU:O	12:f:4131:ASN:N	2.50	0.44
14:j:94:HIS:HA	14:j:101:HIS:HA	1.99	0.44
11:Y:426:PHE:O	11:Y:458:VAL:N	2.50	0.44
12:e:2390:GLY:O	12:e:2394:ALA:N	2.51	0.44
12:e:2963:VAL:O	12:e:3665:GLY:HA2	2.18	0.44
6:P:258:GLY:O	6:P:260:CYS:N	2.48	0.44
12:e:283:ARG:CA	12:f:176:ASP:H	2.29	0.44
12:e:4511:LEU:C	12:e:4513:GLY:H	2.26	0.44
12:f:513:ASP:O	12:f:517:ALA:N	2.37	0.44
12:f:2186:CYS:O	12:f:2191:LEU:N	2.50	0.44
12:f:4554:ASP:C	12:f:4556:CYS:N	2.75	0.44
13:h:480:THR:H	13:h:501:SER:HA	1.82	0.44
1:B:153:THR:O	1:B:173:GLY:N	2.45	0.44
1:D:145:LEU:O	1:D:343:GLY:HA3	2.18	0.44
12:e:804:LEU:HA	12:e:894:SER:O	2.18	0.44
12:e:3950:LYS:O	12:e:3954:ASP:N	2.51	0.44
12:e:4336:GLY:C	12:e:4339:MET:H	2.26	0.44
12:f:1731:THR:C	12:f:1784:ASN:HA	2.43	0.44
12:f:3555:ASN:O	12:f:3556:ALA:C	2.61	0.44
12:f:4307:GLN:O	12:f:4311:LEU:N	2.45	0.44
12:f:4510:CYS:O	12:f:4511:LEU:C	2.61	0.44
12:m:539:SER:O	12:m:543:THR:N	2.40	0.44
12:m:975:ILE:O	12:m:978:CYS:N	2.50	0.44
12:e:286:TYR:CB	12:f:175:GLY:HA2	2.48	0.43
12:e:993:VAL:C	12:e:995:SER:H	2.26	0.43
12:f:1197:LEU:C	12:f:1199:LYS:N	2.76	0.43
12:f:2754:ALA:C	12:f:2756:LEU:N	2.75	0.43
12:f:4239:PRO:O	12:f:4242:ALA:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:g:359:LEU:O	13:g:370:VAL:N	2.51	0.43
14:i:109:LEU:O	14:i:110:ASP:C	2.61	0.43
14:j:216:ASP:C	14:j:218:VAL:N	2.75	0.43
1:A:19:GLY:O	1:A:37:ASN:N	2.41	0.43
12:e:3085:LEU:O	12:e:3089:CYS:N	2.52	0.43
12:f:974:PRO:O	12:f:977:GLU:N	2.51	0.43
12:f:1109:TYR:O	12:f:1112:VAL:N	2.50	0.43
12:f:2379:LEU:C	12:f:2381:ARG:N	2.74	0.43
12:f:2912:PHE:O	12:f:2916:LEU:N	2.51	0.43
12:f:4043:MET:H	12:f:4126:LEU:C	2.25	0.43
12:f:4280:SER:O	12:f:4297:PRO:HA	2.19	0.43
12:f:863:SER:O	12:f:867:CYS:N	2.40	0.43
12:f:2569:VAL:O	12:f:2570:PRO:C	2.61	0.43
13:h:436:SER:N	13:h:450:GLY:O	2.39	0.43
12:e:37:LEU:O	12:e:41:LEU:N	2.39	0.43
12:e:994:LEU:HA	12:e:1019:TYR:O	2.18	0.43
12:e:2162:SER:HA	12:e:2165:PHE:O	2.17	0.43
12:e:4192:GLU:O	12:e:4194:LEU:N	2.51	0.43
12:f:2226:SER:C	12:f:2228:SER:H	2.27	0.43
12:f:2598:GLY:C	12:f:2600:GLY:H	2.26	0.43
12:f:4173:PRO:O	12:f:4176:ARG:N	2.51	0.43
1:C:161:GLY:O	1:C:186:ALA:HB1	2.19	0.43
10:Z:1186:ALA:O	10:Z:1188:SER:N	2.51	0.43
12:e:4459:ILE:HA	12:e:4473:MET:O	2.18	0.43
12:f:1301:LYS:O	12:f:1305:GLU:N	2.51	0.43
12:f:1390:LEU:O	12:f:1393:TYR:N	2.52	0.43
12:f:1680:GLU:C	12:f:1682:GLU:H	2.26	0.43
12:f:1987:SER:O	12:f:1989:ASN:N	2.48	0.43
12:f:4297:PRO:O	12:f:4299:GLY:N	2.51	0.43
14:i:115:HIS:O	14:i:118:LEU:C	2.62	0.43
14:j:82:LYS:O	14:j:83:GLY:C	2.60	0.43
14:j:180:ASP:O	14:j:181:PHE:C	2.62	0.43
15:k:28:ILE:HA	15:k:40:THR:HA	2.00	0.43
12:e:996:LEU:N	12:e:1019:TYR:H	2.15	0.43
12:e:4339:MET:O	12:e:4343:MET:N	2.49	0.43
12:f:3528:LEU:O	12:f:3529:PHE:C	2.62	0.43
12:f:3822:HIS:C	12:f:3824:LEU:H	2.27	0.43
1:F:158:LEU:O	1:F:301:SER:N	2.51	0.43
1:I:200:LYS:O	3:J:98:PRO:HA	2.19	0.43
4:K:154:ILE:N	4:K:179:PHE:O	2.42	0.43
12:e:832:TYR:O	12:e:836:LEU:N	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:e:2593:LEU:O	12:e:2711:ALA:HA	2.19	0.43
12:e:2795:SER:O	12:e:2798:GLU:N	2.51	0.43
12:e:4562:GLY:O	12:e:4645:THR:HA	2.18	0.43
12:f:3626:ALA:HA	12:f:3630:GLY:C	2.43	0.43
14:j:273:SER:O	14:j:276:GLU:C	2.60	0.43
1:D:238:LYS:HA	1:D:252:GLY:HA2	2.00	0.43
6:Q:26:PRO:O	6:Q:28:ASP:N	2.51	0.43
7:R:18:GLU:O	7:R:22:TYR:N	2.52	0.43
12:e:1070:ASN:C	12:e:1073:GLY:H	2.27	0.43
12:e:1838:TRP:O	12:e:1841:GLN:N	2.46	0.43
12:f:2219:GLY:O	12:f:2360:GLY:N	2.44	0.43
14:i:138:ASP:HA	14:i:232:THR:O	2.18	0.43
12:m:25:ALA:N	12:m:125:ILE:O	2.52	0.43
12:e:1554:SER:HA	12:e:1642:GLY:HA2	2.01	0.43
12:e:4288:VAL:HA	12:e:4322:GLY:HA2	2.00	0.43
12:f:1860:GLN:HA	12:f:1865:LYS:HA	2.00	0.43
1:B:51:ALA:HB2	1:D:173:GLY:HA3	2.01	0.42
12:e:2161:LEU:O	12:e:2165:PHE:N	2.49	0.42
12:e:2264:LEU:C	12:e:2279:LEU:H	2.25	0.42
12:e:3538:GLN:C	12:e:3540:ASN:H	2.26	0.42
12:e:3672:SER:C	12:e:3674:SER:H	2.26	0.42
12:e:4274:THR:C	12:e:4277:SER:H	2.27	0.42
12:f:2773:MET:O	12:f:2774:VAL:C	2.61	0.42
12:f:4564:LYS:O	12:f:4642:VAL:CA	2.48	0.42
12:f:4574:LYS:HA	12:f:4625:GLU:O	2.19	0.42
12:e:946:SER:O	12:e:947:HIS:C	2.61	0.42
12:e:1059:CYS:O	12:e:1061:TRP:N	2.52	0.42
12:f:891:HIS:O	12:f:892:SER:C	2.62	0.42
12:f:1368:ASN:O	12:f:1369:GLN:C	2.62	0.42
12:f:2304:ASP:HA	12:f:2344:GLU:O	2.19	0.42
12:f:2759:VAL:C	12:f:2761:SER:H	2.28	0.42
12:f:2770:THR:O	12:f:2771:ALA:C	2.62	0.42
12:e:869:TYR:H	12:e:951:GLY:CA	2.29	0.42
12:e:4219:VAL:O	12:e:4220:ASP:C	2.61	0.42
12:f:945:VAL:O	12:f:946:SER:C	2.62	0.42
12:f:4036:LYS:C	12:f:4038:ASN:H	2.27	0.42
12:f:4182:LEU:O	12:f:4183:LEU:C	2.59	0.42
13:g:480:THR:N	13:g:500:SER:O	2.52	0.42
12:e:993:VAL:C	12:e:995:SER:N	2.77	0.42
12:e:2789:GLN:C	12:e:2791:HIS:N	2.77	0.42
12:e:3637:ASP:HA	12:e:3680:SER:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:2055:TYR:HA	12:f:2059:PHE:O	2.18	0.42
12:f:2600:GLY:O	12:f:2601:LYS:C	2.63	0.42
12:f:2714:PRO:C	12:f:2716:THR:N	2.78	0.42
12:f:2855:LEU:HA	12:f:2858:PHE:O	2.20	0.42
12:f:3498:ASN:C	12:f:3500:MET:N	2.76	0.42
14:i:54:GLY:O	14:i:56:ASN:N	2.53	0.42
14:i:166:PRO:O	14:i:169:GLU:N	2.52	0.42
14:i:268:ALA:HA	14:i:312:ALA:N	2.34	0.42
15:k:25:THR:C	15:k:27:GLY:N	2.77	0.42
12:e:3079:ALA:O	12:e:3080:ALA:C	2.62	0.42
12:e:3537:GLN:CA	12:e:3543:PHE:H	2.30	0.42
12:e:4531:ALA:C	12:e:4533:SER:H	2.27	0.42
12:f:2069:ILE:O	12:f:2073:PHE:N	2.24	0.42
12:f:2555:ILE:O	12:f:2750:THR:HA	2.18	0.42
12:f:4610:TYR:O	12:f:4644:CYS:N	2.52	0.42
12:m:627:TYR:O	12:m:628:PRO:C	2.62	0.42
12:e:809:LYS:C	14:i:357:GLU:N	2.77	0.42
12:e:1136:GLY:HA3	12:e:1207:SER:O	2.19	0.42
12:f:3092:ASN:O	12:f:3094:PHE:N	2.53	0.42
12:f:3626:ALA:HA	12:f:3631:ASN:N	2.33	0.42
12:n:3378:ASN:C	12:n:3380:GLU:H	2.27	0.42
14:r:37:SER:O	14:r:38:SER:C	2.62	0.42
12:e:1029:GLY:C	12:e:1031:VAL:H	2.27	0.42
12:e:2937:GLY:CA	12:e:3095:GLY:H	2.32	0.42
12:f:2593:LEU:HA	12:f:2734:VAL:O	2.20	0.42
12:f:4041:VAL:O	12:f:4125:PHE:HA	2.19	0.42
13:h:455:SER:HA	13:h:472:PHE:O	2.19	0.42
1:F:98:GLN:O	1:F:100:GLN:N	2.53	0.42
12:f:1547:LEU:O	12:f:1551:PHE:N	2.50	0.42
12:f:1626:PHE:O	12:f:1629:PHE:N	2.52	0.42
12:f:3877:HIS:O	12:f:3881:ILE:N	2.53	0.42
12:f:4186:PHE:C	12:f:4188:ALA:N	2.77	0.42
14:i:162:LYS:C	14:i:164:LYS:N	2.77	0.42
14:j:181:PHE:HA	14:j:313:GLY:CA	2.42	0.42
14:j:264:GLN:C	14:j:266:GLY:H	2.28	0.42
15:k:71:ILE:HA	15:l:68:PHE:O	2.20	0.42
12:f:717:ILE:O	12:f:737:VAL:HA	2.19	0.42
12:f:1296:LYS:O	12:f:1297:CYS:C	2.62	0.42
12:f:2188:GLU:C	12:f:2190:TYR:N	2.72	0.42
12:f:2898:LYS:C	12:f:2901:TYR:H	2.28	0.42
12:f:3735:GLN:O	12:f:3738:PHE:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:4112:LYS:O	12:f:4115:SER:C	2.63	0.42
14:i:241:GLU:HA	14:i:246:TYR:O	2.20	0.42
14:j:236:ALA:O	14:j:237:VAL:C	2.62	0.42
12:n:666:GLU:HA	12:n:673:TRP:CB	2.50	0.42
2:H:264:PRO:O	2:H:268:GLY:N	2.53	0.42
12:e:784:SER:CB	12:e:837:ALA:HA	2.49	0.42
12:e:1057:TYR:C	12:e:1059:CYS:N	2.78	0.42
12:e:4172:SER:HA	12:e:4173:PRO:HA	1.88	0.42
12:f:1521:LEU:C	12:f:1523:TRP:N	2.74	0.42
12:f:2943:LYS:C	12:f:2945:THR:N	2.77	0.42
12:f:3482:LEU:O	12:f:3484:ALA:N	2.52	0.42
13:g:313:ALA:O	13:g:329:PHE:N	2.52	0.42
14:i:230:VAL:HA	14:i:270:ILE:O	2.20	0.42
14:i:244:HIS:C	14:i:246:TYR:N	2.77	0.42
14:j:64:GLY:C	14:j:66:GLY:N	2.78	0.42
14:j:113:LEU:C	14:j:115:HIS:N	2.78	0.42
15:k:69:LEU:HA	15:l:72:ARG:H	1.85	0.42
15:l:23:VAL:CA	15:l:29:PRO:HA	2.35	0.42
12:m:137:VAL:O	12:n:139:THR:N	2.53	0.42
5:L:179:THR:N	5:L:187:MET:O	2.31	0.41
12:e:3600:ILE:O	12:e:3604:TYR:N	2.52	0.41
12:f:3945:LYS:C	12:f:3947:LEU:N	2.78	0.41
14:j:241:GLU:HA	14:j:246:TYR:H	1.83	0.41
1:F:20:VAL:HA	1:F:36:PRO:HA	2.02	0.41
10:Z:1150:GLU:HA	10:Z:1153:ALA:HB3	2.02	0.41
12:f:2591:LEU:O	12:f:2709:VAL:HA	2.19	0.41
12:f:2986:LYS:O	12:f:2987:ASN:C	2.63	0.41
12:f:4167:SER:C	12:f:4169:ILE:N	2.77	0.41
12:f:4180:TYR:O	12:f:4181:PHE:C	2.61	0.41
15:l:69:LEU:C	15:l:71:ILE:N	2.77	0.41
12:n:3410:GLU:O	12:n:3411:PRO:C	2.62	0.41
12:f:994:LEU:HA	12:f:1022:ALA:N	2.27	0.41
12:f:3199:MET:C	12:f:3201:LEU:N	2.75	0.41
14:i:132:LEU:O	14:i:134:ILE:N	2.53	0.41
12:m:165:ILE:CA	12:m:171:ALA:H	2.33	0.41
12:m:654:ILE:O	12:m:655:ASP:C	2.63	0.41
12:e:1091:GLY:C	12:e:1093:PHE:H	2.27	0.41
12:e:2055:TYR:HA	12:e:2059:PHE:O	2.21	0.41
12:e:2793:ILE:O	12:e:3087:ASN:N	2.54	0.41
12:e:2836:ARG:HA	12:e:3093:TRP:N	2.33	0.41
12:f:2931:GLY:N	12:f:3059:ILE:O	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:4192:GLU:C	12:f:4195:ARG:H	2.29	0.41
13:h:406:LYS:HA	13:h:423:GLU:HA	2.02	0.41
12:e:3617:ASP:C	12:e:3619:PHE:H	2.28	0.41
12:f:441:LYS:O	12:f:445:ASN:N	2.33	0.41
12:f:1879:LEU:O	12:f:1880:VAL:C	2.62	0.41
12:f:2875:ASN:HA	12:f:2878:SER:O	2.20	0.41
12:f:3576:ASN:O	12:f:3577:ALA:C	2.64	0.41
12:f:3626:ALA:HA	12:f:3630:GLY:CA	2.50	0.41
1:A:156:VAL:HA	1:A:169:PRO:HA	2.02	0.41
12:e:3966:PRO:O	12:e:3968:GLN:N	2.43	0.41
12:f:2667:ASN:O	12:f:2669:PRO:O	2.39	0.41
12:f:2836:ARG:HA	12:f:3091:LEU:O	2.21	0.41
12:f:3757:LYS:C	12:f:3759:ARG:H	2.27	0.41
12:f:4510:CYS:HA	12:f:4561:THR:C	2.45	0.41
14:j:43:VAL:O	14:j:46:ARG:N	2.47	0.41
14:j:218:VAL:C	14:j:220:THR:H	2.28	0.41
12:m:112:LYS:H	12:m:142:GLU:C	2.29	0.41
12:n:803:LEU:CB	12:n:895:ASN:CA	2.98	0.41
1:D:330:ILE:N	6:P:20:TYR:O	2.43	0.41
12:e:349:GLU:O	12:e:353:ILE:N	2.49	0.41
12:f:1026:MET:O	12:f:1028:ASP:N	2.51	0.41
12:f:1818:GLN:O	12:f:1819:ARG:C	2.63	0.41
12:f:3591:ASP:N	12:f:3683:ASP:O	2.53	0.41
14:i:161:ASP:C	14:i:164:LYS:H	2.29	0.41
14:j:117:GLY:C	14:j:119:LEU:N	2.78	0.41
1:A:41:ARG:O	1:A:70:SER:N	2.38	0.41
12:e:720:ILE:HA	12:e:736:LYS:H	1.85	0.41
12:e:2943:LYS:C	12:e:2945:THR:H	2.29	0.41
12:f:914:ARG:HA	12:f:949:PRO:C	2.46	0.41
12:f:3642:ASP:O	12:f:3645:LEU:N	2.53	0.41
12:f:4269:LEU:C	12:f:4273:PHE:H	2.24	0.41
12:e:863:SER:O	12:e:867:CYS:N	2.54	0.41
12:e:964:ILE:HA	12:e:969:ILE:HA	2.03	0.41
12:e:4560:VAL:O	12:e:4587:LEU:HA	2.20	0.41
12:e:4602:ALA:O	12:e:4630:GLU:N	2.46	0.41
12:f:918:GLY:HA2	12:f:950:GLY:HA3	2.03	0.41
12:f:1162:SER:O	12:f:1166:ALA:N	2.35	0.41
12:f:1348:GLU:HA	12:f:1432:GLY:HA2	2.03	0.41
12:f:2225:PRO:O	12:f:2228:SER:N	2.54	0.41
12:f:2242:GLU:HA	12:f:2247:VAL:O	2.21	0.41
12:f:2356:VAL:C	12:f:2359:CYS:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:2983:SER:HA	12:f:2988:GLU:N	2.10	0.41
12:f:3011:LEU:HA	12:f:3016:GLU:O	2.21	0.41
12:f:3498:ASN:C	12:f:3500:MET:H	2.29	0.41
12:f:3993:ILE:C	12:f:3996:PHE:H	2.29	0.41
12:f:4299:GLY:HA2	12:f:4304:GLU:C	2.46	0.41
14:j:66:GLY:O	14:j:67:LYS:C	2.63	0.41
14:j:337:GLU:HA	14:j:340:ILE:O	2.21	0.41
12:n:803:LEU:O	12:n:894:SER:N	2.54	0.41
12:e:21:VAL:HA	12:e:122:ALA:HB1	2.03	0.41
12:e:2066:ALA:C	12:e:2068:LYS:H	2.29	0.41
12:e:4511:LEU:C	12:e:4513:GLY:N	2.79	0.41
12:f:1475:LEU:H	12:f:1587:LEU:CA	2.34	0.41
12:f:2367:ASP:HA	12:f:2370:SER:CA	2.41	0.41
12:f:2677:GLN:C	12:f:2680:ILE:H	2.28	0.41
12:f:4629:LYS:O	12:f:4630:GLU:C	2.63	0.41
14:j:137:ALA:O	14:j:138:ASP:C	2.64	0.41
14:j:311:PRO:O	14:j:313:GLY:N	2.54	0.41
12:n:674:GLU:HA	12:n:679:GLY:HA3	2.03	0.41
12:n:1057:TYR:C	12:n:1059:CYS:N	2.79	0.41
11:Y:343:LEU:HA	11:Y:430:HIS:HA	2.03	0.40
12:e:2299:GLN:O	12:e:2339:VAL:HA	2.21	0.40
12:e:2536:ASP:O	12:e:2548:TRP:N	2.50	0.40
12:f:1908:ALA:HA	12:f:1913:THR:H	1.86	0.40
13:g:364:SER:C	13:g:366:LYS:H	2.29	0.40
13:h:437:MET:HA	13:h:449:VAL:HA	2.03	0.40
14:j:54:GLY:O	14:j:55:LYS:C	2.64	0.40
15:k:66:LEU:HA	15:l:73:SER:HA	2.03	0.40
14:q:46:ARG:O	14:q:47:ALA:C	2.63	0.40
12:f:863:SER:O	12:f:864:LEU:C	2.64	0.40
12:f:1313:SER:O	12:f:1314:GLY:C	2.64	0.40
12:f:2255:ASP:C	12:f:2257:LYS:H	2.27	0.40
12:f:3994:GLN:HA	12:f:3998:PRO:HA	2.03	0.40
12:f:4287:LYS:HA	12:f:4291:HIS:C	2.46	0.40
14:j:110:ASP:C	14:j:112:ASP:N	2.79	0.40
1:F:13:VAL:O	1:F:23:ALA:HA	2.22	0.40
12:e:1938:PHE:O	12:e:1941:MET:N	2.54	0.40
12:e:1980:GLU:O	12:e:1983:ARG:N	2.55	0.40
12:e:2591:LEU:O	12:e:2709:VAL:HA	2.22	0.40
12:e:4537:GLU:O	12:e:4539:LEU:N	2.54	0.40
12:f:1132:GLY:O	12:f:1133:GLN:C	2.64	0.40
12:f:3551:GLU:HA	12:f:3554:SER:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:4601:LYS:N	12:f:4604:VAL:O	2.37	0.40
1:C:200:LYS:O	1:D:117:PRO:HA	2.21	0.40
12:e:1859:ILE:O	12:e:1865:LYS:HA	2.20	0.40
12:e:2983:SER:O	12:e:2987:ASN:HA	2.21	0.40
12:f:2255:ASP:C	12:f:2257:LYS:N	2.79	0.40
12:f:2740:GLY:O	12:f:2741:PRO:C	2.63	0.40
12:f:2845:TRP:O	12:f:2849:ASN:N	2.54	0.40
12:f:4238:ILE:C	12:f:4240:TRP:N	2.80	0.40
4:K:47:ARG:HA	4:K:50:ALA:HB3	2.03	0.40
11:Y:114:CYS:C	11:Y:116:TRP:H	2.28	0.40
12:e:949:PRO:C	12:e:951:GLY:H	2.29	0.40
12:e:2336:PRO:C	12:e:2338:ASN:N	2.79	0.40
12:e:4225:ASP:C	12:e:4227:ALA:N	2.78	0.40
12:f:1892:MET:C	12:f:1894:GLN:N	2.80	0.40
12:f:1908:ALA:C	12:f:1910:THR:H	2.26	0.40
12:f:3509:LEU:O	12:f:3513:PHE:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	368/376 (98%)	359 (98%)	9 (2%)	0	100	100
1	B	368/376 (98%)	356 (97%)	12 (3%)	0	100	100
1	C	373/376 (99%)	361 (97%)	12 (3%)	0	100	100
1	D	368/376 (98%)	356 (97%)	12 (3%)	0	100	100
1	E	368/376 (98%)	356 (97%)	12 (3%)	0	100	100
1	F	368/376 (98%)	357 (97%)	11 (3%)	0	100	100
1	G	368/376 (98%)	357 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	368/376 (98%)	354 (96%)	14 (4%)	0	100	100
2	H	368/375 (98%)	357 (97%)	11 (3%)	0	100	100
3	J	377/417 (90%)	365 (97%)	12 (3%)	0	100	100
4	K	276/286 (96%)	268 (97%)	8 (3%)	0	100	100
5	L	267/272 (98%)	261 (98%)	6 (2%)	0	100	100
6	M	330/405 (82%)	311 (94%)	18 (6%)	1 (0%)	36	72
6	N	270/405 (67%)	262 (97%)	7 (3%)	1 (0%)	30	67
6	P	319/405 (79%)	312 (98%)	7 (2%)	0	100	100
6	Q	335/405 (83%)	318 (95%)	17 (5%)	0	100	100
7	O	177/186 (95%)	165 (93%)	12 (7%)	0	100	100
7	R	168/186 (90%)	160 (95%)	8 (5%)	0	100	100
8	U	165/190 (87%)	157 (95%)	8 (5%)	0	100	100
9	V	177/182 (97%)	172 (97%)	5 (3%)	0	100	100
10	W	144/1281 (11%)	138 (96%)	5 (4%)	1 (1%)	18	56
10	Z	190/1281 (15%)	185 (97%)	5 (3%)	0	100	100
11	Y	404/467 (86%)	377 (93%)	24 (6%)	3 (1%)	18	56
12	e	4559/4646 (98%)	4166 (91%)	378 (8%)	15 (0%)	36	72
12	f	4555/4646 (98%)	3899 (86%)	583 (13%)	73 (2%)	7	38
12	m	4552/4646 (98%)	4431 (97%)	115 (2%)	6 (0%)	48	83
12	n	4514/4646 (97%)	4402 (98%)	110 (2%)	2 (0%)	100	100
13	g	356/612 (58%)	352 (99%)	4 (1%)	0	100	100
13	h	356/612 (58%)	346 (97%)	10 (3%)	0	100	100
13	o	356/612 (58%)	350 (98%)	6 (2%)	0	100	100
13	p	356/612 (58%)	350 (98%)	6 (2%)	0	100	100
14	i	291/492 (59%)	248 (85%)	40 (14%)	3 (1%)	12	49
14	j	306/492 (62%)	233 (76%)	61 (20%)	12 (4%)	2	19
14	q	301/492 (61%)	293 (97%)	8 (3%)	0	100	100
14	r	291/492 (59%)	277 (95%)	14 (5%)	0	100	100
15	k	91/96 (95%)	69 (76%)	22 (24%)	0	100	100
15	l	91/96 (95%)	69 (76%)	21 (23%)	1 (1%)	11	46
15	s	91/96 (95%)	84 (92%)	7 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	t	91/96 (95%)	86 (94%)	5 (6%)	0	100	100
All	All	28073/33135 (85%)	26319 (94%)	1636 (6%)	118 (0%)	31	67

All (118) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	M	217	PRO
10	W	1142	PRO
11	Y	175	PRO
11	Y	441	PRO
12	e	4550	SER
12	f	38	VAL
12	f	203	PRO
12	f	2190	TYR
12	f	2429	PRO
12	f	3925	PRO
14	j	63	ASP
14	j	377	PRO
12	m	870	ASP
12	m	1309	THR
12	e	819	GLY
12	e	928	GLY
12	e	1040	VAL
12	e	1862	ALA
12	e	4193	ARG
12	f	716	ARG
12	f	1198	GLU
12	f	1208	TRP
12	f	1310	GLY
12	f	1314	GLY
12	f	1957	PHE
12	f	1984	GLU
12	f	4168	ARG
14	j	54	GLY
12	n	21	VAL
12	n	1309	THR
12	e	726	ARG
12	e	994	LEU
12	e	4318	PRO
12	f	717	ILE
12	f	930	ALA
12	f	1412	HIS

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Mol	Chain	Res	Type
12	f	1656	LYS
12	f	1758	TRP
12	f	1899	ARG
12	f	1931	ASN
12	f	2172	ARG
12	f	2246	GLY
12	f	2366	GLU
12	f	2598	GLY
12	f	2715	PRO
12	f	2754	ALA
12	f	2900	PHE
12	f	3499	GLN
12	f	3513	PHE
12	f	3619	PHE
12	f	3682	ARG
12	f	3774	LYS
12	f	4377	MET
14	i	364	MET
14	j	217	ASN
12	m	976	GLU
12	f	869	TYR
12	f	1058	GLN
12	f	1119	LYS
12	f	1197	LEU
12	f	1312	LEU
12	f	1682	GLU
12	f	1759	SER
12	f	1799	GLU
12	f	2298	ARG
12	f	2504	GLY
12	f	2755	MET
12	f	3189	GLU
12	f	3482	LEU
12	f	3670	ASP
12	f	3671	LEU
12	f	3701	PHE
12	f	3870	ARG
14	i	181	PHE
14	j	138	ASP
14	j	236	ALA
15	l	54	ARG
12	m	210	HIS

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Mol	Chain	Res	Type
12	e	4632	PRO
12	f	1390	LEU
12	f	2645	PRO
12	f	3217	GLU
12	f	3755	GLU
14	j	68	THR
14	j	114	TYR
14	j	344	PRO
12	m	654	ILE
6	N	163	ASP
12	e	2161	LEU
12	e	4326	ASN
12	f	1842	MET
12	f	2883	PRO
12	f	3848	GLY
14	i	57	ILE
14	j	39	ILE
12	f	1396	ILE
12	f	1487	ILE
12	f	2931	GLY
12	f	1103	GLY
12	f	1206	PRO
12	f	1997	ILE
12	f	2360	GLY
12	f	2613	PRO
12	f	3212	VAL
12	f	4132	PRO
14	j	374	PRO
12	e	732	VAL
12	e	4151	PRO
12	f	805	VAL
12	f	1511	PRO
12	f	2291	VAL
12	f	3981	THR
12	m	627	TYR
11	Y	77	PRO
12	e	3736	GLY
12	f	1211	ILE
14	j	51	LEU
12	f	2570	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

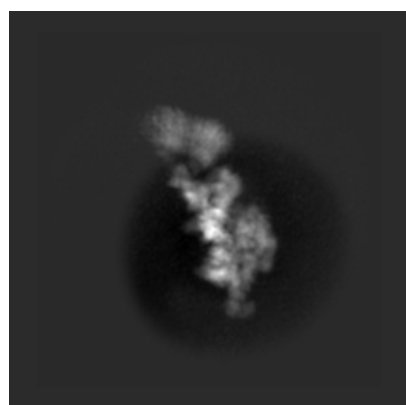
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46845. These allow visual inspection of the internal detail of the map and identification of artifacts.

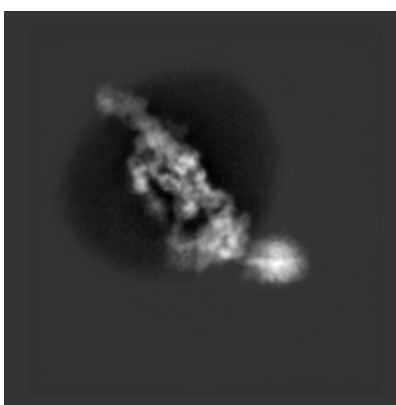
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

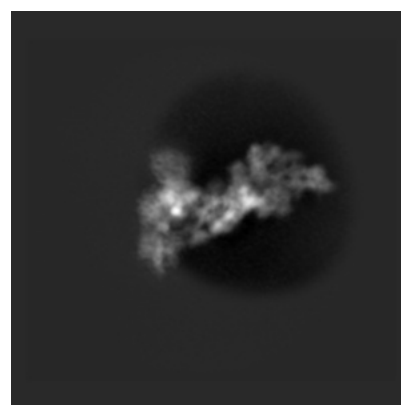
6.1.1 Primary map



X



Y

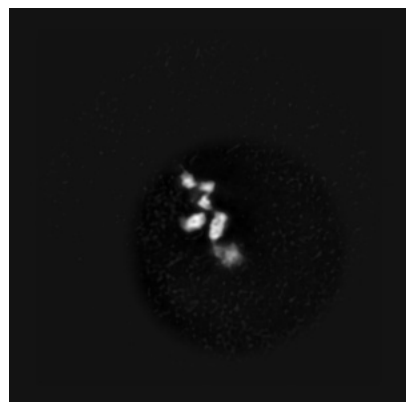


Z

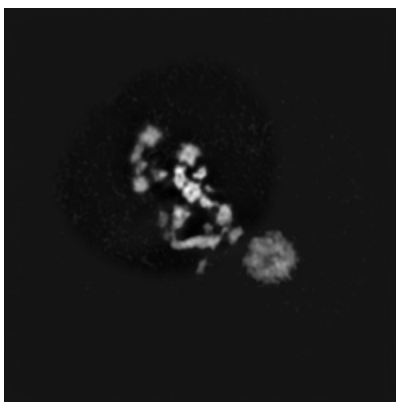
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

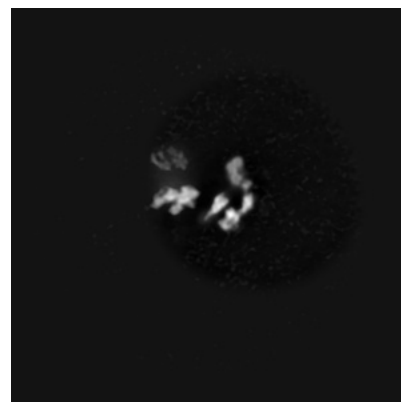
6.2.1 Primary map



X Index: 150



Y Index: 150

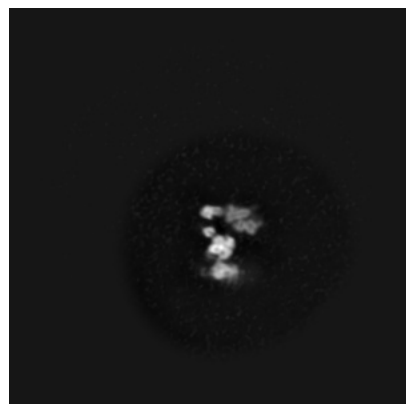


Z Index: 150

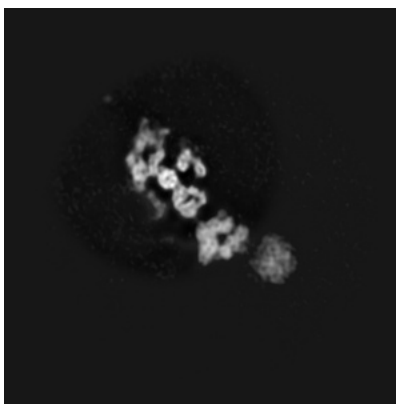
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

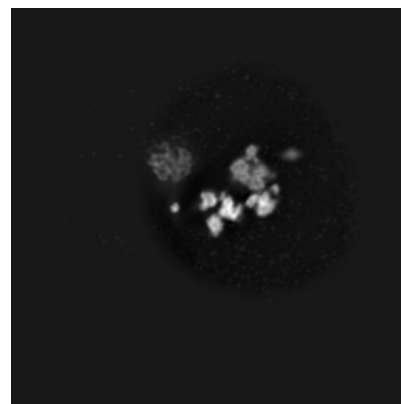
6.3.1 Primary map



X Index: 174



Y Index: 157

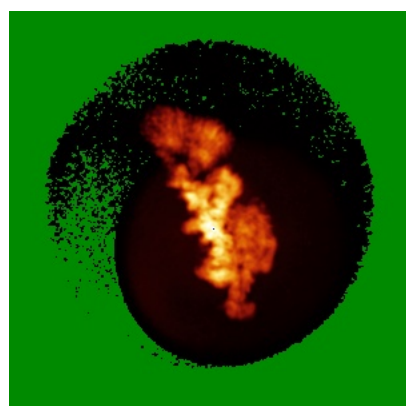


Z Index: 136

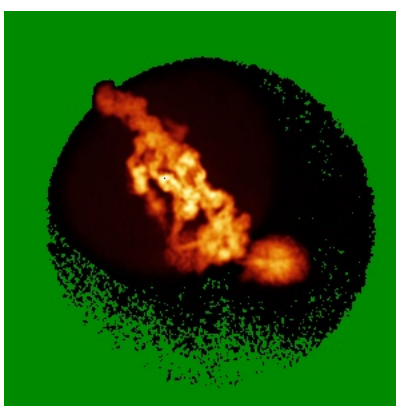
The images above show the largest variance slices of the map in three orthogonal directions.

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

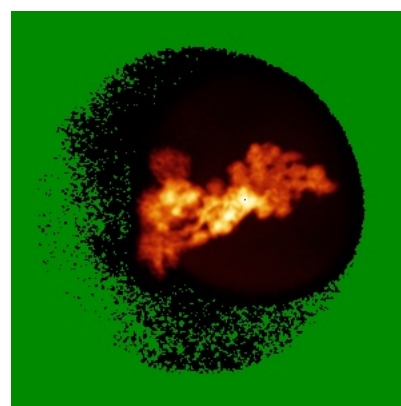
6.4.1 Primary map



X



Y

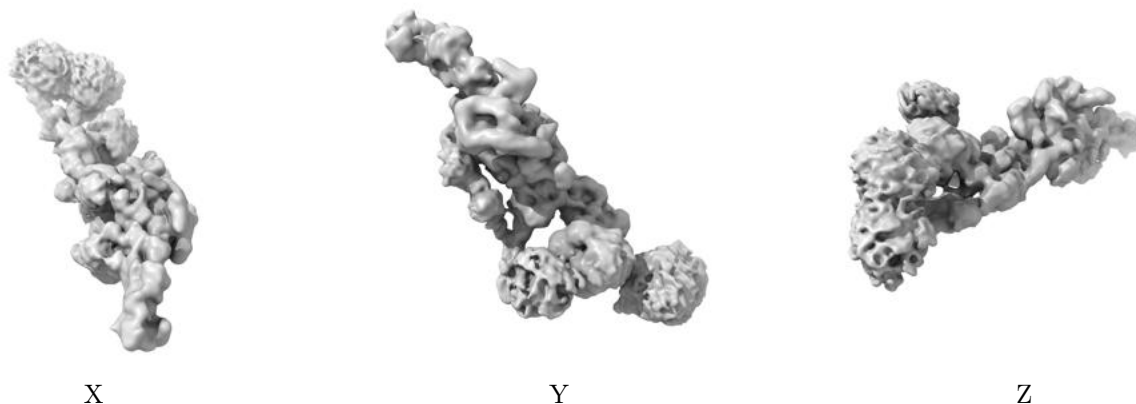


Z

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

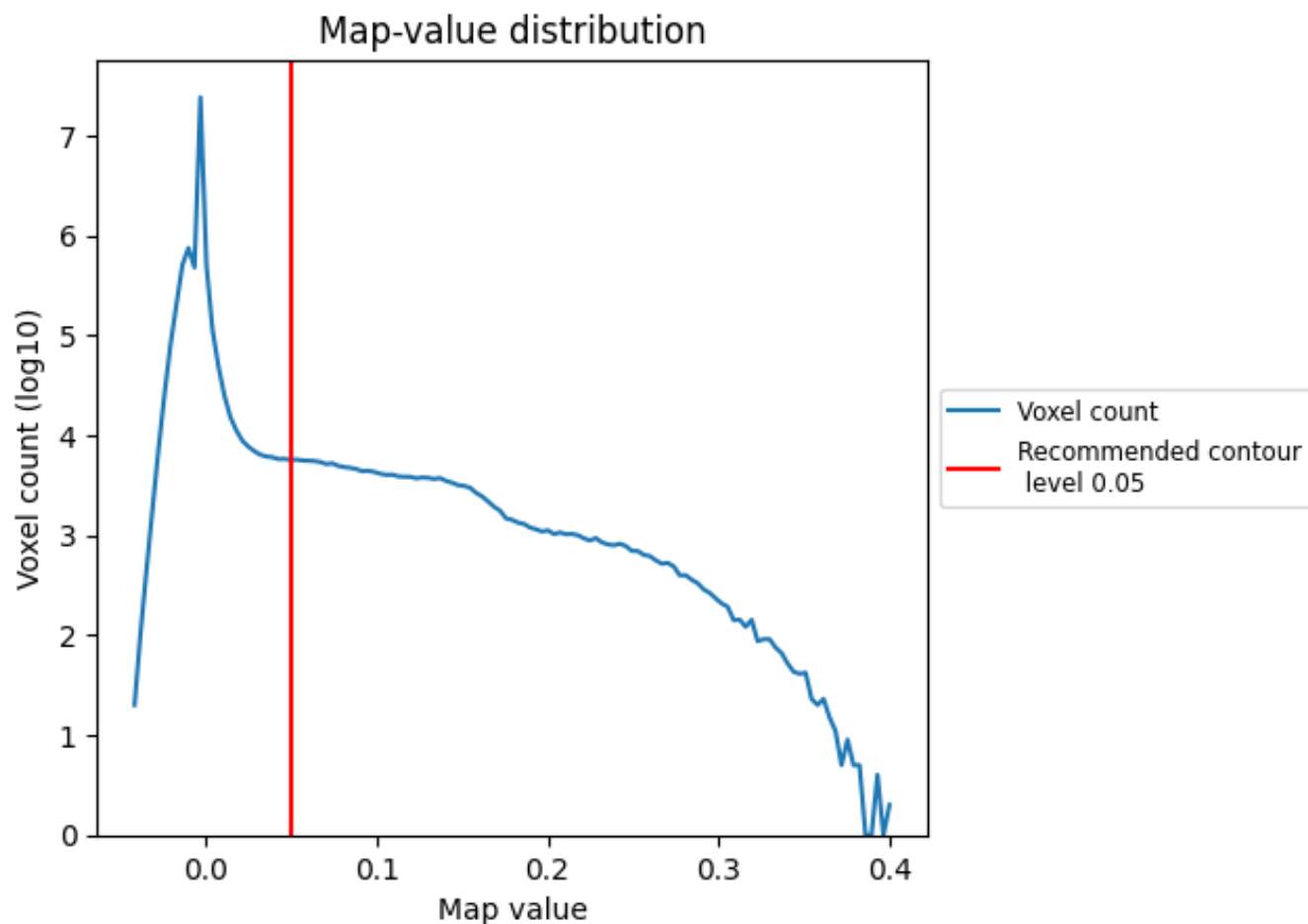
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

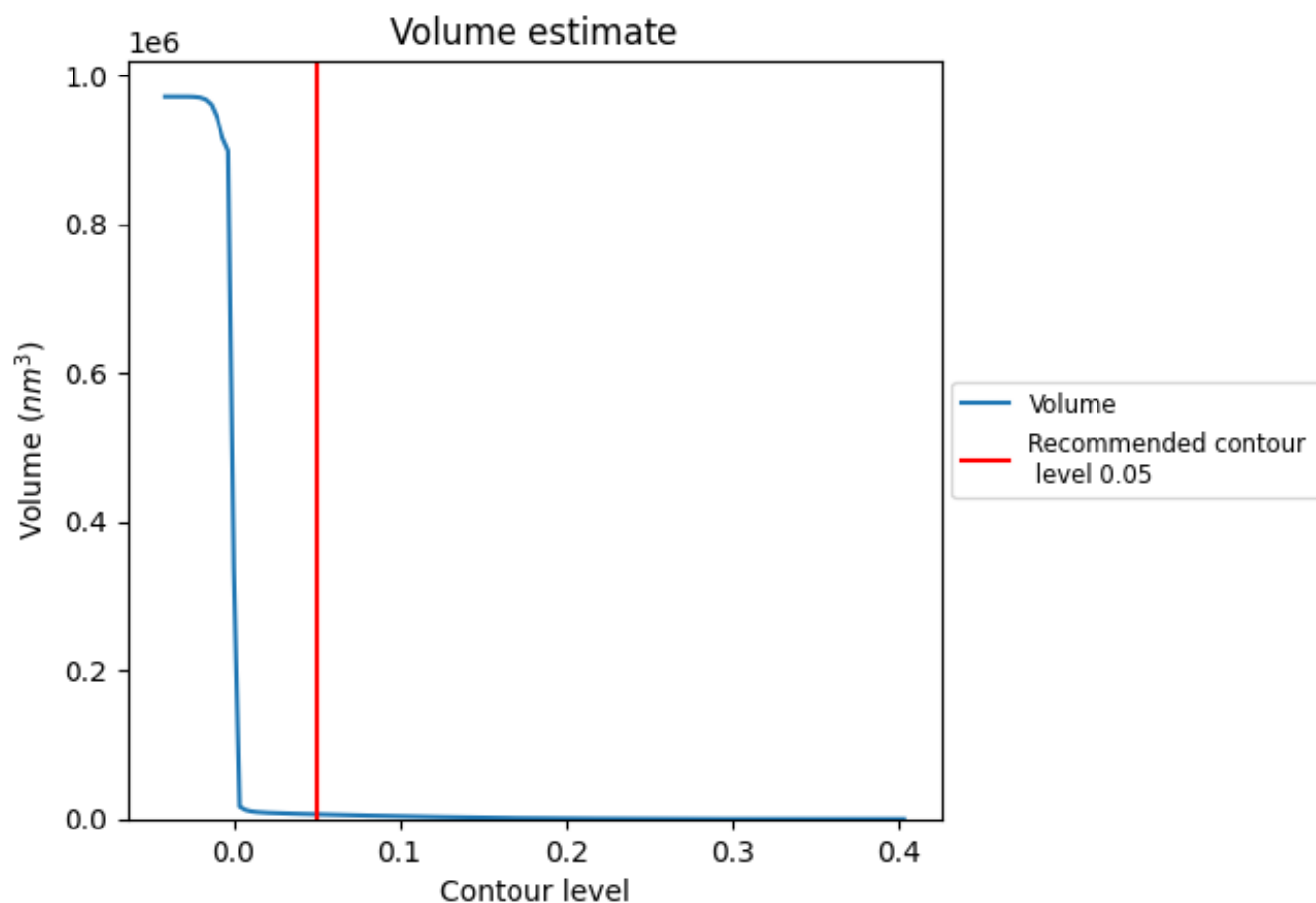
This section contains the results of statistical analysis of the map.

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.

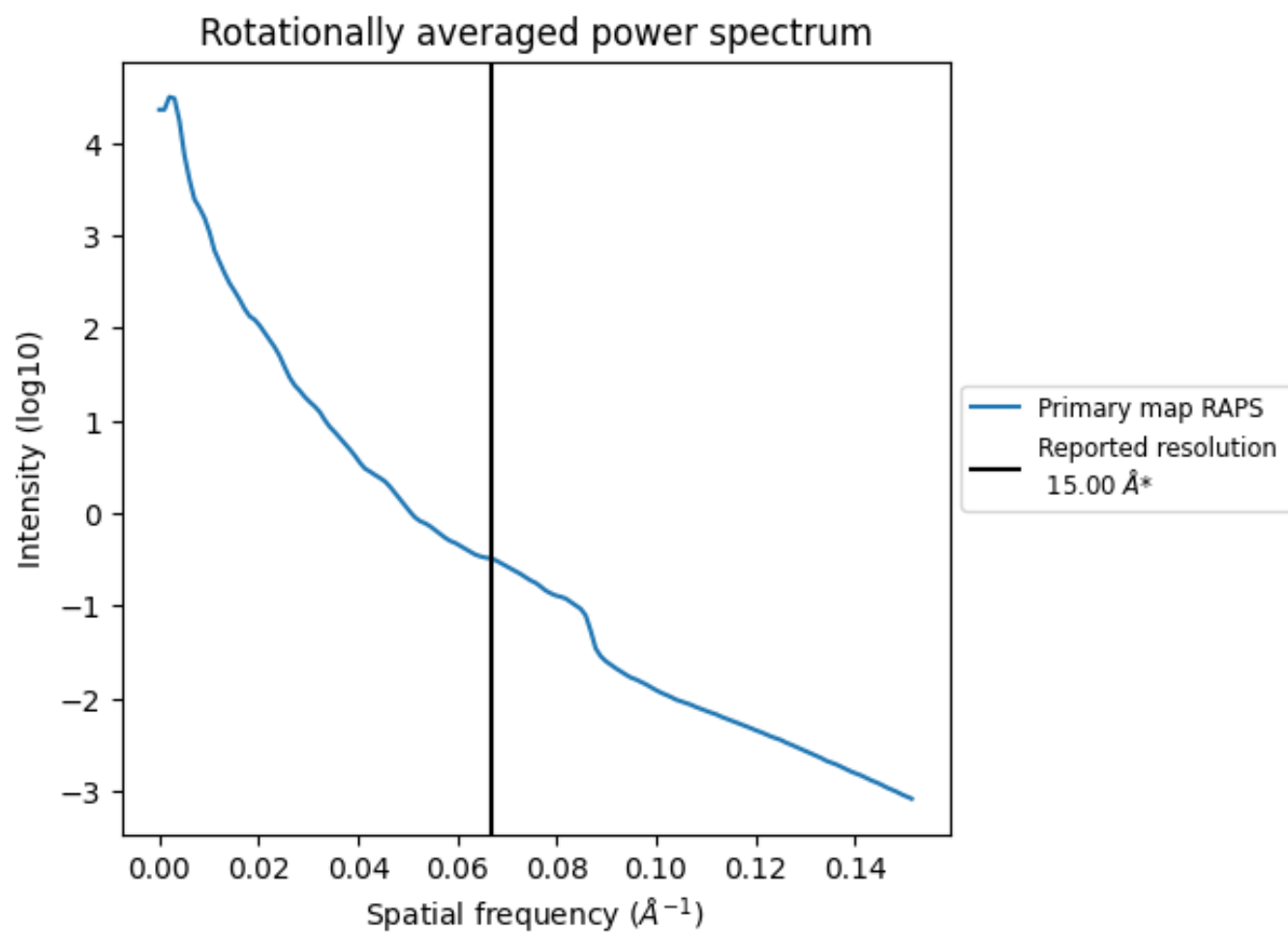
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6296 nm^3 ; this corresponds to an approximate mass of 5688 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 0.067 Å⁻¹

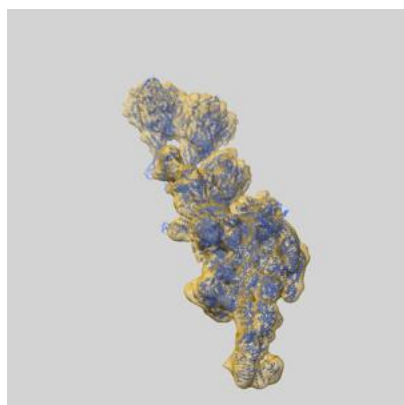
8 Fourier-Shell correlation

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

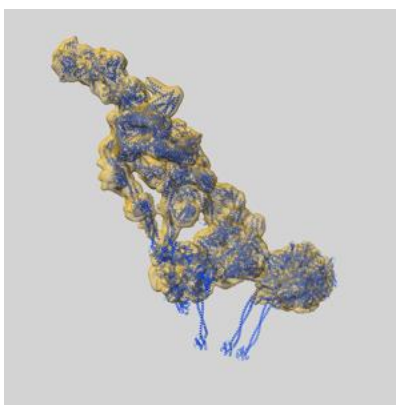
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46845 and PDB model 9DGR. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

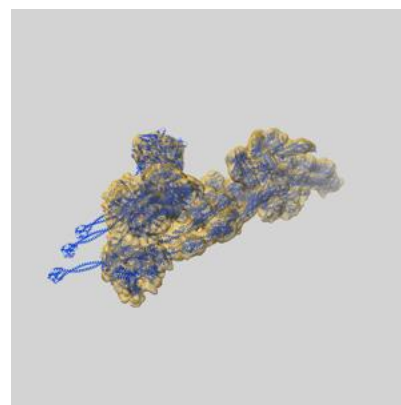
9.1 Map-model overlay [i](#)



X



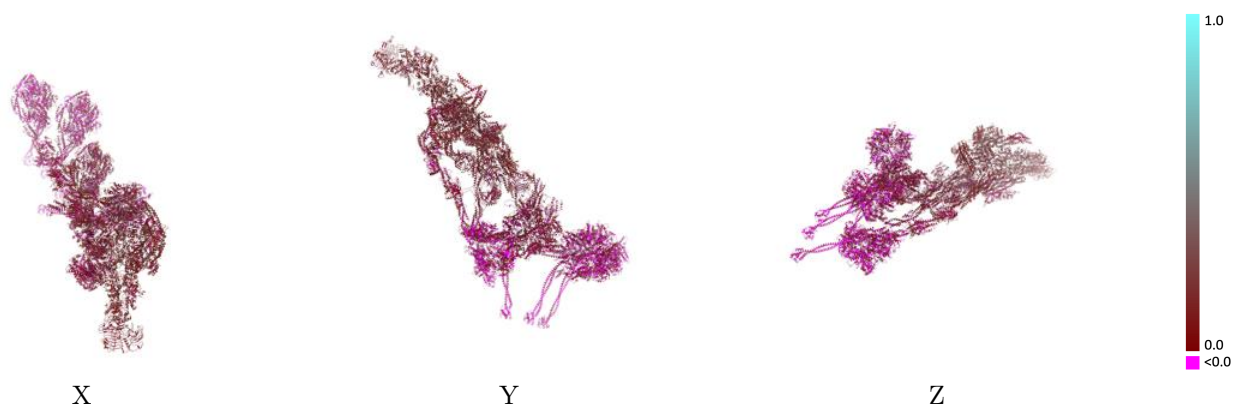
Y



Z

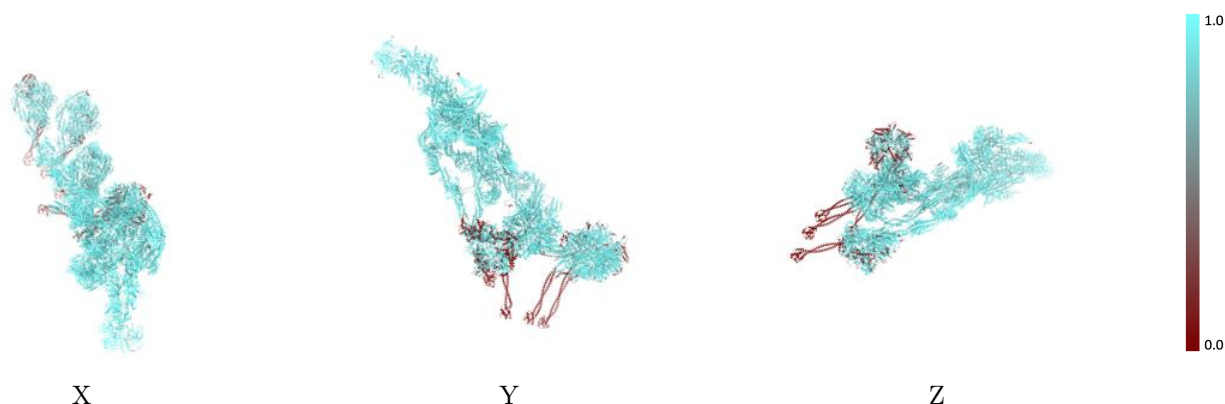
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



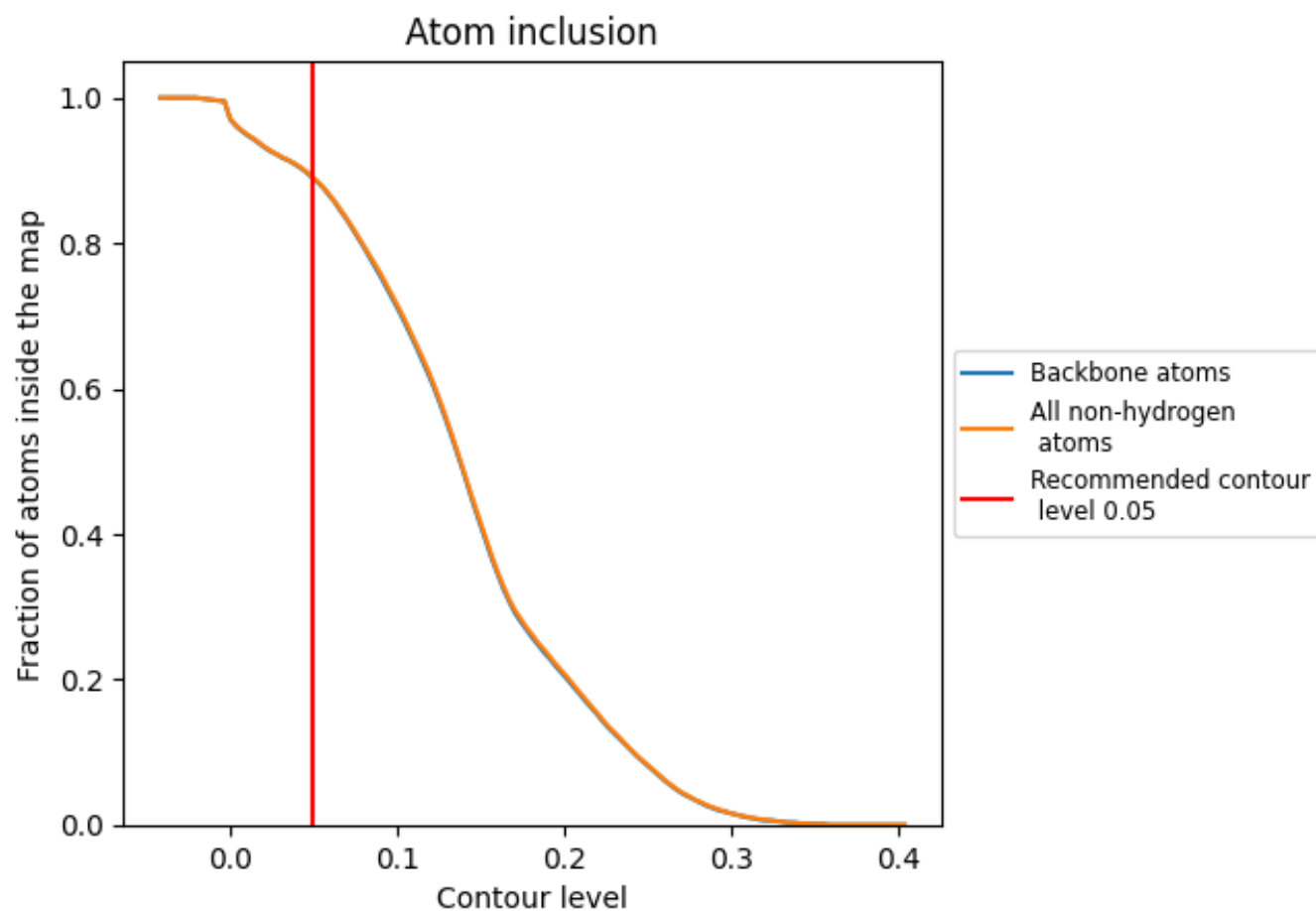
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary











The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8900	 0.0960
A	 1.0000	 0.1630
B	 1.0000	 0.1730
C	 1.0000	 0.1720
D	 1.0000	 0.1690
E	 1.0000	 0.1690
F	 1.0000	 0.1710
G	 1.0000	 0.1720
H	 1.0000	 0.1580
I	 0.9900	 0.1630
J	 0.9970	 0.1600
K	 1.0000	 0.1540
L	 0.9990	 0.1650
M	 0.9950	 0.1500
N	 0.9800	 0.1540
O	 1.0000	 0.1550
P	 0.9960	 0.1750
Q	 0.9780	 0.1660
R	 1.0000	 0.1550
U	 0.9780	 0.1210
V	 1.0000	 0.1350
W	 1.0000	 0.1400
Y	 0.9580	 0.1330
Z	 0.9990	 0.1740
e	 0.6470	 0.0500
f	 0.9470	 0.1060
g	 1.0000	 0.0740
h	 1.0000	 0.0950
i	 0.9600	 0.0840
j	 1.0000	 0.1310
k	 1.0000	 0.1220
l	 1.0000	 0.0990
m	 0.8960	 0.0640
n	 0.8400	 0.0540
o	 1.0000	 0.0970



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Chain	Atom inclusion	Q-score
p	 0.9990	 0.0840
q	 1.0000	 0.1170
r	 0.9970	 0.0810
s	 0.9950	 0.0960
t	 1.0000	 0.1000