



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 06:43 PM UTC

PDB ID : 5YFP / pdb_00005yfp
EMDB ID : EMD-6827
Title : Cryo-EM Structure of the Exocyst Complex
Authors : Mei, K.; Li, Y.; Wang, S.; Shao, G.; Wang, J.; Ding, Y.; Luo, G.; Yue, P.; Liu, J.J.; Wang, X.; Dong, M.Q.; Guo, W.; Wang, H.W.
Deposited on : 2017-09-21
Resolution : 4.40 Å(reported)
Based on initial models : ?, 2A2F, 2B1E, 2FJI, 2D2S, 1ZC4, 5H11

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:

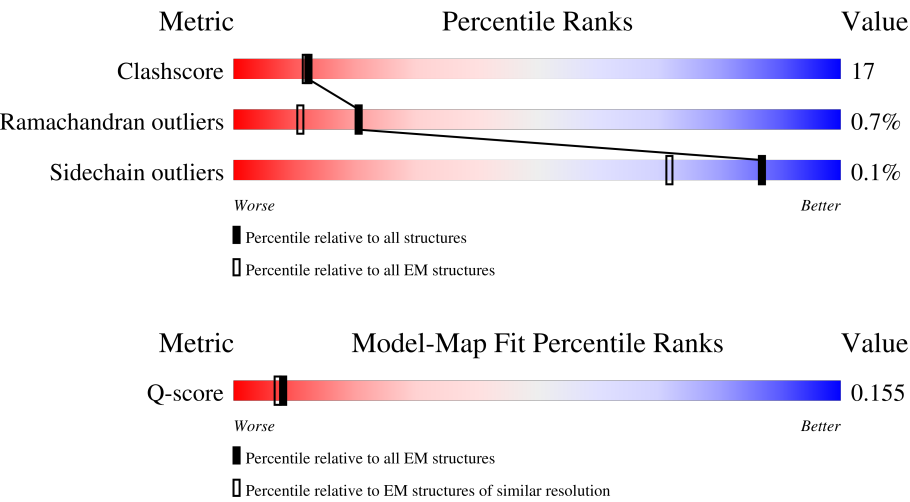
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3132 (3.91 - 4.90)

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 <=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	1336	15% 40% 10% 50%
2	B	971	12% 73% 21% ..
3	C	805	21% 67% 31% ..
4	D	1065	5% 68% 19% 10%

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Mol	Chain	Length	Quality of chain
5	E	871	13% 64% 25% 11%
6	F	910	8% 61% 18% 20%
7	G	623	17% 59% 39% ..
8	H	753	7% 48% 20% 31%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 33096 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 Exocyst complex component SEC3.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	672	Total	C	N	O	0	0
			3345	2001	672	672		

- Molecule 2 is a protein called Exocyst complex component SEC5.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	928	Total	C	N	O	0	0
			4610	2755	927	928		

- Molecule 3 is a protein called Exocyst complex component SEC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	794	Total	C	N	O	S	0	0
			4994	3097	892	989	16		

- Molecule 4 is a protein called Exocyst complex component SEC8.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	954	Total	C	N	O	0	0
			4739	2831	954	954		

- Molecule 5 is a protein called Exocyst complex component SEC10.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	776	Total	C	N	O	0	0
			3860	2308	776	776		

- Molecule 6 is a protein called Exocyst complex component SEC15.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	725	Total	C	N	O	0	0
			3612	2162	725	725		

- Molecule 7 is a protein called Exocyst complex component EXO70.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	615	Total	C	N	O	S	0	0
			4696	2968	809	902	17		

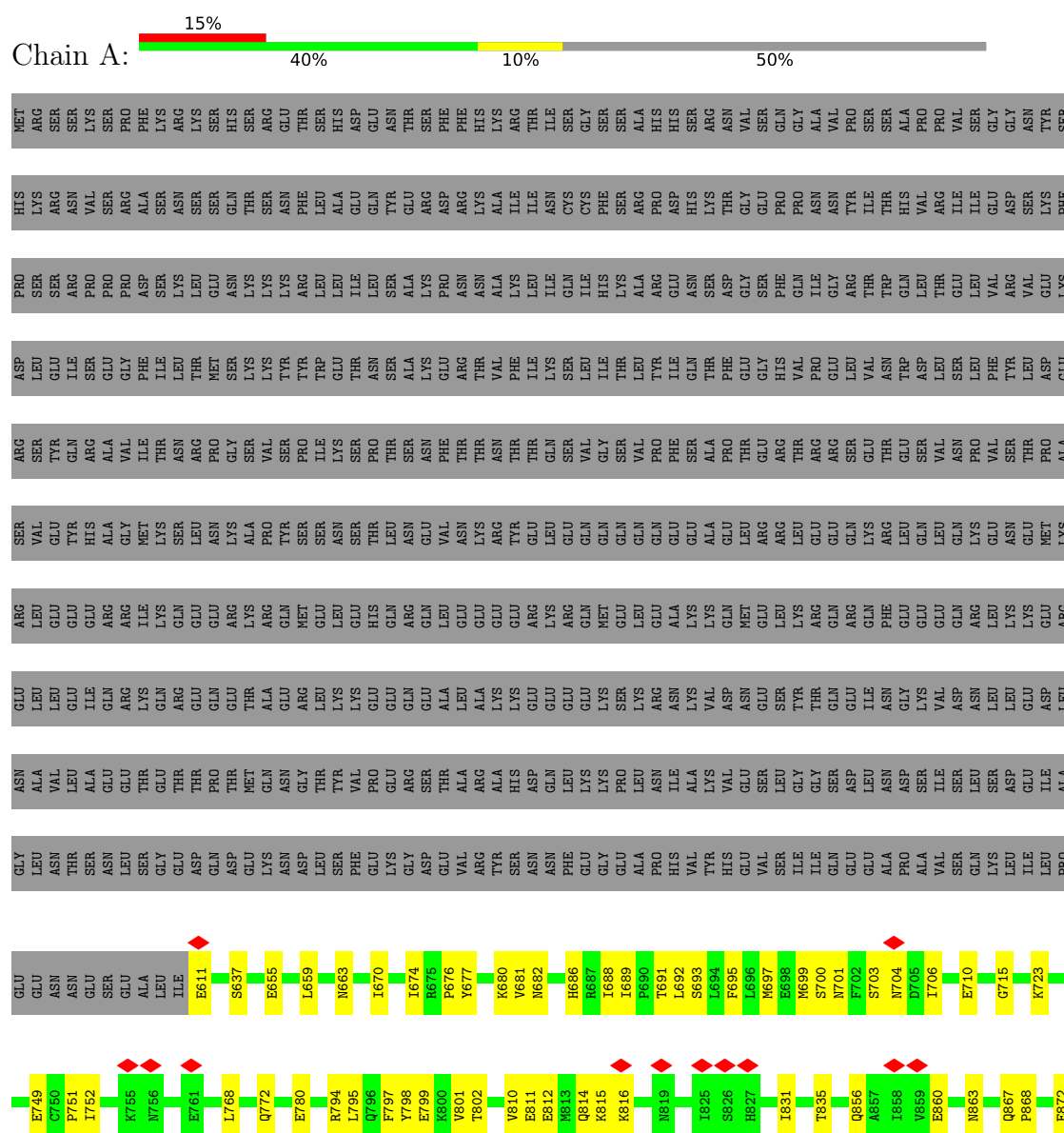
- Molecule 8 is a protein called Exocyst complex component EXO84.

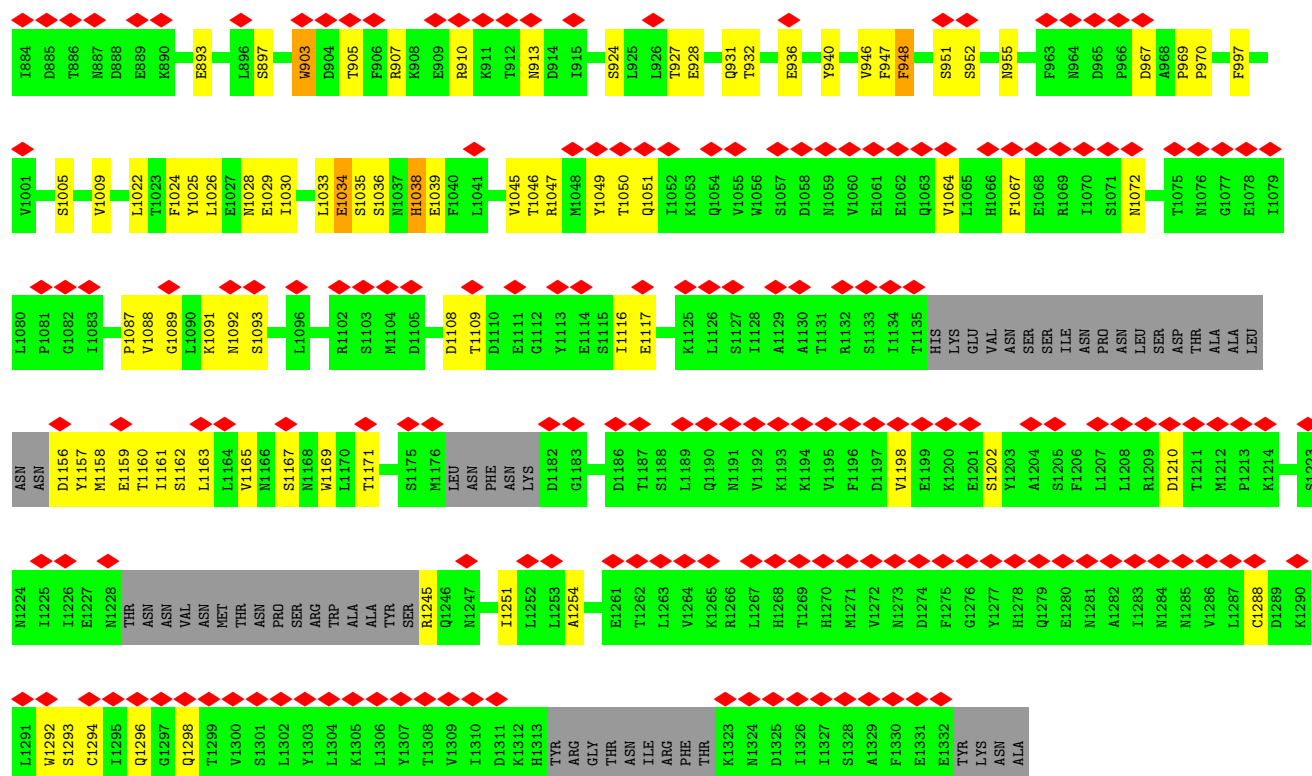
Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	518	Total	C	N	O	S	0	0
			3240	2002	591	643	4		

3 Residue-property plots

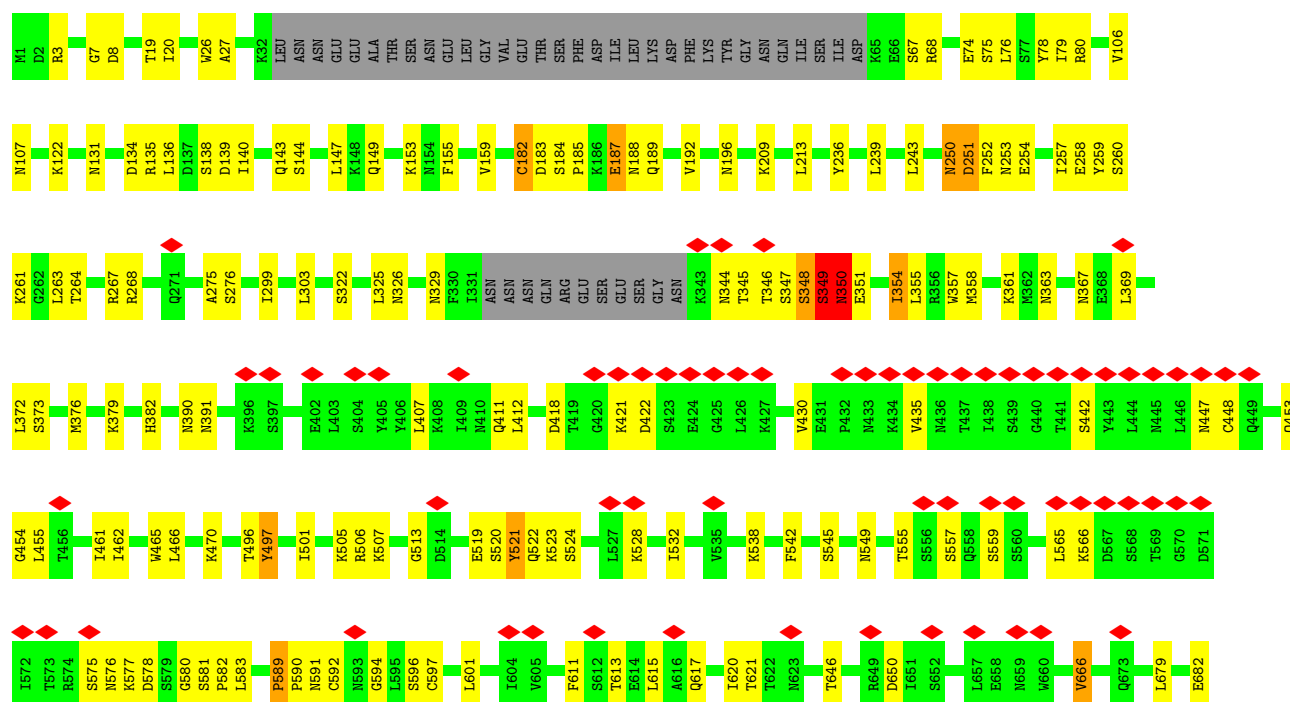
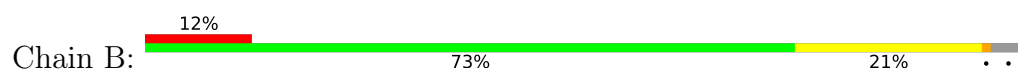
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

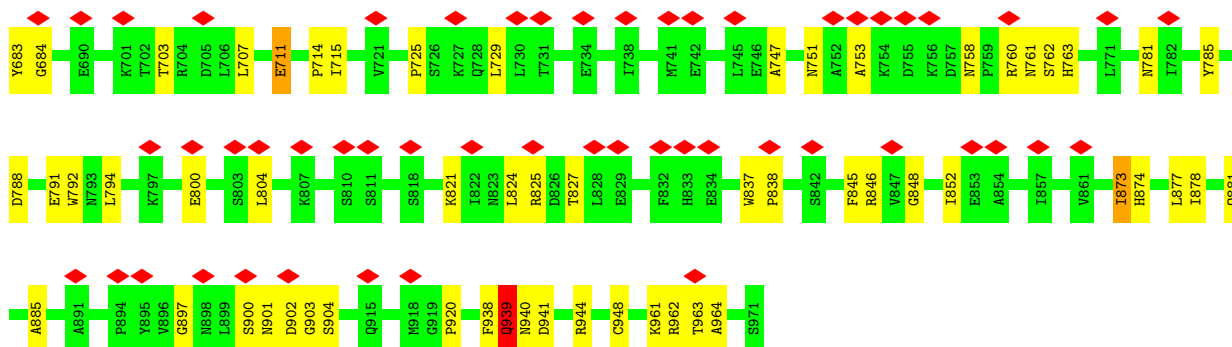
• Molecule 1: Exocyst complex component SEC3



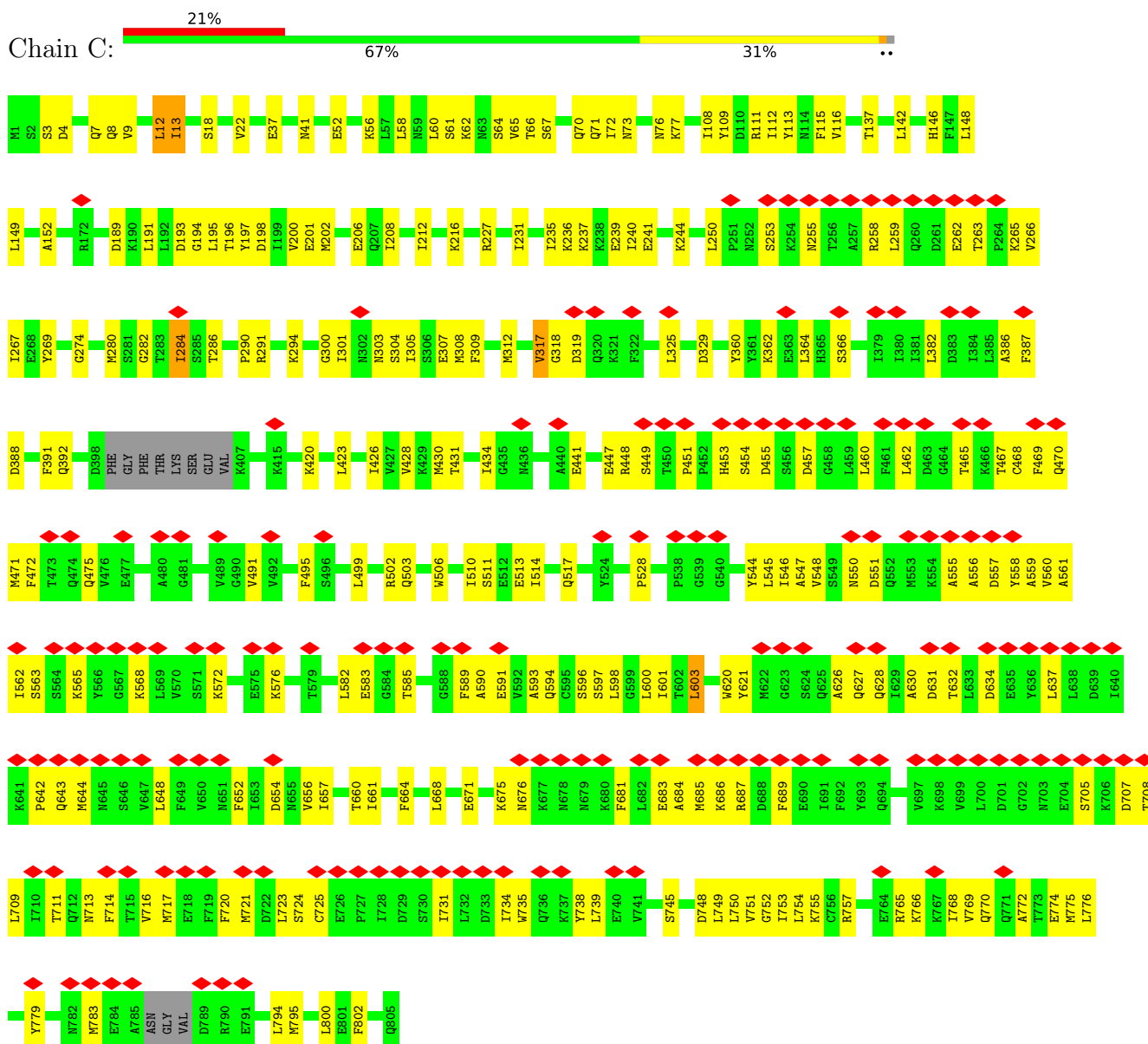


• Molecule 2: Exocyst complex component SEC5



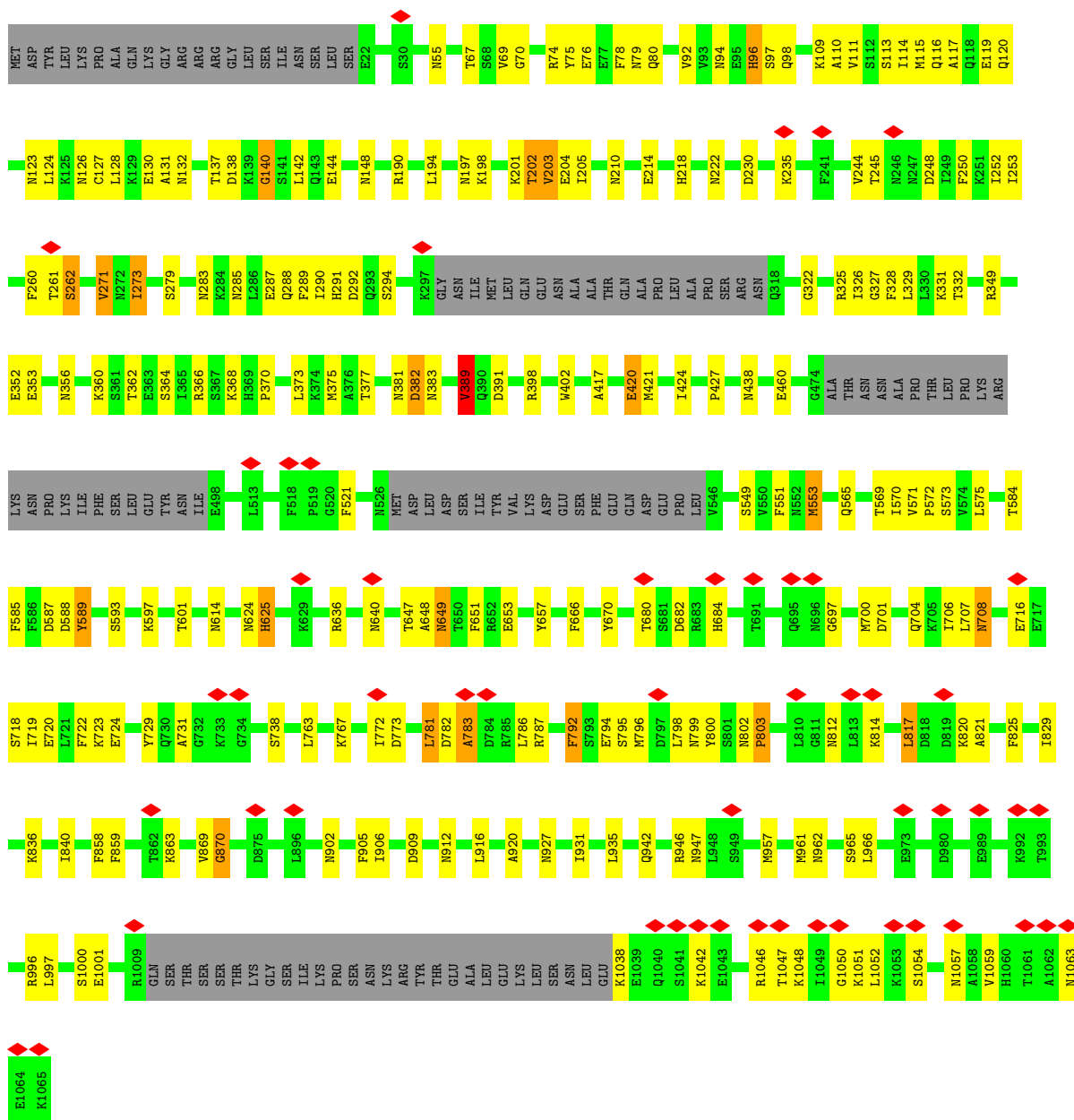


• Molecule 3: Exocyst complex component SEC6

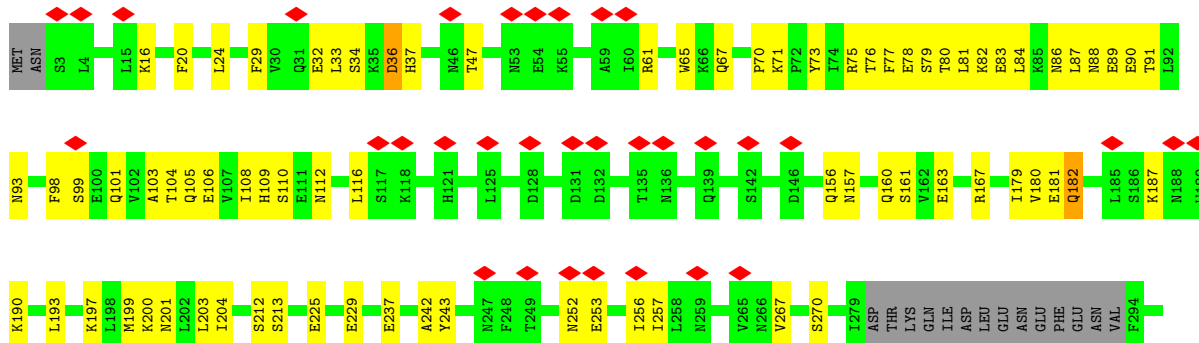


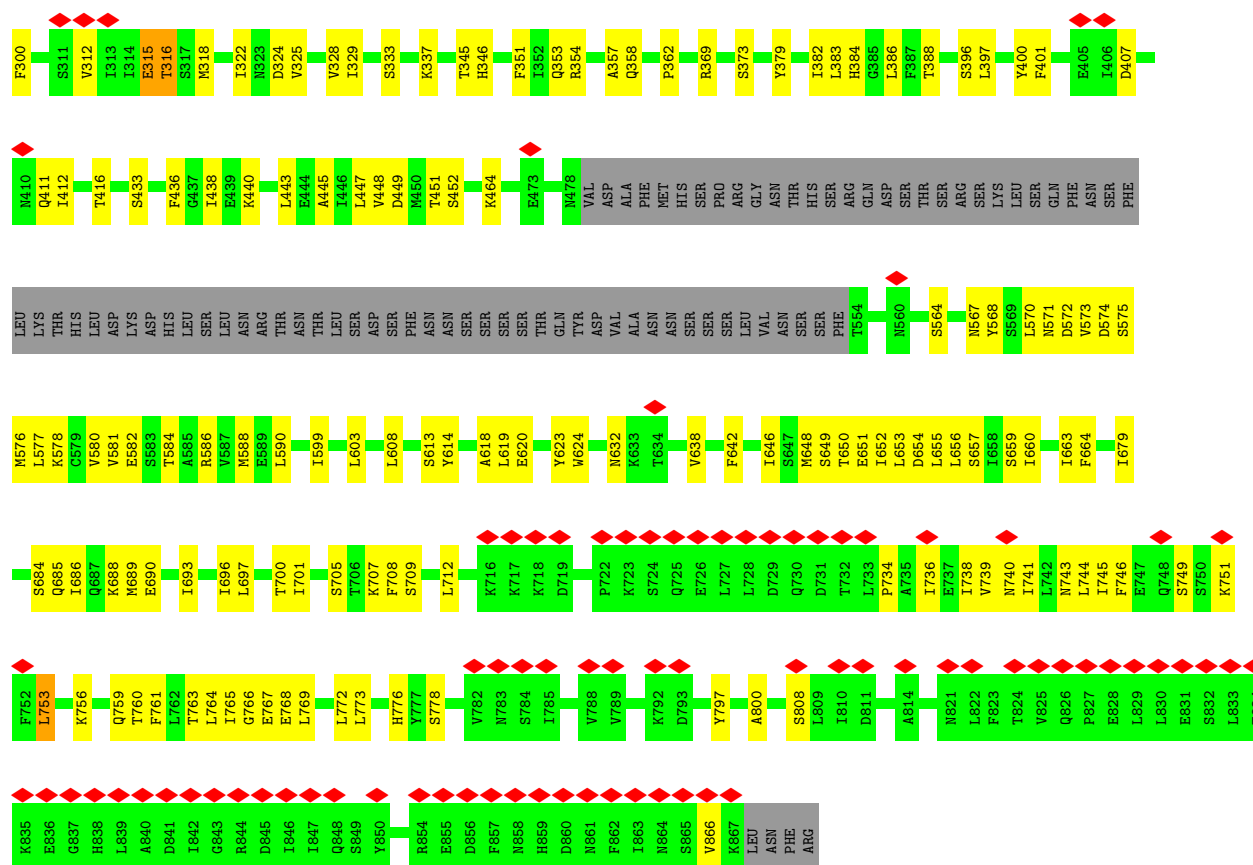
• Molecule 4: Exocyst complex component SEC8



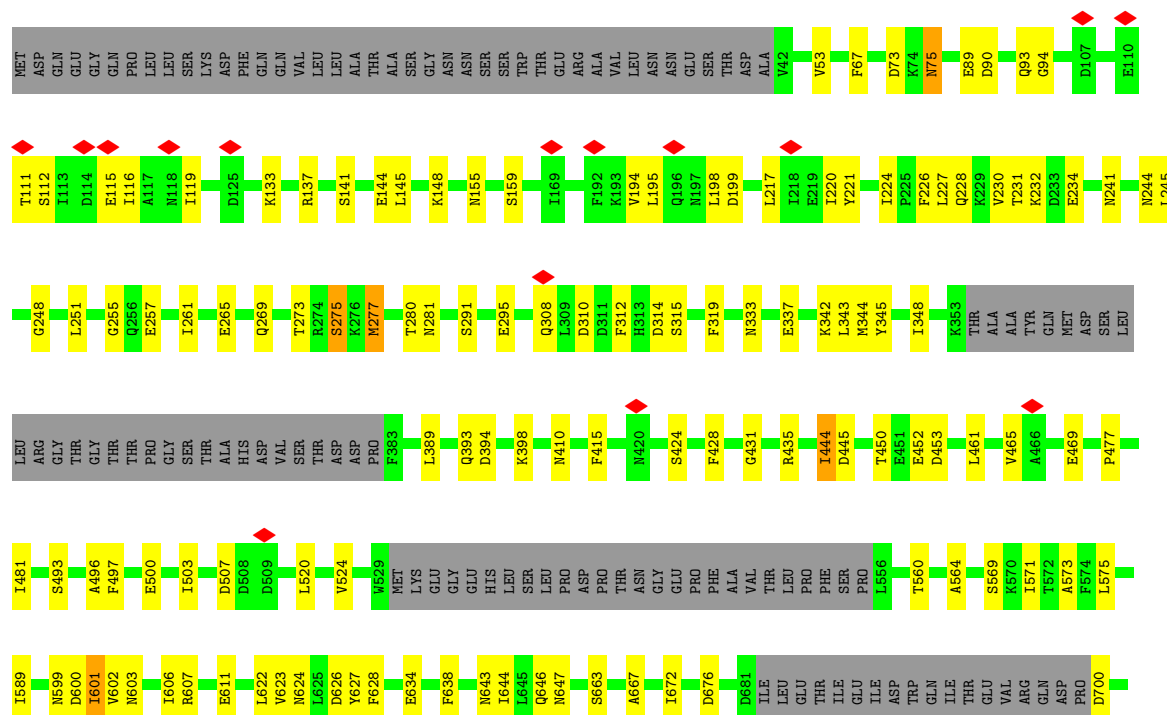


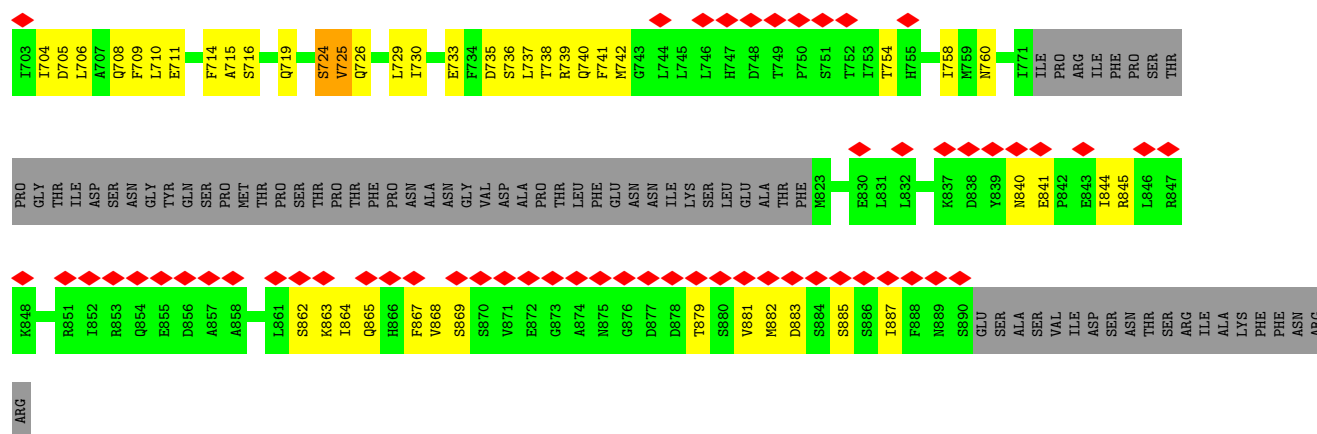
• Molecule 5: Exocyst complex component SEC10



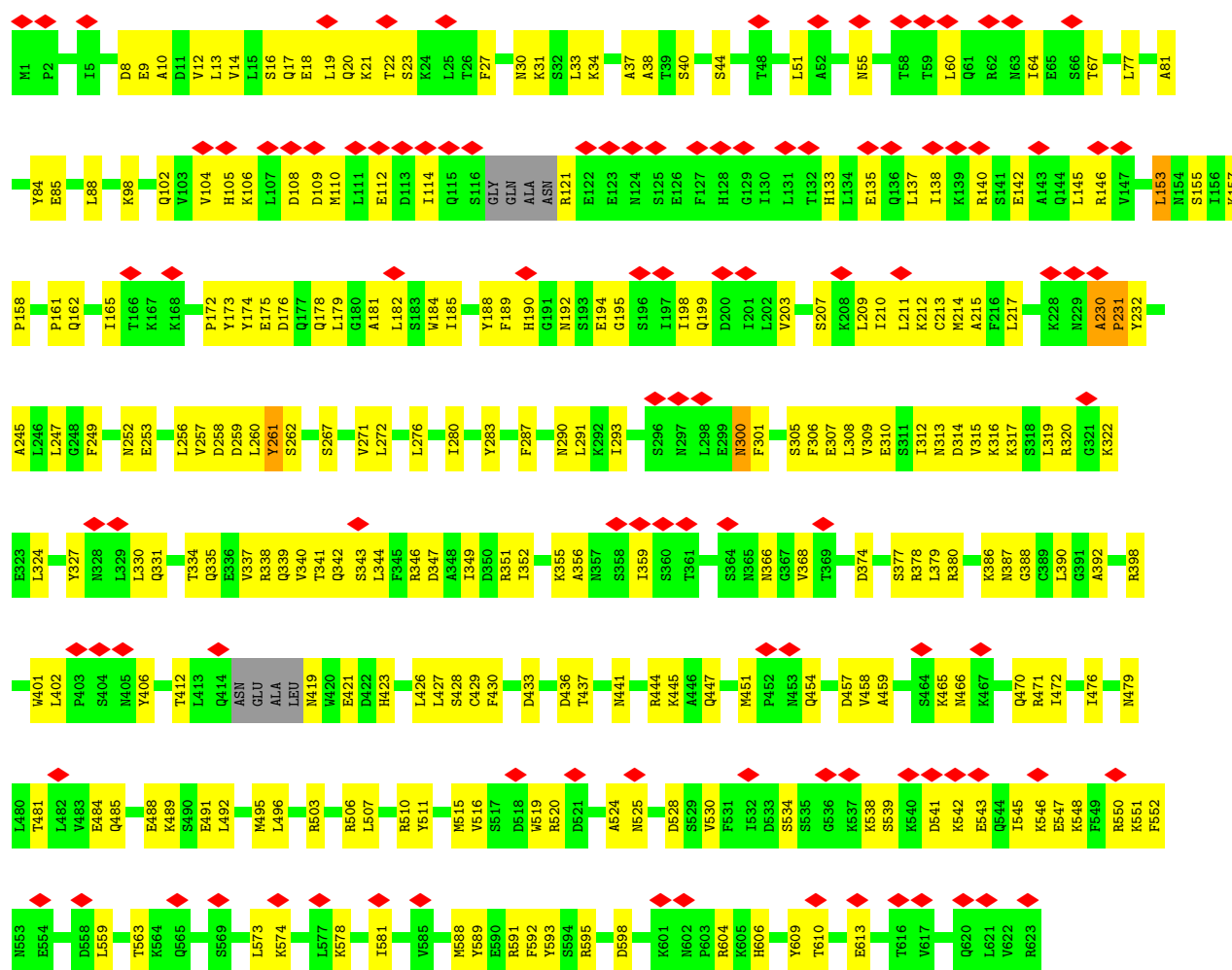


• Molecule 6: Exocyst complex component SEC15





• Molecule 7: Exocyst complex component EXO70



• Molecule 8: Exocyst complex component EXO84





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	343342	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; The defocus value of each image was determined by CTFFIND3.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.088	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0203	Depositor
Map size ($\text{\AA}$)	470.3544, 470.3544, 470.3544	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.30654, 1.30654, 1.30654	Depositor

5 Model quality

5.1 Standard geometry

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	0.30	0/3340	0.90	24/4659 (0.5%)
2	B	0.37	0/4607	1.02	53/6427 (0.8%)
3	C	0.28	0/5043	0.77	20/6885 (0.3%)
4	D	0.38	0/4734	1.06	61/6601 (0.9%)
5	E	0.26	0/3857	0.78	17/5383 (0.3%)
6	F	0.31	0/3607	0.85	15/5034 (0.3%)
7	G	0.32	0/4768	0.74	4/6443 (0.1%)
8	H	0.39	0/3253	0.81	9/4443 (0.2%)
All	All	0.33	0/33209	0.88	203/45875 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
2	B	0	41
3	C	0	8
4	D	0	43
5	E	0	6
6	F	0	13
7	G	0	9
8	H	0	12
All	All	0	143

There are no bond length outliers.

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	758	ASN	CA-C-N	11.84	155.41	127.00
2	B	758	ASN	C-N-CA	11.84	155.41	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1116	ILE	CA-C-N	10.79	141.13	121.70
1	A	1116	ILE	C-N-CA	10.79	141.13	121.70
6	F	444	ILE	CA-C-N	10.00	139.70	121.70
6	F	444	ILE	C-N-CA	10.00	139.70	121.70
4	D	649	ASN	CA-C-N	8.86	137.65	121.70
4	D	649	ASN	C-N-CA	8.86	137.65	121.70
6	F	275	SER	CA-C-N	8.78	137.51	121.70
6	F	275	SER	C-N-CA	8.78	137.51	121.70
8	H	472	GLN	CA-C-N	8.28	136.61	121.70
8	H	472	GLN	C-N-CA	8.28	136.61	121.70
4	D	708	ASN	N-CA-C	-8.23	99.08	111.34
5	E	243	TYR	CA-C-N	8.20	136.45	121.70
5	E	243	TYR	C-N-CA	8.20	136.45	121.70
2	B	496	THR	CA-C-N	8.16	136.39	121.70
2	B	496	THR	C-N-CA	8.16	136.39	121.70
5	E	316	THR	CA-C-N	8.11	136.30	121.70
5	E	316	THR	C-N-CA	8.11	136.30	121.70
7	G	300	ASN	CA-C-N	8.04	136.18	121.70
7	G	300	ASN	C-N-CA	8.04	136.18	121.70
1	A	1038	HIS	CA-C-N	8.02	136.13	121.70
1	A	1038	HIS	C-N-CA	8.02	136.13	121.70
4	D	382	ASP	CA-C-N	7.80	135.75	121.70
4	D	382	ASP	C-N-CA	7.80	135.75	121.70
4	D	782	ASP	CA-C-N	7.80	135.75	121.70
4	D	782	ASP	C-N-CA	7.80	135.75	121.70
4	D	260	PHE	CA-C-N	7.52	135.91	121.54
4	D	260	PHE	C-N-CA	7.52	135.91	121.54
6	F	348	ILE	N-CA-C	-7.49	105.25	112.29
1	A	752	ILE	N-CA-C	-7.48	105.55	112.43
1	A	1109	THR	CA-C-N	7.45	135.11	121.70
1	A	1109	THR	C-N-CA	7.45	135.11	121.70
2	B	513	GLY	CA-C-N	7.38	134.98	121.70
2	B	513	GLY	C-N-CA	7.38	134.98	121.70
8	H	338	PHE	N-CA-C	-7.31	102.36	110.91
2	B	187	GLU	CA-C-N	7.29	134.82	121.70
2	B	187	GLU	C-N-CA	7.29	134.82	121.70
4	D	262	SER	N-CA-C	-7.28	95.29	110.80
1	A	903	TRP	CA-C-N	7.12	134.52	121.70
1	A	903	TRP	C-N-CA	7.12	134.52	121.70
2	B	523	LYS	CA-C-N	7.09	134.46	121.70
2	B	523	LYS	C-N-CA	7.09	134.46	121.70
2	B	252	PHE	CA-C-N	7.07	134.42	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	252	PHE	C-N-CA	7.07	134.42	121.70
2	B	497	TYR	CA-C-N	7.03	134.96	121.54
2	B	497	TYR	C-N-CA	7.03	134.96	121.54
4	D	271	VAL	CA-C-N	7.02	134.34	121.70
4	D	271	VAL	C-N-CA	7.02	134.34	121.70
2	B	679	LEU	CA-C-N	7.01	134.32	121.70
2	B	679	LEU	C-N-CA	7.01	134.32	121.70
2	B	122	LYS	CA-C-N	6.99	134.27	121.70
2	B	122	LYS	C-N-CA	6.99	134.27	121.70
2	B	555	THR	CA-C-N	6.97	134.86	121.54
2	B	555	THR	C-N-CA	6.97	134.86	121.54
6	F	469	GLU	CA-C-N	6.96	134.23	121.70
6	F	469	GLU	C-N-CA	6.96	134.23	121.70
1	A	907	ARG	CA-C-N	6.94	134.20	121.70
1	A	907	ARG	C-N-CA	6.94	134.20	121.70
1	A	948	PHE	N-CA-C	-6.93	102.84	112.12
3	C	286	THR	CA-C-N	6.86	134.05	121.70
3	C	286	THR	C-N-CA	6.86	134.05	121.70
4	D	870	GLY	CA-C-N	6.79	133.92	121.70
4	D	870	GLY	C-N-CA	6.79	133.92	121.70
1	A	913	ASN	CA-C-N	6.78	133.91	121.70
1	A	913	ASN	C-N-CA	6.78	133.91	121.70
1	A	948	PHE	CA-C-N	6.78	133.90	121.70
1	A	948	PHE	C-N-CA	6.78	133.90	121.70
5	E	47	THR	CA-C-N	6.75	133.84	121.70
5	E	47	THR	C-N-CA	6.75	133.84	121.70
2	B	250	ASN	CA-C-N	6.74	133.83	121.70
2	B	250	ASN	C-N-CA	6.74	133.83	121.70
8	H	387	GLN	CA-C-N	6.71	133.78	121.70
8	H	387	GLN	C-N-CA	6.71	133.78	121.70
2	B	521	TYR	CA-C-N	6.70	133.76	121.70
2	B	521	TYR	C-N-CA	6.70	133.76	121.70
2	B	794	LEU	CA-C-N	6.69	133.75	121.70
2	B	794	LEU	C-N-CA	6.69	133.75	121.70
4	D	589	TYR	N-CA-C	-6.65	104.33	113.18
4	D	575	LEU	CA-C-N	6.65	133.67	121.70
4	D	575	LEU	C-N-CA	6.65	133.67	121.70
2	B	3	ARG	CA-C-N	6.62	133.62	121.70
2	B	3	ARG	C-N-CA	6.62	133.62	121.70
4	D	197	ASN	CA-C-N	6.61	133.59	121.70
4	D	197	ASN	C-N-CA	6.61	133.59	121.70
3	C	253	SER	CA-C-N	6.59	133.57	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	253	SER	C-N-CA	6.59	133.57	121.70
1	A	910	ARG	CA-C-N	6.56	133.51	121.70
1	A	910	ARG	C-N-CA	6.56	133.51	121.70
5	E	315	GLU	CA-C-N	6.52	133.44	121.70
5	E	315	GLU	C-N-CA	6.52	133.44	121.70
1	A	1210	ASP	CA-C-N	6.51	133.42	121.70
1	A	1210	ASP	C-N-CA	6.51	133.42	121.70
3	C	263	THR	CA-C-N	6.49	142.57	127.00
3	C	263	THR	C-N-CA	6.49	142.57	127.00
4	D	781	LEU	CA-C-N	6.48	133.37	121.70
4	D	781	LEU	C-N-CA	6.48	133.37	121.70
4	D	584	THR	CA-C-N	6.48	133.36	121.70
4	D	584	THR	C-N-CA	6.48	133.36	121.70
4	D	614	ASN	CA-C-N	6.27	142.05	127.00
4	D	614	ASN	C-N-CA	6.27	142.05	127.00
2	B	447	ASN	CA-C-N	6.21	132.88	121.70
2	B	447	ASN	C-N-CA	6.21	132.88	121.70
4	D	814	LYS	CA-C-N	6.14	132.75	121.70
4	D	814	LYS	C-N-CA	6.14	132.75	121.70
6	F	75	ASN	CA-C-N	6.14	132.75	121.70
6	F	75	ASN	C-N-CA	6.14	132.75	121.70
4	D	680	THR	CA-C-N	6.12	132.71	121.70
4	D	680	THR	C-N-CA	6.12	132.71	121.70
4	D	273	ILE	CA-C-N	6.10	132.68	121.70
4	D	273	ILE	C-N-CA	6.10	132.68	121.70
8	H	335	ALA	CA-C-N	6.09	132.66	121.70
8	H	335	ALA	C-N-CA	6.09	132.66	121.70
4	D	198	LYS	CA-C-N	6.06	132.60	121.70
4	D	198	LYS	C-N-CA	6.06	132.60	121.70
4	D	201	LYS	CA-C-N	6.05	132.58	121.70
4	D	201	LYS	C-N-CA	6.05	132.58	121.70
5	E	182	GLN	CA-C-N	6.04	132.58	121.70
5	E	182	GLN	C-N-CA	6.04	132.58	121.70
6	F	291	SER	CA-C-N	6.02	132.54	121.70
6	F	291	SER	C-N-CA	6.02	132.54	121.70
1	A	715	GLY	CA-C-N	5.96	132.42	121.70
1	A	715	GLY	C-N-CA	5.96	132.42	121.70
3	C	255	ASN	CA-C-N	5.93	132.38	121.70
3	C	255	ASN	C-N-CA	5.93	132.38	121.70
3	C	267	ILE	CA-C-N	5.93	132.38	121.70
3	C	267	ILE	C-N-CA	5.93	132.38	121.70
4	D	55	ASN	CA-C-N	5.92	141.21	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	55	ASN	C-N-CA	5.92	141.21	127.00
4	D	729	TYR	CA-C-N	5.89	132.31	121.70
4	D	729	TYR	C-N-CA	5.89	132.31	121.70
2	B	715	ILE	N-CA-C	5.85	127.37	111.00
2	B	344	ASN	CA-C-N	5.80	132.14	121.70
2	B	344	ASN	C-N-CA	5.80	132.14	121.70
4	D	1038	LYS	CA-C-N	5.79	132.12	121.70
4	D	1038	LYS	C-N-CA	5.79	132.12	121.70
3	C	317	VAL	CA-C-N	5.73	132.02	121.70
3	C	317	VAL	C-N-CA	5.73	132.02	121.70
2	B	345	THR	CA-C-N	5.72	132.00	121.70
2	B	345	THR	C-N-CA	5.72	132.00	121.70
4	D	230	ASP	CA-C-N	5.71	131.99	121.70
4	D	230	ASP	C-N-CA	5.71	131.99	121.70
6	F	450	THR	CA-C-N	5.71	132.46	121.54
6	F	450	THR	C-N-CA	5.71	132.46	121.54
4	D	67	THR	CA-C-N	5.69	131.94	121.70
4	D	67	THR	C-N-CA	5.69	131.94	121.70
5	E	638	VAL	N-CA-C	-5.67	107.21	112.43
3	C	250	LEU	CA-C-N	5.65	140.56	127.00
3	C	250	LEU	C-N-CA	5.65	140.56	127.00
2	B	578	ASP	CA-C-N	5.59	131.76	121.70
2	B	578	ASP	C-N-CA	5.59	131.76	121.70
7	G	232	TYR	CA-C-N	5.59	131.75	121.70
7	G	232	TYR	C-N-CA	5.59	131.75	121.70
4	D	792	PHE	CA-C-N	5.57	131.72	121.70
4	D	792	PHE	C-N-CA	5.57	131.72	121.70
8	H	336	GLN	CA-C-N	5.56	132.16	121.54
8	H	336	GLN	C-N-CA	5.56	132.16	121.54
2	B	939	GLN	CA-C-N	5.54	131.67	121.70
2	B	939	GLN	C-N-CA	5.54	131.67	121.70
4	D	803	PRO	CA-C-N	5.51	131.62	121.70
4	D	803	PRO	C-N-CA	5.51	131.62	121.70
3	C	137	THR	CA-C-N	5.50	131.61	121.70
3	C	137	THR	C-N-CA	5.50	131.61	121.70
3	C	284	ILE	CA-C-N	5.46	131.53	121.70
3	C	284	ILE	C-N-CA	5.46	131.53	121.70
4	D	389	VAL	CA-C-N	5.44	131.49	121.70
4	D	389	VAL	C-N-CA	5.44	131.49	121.70
2	B	714	PRO	CA-C-N	5.43	131.47	121.70
2	B	714	PRO	C-N-CA	5.43	131.47	121.70
2	B	760	ARG	CA-C-N	5.42	131.90	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	760	ARG	C-N-CA	5.42	131.90	121.54
4	D	203	VAL	N-CA-C	5.39	120.55	109.34
2	B	182	CYS	CA-C-N	5.39	131.40	121.70
2	B	182	CYS	C-N-CA	5.39	131.40	121.70
5	E	464	LYS	CA-C-N	5.37	131.37	121.70
5	E	464	LYS	C-N-CA	5.37	131.37	121.70
4	D	370	PRO	CA-C-N	5.35	131.34	121.70
4	D	370	PRO	C-N-CA	5.35	131.34	121.70
2	B	940	ASN	N-CA-C	5.29	125.83	111.00
3	C	206	GLU	CA-C-N	5.26	131.17	121.70
3	C	206	GLU	C-N-CA	5.26	131.17	121.70
2	B	506	ARG	CA-C-N	5.25	131.57	121.54
2	B	506	ARG	C-N-CA	5.25	131.57	121.54
2	B	346	THR	N-CA-C	5.25	125.69	111.00
2	B	711	GLU	CA-C-N	5.24	131.12	121.70
2	B	711	GLU	C-N-CA	5.24	131.12	121.70
4	D	205	ILE	CA-C-N	5.24	134.14	124.82
4	D	205	ILE	C-N-CA	5.24	134.14	124.82
4	D	786	LEU	CA-C-N	5.21	131.49	121.54
4	D	786	LEU	C-N-CA	5.21	131.49	121.54
2	B	455	LEU	N-CA-C	5.15	117.31	111.02
6	F	277	MET	N-CA-C	-5.14	108.27	114.75
5	E	300	PHE	CA-C-N	5.14	130.95	121.70
5	E	300	PHE	C-N-CA	5.14	130.95	121.70
5	E	312	VAL	CA-C-N	5.13	131.21	121.97
5	E	312	VAL	C-N-CA	5.13	131.21	121.97
6	F	281	ASN	N-CA-C	5.13	125.37	111.00
1	A	997	PHE	N-CA-C	5.08	118.94	112.34
4	D	783	ALA	N-CA-C	5.05	125.13	111.00
2	B	350	ASN	N-CA-C	5.04	121.54	110.80
1	A	637	SER	N-CA-C	5.03	116.80	110.91
4	D	795	SER	CA-C-N	5.02	131.13	121.54
4	D	795	SER	C-N-CA	5.02	131.13	121.54

There are no chirality outliers.

All (143) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1034	GLU	Peptide
1	A	1039	GLU	Peptide
1	A	1064	VAL	Peptide
1	A	1117	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	A	749	GLU	Peptide
1	A	780	GLU	Peptide
1	A	946	VAL	Peptide
1	A	947	PHE	Peptide
1	A	948	PHE	Peptide
1	A	955	ASN	Peptide
1	A	967	ASP	Peptide
2	B	184	SER	Peptide
2	B	187	GLU	Peptide
2	B	236	TYR	Peptide
2	B	251	ASP	Peptide
2	B	268	ARG	Peptide
2	B	347	SER	Peptide
2	B	348	SER	Peptide
2	B	349	SER	Peptide
2	B	350	ASN	Peptide
2	B	354	ILE	Peptide
2	B	407	LEU	Peptide
2	B	411	GLN	Peptide
2	B	418	ASP	Peptide
2	B	430	VAL	Peptide
2	B	435	VAL	Peptide
2	B	442	SER	Peptide
2	B	448	CYS	Peptide
2	B	453	GLN	Peptide
2	B	454	GLY	Peptide
2	B	507	LYS	Peptide
2	B	519	GLU	Peptide
2	B	524	SER	Peptide
2	B	557	SER	Peptide
2	B	559	SER	Peptide
2	B	577	LYS	Peptide
2	B	580	GLY	Peptide
2	B	581	SER	Peptide
2	B	589	PRO	Peptide
2	B	591	ASN	Peptide
2	B	592	CYS	Peptide
2	B	666	VAL	Peptide
2	B	703	THR	Peptide
2	B	711	GLU	Peptide
2	B	753	ALA	Peptide
2	B	761	ASN	Peptide

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Mol	Chain	Res	Type	Group
2	B	763	HIS	Peptide
2	B	788	ASP	Peptide
2	B	791	GLU	Peptide
2	B	792	TRP	Peptide
2	B	873	ILE	Peptide
2	B	939	GLN	Peptide
3	C	12	LEU	Peptide
3	C	13	ILE	Peptide
3	C	284	ILE	Peptide
3	C	294	LYS	Peptide
3	C	319	ASP	Peptide
3	C	453	HIS	Peptide
3	C	454	SER	Peptide
3	C	603	LEU	Peptide
4	D	1057	ASN	Peptide
4	D	137	THR	Peptide
4	D	138	ASP	Peptide
4	D	140	GLY	Peptide
4	D	142	LEU	Peptide
4	D	202	THR	Peptide
4	D	235	LYS	Peptide
4	D	244	VAL	Peptide
4	D	248	ASP	Peptide
4	D	250	PHE	Peptide
4	D	261	THR	Peptide
4	D	262	SER	Peptide
4	D	271	VAL	Peptide
4	D	273	ILE	Peptide
4	D	373	LEU	Peptide
4	D	375	MET	Peptide
4	D	377	THR	Peptide
4	D	383	ASN	Peptide
4	D	389	VAL	Peptide
4	D	420	GLU	Peptide
4	D	438	ASN	Peptide
4	D	460	GLU	Peptide
4	D	549	SER	Peptide
4	D	551	PHE	Peptide
4	D	553	MET	Peptide
4	D	570	ILE	Peptide
4	D	571	VAL	Peptide
4	D	585	PHE	Peptide

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Mol	Chain	Res	Type	Group
4	D	624	ASN	Peptide
4	D	625	HIS	Peptide
4	D	651	PHE	Peptide
4	D	682	ASP	Peptide
4	D	707	LEU	Peptide
4	D	731	ALA	Peptide
4	D	781	LEU	Peptide
4	D	787	ARG	Peptide
4	D	792	PHE	Peptide
4	D	799	ASN	Peptide
4	D	802	ASN	Peptide
4	D	812	ASN	Peptide
4	D	817	LEU	Peptide
4	D	863	LYS	Peptide
4	D	96	HIS	Peptide
5	E	179	ILE	Peptide
5	E	24	LEU	Peptide
5	E	315	GLU	Peptide
5	E	36	ASP	Peptide
5	E	564	SER	Peptide
5	E	753	LEU	Peptide
6	F	280	THR	Peptide
6	F	295	GLU	Peptide
6	F	345	TYR	Peptide
6	F	410	ASN	Peptide
6	F	415	PHE	Peptide
6	F	444	ILE	Peptide
6	F	445	ASP	Peptide
6	F	53	VAL	Peptide
6	F	599	ASN	Peptide
6	F	600	ASP	Peptide
6	F	601	ILE	Peptide
6	F	643	ASN	Peptide
6	F	75	ASN	Peptide
7	G	153	LEU	Peptide
7	G	175	GLU	Peptide
7	G	190	HIS	Peptide
7	G	230	ALA	Peptide
7	G	259	ASP	Peptide
7	G	261	TYR	Peptide
7	G	262	SER	Peptide
7	G	300	ASN	Peptide

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Mol	Chain	Res	Type	Group
7	G	317	LYS	Peptide
8	H	314	VAL	Peptide
8	H	315	LEU	Peptide
8	H	336	GLN	Peptide
8	H	337	LYS	Peptide
8	H	338	PHE	Peptide
8	H	339	ILE	Peptide
8	H	348	LEU	Peptide
8	H	387	GLN	Peptide
8	H	454	GLU	Peptide
8	H	470	SER	Peptide
8	H	652	ASN	Peptide
8	H	708	GLN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3345	0	1403	67	0
2	B	4610	0	1926	84	0
3	C	4994	0	3576	173	0
4	D	4739	0	2011	91	0
5	E	3860	0	1635	120	0
6	F	3612	0	1508	84	0
7	G	4696	0	4483	192	0
8	H	3240	0	2433	86	0
All	All	33096	0	18975	886	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (886) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:506:TRP:O	3:C:510:ILE:HB	1.54	1.06
3:C:558:TYR:O	3:C:562:ILE:HB	1.60	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:714:PHE:CD2	3:C:714:PHE:CZ	2.38	0.99
3:C:544:TYR:CG	3:C:544:TYR:CE2	2.40	0.97
3:C:557:ASP:O	3:C:561:ALA:HB3	1.66	0.96
8:H:530:ALA:O	8:H:534:LYS:HB2	1.69	0.92
7:G:546:LYS:O	7:G:550:ARG:HB3	1.68	0.92
3:C:555:ALA:O	3:C:559:ALA:HB3	1.70	0.91
7:G:589:TYR:O	7:G:593:TYR:HB3	1.71	0.91
7:G:33:LEU:O	7:G:37:ALA:HB3	1.74	0.87
3:C:561:ALA:O	3:C:565:LYS:HB2	1.74	0.87
4:D:127:CYS:O	4:D:131:ALA:HB3	1.74	0.86
7:G:543:GLU:O	7:G:547:GLU:HB2	1.75	0.86
7:G:106:LYS:O	7:G:110:MET:HB2	1.73	0.86
7:G:210:ILE:O	7:G:214:MET:HB2	1.77	0.85
3:C:457:ASP:CA	3:C:457:ASP:CG	2.51	0.83
7:G:105:HIS:O	7:G:109:ASP:HB2	1.78	0.83
7:G:351:ARG:O	7:G:355:LYS:HB2	1.78	0.82
7:G:307:GLU:O	7:G:310:GLU:HB3	1.79	0.82
3:C:774:GLU:CG	3:C:774:GLU:CA	2.56	0.82
3:C:766:LYS:O	3:C:770:GLN:HB2	1.80	0.82
8:H:380:ALA:HA	8:H:392:VAL:O	1.81	0.80
8:H:351:SER:HA	8:H:370:ILE:O	1.81	0.79
7:G:84:TYR:O	7:G:88:LEU:HB2	1.83	0.77
7:G:588:MET:O	7:G:592:PHE:HB3	1.84	0.77
3:C:556:ALA:O	3:C:560:VAL:HB	1.84	0.76
3:C:765:ARG:O	3:C:769:VAL:HB	1.86	0.74
7:G:331:GLN:O	7:G:335:GLN:HB2	1.88	0.73
7:G:287:PHE:O	7:G:291:LEU:HB2	1.89	0.72
7:G:253:GLU:O	7:G:257:VAL:HB	1.89	0.71
7:G:211:LEU:O	7:G:215:ALA:HB2	1.89	0.71
7:G:347:ASP:O	7:G:351:ARG:HB2	1.92	0.70
3:C:630:ALA:O	3:C:634:ASP:HB2	1.92	0.70
3:C:471:MET:CB	3:C:471:MET:SD	2.81	0.69
3:C:546:ILE:HG21	3:C:644:MET:HA	1.73	0.69
7:G:340:VAL:O	7:G:344:LEU:HB2	1.93	0.69
3:C:559:ALA:O	3:C:563:SER:HB2	1.93	0.68
3:C:572:LYS:O	3:C:576:LYS:HB2	1.93	0.68
7:G:520:ARG:O	7:G:524:ALA:HB2	1.92	0.68
7:G:591:ARG:O	7:G:595:ARG:HB2	1.92	0.68
3:C:648:LEU:O	3:C:652:PHE:HB2	1.94	0.67
3:C:671:GLU:HG2	3:C:755:LYS:HB3	1.78	0.65
3:C:491:VAL:O	3:C:495:PHE:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:158:PRO:HG3	7:G:212:LYS:HD3	1.78	0.65
7:G:319:LEU:HB3	7:G:322:LYS:HZ1	1.62	0.64
7:G:98:LYS:O	7:G:102:GLN:HB3	1.97	0.64
3:C:686:LYS:O	3:C:689:PHE:HB3	1.98	0.64
7:G:390:LEU:O	7:G:423:HIS:ND1	2.30	0.64
3:C:661:ILE:HD12	3:C:713:ASN:HB3	1.80	0.64
7:G:470:GLN:HA	7:G:515:MET:HG2	1.80	0.63
3:C:561:ALA:O	3:C:565:LYS:CB	2.46	0.63
8:H:533:LEU:HA	8:H:536:LEU:HB2	1.81	0.63
7:G:184:TRP:O	7:G:188:TYR:CB	2.47	0.63
3:C:716:VAL:O	3:C:720:PHE:HB3	1.99	0.63
6:F:711:GLU:HA	6:F:715:ALA:HB3	1.81	0.63
3:C:517:GLN:HB3	3:C:603:LEU:HD13	1.80	0.62
7:G:98:LYS:O	7:G:102:GLN:CB	2.47	0.62
2:B:357:TRP:O	2:B:361:LYS:N	2.25	0.62
7:G:324:LEU:HG	7:G:327:TYR:HB2	1.81	0.62
7:G:359:ILE:O	7:G:445:LYS:NZ	2.32	0.62
8:H:403:VAL:HA	8:H:416:LYS:HA	1.80	0.62
3:C:317:VAL:H	3:C:318:GLY:HA2	1.64	0.62
7:G:290:ASN:HA	7:G:293:ILE:HG22	1.82	0.62
3:C:491:VAL:O	3:C:495:PHE:CB	2.48	0.61
3:C:716:VAL:O	3:C:720:PHE:CB	2.48	0.61
7:G:488:GLU:HG2	7:G:489:LYS:HG3	1.82	0.61
4:D:140:GLY:O	4:D:144:GLU:N	2.29	0.61
7:G:283:TYR:O	7:G:287:PHE:HB2	2.00	0.61
1:A:611:GLU:N	2:B:261:LYS:O	2.33	0.61
7:G:142:GLU:HA	7:G:145:LEU:HD12	1.83	0.61
7:G:306:PHE:O	7:G:309:VAL:HB	2.01	0.61
3:C:423:LEU:HD23	3:C:491:VAL:HG23	1.83	0.60
6:F:90:ASP:O	6:F:94:GLY:HA3	2.00	0.60
3:C:72:ILE:O	3:C:76:ASN:CB	2.49	0.60
7:G:305:SER:O	7:G:308:LEU:HB2	2.00	0.60
7:G:330:LEU:O	7:G:334:THR:CB	2.49	0.60
4:D:716:GLU:O	4:D:720:GLU:CB	2.50	0.60
7:G:546:LYS:O	7:G:550:ARG:CB	2.47	0.60
8:H:528:SER:O	8:H:532:ARG:HB2	2.01	0.60
3:C:66:THR:O	3:C:70:GLN:CB	2.50	0.60
7:G:352:ILE:HG22	7:G:441:ASN:HD22	1.67	0.60
6:F:315:SER:O	6:F:319:PHE:CB	2.49	0.60
3:C:585:THR:O	3:C:589:PHE:N	2.35	0.60
5:E:267:VAL:O	5:E:270:SER:C	2.45	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:252:ASN:O	7:G:256:LEU:HB3	2.03	0.59
7:G:283:TYR:O	7:G:287:PHE:CB	2.50	0.59
1:A:1288:CYS:O	1:A:1292:TRP:N	2.35	0.59
3:C:430:MET:O	3:C:434:ILE:HB	2.01	0.59
5:E:108:ILE:O	5:E:112:ASN:CB	2.51	0.59
7:G:287:PHE:O	7:G:291:LEU:CB	2.50	0.59
8:H:321:TRP:O	8:H:325:LEU:CB	2.50	0.59
7:G:441:ASN:OD1	7:G:444:ARG:NH1	2.35	0.59
7:G:447:GLN:HE22	7:G:458:VAL:HA	1.67	0.59
4:D:116:GLN:O	4:D:120:GLN:N	2.34	0.59
2:B:725:PRO:O	2:B:729:LEU:N	2.35	0.59
8:H:543:ILE:HG23	8:H:555:ALA:HB1	1.84	0.59
3:C:734:ILE:O	3:C:738:TYR:HB3	2.02	0.59
5:E:200:LYS:O	5:E:204:ILE:CB	2.51	0.59
4:D:287:GLU:O	4:D:291:HIS:CB	2.51	0.58
3:C:468:CYS:SG	3:C:502:ARG:NH1	2.76	0.58
4:D:109:LYS:O	4:D:113:SER:N	2.35	0.58
3:C:676:ASN:ND2	3:C:725:CYS:O	2.36	0.58
7:G:34:LYS:O	7:G:38:ALA:HB2	2.03	0.58
7:G:184:TRP:O	7:G:188:TYR:HB2	2.03	0.58
4:D:349:ARG:O	4:D:353:GLU:CB	2.52	0.58
7:G:388:GLY:O	7:G:392:ALA:HB2	2.03	0.58
3:C:73:ASN:O	3:C:77:LYS:CB	2.52	0.58
4:D:144:GLU:O	4:D:148:ASN:N	2.34	0.58
3:C:565:LYS:O	3:C:568:LYS:NZ	2.33	0.58
8:H:207:LEU:O	8:H:211:SER:CB	2.51	0.58
3:C:745:SER:HB2	3:C:795:MET:HB3	1.86	0.58
4:D:947:ASN:O	8:H:707:LYS:NZ	2.34	0.58
5:E:99:SER:O	5:E:103:ALA:HB2	2.04	0.58
6:F:624:ASN:O	6:F:628:PHE:CB	2.52	0.57
3:C:559:ALA:O	3:C:563:SER:CB	2.52	0.57
3:C:735:TRP:O	3:C:739:LEU:CB	2.52	0.57
4:D:916:LEU:O	4:D:920:ALA:HB2	2.05	0.57
4:D:957:MET:O	4:D:961:MET:CB	2.51	0.57
6:F:700:ASP:N	6:F:760:ASN:O	2.37	0.57
7:G:516:VAL:HG13	7:G:581:ILE:HG12	1.87	0.57
2:B:781:ASN:O	2:B:785:TYR:CB	2.52	0.57
4:D:521:PHE:HA	5:E:756:LYS:HA	1.87	0.57
5:E:653:LEU:O	5:E:657:SER:CB	2.53	0.57
7:G:146:ARG:NH2	7:G:194:GLU:OE1	2.37	0.57
8:H:331:ASN:O	8:H:335:ALA:N	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:468:CYS:O	3:C:472:PHE:HB3	2.05	0.57
4:D:653:GLU:O	4:D:657:TYR:N	2.38	0.57
6:F:394:ASP:O	6:F:398:LYS:CB	2.53	0.57
7:G:85:GLU:OE1	7:G:133:HIS:NE2	2.37	0.57
7:G:419:ASN:HB3	7:G:421:GLU:HG2	1.86	0.57
7:G:610:THR:HG1	7:G:613:GLU:H	1.50	0.57
3:C:590:ALA:O	3:C:593:ALA:HB3	2.04	0.57
4:D:565:GLN:O	4:D:569:THR:N	2.37	0.57
4:D:700:MET:O	4:D:704:GLN:N	2.38	0.56
8:H:355:MET:HA	8:H:367:MET:HA	1.85	0.56
8:H:443:ALA:O	8:H:447:LEU:CB	2.53	0.56
3:C:4:ASP:O	3:C:8:GLN:N	2.36	0.56
5:E:73:TYR:O	5:E:77:PHE:CB	2.53	0.56
5:E:75:ARG:O	5:E:79:SER:N	2.37	0.56
7:G:27:PHE:O	7:G:31:LYS:CB	2.53	0.56
7:G:189:PHE:HA	7:G:192:ASN:HB2	1.87	0.56
7:G:346:ARG:HG2	7:G:401:TRP:HA	1.87	0.56
5:E:112:ASN:O	5:E:116:LEU:CB	2.54	0.56
2:B:873:ILE:O	2:B:877:LEU:CB	2.54	0.56
3:C:60:LEU:O	3:C:64:SER:CB	2.53	0.56
4:D:706:ILE:N	4:D:708:ASN:O	2.39	0.56
6:F:864:ILE:O	6:F:868:VAL:CB	2.54	0.56
7:G:9:GLU:O	7:G:13:LEU:CB	2.53	0.56
7:G:330:LEU:O	7:G:334:THR:HB	2.05	0.56
2:B:646:THR:O	2:B:650:ASP:CB	2.54	0.56
3:C:208:ILE:H	3:C:212:ILE:H	1.54	0.56
3:C:627:GLN:NE2	3:C:631:ASP:OD2	2.38	0.56
7:G:447:GLN:NE2	7:G:457:ASP:O	2.39	0.56
8:H:219:LYS:O	8:H:223:ASN:CB	2.54	0.56
1:A:682:ASN:O	1:A:686:HIS:CB	2.54	0.56
2:B:538:LYS:O	2:B:542:PHE:CB	2.54	0.56
2:B:800:GLU:O	2:B:804:LEU:N	2.33	0.56
5:E:433:SER:O	5:E:438:ILE:N	2.37	0.56
6:F:607:ARG:O	6:F:611:GLU:N	2.38	0.56
7:G:352:ILE:O	7:G:356:ALA:CB	2.54	0.56
8:H:215:GLN:O	8:H:219:LYS:CB	2.54	0.55
8:H:546:GLU:HB3	8:H:555:ALA:HB2	1.87	0.55
3:C:752:GLY:HA3	3:C:800:LEU:HD23	1.87	0.55
4:D:126:ASN:O	4:D:130:GLU:CB	2.53	0.55
5:E:599:ILE:O	5:E:603:LEU:CB	2.54	0.55
7:G:589:TYR:OH	7:G:609:TYR:O	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1072:ASN:O	1:A:1245:ARG:N	2.39	0.55
3:C:62:LYS:O	3:C:66:THR:CB	2.54	0.55
3:C:685:MET:HB3	3:C:721:MET:HG2	1.89	0.55
4:D:666:PHE:O	4:D:670:TYR:CB	2.54	0.55
6:F:217:LEU:O	6:F:221:TYR:CB	2.55	0.55
5:E:685:GLN:O	5:E:689:MET:CB	2.54	0.55
3:C:705:SER:HA	3:C:708:THR:HB	1.88	0.55
6:F:725:VAL:O	6:F:729:LEU:N	2.39	0.55
5:E:749:SER:O	5:E:753:LEU:N	2.38	0.55
7:G:347:ASP:O	7:G:351:ARG:CB	2.55	0.55
1:A:1251:ILE:HA	1:A:1254:ALA:HB2	1.89	0.55
5:E:83:GLU:O	5:E:87:LEU:N	2.37	0.55
7:G:352:ILE:O	7:G:356:ALA:HB3	2.07	0.55
8:H:444:LYS:HA	8:H:448:CYS:H	1.70	0.55
8:H:533:LEU:O	8:H:537:ASP:N	2.39	0.55
3:C:388:ASP:O	3:C:392:GLN:CB	2.55	0.55
4:D:1047:THR:O	4:D:1051:LYS:CB	2.55	0.55
5:E:33:LEU:O	5:E:37:HIS:N	2.40	0.55
5:E:163:GLU:O	5:E:167:ARG:CB	2.55	0.55
7:G:114:ILE:O	7:G:121:ARG:N	2.39	0.55
8:H:434:SER:O	8:H:438:ASP:CB	2.55	0.55
4:D:697:GLY:O	4:D:701:ASP:CB	2.55	0.55
7:G:16:SER:O	7:G:20:GLN:N	2.38	0.55
7:G:507:LEU:HD23	7:G:510:ARG:HH12	1.72	0.55
1:A:1067:PHE:O	1:A:1245:ARG:N	2.40	0.54
3:C:240:ILE:O	3:C:244:LYS:N	2.39	0.54
3:C:280:MET:HA	3:C:282:GLY:HA3	1.88	0.54
5:E:576:MET:O	5:E:580:VAL:CB	2.55	0.54
6:F:275:SER:HA	6:F:277:MET:H	1.71	0.54
7:G:377:SER:HA	7:G:380:ARG:HG2	1.88	0.54
1:A:1030:ILE:O	1:A:1035:SER:N	2.35	0.54
3:C:8:GLN:O	3:C:12:LEU:CB	2.54	0.54
5:E:736:ILE:O	5:E:740:ASN:CB	2.55	0.54
8:H:528:SER:HA	8:H:531:GLN:HB3	1.89	0.54
8:H:608:GLU:OE1	8:H:610:VAL:N	2.40	0.54
1:A:1156:ASP:O	1:A:1160:THR:N	2.40	0.54
4:D:763:LEU:O	4:D:767:LYS:CB	2.56	0.54
5:E:105:GLN:O	5:E:109:HIS:CB	2.55	0.54
6:F:244:ASN:O	6:F:248:GLY:N	2.41	0.54
8:H:269:GLN:O	8:H:273:GLN:CB	2.55	0.54
4:D:285:ASN:O	4:D:289:PHE:CB	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:461:LEU:O	6:F:465:VAL:N	2.40	0.54
2:B:131:ASN:O	2:B:135:ARG:N	2.40	0.54
2:B:259:TYR:O	2:B:263:LEU:CB	2.56	0.54
3:C:304:SER:O	3:C:308:MET:CB	2.55	0.54
4:D:124:LEU:O	4:D:128:LEU:CB	2.55	0.54
4:D:364:SER:O	4:D:368:LYS:CB	2.55	0.54
5:E:78:GLU:O	5:E:82:LYS:N	2.39	0.54
1:A:1046:THR:O	1:A:1050:THR:CB	2.55	0.54
2:B:149:GLN:HA	2:B:153:LYS:H	1.71	0.54
2:B:939:GLN:HA	2:B:941:ASP:H	1.72	0.54
3:C:300:GLY:O	3:C:304:SER:CB	2.55	0.54
5:E:797:TYR:HA	5:E:800:ALA:HB3	1.90	0.54
7:G:34:LYS:O	7:G:38:ALA:CB	2.56	0.54
7:G:19:LEU:O	7:G:23:SER:N	2.41	0.54
7:G:174:TYR:HD1	7:G:178:GLN:HE22	1.55	0.54
5:E:740:ASN:O	5:E:744:LEU:CB	2.56	0.54
7:G:589:TYR:O	7:G:593:TYR:CB	2.50	0.54
3:C:462:LEU:N	3:C:551:ASP:OD2	2.41	0.54
3:C:598:LEU:HA	3:C:601:ILE:HD12	1.89	0.54
3:C:668:LEU:HD13	3:C:749:LEU:HD11	1.90	0.54
3:C:751:VAL:O	3:C:755:LYS:N	2.41	0.54
6:F:737:LEU:O	6:F:741:PHE:CB	2.55	0.54
7:G:451:MET:HE2	7:G:454:GLN:HG3	1.90	0.54
3:C:142:LEU:O	3:C:146:HIS:CB	2.56	0.54
5:E:708:PHE:O	5:E:712:LEU:CB	2.56	0.54
6:F:711:GLU:O	6:F:716:SER:N	2.40	0.54
6:F:754:THR:H	6:F:758:ILE:H	1.54	0.54
8:H:744:PHE:O	8:H:748:ASN:HB2	2.08	0.54
2:B:134:ASP:O	2:B:138:SER:CB	2.57	0.53
6:F:389:LEU:O	6:F:393:GLN:N	2.41	0.53
3:C:572:LYS:O	3:C:576:LYS:CB	2.57	0.53
4:D:905:PHE:O	4:D:909:ASP:CB	2.57	0.53
5:E:412:ILE:O	5:E:416:THR:N	2.41	0.53
5:E:701:ILE:O	5:E:705:SER:CB	2.56	0.53
5:E:769:LEU:O	5:E:773:LEU:N	2.40	0.53
7:G:195:GLY:O	7:G:199:GLN:CB	2.55	0.53
8:H:706:ASP:HA	8:H:709:LEU:HD13	1.90	0.53
2:B:139:ASP:O	2:B:143:GLN:CB	2.57	0.53
4:D:389:VAL:HA	4:D:391:ASP:H	1.73	0.53
5:E:79:SER:O	5:E:83:GLU:N	2.42	0.53
5:E:318:MET:O	5:E:322:ILE:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:705:SER:O	5:E:709:SER:CB	2.56	0.53
6:F:738:THR:O	6:F:742:MET:CB	2.56	0.53
3:C:18:SER:O	3:C:22:VAL:N	2.36	0.53
3:C:648:LEU:O	3:C:652:PHE:CB	2.57	0.53
6:F:133:LYS:O	6:F:137:ARG:CB	2.56	0.53
1:A:1025:TYR:O	1:A:1029:GLU:N	2.40	0.53
2:B:747:ALA:O	2:B:751:ASN:CB	2.56	0.53
4:D:325:ARG:O	4:D:329:LEU:CB	2.57	0.53
8:H:461:ILE:O	8:H:465:PHE:CB	2.57	0.53
1:A:706:ILE:O	1:A:710:GLU:CB	2.56	0.53
5:E:199:MET:O	5:E:203:LEU:CB	2.57	0.53
3:C:194:GLY:O	3:C:198:ASP:CB	2.57	0.53
3:C:236:LYS:O	3:C:240:ILE:CB	2.57	0.53
3:C:628:GLN:O	3:C:632:THR:HB	2.08	0.53
4:D:123:ASN:O	4:D:127:CYS:CB	2.56	0.53
4:D:417:ALA:O	4:D:421:MET:CB	2.57	0.53
5:E:104:THR:O	5:E:108:ILE:CB	2.57	0.53
5:E:187:LYS:N	5:E:190:LYS:O	2.41	0.53
5:E:396:SER:O	5:E:400:TYR:CB	2.57	0.53
7:G:184:TRP:O	7:G:188:TYR:HB3	2.09	0.53
4:D:352:GLU:O	4:D:356:ASN:CB	2.57	0.53
5:E:608:LEU:O	5:E:613:SER:N	2.38	0.53
6:F:257:GLU:O	6:F:261:ILE:CB	2.57	0.53
5:E:316:THR:HA	5:E:318:MET:H	1.74	0.53
8:H:456:GLU:O	8:H:460:ARG:CB	2.57	0.53
2:B:944:ARG:O	2:B:948:CYS:CB	2.57	0.53
4:D:362:THR:O	4:D:366:ARG:CB	2.57	0.53
5:E:86:ASN:O	5:E:90:GLU:N	2.42	0.53
6:F:840:ASN:O	6:F:844:ILE:CB	2.57	0.53
7:G:466:ASN:HD21	7:G:472:ILE:HD12	1.74	0.53
5:E:773:LEU:O	5:E:778:SER:N	2.36	0.52
7:G:195:GLY:O	7:G:199:GLN:HB2	2.09	0.52
7:G:161:PRO:HG3	7:G:213:CYS:HB3	1.91	0.52
1:A:688:ILE:O	1:A:692:LEU:N	2.39	0.52
1:A:1159:GLU:O	1:A:1163:LEU:CB	2.57	0.52
2:B:239:LEU:O	2:B:243:LEU:CB	2.58	0.52
5:E:684:SER:O	5:E:688:LYS:CB	2.57	0.52
6:F:194:VAL:O	6:F:198:LEU:CB	2.57	0.52
2:B:136:LEU:O	2:B:140:ILE:CB	2.57	0.52
3:C:555:ALA:O	3:C:559:ALA:CB	2.52	0.52
4:D:279:SER:O	4:D:283:ASN:CB	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:720:GLU:O	4:D:724:GLU:CB	2.58	0.52
4:D:912:ASN:O	4:D:916:LEU:CB	2.57	0.52
5:E:660:ILE:O	5:E:664:PHE:CB	2.57	0.52
6:F:308:GLN:O	6:F:312:PHE:N	2.40	0.52
8:H:171:THR:O	8:H:175:LYS:CB	2.57	0.52
1:A:693:SER:O	1:A:697:MET:CB	2.58	0.52
2:B:363:ASN:O	2:B:367:ASN:CB	2.57	0.52
3:C:61:SER:O	3:C:65:VAL:CB	2.58	0.52
7:G:427:LEU:HG	7:G:496:LEU:HD23	1.91	0.52
5:E:379:TYR:O	5:E:383:LEU:CB	2.58	0.52
5:E:620:GLU:O	5:E:624:TRP:N	2.42	0.52
7:G:104:VAL:O	7:G:108:ASP:HB2	2.09	0.52
7:G:203:VAL:O	7:G:207:SER:OG	2.27	0.52
8:H:749:SER:HA	8:H:752:ILE:HD12	1.91	0.52
6:F:141:SER:O	6:F:145:LEU:CB	2.57	0.52
5:E:586:ARG:O	5:E:590:LEU:CB	2.58	0.52
7:G:492:LEU:HA	7:G:495:MET:HB2	1.92	0.52
2:B:597:CYS:O	2:B:601:LEU:CB	2.58	0.52
3:C:735:TRP:O	3:C:739:LEU:HB3	2.09	0.52
4:D:996:ARG:O	4:D:1000:SER:CB	2.58	0.52
5:E:369:ARG:O	5:E:373:SER:CB	2.58	0.52
6:F:863:LYS:O	6:F:867:PHE:CB	2.58	0.52
7:G:203:VAL:O	7:G:207:SER:CB	2.58	0.52
8:H:187:PHE:O	8:H:191:LYS:N	2.38	0.52
8:H:357:LEU:HA	8:H:364:PRO:HA	1.91	0.52
8:H:432:GLU:O	8:H:436:LEU:CB	2.58	0.52
4:D:821:ALA:O	4:D:825:PHE:CB	2.58	0.51
6:F:603:ASN:O	6:F:607:ARG:N	2.44	0.51
2:B:143:GLN:O	2:B:147:LEU:CB	2.59	0.51
2:B:192:VAL:O	2:B:196:ASN:N	2.40	0.51
3:C:191:LEU:O	3:C:195:LEU:CB	2.58	0.51
5:E:650:THR:O	5:E:654:ASP:CB	2.59	0.51
6:F:841:GLU:O	6:F:845:ARG:CB	2.58	0.51
6:F:881:VAL:O	6:F:885:SER:CB	2.58	0.51
7:G:8:ASP:O	7:G:12:VAL:CB	2.58	0.51
7:G:272:LEU:HD23	7:G:322:LYS:HG2	1.92	0.51
7:G:316:LYS:O	7:G:320:ARG:NH1	2.43	0.51
7:G:374:ASP:O	7:G:378:ARG:HB2	2.10	0.51
3:C:387:PHE:O	3:C:391:PHE:CB	2.58	0.51
3:C:426:ILE:HG23	3:C:475:GLN:HE21	1.76	0.51
3:C:448:ARG:HH22	3:C:513:GLU:HB3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:768:ILE:O	3:C:772:ALA:CB	2.58	0.51
5:E:619:LEU:O	5:E:623:TYR:N	2.44	0.51
5:E:655:LEU:O	5:E:659:SER:CB	2.59	0.51
6:F:226:PHE:O	6:F:230:VAL:CB	2.58	0.51
8:H:226:TYR:O	8:H:230:MET:CB	2.58	0.51
8:H:318:GLU:O	8:H:322:ASP:CB	2.58	0.51
3:C:499:LEU:HD23	3:C:502:ARG:HD3	1.92	0.51
3:C:627:GLN:O	3:C:631:ASP:HB2	2.11	0.51
7:G:543:GLU:O	7:G:547:GLU:CB	2.53	0.51
8:H:170:SER:O	8:H:174:ARG:CB	2.59	0.51
8:H:557:GLU:OE2	8:H:621:LYS:NZ	2.40	0.51
2:B:354:ILE:HA	2:B:357:TRP:H	1.76	0.51
3:C:112:ILE:O	3:C:116:VAL:CB	2.58	0.51
3:C:465:THR:HG23	3:C:502:ARG:HH22	1.74	0.51
5:E:739:VAL:O	5:E:743:ASN:CB	2.59	0.51
8:H:348:LEU:HA	8:H:373:LEU:HA	1.92	0.51
4:D:113:SER:O	4:D:117:ALA:N	2.40	0.51
5:E:82:LYS:O	5:E:86:ASN:N	2.42	0.51
6:F:111:THR:O	6:F:115:GLU:CB	2.58	0.51
7:G:520:ARG:O	7:G:524:ALA:CB	2.59	0.51
7:G:588:MET:O	7:G:592:PHE:CB	2.56	0.51
8:H:233:ASN:O	8:H:237:ASN:CB	2.59	0.51
1:A:1288:CYS:O	1:A:1293:SER:N	2.42	0.51
2:B:613:THR:O	2:B:617:GLN:CB	2.59	0.51
3:C:559:ALA:HB1	3:C:582:LEU:HD22	1.93	0.51
4:D:128:LEU:O	4:D:132:ASN:CB	2.59	0.51
8:H:404:THR:N	8:H:415:PHE:O	2.43	0.51
4:D:927:ASN:O	4:D:931:ILE:N	2.42	0.51
2:B:611:PHE:O	2:B:615:LEU:CB	2.59	0.51
4:D:997:LEU:O	4:D:1001:GLU:CB	2.59	0.51
5:E:346:HIS:O	5:E:351:PHE:N	2.44	0.51
5:E:642:PHE:O	5:E:646:ILE:CB	2.58	0.51
6:F:865:GLN:O	6:F:869:SER:CB	2.58	0.51
7:G:30:ASN:O	7:G:34:LYS:CB	2.59	0.51
7:G:114:ILE:HA	7:G:121:ARG:HG2	1.93	0.51
7:G:310:GLU:O	7:G:313:ASN:HB2	2.11	0.51
1:A:1024:PHE:O	1:A:1028:ASN:N	2.43	0.50
3:C:67:SER:O	3:C:71:GLN:CB	2.58	0.50
5:E:686:ILE:O	5:E:690:GLU:CB	2.59	0.50
6:F:269:GLN:O	6:F:273:THR:CB	2.59	0.50
8:H:225:SER:O	8:H:229:ILE:CB	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:260:SER:O	2:B:264:THR:CB	2.59	0.50
4:D:92:VAL:O	4:D:96:HIS:N	2.36	0.50
4:D:322:GLY:O	4:D:326:ILE:CB	2.59	0.50
5:E:578:LYS:O	5:E:582:GLU:CB	2.59	0.50
7:G:330:LEU:O	7:G:334:THR:OG1	2.29	0.50
1:A:1158:MET:O	1:A:1162:SER:CB	2.60	0.50
4:D:110:ALA:O	4:D:114:ILE:N	2.42	0.50
6:F:333:ASN:O	6:F:337:GLU:CB	2.59	0.50
7:G:161:PRO:HD2	7:G:217:LEU:HG	1.94	0.50
8:H:208:THR:O	8:H:212:ILE:CB	2.59	0.50
2:B:140:ILE:O	2:B:144:SER:CB	2.59	0.50
3:C:262:GLU:H	3:C:265:LYS:H	1.58	0.50
3:C:305:ILE:O	3:C:309:PHE:CB	2.60	0.50
4:D:328:PHE:O	4:D:332:THR:CB	2.60	0.50
6:F:735:ASP:O	6:F:739:ARG:N	2.43	0.50
7:G:339:GLN:O	7:G:343:SER:CB	2.59	0.50
8:H:214:VAL:O	8:H:218:VAL:CB	2.59	0.50
8:H:460:ARG:O	8:H:464:SER:CB	2.60	0.50
1:A:794:ARG:O	1:A:798:TYR:CB	2.59	0.50
2:B:349:SER:O	2:B:351:GLU:N	2.36	0.50
3:C:637:LEU:HD21	3:C:652:PHE:HE2	1.75	0.50
5:E:397:LEU:O	5:E:401:PHE:CB	2.60	0.50
5:E:768:GLU:O	5:E:772:LEU:N	2.41	0.50
7:G:162:GLN:HB2	7:G:217:LEU:HD21	1.93	0.50
8:H:703:LYS:O	8:H:707:LYS:HB2	2.10	0.50
1:A:1087:PRO:O	1:A:1091:LYS:CB	2.59	0.50
5:E:156:GLN:O	5:E:160:GLN:CB	2.60	0.50
6:F:634:GLU:O	6:F:638:PHE:N	2.42	0.50
7:G:13:LEU:O	7:G:17:GLN:N	2.41	0.50
8:H:529:THR:HG22	8:H:569:LEU:HD13	1.93	0.50
1:A:893:GLU:O	1:A:897:SER:CB	2.59	0.50
3:C:428:VAL:O	3:C:431:THR:OG1	2.24	0.50
5:E:384:HIS:O	5:E:388:THR:CB	2.60	0.50
5:E:574:ASP:O	5:E:578:LYS:CB	2.60	0.50
7:G:199:GLN:NE2	7:G:267:SER:OG	2.45	0.50
7:G:258:ASP:HA	7:G:261:TYR:HE2	1.77	0.50
7:G:339:GLN:O	7:G:343:SER:HB2	2.12	0.50
1:A:697:MET:O	1:A:701:ASN:CB	2.59	0.50
1:A:812:GLU:O	1:A:816:LYS:CB	2.60	0.50
3:C:108:ILE:O	3:C:112:ILE:CB	2.59	0.50
3:C:661:ILE:HA	3:C:664:PHE:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1047:ARG:O	1:A:1051:GLN:CB	2.60	0.50
2:B:897:GLY:O	2:B:938:PHE:N	2.44	0.50
3:C:360:TYR:O	3:C:364:LEU:CB	2.59	0.50
5:E:696:ILE:O	5:E:700:THR:CB	2.60	0.50
5:E:697:LEU:O	5:E:701:ILE:CB	2.60	0.50
3:C:235:ILE:O	3:C:239:GLU:CB	2.59	0.49
3:C:597:SER:O	3:C:600:LEU:HB2	2.12	0.49
4:D:647:THR:O	4:D:649:ASN:N	2.42	0.49
8:H:446:ASP:O	8:H:450:ILE:CB	2.59	0.49
1:A:1045:VAL:O	1:A:1049:TYR:CB	2.60	0.49
2:B:263:LEU:O	2:B:267:ARG:N	2.43	0.49
7:G:109:ASP:HA	7:G:112:GLU:HB2	1.94	0.49
7:G:340:VAL:O	7:G:344:LEU:CB	2.60	0.49
3:C:362:LYS:O	3:C:366:SER:CB	2.60	0.49
7:G:334:THR:HA	7:G:337:VAL:HG12	1.94	0.49
7:G:388:GLY:O	7:G:392:ALA:CB	2.61	0.49
8:H:444:LYS:O	8:H:448:CYS:CB	2.61	0.49
8:H:667:THR:O	8:H:671:THR:OG1	2.26	0.49
1:A:1161:ILE:O	1:A:1165:VAL:CB	2.61	0.49
2:B:369:LEU:O	2:B:373:SER:CB	2.61	0.49
2:B:466:LEU:O	2:B:470:LYS:CB	2.60	0.49
3:C:503:GLN:HA	3:C:506:TRP:HD1	1.78	0.49
5:E:77:PHE:O	5:E:81:LEU:N	2.42	0.49
6:F:879:THR:O	6:F:883:ASP:CB	2.61	0.49
7:G:470:GLN:HE22	7:G:563:THR:HA	1.77	0.49
1:A:1198:VAL:O	1:A:1202:SER:CB	2.61	0.49
2:B:8:ASP:HA	3:C:142:LEU:HA	1.95	0.49
3:C:734:ILE:O	3:C:738:TYR:CB	2.60	0.49
6:F:144:GLU:O	6:F:148:LYS:CB	2.61	0.49
7:G:481:THR:O	7:G:485:GLN:HB2	2.13	0.49
7:G:539:SER:OG	7:G:541:ASP:O	2.31	0.49
8:H:527:SER:O	8:H:531:GLN:N	2.38	0.49
1:A:797:PHE:O	1:A:801:VAL:CB	2.61	0.49
2:B:501:ILE:O	2:B:505:LYS:CB	2.61	0.49
5:E:760:THR:O	5:E:764:LEU:CB	2.61	0.49
6:F:623:VAL:O	6:F:627:TYR:CB	2.60	0.49
7:G:142:GLU:HB3	7:G:146:ARG:HH12	1.77	0.49
4:D:719:ILE:O	4:D:723:LYS:CB	2.60	0.49
5:E:679:ILE:O	5:E:684:SER:N	2.44	0.49
6:F:115:GLU:O	6:F:119:ILE:CB	2.60	0.49
6:F:726:GLN:O	6:F:730:ILE:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:10:ALA:O	7:G:14:VAL:CB	2.61	0.49
7:G:209:LEU:HA	7:G:212:LYS:HD2	1.95	0.49
8:H:212:ILE:O	8:H:216:GLU:CB	2.61	0.49
4:D:772:ILE:HA	4:D:773:ASP:HA	1.59	0.49
5:E:651:GLU:O	5:E:655:LEU:CB	2.61	0.49
7:G:386:LYS:HG3	7:G:495:MET:HE2	1.95	0.49
7:G:525:ASN:HA	7:G:528:ASP:HB2	1.94	0.49
1:A:699:MET:O	1:A:703:SER:CB	2.61	0.48
1:A:1165:VAL:O	1:A:1169:TRP:CB	2.60	0.48
5:E:61:ARG:O	5:E:65:TRP:N	2.46	0.48
6:F:706:LEU:O	6:F:710:LEU:N	2.44	0.48
8:H:213:GLN:O	8:H:217:GLU:CB	2.61	0.48
3:C:52:GLU:O	3:C:56:LYS:CB	2.61	0.48
5:E:106:GLU:O	5:E:110:SER:CB	2.61	0.48
6:F:424:SER:O	6:F:428:PHE:CB	2.62	0.48
7:G:40:SER:O	7:G:44:SER:CB	2.61	0.48
7:G:51:LEU:O	7:G:55:ASN:CB	2.61	0.48
7:G:338:ARG:O	7:G:342:GLN:HB2	2.13	0.48
8:H:536:LEU:O	8:H:540:VAL:N	2.44	0.48
3:C:547:ALA:HA	3:C:550:ASN:HD22	1.79	0.48
5:E:333:SER:O	5:E:337:LYS:CB	2.61	0.48
5:E:353:GLN:O	5:E:357:ALA:CB	2.62	0.48
5:E:759:GLN:O	5:E:763:THR:CB	2.62	0.48
6:F:730:ILE:O	6:F:735:ASP:N	2.46	0.48
7:G:436:ASP:OD2	7:G:503:ARG:NH2	2.46	0.48
8:H:223:ASN:O	8:H:227:ASN:CB	2.61	0.48
8:H:328:LEU:O	8:H:332:VAL:CB	2.61	0.48
8:H:547:LEU:HD21	8:H:595:ILE:HG12	1.95	0.48
3:C:382:LEU:O	3:C:386:ALA:HB3	2.13	0.48
3:C:467:THR:O	3:C:471:MET:CB	2.62	0.48
3:C:735:TRP:CD1	3:C:772:ALA:HB1	2.48	0.48
4:D:74:ARG:O	4:D:78:PHE:CB	2.62	0.48
4:D:111:VAL:O	4:D:115:MET:N	2.39	0.48
5:E:252:ASN:O	5:E:256:ILE:CB	2.62	0.48
5:E:567:ASN:H	5:E:570:LEU:H	1.60	0.48
6:F:261:ILE:O	6:F:265:GLU:CB	2.61	0.48
7:G:249:PHE:O	7:G:253:GLU:HB3	2.14	0.48
3:C:269:TYR:O	3:C:274:GLY:N	2.47	0.48
5:E:652:ILE:O	5:E:656:LEU:CB	2.62	0.48
1:A:700:SER:O	1:A:704:ASN:CB	2.61	0.48
4:D:961:MET:O	4:D:965:SER:CB	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:231:PRO:O	7:G:301:PHE:N	2.39	0.48
7:G:542:LYS:HG2	7:G:545:ILE:HD12	1.95	0.48
8:H:739:TYR:OH	8:H:740:LYS:NZ	2.47	0.48
1:A:798:TYR:O	1:A:802:THR:CB	2.61	0.48
2:B:325:LEU:O	2:B:329:ASN:CB	2.62	0.48
5:E:568:TYR:H	5:E:572:ASP:H	1.61	0.48
5:E:741:ILE:O	5:E:745:ILE:CB	2.62	0.48
7:G:18:GLU:O	7:G:22:THR:N	2.43	0.48
7:G:249:PHE:O	7:G:253:GLU:CB	2.61	0.48
8:H:266:LYS:O	8:H:270:LEU:CB	2.62	0.48
5:E:325:VAL:O	5:E:329:ILE:CB	2.62	0.48
6:F:672:ILE:O	6:F:676:ASP:CB	2.62	0.48
1:A:868:PRO:O	1:A:872:GLU:CB	2.62	0.47
2:B:824:LEU:O	2:B:827:THR:CB	2.61	0.47
5:E:180:VAL:HA	5:E:181:GLU:HA	1.66	0.47
7:G:433:ASP:OD1	7:G:503:ARG:NH2	2.35	0.47
1:A:670:ILE:O	1:A:674:ILE:N	2.46	0.47
2:B:155:PHE:O	2:B:159:VAL:N	2.44	0.47
2:B:351:GLU:O	2:B:355:LEU:N	2.47	0.47
3:C:597:SER:HA	3:C:600:LEU:HD22	1.95	0.47
4:D:825:PHE:O	4:D:829:ILE:CB	2.61	0.47
4:D:902:ASN:O	4:D:906:ILE:CB	2.62	0.47
5:E:87:LEU:O	5:E:91:THR:N	2.47	0.47
7:G:426:LEU:HA	7:G:429:CYS:HB3	1.96	0.47
7:G:591:ARG:HD3	7:G:595:ARG:HH22	1.79	0.47
1:A:856:GLN:O	1:A:860:GLU:N	2.47	0.47
1:A:928:GLU:O	1:A:932:THR:CB	2.62	0.47
3:C:148:LEU:O	3:C:152:ALA:N	2.47	0.47
3:C:193:ASP:O	3:C:197:TYR:CB	2.62	0.47
3:C:198:ASP:O	3:C:202:MET:N	2.47	0.47
3:C:723:LEU:HB3	3:C:753:ILE:HD13	1.95	0.47
4:D:288:GLN:O	4:D:292:ASP:CB	2.62	0.47
4:D:381:ASN:HA	4:D:382:ASP:HA	1.62	0.47
5:E:29:PHE:O	5:E:34:SER:N	2.40	0.47
8:H:218:VAL:O	8:H:222:ILE:CB	2.62	0.47
8:H:563:GLU:O	8:H:567:GLU:HB2	2.14	0.47
1:A:677:TYR:O	1:A:681:VAL:CB	2.62	0.47
2:B:74:GLU:O	2:B:78:TYR:CB	2.62	0.47
5:E:445:ALA:O	5:E:449:ASP:CB	2.63	0.47
5:E:577:LEU:O	5:E:581:VAL:CB	2.62	0.47
2:B:372:LEU:O	2:B:376:MET:CB	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:109:TYR:O	3:C:113:TYR:CB	2.62	0.47
4:D:327:GLY:O	4:D:331:LYS:CB	2.62	0.47
5:E:443:LEU:O	5:E:447:LEU:CB	2.63	0.47
7:G:104:VAL:O	7:G:108:ASP:CB	2.63	0.47
7:G:312:ILE:HD12	7:G:315:VAL:HB	1.96	0.47
2:B:821:LYS:O	2:B:825:ARG:N	2.47	0.47
3:C:111:ARG:O	3:C:115:PHE:CB	2.62	0.47
3:C:196:THR:O	3:C:200:VAL:CB	2.63	0.47
3:C:582:LEU:O	3:C:585:THR:OG1	2.33	0.47
3:C:775:MET:O	3:C:779:TYR:CB	2.63	0.47
4:D:119:GLU:O	4:D:124:LEU:N	2.48	0.47
4:D:218:HIS:O	4:D:222:ASN:CB	2.63	0.47
6:F:497:PHE:O	6:F:500:GLU:N	2.43	0.47
8:H:227:ASN:O	8:H:231:THR:CB	2.63	0.47
8:H:253:LEU:O	8:H:257:LEU:N	2.43	0.47
3:C:707:ASP:O	3:C:711:THR:N	2.48	0.47
6:F:560:THR:O	6:F:564:ALA:HB3	2.15	0.47
8:H:243:LEU:O	8:H:247:ARG:CB	2.63	0.47
1:A:1089:GLY:O	1:A:1093:SER:CB	2.62	0.47
2:B:19:THR:HA	2:B:20:ILE:HA	1.64	0.47
5:E:76:THR:O	5:E:80:THR:N	2.44	0.47
5:E:225:GLU:O	5:E:229:GLU:CB	2.63	0.47
5:E:447:LEU:O	5:E:451:THR:CB	2.63	0.47
4:D:190:ARG:O	4:D:194:LEU:CB	2.63	0.47
5:E:571:ASN:O	5:E:575:SER:N	2.48	0.47
8:H:172:SER:O	8:H:176:MET:CB	2.63	0.47
1:A:1294:CYS:O	1:A:1298:GLN:N	2.48	0.46
2:B:379:LYS:O	2:B:382:HIS:C	2.58	0.46
3:C:716:VAL:HG23	3:C:738:TYR:HE1	1.81	0.46
4:D:942:GLN:O	4:D:946:ARG:CB	2.63	0.46
6:F:705:ASP:O	6:F:709:PHE:N	2.43	0.46
7:G:374:ASP:O	7:G:378:ARG:CB	2.63	0.46
2:B:7:GLY:HA3	3:C:146:HIS:HA	1.98	0.46
3:C:37:GLU:O	3:C:41:ASN:CB	2.64	0.46
5:E:648:MET:O	5:E:652:ILE:CB	2.64	0.46
6:F:493:SER:HA	6:F:496:ALA:HB3	1.97	0.46
1:A:676:PRO:O	1:A:680:LYS:CB	2.64	0.46
3:C:628:GLN:O	3:C:632:THR:CB	2.63	0.46
3:C:731:ILE:HG13	3:C:768:ILE:HG21	1.96	0.46
5:E:84:LEU:O	5:E:88:ASN:N	2.45	0.46
3:C:3:SER:O	3:C:7:GLN:N	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:735:TRP:O	3:C:739:LEU:HB2	2.15	0.46
4:D:252:ILE:HA	4:D:253:ILE:HA	1.61	0.46
5:E:253:GLU:O	5:E:257:ILE:CB	2.64	0.46
5:E:584:THR:O	5:E:588:MET:CB	2.64	0.46
6:F:112:SER:O	6:F:116:ILE:CB	2.63	0.46
7:G:387:ASN:HA	7:G:390:LEU:HD12	1.97	0.46
8:H:358:ASN:N	8:H:363:LYS:O	2.47	0.46
8:H:475:PRO:HA	8:H:476:GLY:HA3	1.56	0.46
2:B:545:SER:O	2:B:549:ASN:CB	2.63	0.46
2:B:707:LEU:HA	7:G:604:ARG:HH21	1.79	0.46
2:B:961:LYS:HA	2:B:964:ALA:HB2	1.98	0.46
3:C:301:ILE:O	3:C:305:ILE:CB	2.64	0.46
3:C:308:MET:O	3:C:312:MET:CB	2.63	0.46
5:E:354:ARG:O	5:E:358:GLN:CB	2.64	0.46
5:E:746:PHE:O	5:E:751:LYS:N	2.48	0.46
7:G:267:SER:O	7:G:271:VAL:N	2.40	0.46
8:H:563:GLU:O	8:H:567:GLU:CB	2.62	0.46
1:A:1029:GLU:O	1:A:1033:LEU:N	2.46	0.46
2:B:881:GLN:O	2:B:885:ALA:CB	2.64	0.46
3:C:470:GLN:HG2	3:C:558:TYR:HE2	1.80	0.46
4:D:916:LEU:O	4:D:920:ALA:CB	2.63	0.46
8:H:383:SER:HA	8:H:384:ARG:HA	1.74	0.46
8:H:642:ASP:HA	8:H:645:LEU:HD13	1.98	0.46
8:H:685:LYS:O	8:H:688:SER:OG	2.29	0.46
2:B:75:SER:O	2:B:79:ILE:CB	2.63	0.46
2:B:421:LYS:HA	2:B:422:ASP:HA	1.70	0.46
2:B:461:ILE:O	2:B:465:TRP:CB	2.63	0.46
7:G:341:THR:OG1	7:G:342:GLN:N	2.49	0.46
2:B:462:ILE:O	2:B:466:LEU:CB	2.64	0.46
1:A:927:THR:O	1:A:931:GLN:N	2.38	0.46
2:B:254:GLU:HA	2:B:258:GLU:H	1.80	0.46
2:B:901:ASN:HA	2:B:902:ASP:HA	1.60	0.46
3:C:227:ARG:O	3:C:231:ILE:CB	2.64	0.46
3:C:265:LYS:HA	3:C:266:VAL:HA	1.57	0.46
3:C:303:ASN:O	3:C:307:GLU:CB	2.63	0.46
5:E:353:GLN:O	5:E:357:ALA:HB3	2.16	0.46
6:F:704:ILE:O	6:F:708:GLN:N	2.48	0.46
7:G:33:LEU:O	7:G:37:ALA:CB	2.56	0.46
7:G:77:LEU:O	7:G:81:ALA:CB	2.64	0.46
7:G:459:ALA:HA	7:G:510:ARG:HD3	1.98	0.46
1:A:689:ILE:O	1:A:693:SER:CB	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:795:LEU:O	1:A:799:GLU:CB	2.64	0.46
2:B:250:ASN:H	2:B:251:ASP:C	2.24	0.46
2:B:848:GLY:O	2:B:852:ILE:N	2.45	0.46
2:B:962:ARG:HA	2:B:963:THR:HA	1.75	0.46
3:C:620:TRP:HE1	3:C:626:ALA:HB2	1.80	0.46
4:D:858:PHE:HA	4:D:859:PHE:HA	1.81	0.46
5:E:573:VAL:O	5:E:577:LEU:CB	2.64	0.46
2:B:182:CYS:H	2:B:183:ASP:HA	1.81	0.45
4:D:75:TYR:O	4:D:79:ASN:CB	2.65	0.45
4:D:290:ILE:O	4:D:294:SER:CB	2.64	0.45
4:D:420:GLU:O	4:D:424:ILE:N	2.39	0.45
5:E:345:THR:HA	5:E:346:HIS:HA	1.60	0.45
7:G:485:GLN:HA	7:G:488:GLU:HB2	1.99	0.45
2:B:76:LEU:O	2:B:80:ARG:CB	2.64	0.45
3:C:197:TYR:O	3:C:201:GLU:CB	2.64	0.45
4:D:210:ASN:O	4:D:214:GLU:CB	2.65	0.45
5:E:89:GLU:O	5:E:93:ASN:CB	2.65	0.45
7:G:574:LYS:O	7:G:578:LYS:HB2	2.15	0.45
1:A:831:ILE:O	1:A:835:THR:CB	2.63	0.45
1:A:863:ASN:O	1:A:867:GLN:N	2.49	0.45
3:C:258:ARG:HA	3:C:259:LEU:HA	1.68	0.45
3:C:469:PHE:HB3	3:C:558:TYR:CD2	2.51	0.45
5:E:659:SER:O	5:E:663:ILE:CB	2.64	0.45
6:F:569:SER:O	6:F:573:ALA:CB	2.64	0.45
6:F:601:ILE:O	6:F:603:ASN:N	2.49	0.45
7:G:247:LEU:HD11	7:G:314:ASP:HB3	1.98	0.45
8:H:259:GLN:O	8:H:263:ILE:N	2.49	0.45
1:A:810:VAL:O	1:A:814:GLN:CB	2.64	0.45
7:G:195:GLY:HA2	7:G:198:ILE:HG22	1.98	0.45
7:G:542:LYS:HB3	7:G:546:LYS:HZ1	1.81	0.45
8:H:673:GLU:O	8:H:677:ASP:HB2	2.16	0.45
1:A:1022:LEU:O	1:A:1026:LEU:N	2.48	0.45
3:C:714:PHE:HA	3:C:717:MET:HB2	1.98	0.45
4:D:572:PRO:HA	4:D:573:SER:HA	1.50	0.45
4:D:931:ILE:O	4:D:935:LEU:CB	2.64	0.45
6:F:230:VAL:O	6:F:234:GLU:CB	2.65	0.45
6:F:602:VAL:O	6:F:606:ILE:N	2.48	0.45
7:G:135:GLU:HA	7:G:138:ILE:HD12	1.98	0.45
1:A:936:GLU:O	1:A:940:TYR:N	2.50	0.45
3:C:751:VAL:HA	3:C:765:ARG:HD2	1.98	0.45
5:E:649:SER:O	5:E:653:LEU:CB	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:417:PHE:HA	8:H:422:SER:HA	1.99	0.45
2:B:881:GLN:O	2:B:885:ALA:HB2	2.17	0.45
3:C:58:LEU:O	3:C:62:LYS:CB	2.64	0.45
6:F:195:LEU:O	6:F:199:ASP:CB	2.64	0.45
4:D:718:SER:O	4:D:722:PHE:CB	2.64	0.45
6:F:228:GLN:O	6:F:232:LYS:CB	2.65	0.45
8:H:585:SER:HA	8:H:588:ILE:HD12	1.98	0.45
8:H:614:SER:OG	8:H:615:GLY:N	2.50	0.45
3:C:506:TRP:HB3	3:C:510:ILE:HD12	1.97	0.45
7:G:211:LEU:O	7:G:215:ALA:CB	2.62	0.45
7:G:538:LYS:NZ	7:G:598:ASP:O	2.50	0.45
6:F:714:PHE:O	6:F:719:GLN:N	2.50	0.44
7:G:179:LEU:HD23	7:G:182:LEU:HD12	1.99	0.44
1:A:1009:VAL:HA	1:A:1108:ASP:HA	1.98	0.44
4:D:1048:LYS:O	4:D:1052:LEU:CB	2.65	0.44
5:E:632:ASN:HA	5:E:707:LYS:HA	2.00	0.44
2:B:106:VAL:HA	2:B:107:ASN:HA	1.58	0.44
3:C:546:ILE:O	3:C:550:ASN:ND2	2.51	0.44
4:D:1059:VAL:H	4:D:1063:ASN:HA	1.83	0.44
7:G:105:HIS:O	7:G:109:ASP:CB	2.59	0.44
7:G:339:GLN:HA	7:G:342:GLN:HB3	1.98	0.44
1:A:659:LEU:O	1:A:663:ASN:CB	2.66	0.44
3:C:448:ARG:NH2	3:C:513:GLU:OE1	2.51	0.44
4:D:76:GLU:O	4:D:80:GLN:CB	2.66	0.44
1:A:655:GLU:O	1:A:659:LEU:CB	2.65	0.44
3:C:511:SER:HA	3:C:514:ILE:HD12	1.98	0.44
4:D:869:VAL:HA	4:D:870:GLY:HA2	1.70	0.44
4:D:1042:LYS:O	4:D:1046:ARG:N	2.51	0.44
6:F:622:LEU:O	6:F:626:ASP:N	2.37	0.44
7:G:203:VAL:O	7:G:207:SER:HB3	2.17	0.44
6:F:220:ILE:O	6:F:224:ILE:CB	2.66	0.44
6:F:883:ASP:O	6:F:887:ILE:CB	2.66	0.44
7:G:155:SER:O	7:G:157:LYS:NZ	2.50	0.44
3:C:591:GLU:O	3:C:594:GLN:HB2	2.17	0.44
4:D:684:HIS:HA	5:E:866:VAL:HA	2.00	0.44
6:F:310:ASP:O	6:F:314:ASP:CB	2.66	0.44
7:G:412:THR:O	7:G:503:ARG:NE	2.48	0.44
8:H:657:LEU:HD11	8:H:705:ILE:HG12	2.00	0.44
3:C:212:ILE:O	3:C:216:LYS:CB	2.66	0.44
3:C:681:PHE:O	3:C:684:ALA:HB3	2.17	0.44
5:E:761:PHE:O	5:E:765:ILE:CB	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:862:SER:HA	6:F:882:MET:HA	2.00	0.44
8:H:440:ILE:HA	8:H:443:ALA:HB3	1.99	0.44
1:A:1005:SER:O	1:A:1009:VAL:CB	2.66	0.44
2:B:575:SER:HA	2:B:576:ASN:HA	1.67	0.44
3:C:562:ILE:HA	3:C:565:LYS:HB3	2.00	0.44
5:E:693:ILE:O	5:E:697:LEU:N	2.51	0.44
6:F:733:GLU:O	6:F:737:LEU:N	2.51	0.44
2:B:322:SER:O	2:B:326:ASN:CB	2.66	0.43
4:D:398:ARG:O	4:D:402:TRP:CB	2.65	0.43
5:E:197:LYS:O	5:E:201:ASN:N	2.51	0.43
2:B:845:PHE:HA	2:B:846:ARG:HA	1.75	0.43
1:A:691:THR:O	1:A:695:PHE:CB	2.66	0.43
2:B:582:PRO:HA	2:B:583:LEU:HA	1.47	0.43
5:E:182:GLN:O	5:E:193:LEU:N	2.44	0.43
5:E:212:SER:H	6:F:67:PHE:HA	1.83	0.43
5:E:763:THR:O	5:E:767:GLU:CB	2.66	0.43
6:F:724:SER:O	6:F:726:GLN:N	2.51	0.43
7:G:312:ILE:HG13	7:G:316:LYS:HE2	2.00	0.43
8:H:252:ASP:O	8:H:256:VAL:N	2.50	0.43
1:A:1167:SER:O	1:A:1171:THR:N	2.49	0.43
3:C:510:ILE:HD11	3:C:548:VAL:HG21	2.00	0.43
3:C:768:ILE:O	3:C:772:ALA:HB2	2.18	0.43
7:G:77:LEU:HD22	7:G:110:MET:HG3	2.00	0.43
2:B:528:LYS:O	2:B:532:ILE:N	2.52	0.43
3:C:325:LEU:O	3:C:329:ASP:CB	2.66	0.43
3:C:657:ILE:HG22	3:C:713:ASN:HD22	1.84	0.43
4:D:202:THR:O	4:D:204:GLU:N	2.51	0.43
5:E:16:LYS:O	5:E:20:PHE:N	2.44	0.43
5:E:32:GLU:O	5:E:36:ASP:N	2.38	0.43
5:E:67:GLN:O	5:E:71:LYS:CB	2.66	0.43
5:E:407:ASP:O	5:E:411:GLN:N	2.51	0.43
6:F:89:GLU:O	6:F:93:GLN:CB	2.66	0.43
6:F:155:ASN:O	6:F:159:SER:CB	2.67	0.43
1:A:1157:TYR:O	1:A:1161:ILE:CB	2.67	0.43
2:B:521:TYR:H	2:B:522:GLN:C	2.27	0.43
4:D:836:LYS:O	4:D:840:ILE:CB	2.66	0.43
5:E:734:PRO:O	5:E:738:ILE:CB	2.67	0.43
7:G:153:LEU:HD23	7:G:153:LEU:HA	1.81	0.43
7:G:162:GLN:HA	7:G:165:ILE:HB	2.01	0.43
7:G:312:ILE:HD11	7:G:330:LEU:HB3	2.00	0.43
7:G:588:MET:HE3	7:G:588:MET:HB2	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:614:TYR:HA	5:E:618:ALA:HB3	2.01	0.43
7:G:17:GLN:O	7:G:21:LYS:N	2.41	0.43
7:G:573:LEU:HD23	7:G:573:LEU:HA	1.91	0.43
3:C:716:VAL:O	3:C:720:PHE:HB2	2.17	0.43
3:C:748:ASP:HB3	3:C:802:PHE:HB3	2.00	0.43
7:G:60:LEU:O	7:G:64:ILE:CB	2.67	0.43
3:C:621:TYR:HE2	3:C:675:LYS:HD3	1.83	0.43
3:C:724:SER:O	3:C:757:ARG:NH2	2.52	0.43
4:D:69:VAL:HA	4:D:70:GLY:HA2	1.77	0.43
6:F:227:LEU:O	6:F:231:THR:CB	2.67	0.43
6:F:571:ILE:O	6:F:575:LEU:N	2.52	0.43
7:G:231:PRO:C	7:G:301:PHE:H	2.27	0.43
8:H:612:LEU:O	8:H:616:THR:OG1	2.22	0.43
8:H:711:ASN:OD1	8:H:711:ASN:N	2.52	0.43
2:B:620:ILE:HA	2:B:621:THR:HA	1.75	0.43
3:C:189:ASP:O	3:C:193:ASP:N	2.42	0.43
4:D:356:ASN:O	4:D:360:LYS:CB	2.67	0.43
5:E:436:PHE:O	5:E:440:LYS:N	2.47	0.43
7:G:349:ILE:HG23	7:G:437:THR:HG21	1.99	0.43
1:A:1292:TRP:O	1:A:1296:GLN:N	2.52	0.42
2:B:275:ALA:HA	2:B:276:SER:HA	1.62	0.42
3:C:451:PRO:HA	3:C:544:TYR:HE1	1.84	0.42
3:C:642:PRO:HG2	3:C:643:GLN:HG3	2.00	0.42
4:D:962:ASN:O	4:D:966:LEU:CB	2.67	0.42
7:G:491:GLU:O	7:G:495:MET:N	2.52	0.42
2:B:354:ILE:O	2:B:358:MET:N	2.39	0.42
3:C:735:TRP:HZ2	3:C:776:LEU:HD13	1.84	0.42
3:C:750:LEU:O	3:C:754:LEU:N	2.50	0.42
4:D:636:ARG:O	4:D:640:ASN:CB	2.67	0.42
5:E:213:SER:HA	6:F:73:ASP:H	1.83	0.42
6:F:251:LEU:O	6:F:255:GLY:N	2.38	0.42
7:G:98:LYS:O	7:G:102:GLN:HB2	2.19	0.42
7:G:176:ASP:HA	7:G:179:LEU:HB2	2.01	0.42
7:G:327:TYR:HA	7:G:330:LEU:HD12	2.00	0.42
7:G:368:VAL:HG13	7:G:479:ASN:HD22	1.84	0.42
6:F:431:GLY:O	6:F:435:ARG:CB	2.67	0.42
3:C:775:MET:O	3:C:779:TYR:HB3	2.19	0.42
7:G:67:THR:OG1	8:H:178:ALA:O	2.37	0.42
7:G:137:LEU:HD13	7:G:140:ARG:HH21	1.84	0.42
2:B:67:SER:HA	2:B:68:ARG:HA	1.72	0.42
2:B:209:LYS:O	2:B:213:LEU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:503:ILE:O	6:F:507:ASP:N	2.50	0.42
6:F:624:ASN:C	6:F:628:PHE:H	2.27	0.42
6:F:663:SER:O	6:F:667:ALA:HB2	2.19	0.42
7:G:339:GLN:O	7:G:343:SER:OG	2.36	0.42
7:G:426:LEU:O	7:G:430:PHE:HB3	2.19	0.42
3:C:149:LEU:HA	3:C:152:ALA:HB3	2.02	0.42
3:C:382:LEU:O	3:C:386:ALA:CB	2.67	0.42
3:C:441:GLU:OE2	3:C:465:THR:N	2.53	0.42
3:C:654:ASP:HB2	3:C:709:LEU:HD13	2.02	0.42
5:E:98:PHE:O	5:E:101:GLN:N	2.52	0.42
6:F:520:LEU:O	6:F:524:VAL:N	2.47	0.42
6:F:569:SER:O	6:F:573:ALA:HB2	2.19	0.42
2:B:188:ASN:HA	2:B:189:GLN:HA	1.88	0.42
2:B:682:GLU:HA	2:B:683:TYR:HA	1.77	0.42
5:E:382:ILE:O	5:E:386:LEU:CB	2.68	0.42
5:E:772:LEU:O	5:E:776:HIS:N	2.48	0.42
6:F:560:THR:O	6:F:564:ALA:CB	2.67	0.42
6:F:646:GLN:HA	6:F:647:ASN:HA	1.83	0.42
7:G:519:TRP:CZ2	7:G:559:LEU:HB3	2.55	0.42
1:A:969:PRO:HA	1:A:970:PRO:HA	1.70	0.42
1:A:1036:SER:O	1:A:1038:HIS:N	2.47	0.42
7:G:165:ILE:HD11	7:G:245:ALA:HB2	2.02	0.42
7:G:276:LEU:O	7:G:280:ILE:N	2.35	0.42
7:G:428:SER:HA	7:G:496:LEU:HD22	2.02	0.42
1:A:1030:ILE:HA	1:A:1034:GLU:H	1.84	0.42
3:C:545:LEU:HD13	3:C:596:SER:HB2	2.00	0.42
3:C:560:VAL:HG22	3:C:583:GLU:HA	2.01	0.42
3:C:750:LEU:HA	3:C:753:ILE:HB	2.01	0.42
7:G:338:ARG:O	7:G:342:GLN:CB	2.68	0.42
7:G:366:ASN:HD21	7:G:471:ARG:HH21	1.67	0.42
7:G:398:ARG:HG2	7:G:402:LEU:HD11	2.00	0.42
1:A:768:LEU:O	1:A:772:GLN:N	2.50	0.42
2:B:299:ILE:O	2:B:303:LEU:CB	2.68	0.42
3:C:237:LYS:O	3:C:241:GLU:CB	2.68	0.42
3:C:441:GLU:OE2	3:C:465:THR:OG1	2.32	0.42
4:D:794:GLU:O	4:D:798:LEU:N	2.53	0.42
7:G:402:LEU:HD13	7:G:406:TYR:CZ	2.54	0.42
7:G:484:GLU:O	7:G:488:GLU:N	2.53	0.42
7:G:546:LYS:HD3	7:G:606:HIS:HD2	1.85	0.42
8:H:662:VAL:O	8:H:666:GLN:HB3	2.20	0.42
1:A:903:TRP:HA	1:A:905:THR:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:932:THR:O	1:A:936:GLU:N	2.53	0.41
2:B:900:SER:O	2:B:904:SER:N	2.43	0.41
3:C:420:LYS:HA	3:C:423:LEU:HD12	2.02	0.41
4:D:597:LYS:O	4:D:601:THR:CB	2.68	0.41
5:E:157:ASN:O	5:E:161:SER:CB	2.68	0.41
7:G:181:ALA:O	7:G:185:ILE:HB	2.20	0.41
7:G:547:GLU:O	7:G:551:LYS:HB2	2.19	0.41
7:G:574:LYS:O	7:G:578:LYS:CB	2.68	0.41
1:A:723:LYS:N	4:D:94:ASN:O	2.53	0.41
8:H:338:PHE:N	8:H:339:ILE:O	2.53	0.41
2:B:253:ASN:O	2:B:257:ILE:N	2.36	0.41
2:B:594:GLY:O	2:B:596:SER:N	2.51	0.41
8:H:662:VAL:O	8:H:666:GLN:CB	2.68	0.41
4:D:389:VAL:HA	4:D:391:ASP:N	2.35	0.41
7:G:343:SER:O	7:G:347:ASP:CB	2.69	0.41
1:A:1088:VAL:O	1:A:1092:ASN:CB	2.69	0.41
7:G:179:LEU:HD22	7:G:260:LEU:HD11	2.03	0.41
7:G:379:LEU:HD23	7:G:379:LEU:HA	1.90	0.41
5:E:448:VAL:O	5:E:452:SER:CB	2.68	0.41
6:F:342:LYS:HA	6:F:343:LEU:HA	1.75	0.41
2:B:874:HIS:O	2:B:878:ILE:CB	2.67	0.41
7:G:195:GLY:O	7:G:199:GLN:HB3	2.20	0.41
7:G:412:THR:HB	7:G:506:ARG:HE	1.86	0.41
3:C:447:GLU:O	3:C:449:SER:N	2.52	0.41
7:G:476:ILE:HG21	7:G:511:TYR:CZ	2.56	0.41
7:G:548:LYS:O	7:G:552:PHE:CB	2.68	0.41
2:B:520:SER:HA	2:B:521:TYR:HA	1.59	0.41
3:C:455:ASP:H	3:C:460:LEU:HD23	1.84	0.41
4:D:589:TYR:HA	4:D:593:SER:H	1.86	0.41
4:D:1050:GLY:O	4:D:1054:SER:N	2.54	0.41
5:E:324:ASP:O	5:E:328:VAL:CB	2.69	0.41
5:E:766:GLY:HA3	5:E:808:SER:H	1.86	0.41
6:F:241:ASN:O	6:F:245:LEU:N	2.51	0.41
7:G:344:LEU:HA	7:G:347:ASP:HB3	2.02	0.41
7:G:530:VAL:O	7:G:534:SER:OG	2.31	0.41
2:B:390:ASN:HA	2:B:391:ASN:HA	1.73	0.41
2:B:838:PRO:HA	2:B:903:GLY:N	2.36	0.41
3:C:290:PRO:HA	3:C:291:ARG:HA	1.56	0.41
3:C:656:VAL:O	3:C:660:THR:OG1	2.30	0.41
4:D:587:ASP:C	4:D:589:TYR:H	2.28	0.41
7:G:173:TYR:HA	7:G:256:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:657:LEU:HD12	8:H:657:LEU:HA	1.88	0.41
1:A:811:GLU:O	1:A:815:LYS:CB	2.69	0.40
2:B:565:LEU:HA	2:B:566:LYS:HA	1.80	0.40
4:D:817:LEU:O	4:D:820:LYS:N	2.54	0.40
7:G:465:LYS:HE2	7:G:465:LYS:HB2	1.90	0.40
2:B:26:TRP:HA	2:B:27:ALA:HA	1.79	0.40
3:C:637:LEU:HD23	3:C:637:LEU:HA	1.93	0.40
3:C:683:GLU:O	3:C:687:ARG:N	2.53	0.40
7:G:172:PRO:HD2	7:G:249:PHE:HE1	1.86	0.40
8:H:702:PHE:HA	8:H:705:ILE:HD12	2.03	0.40
1:A:951:SER:HA	1:A:952:SER:HA	1.92	0.40
4:D:96:HIS:O	4:D:98:GLN:N	2.54	0.40
6:F:736:SER:O	6:F:740:GLN:CB	2.68	0.40
7:G:105:HIS:HA	7:G:108:ASP:HB3	2.03	0.40
1:A:924:SER:O	1:A:928:GLU:N	2.54	0.40
3:C:9:VAL:O	3:C:13:ILE:N	2.55	0.40
3:C:779:TYR:O	3:C:783:MET:N	2.39	0.40
3:C:794:LEU:HG	3:C:795:MET:HG2	2.04	0.40
5:E:237:GLU:O	5:E:242:ALA:N	2.44	0.40
6:F:477:PRO:O	6:F:481:ILE:CB	2.70	0.40
7:G:309:VAL:HA	7:G:312:ILE:HG22	2.03	0.40
8:H:715:LEU:N	8:H:751:LYS:HE2	2.36	0.40
8:H:682:LEU:HD13	8:H:682:LEU:HA	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	662/1336 (50%)	518 (78%)	143 (22%)	1 (0%)	43	77
2	B	922/971 (95%)	707 (77%)	202 (22%)	13 (1%)	9	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	788/805 (98%)	673 (85%)	114 (14%)	1 (0%)	48	83
4	D	944/1065 (89%)	718 (76%)	213 (23%)	13 (1%)	9	39
5	E	770/871 (88%)	641 (83%)	127 (16%)	2 (0%)	36	71
6	F	715/910 (79%)	578 (81%)	130 (18%)	7 (1%)	12	47
7	G	609/623 (98%)	555 (91%)	52 (8%)	2 (0%)	36	71
8	H	506/753 (67%)	431 (85%)	73 (14%)	2 (0%)	30	66
All	All	5916/7334 (81%)	4821 (82%)	1054 (18%)	41 (1%)	20	55

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	349	SER
2	B	350	ASN
2	B	590	PRO
2	B	762	SER
4	D	97	SER
6	F	453	ASP
7	G	231	PRO
8	H	337	LYS
4	D	203	VAL
6	F	725	VAL
1	A	751	PRO
4	D	245	THR
4	D	553	MET
4	D	588	ASP
4	D	783	ALA
4	D	803	PRO
6	F	344	MET
6	F	452	GLU
6	F	589	ILE
2	B	348	SER
2	B	497	TYR
2	B	589	PRO
4	D	648	ALA
4	D	738	SER
4	D	796	MET
4	D	800	TYR
6	F	644	ILE
6	F	724	SER
7	G	230	ALA

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Mol	Chain	Res	Type
8	H	315	LEU
2	B	666	VAL
2	B	837	TRP
2	B	920	PRO
4	D	427	PRO
2	B	412	LEU
4	D	625	HIS
2	B	185	PRO
2	B	684	GLY
5	E	362	PRO
3	C	528	PRO
5	E	70	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	300/740 (40%)	300 (100%)	0	100	100
7	G	480/570 (84%)	480 (100%)	0	100	100
8	H	202/697 (29%)	201 (100%)	1 (0%)	81	81
All	All	982/2007 (49%)	981 (100%)	1 (0%)	87	88

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

Mol	Chain	Res	Type
8	H	545	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	475	GLN
3	C	505	ASN
3	C	550	ASN
3	C	594	GLN

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Mol	Chain	Res	Type
3	C	625	GLN
3	C	643	GLN
3	C	655	ASN
3	C	679	ASN
3	C	694	GLN
3	C	713	ASN
7	G	89	GLN
7	G	190	HIS
7	G	290	ASN
7	G	313	ASN
7	G	366	ASN
7	G	395	ASN
7	G	468	HIS
7	G	470	GLN
7	G	606	HIS
8	H	531	GLN
8	H	638	ASN
8	H	646	GLN
8	H	659	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6827. These allow visual inspection of the internal detail of the map and identification of artifacts.

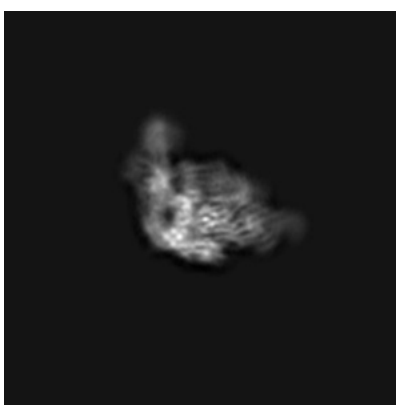
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

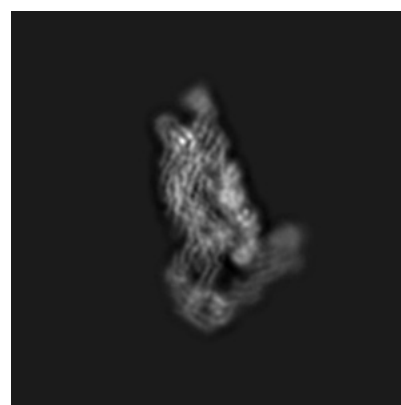
6.1.1 Primary map



X



Y

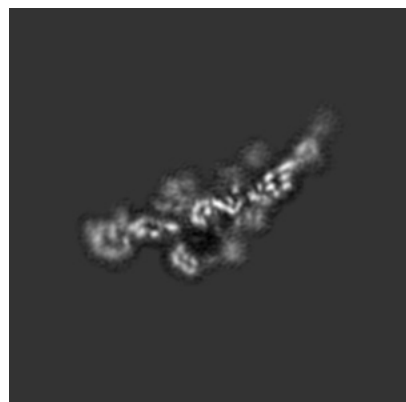


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 180



Y Index: 180

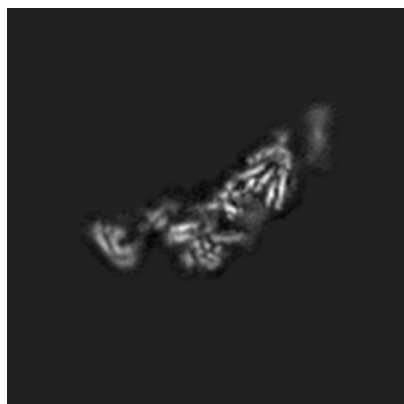


Z Index: 180

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

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 161



Y Index: 193



Z Index: 163

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

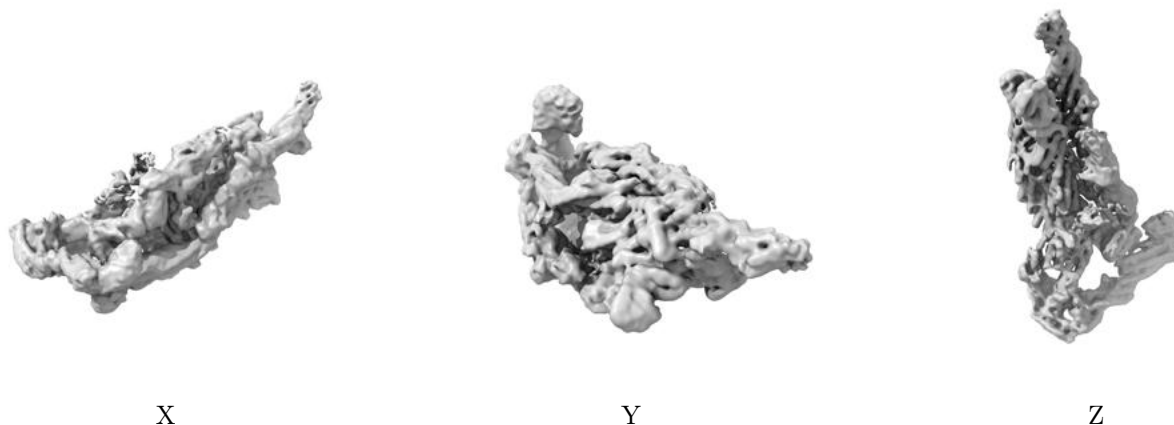


Z

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 0.0203. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

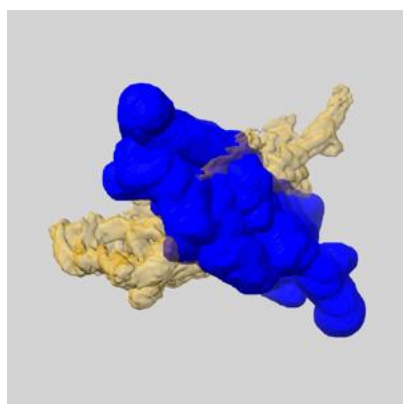
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

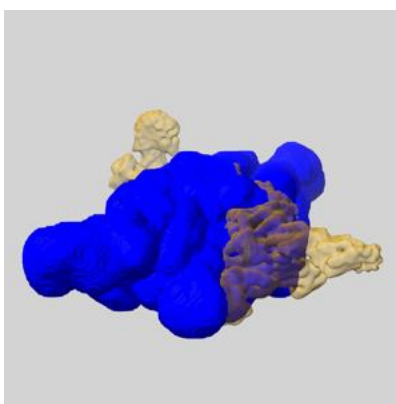
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

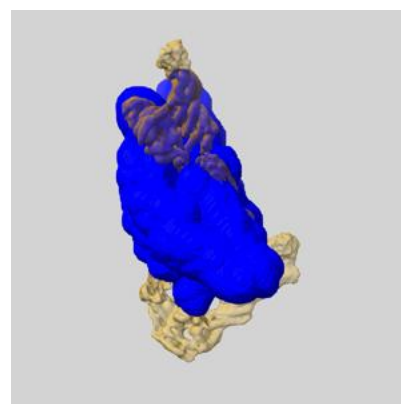
6.6.1 emd_6827_msk_5.map [i](#)



X

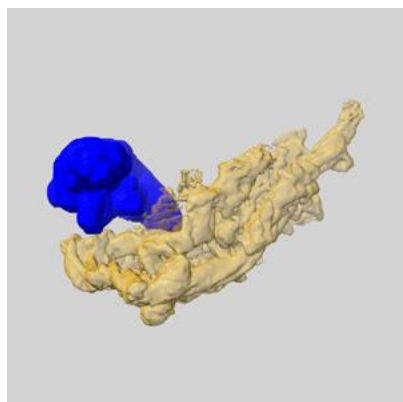


Y

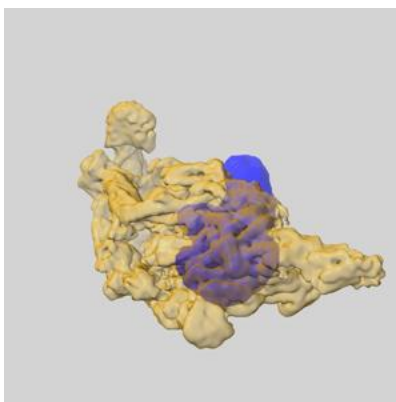


Z

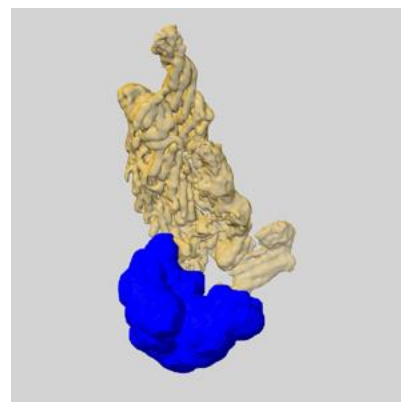
6.6.2 emd_6827_msk_4.map [i](#)



X

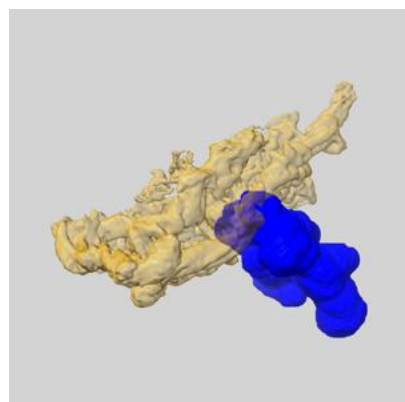


Y

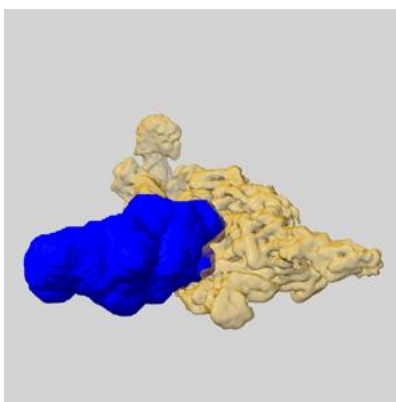


Z

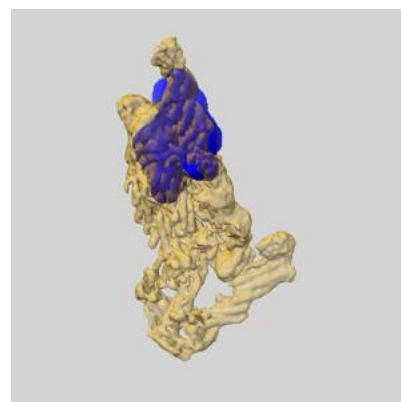
6.6.3 emd_6827_msk_3.map [i](#)



X

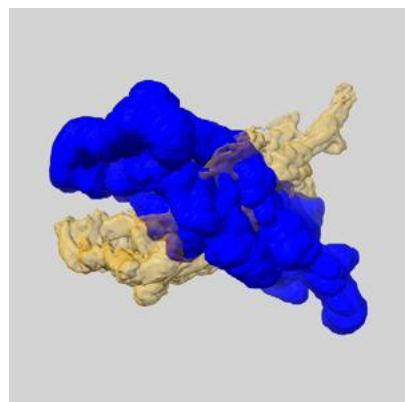


Y

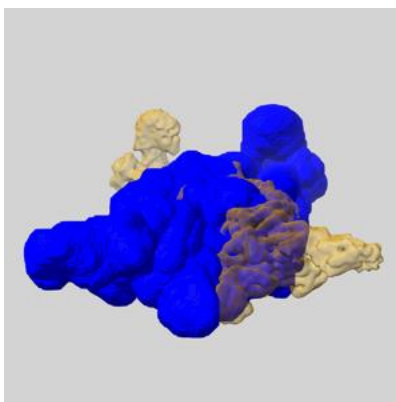


Z

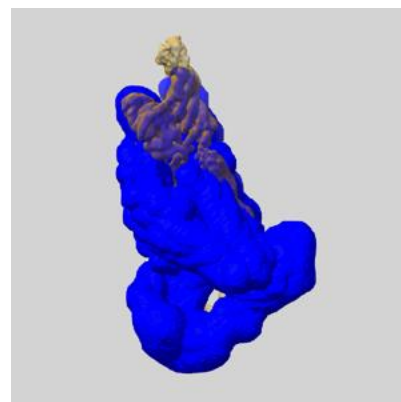
6.6.4 emd_6827_msk_2.map [i](#)



X

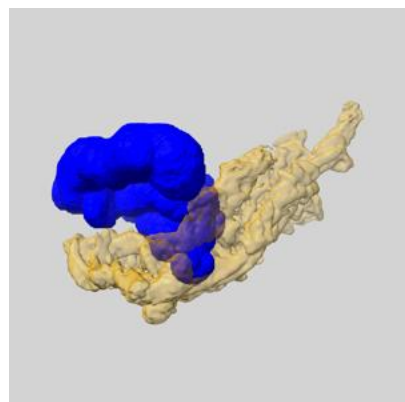


Y

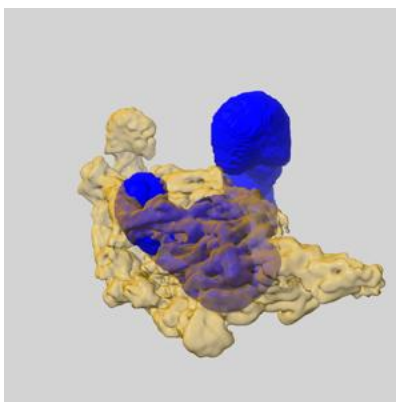


Z

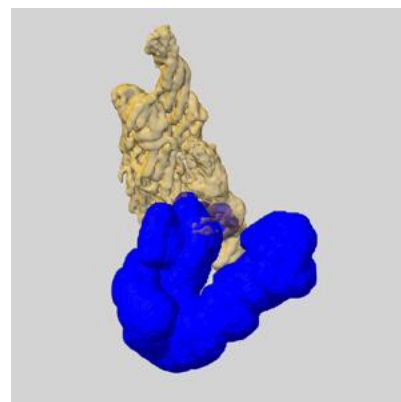
6.6.5 emd_6827_msk_1.map [i](#)



X



Y

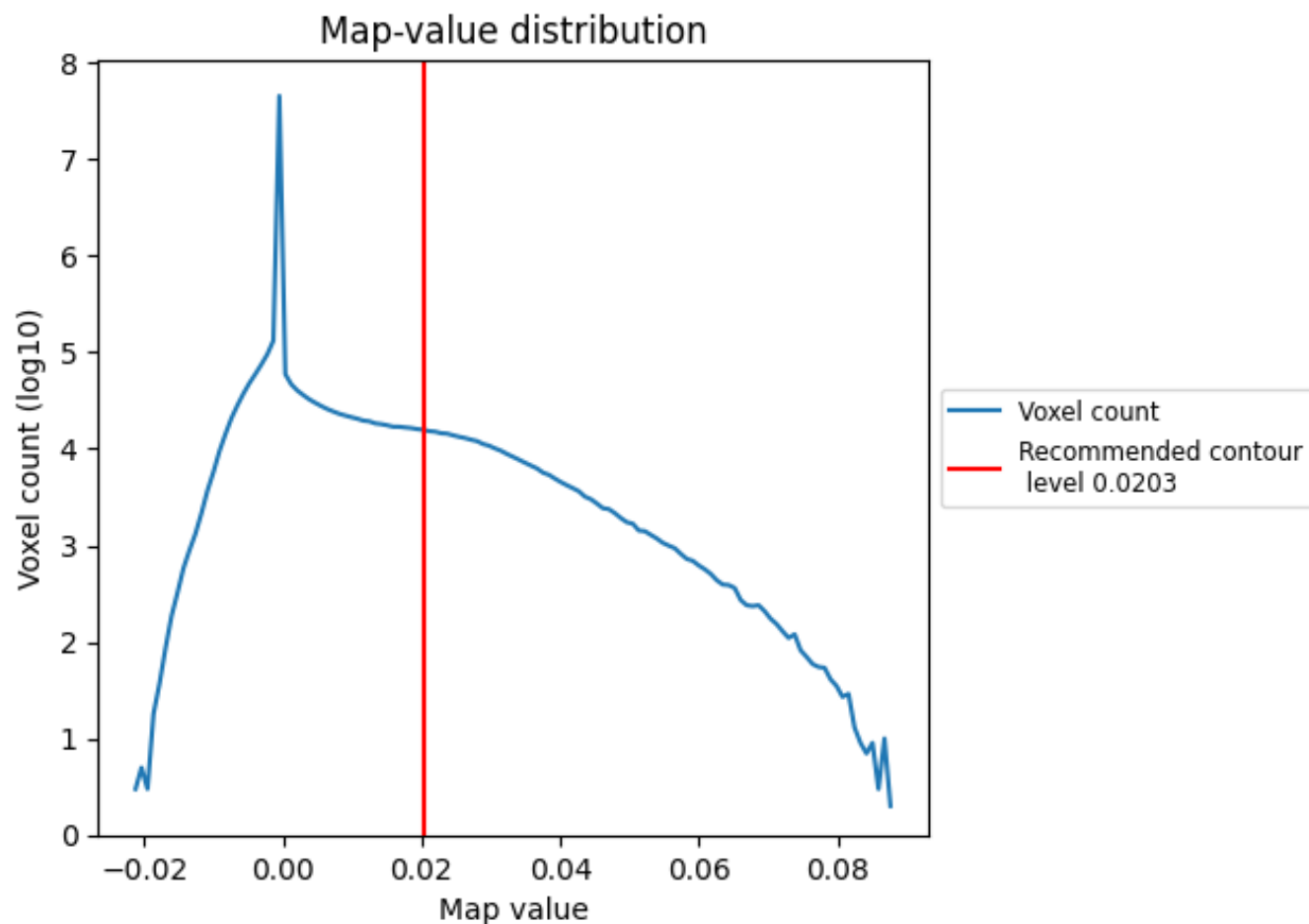


Z

7 Map analysis [i](#)

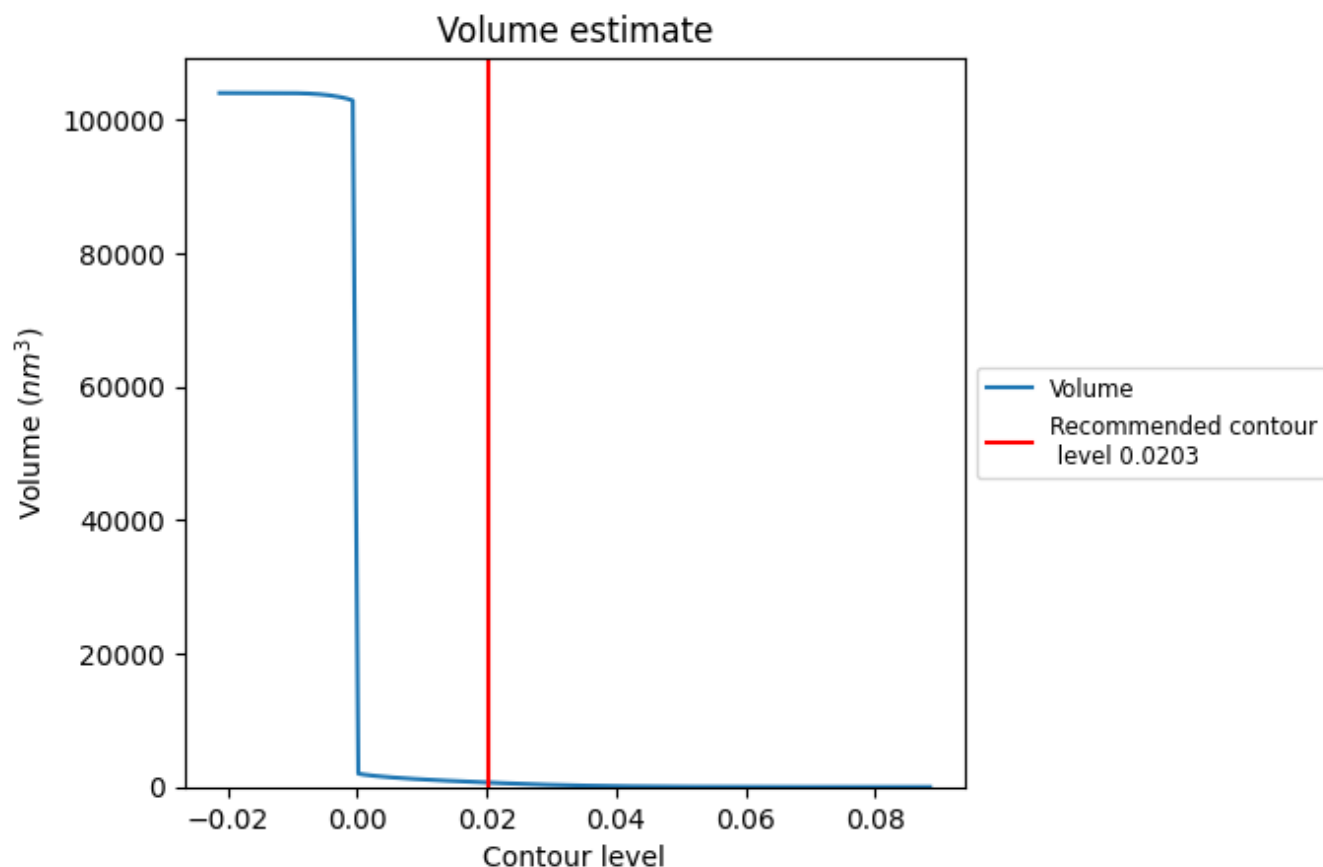
This section contains the results of statistical analysis of the map.

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.

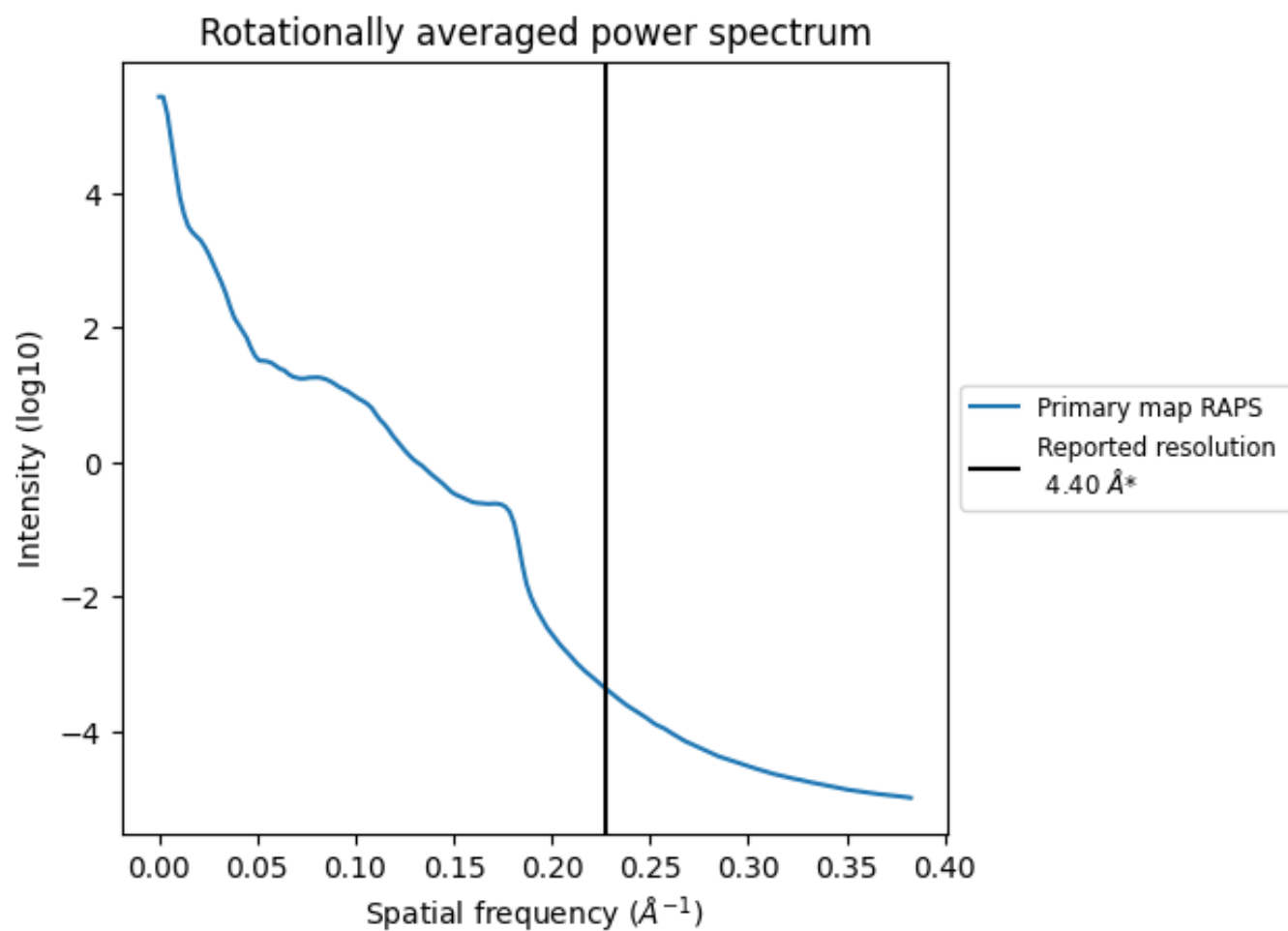
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 656 nm^3 ; this corresponds to an approximate mass of 593 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 ⓘ

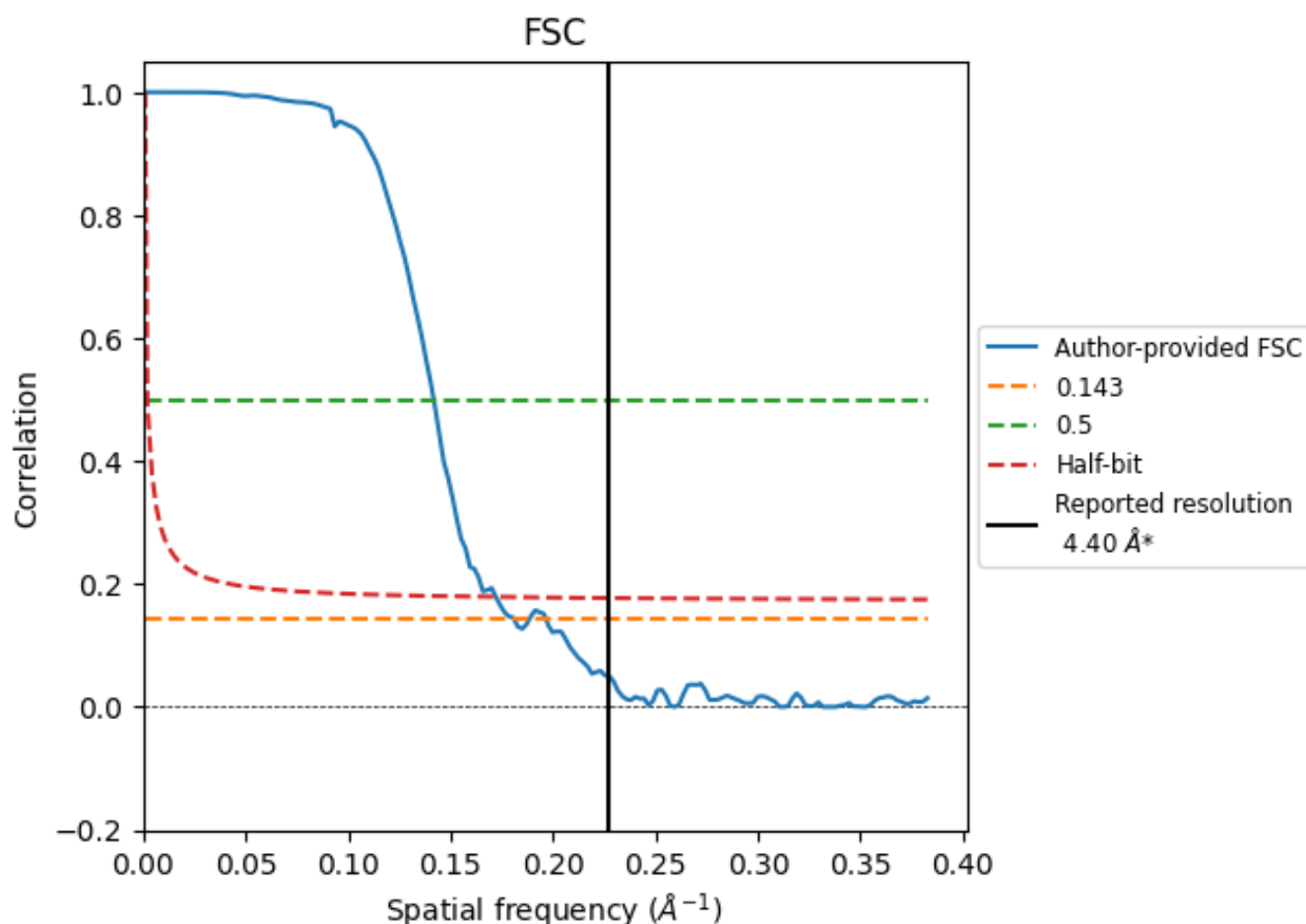


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

8.2 Resolution estimates [i](#)

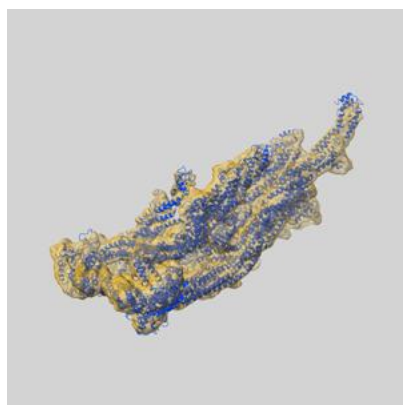
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	5.52	7.05	5.81
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 5.52 differs from the reported value 4.4 by more than 10 %

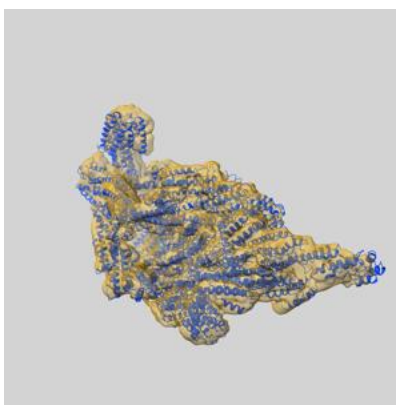
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6827 and PDB model 5YFP. Per-residue inclusion information can be found in section 3 on page 6.

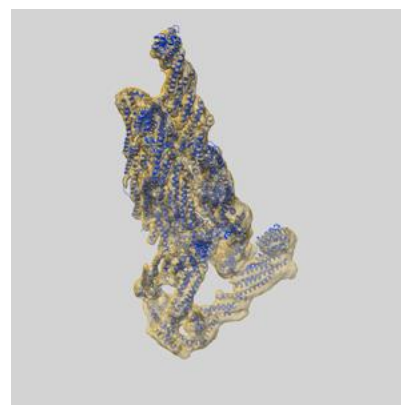
9.1 Map-model overlay [i](#)



X



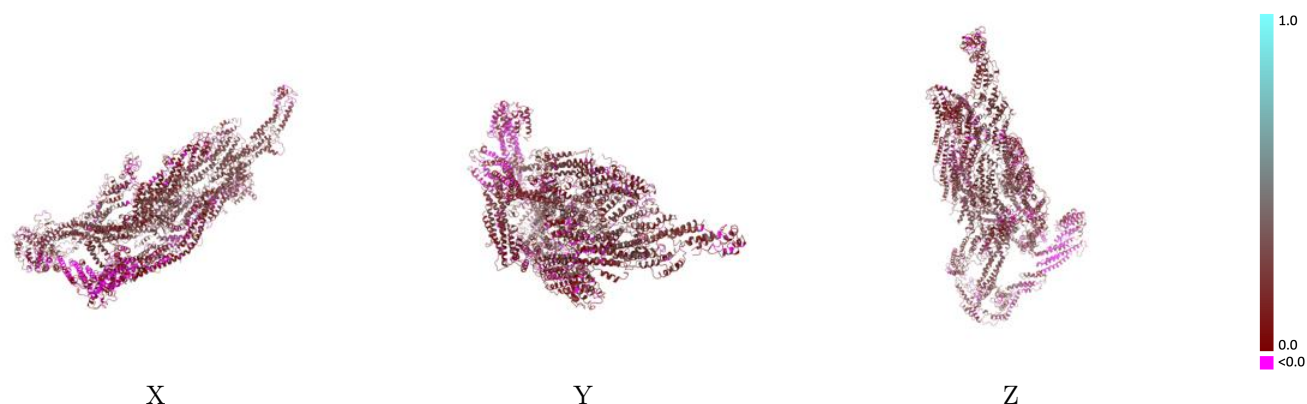
Y



Z

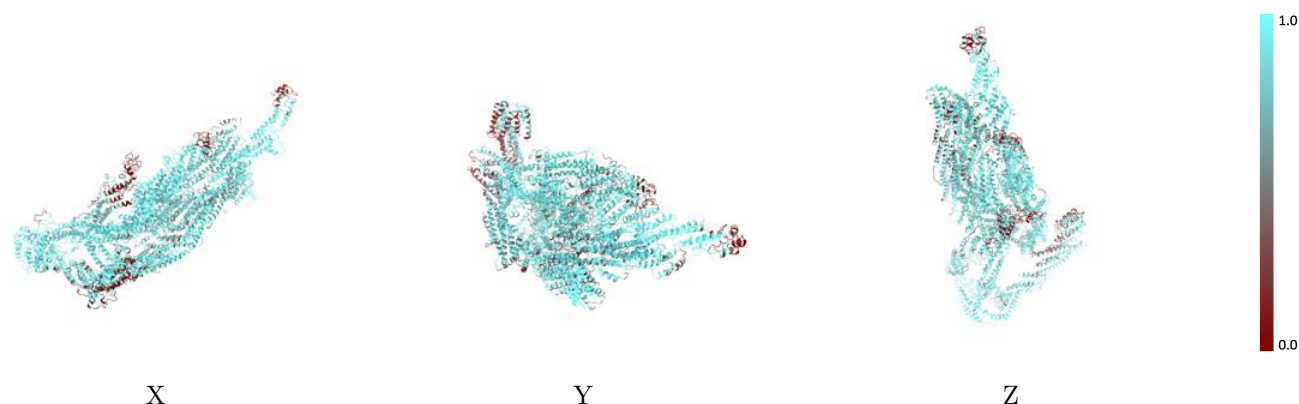
The images above show the 3D surface view of the map at the recommended contour level 0.0203 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



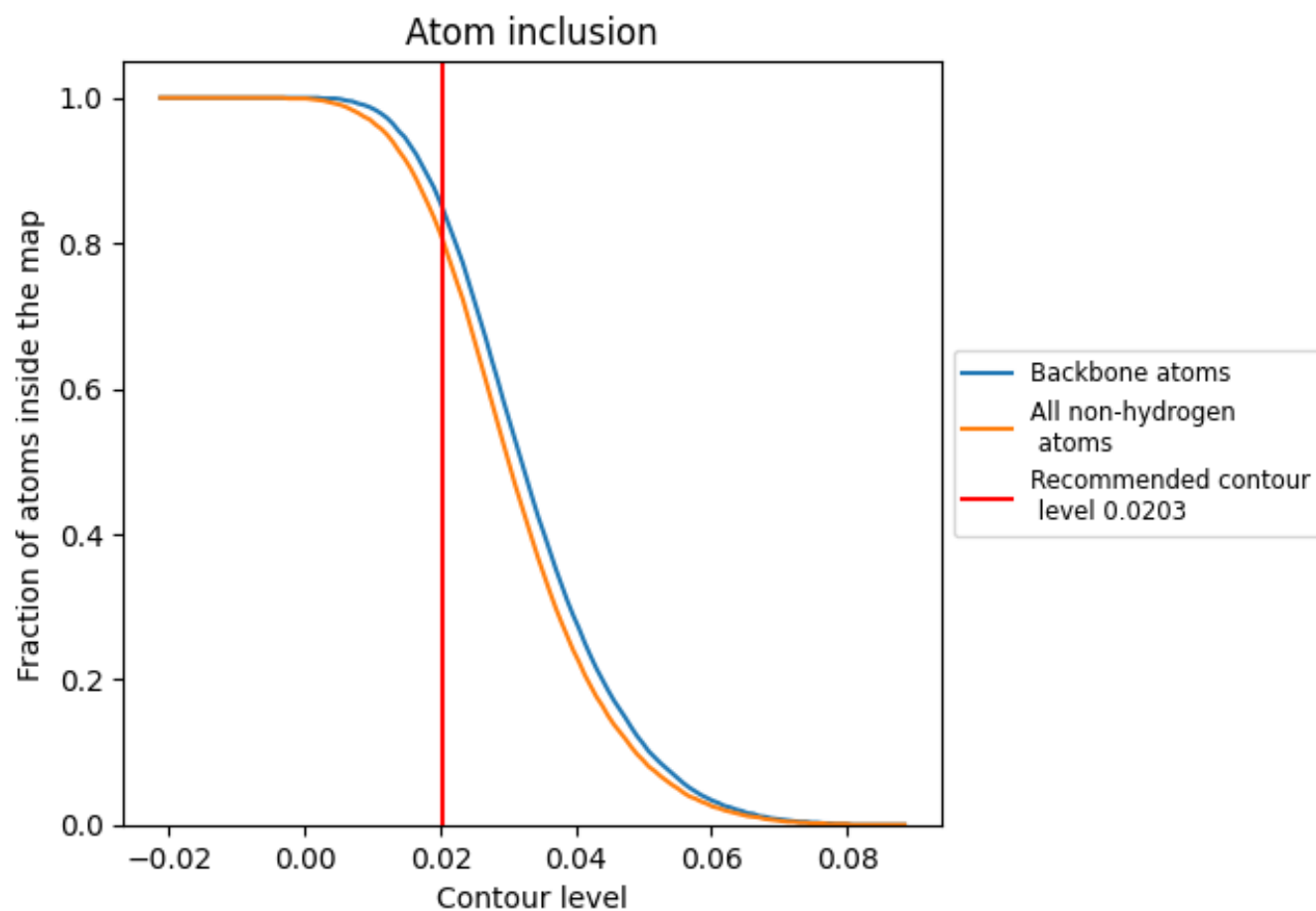
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0203).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 81% 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 (0.0203) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8060	0.1550
A	0.6810	0.1830
B	0.8570	0.1700
C	0.7260	0.0710
D	0.9120	0.2150
E	0.8330	0.1590
F	0.8680	0.2050
G	0.7480	0.1070
H	0.8070	0.1530

1.0

0.0

<0.0