



Full wwPDB EM Validation Report ⓘ

Sep 28, 2026 – 11:43 AM JST

PDB ID : 21WD / pdb_000021wd
EMDB ID : EMD-68043
Title : In situ structure of the bis-trans-lumenal/trans-stromal PSII-LHCII tetramer (TL-TS-TL tetramer) from *Oryza sativa*
Authors : Li, J.; Elias, E.; Zhang, K.; Croce, R.; Zhu, J.
Deposited on : 2025-12-31
Resolution : 4.24 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:

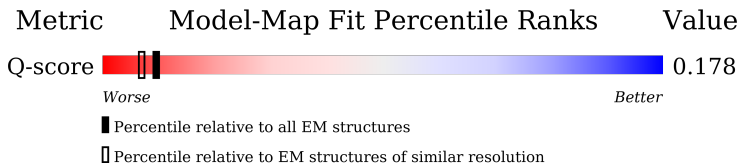
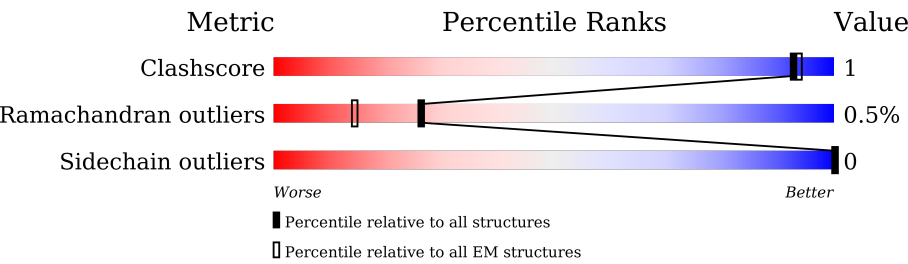
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.2
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

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 4.24 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	4688 (3.74 - 4.74)

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	00	219	95%
1	01	219	98%
1	02	219	11% 94%
1	05	219	6% 95%

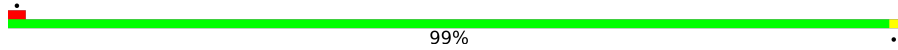
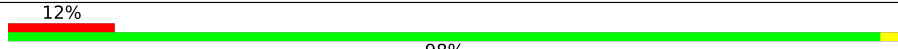
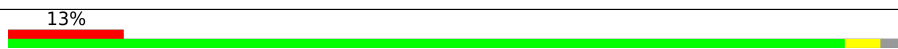
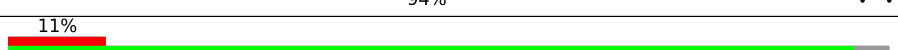
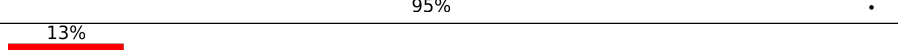
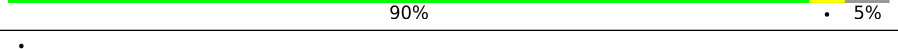
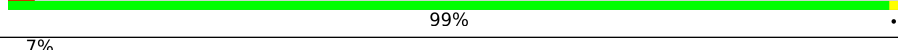
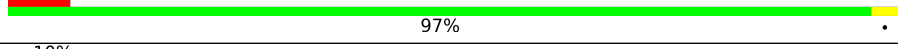
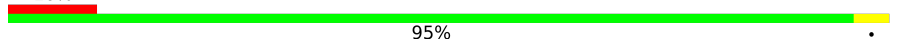
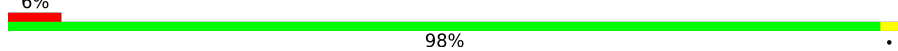
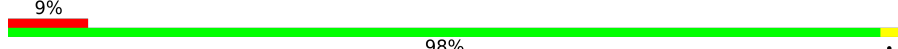
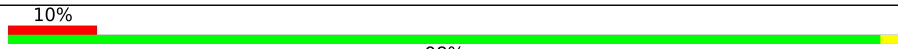
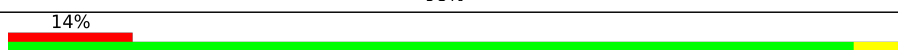
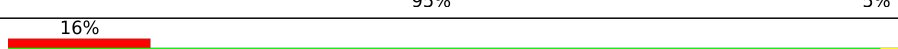
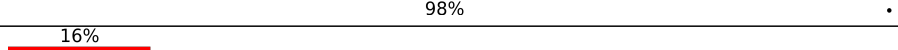
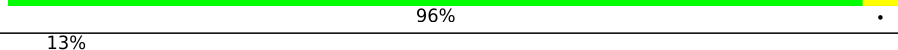
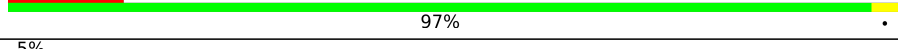
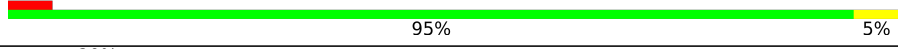
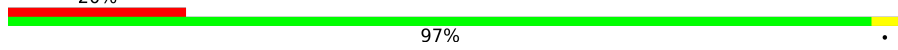
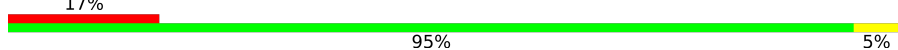
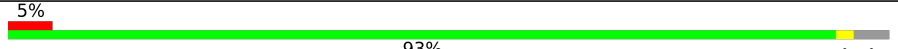
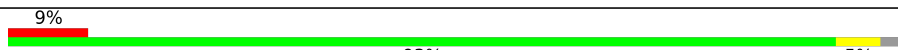
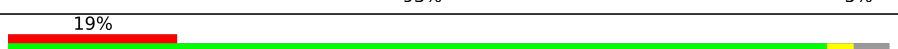
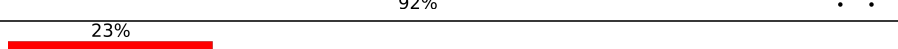
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Mol	Chain	Length	Quality of chain
1	06	219	
1	09	219	
1	10	219	
1	11	219	
1	12	219	
1	15	219	
1	16	219	
1	19	219	
1	1G	219	
1	1N	219	
1	1g	219	
1	1n	219	
1	2G	219	
1	2N	219	
1	2g	219	
1	2n	219	
1	30	219	
1	31	219	
1	32	219	
1	35	219	
1	36	219	
1	39	219	
1	3G	219	
1	3N	219	
1	3g	219	

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Mol	Chain	Length	Quality of chain
1	3n	219	
1	40	219	
1	41	219	
1	42	219	
1	45	219	
1	46	219	
1	49	219	
1	4G	219	
1	4N	219	
1	4g	219	
1	4n	219	
2	03	220	
2	07	220	
2	13	220	
2	17	220	
2	33	220	
2	37	220	
2	43	220	
2	47	220	
3	04	209	
3	08	209	
3	14	209	
3	18	209	
3	34	209	
3	38	209	

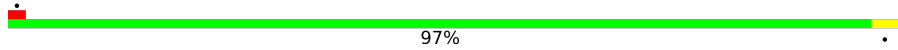
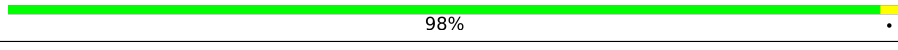
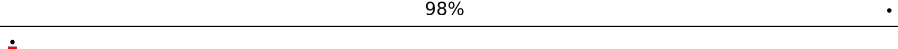
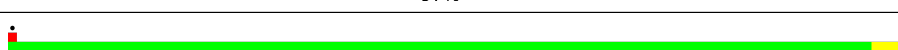
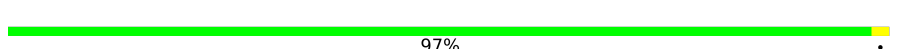
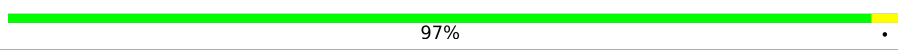
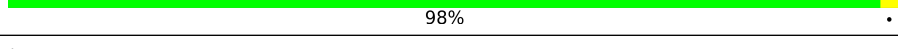
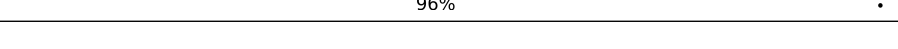
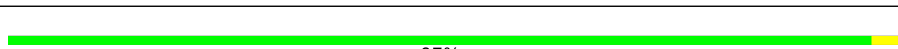
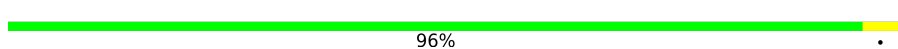
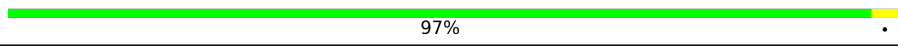
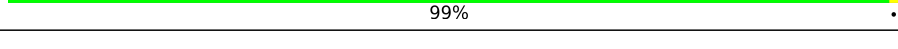
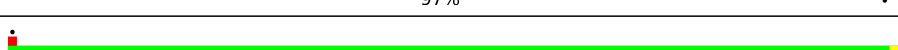
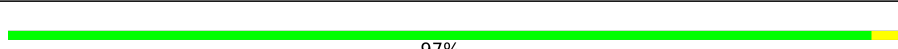
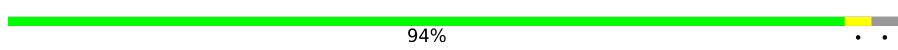
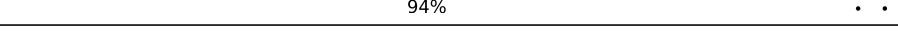
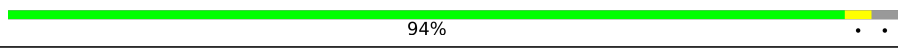
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Mol	Chain	Length	Quality of chain
3	44	209	
3	48	209	
4	1A	334	
4	1a	334	
4	2A	334	
4	2a	334	
4	3A	334	
4	3a	334	
4	4A	334	
4	4a	334	
5	1B	503	
5	1b	503	
5	2B	503	
5	2b	503	
5	3B	503	
5	3b	503	
5	4B	503	
5	4b	503	
6	1C	450	
6	1c	450	
6	2C	450	
6	2c	450	
6	3C	450	
6	3c	450	
6	4C	450	

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Mol	Chain	Length	Quality of chain
6	4c	450	
7	1D	341	
7	1d	341	
7	2D	341	
7	2d	341	
7	3D	341	
7	3d	341	
7	4D	341	
7	4d	341	
8	1E	75	
8	1e	75	
8	2E	75	
8	2e	75	
8	3E	75	
8	3e	75	
8	4E	75	
8	4e	75	
9	1F	36	
9	1f	36	
9	2F	36	
9	2f	36	
9	3F	36	
9	3f	36	
9	4F	36	
9	4f	36	

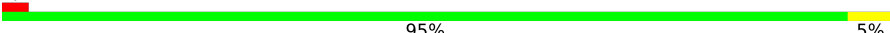
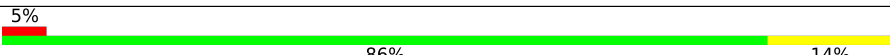
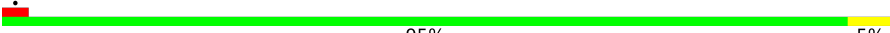
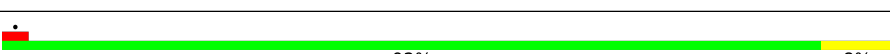
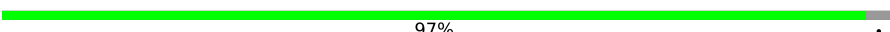
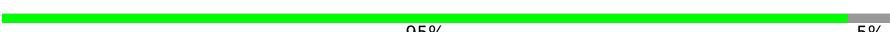
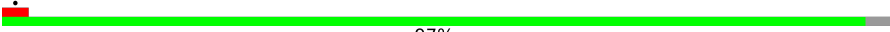
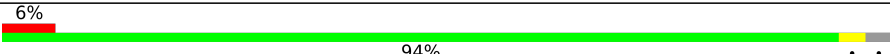
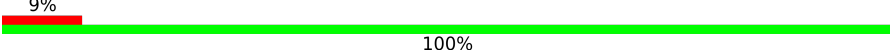
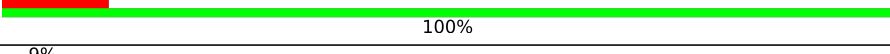
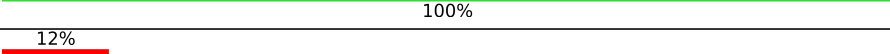
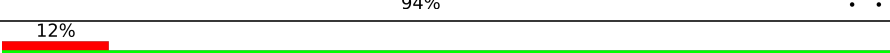
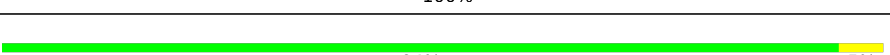
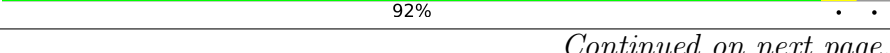
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Mol	Chain	Length	Quality of chain
10	1H	60	100%
10	1h	60	100%
10	2H	60	100%
10	2h	60	8% 100%
10	3H	60	100%
10	3h	60	8% 100%
10	4H	60	8% 100%
10	4h	60	8% 100%
11	1I	34	62% 21% 18%
11	1i	34	100%
11	2I	34	62% 32% 6%
11	2i	34	100%
11	3I	34	56% 26% 18%
11	3i	34	100%
11	4I	34	56% 26% 18%
11	4i	34	100%
12	1J	35	100%
12	1j	35	97% .
12	2J	35	100%
12	2j	35	97% .
12	3J	35	100%
12	3j	35	97% .
12	4J	35	6% 100%
12	4j	35	97% .
13	1K	37	100%

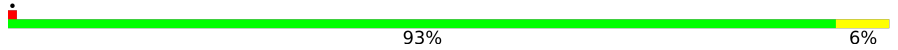
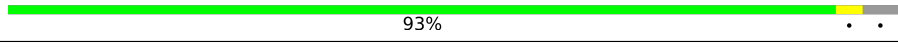
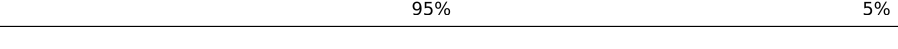
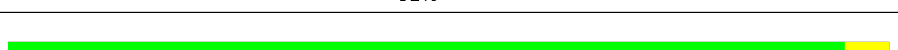
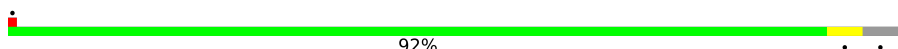
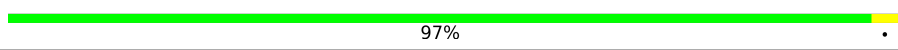
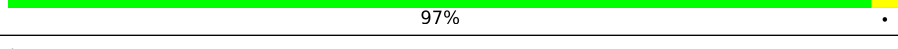
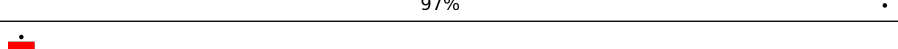
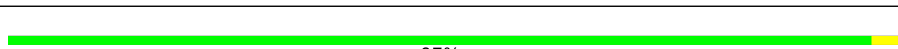
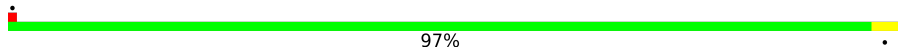
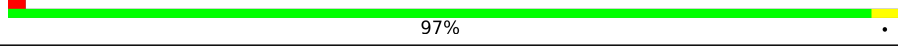
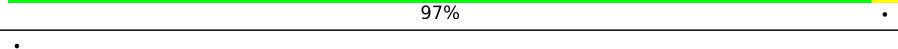
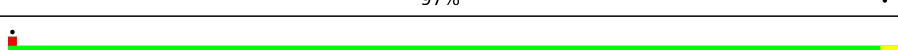
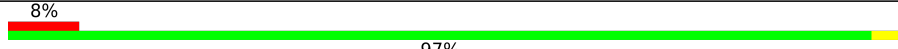
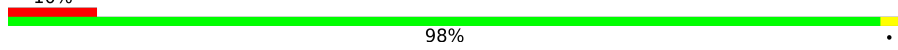
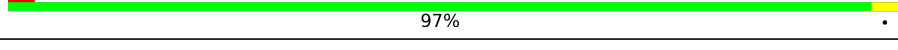
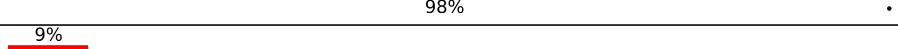
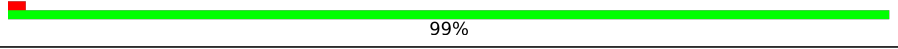
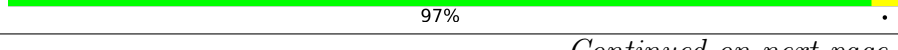
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Mol	Chain	Length	Quality of chain
13	1k	37	
13	2K	37	
13	2k	37	
13	3K	37	
13	3k	37	
13	4K	37	
13	4k	37	
14	1L	37	
14	1l	37	
14	2L	37	
14	2l	37	
14	3L	37	
14	3l	37	
14	4L	37	
14	4l	37	
15	1M	33	
15	1m	33	
15	2M	33	
15	2m	33	
15	3M	33	
15	3m	33	
15	4M	33	
15	4m	33	
16	1O	248	
16	1o	248	

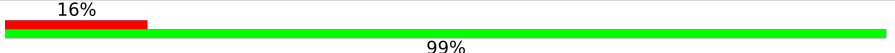
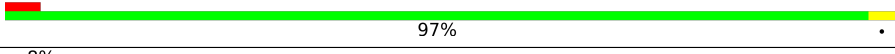
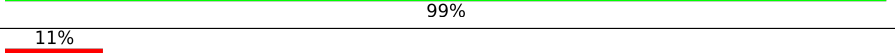
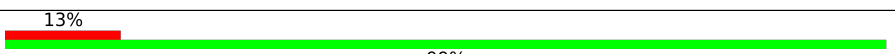
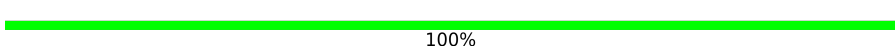
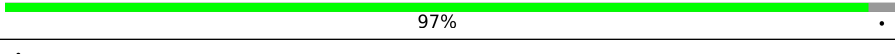
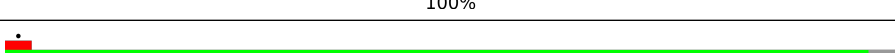
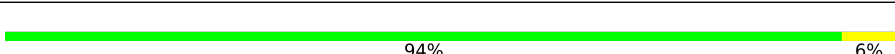
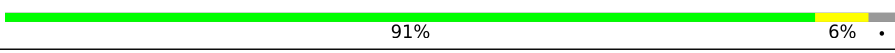
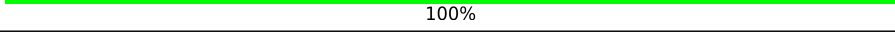
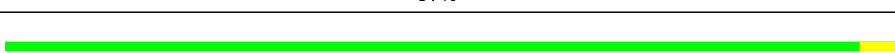
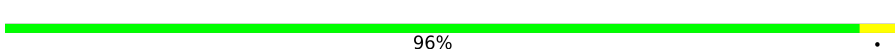
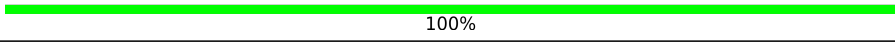
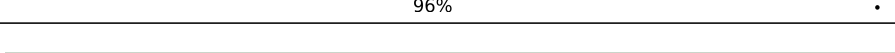
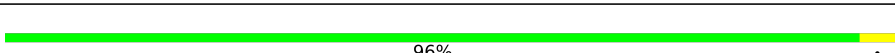
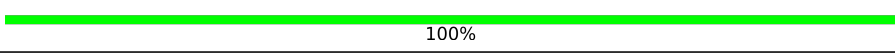
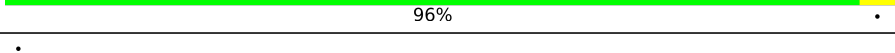
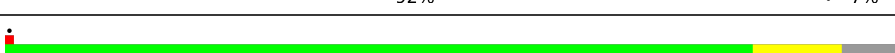
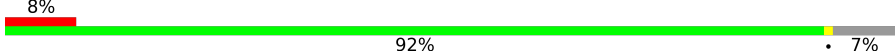
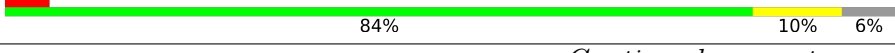
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Mol	Chain	Length	Quality of chain
16	2O	248	
16	2o	248	
16	3O	248	
16	3o	248	
16	4O	248	
16	4o	248	
17	1P	186	
17	1p	186	
17	2P	186	
17	2p	186	
17	3P	186	
17	3p	186	
17	4P	186	
17	4p	186	
18	1R	234	
18	1r	234	
18	2R	234	
18	2r	234	
18	3R	234	
18	3r	234	
18	4R	234	
18	4r	234	
19	1S	218	
19	1s	218	
19	2S	218	

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Mol	Chain	Length	Quality of chain
19	2s	218	
19	3S	218	
19	3s	218	
19	4S	218	
19	4s	218	
20	1T	32	
20	1t	32	
20	2T	32	
20	2t	32	
20	3T	32	
20	3t	32	
20	4T	32	
20	4t	32	
21	1U	27	
21	1u	27	
21	2U	27	
21	2u	27	
21	3U	27	
21	3u	27	
21	4U	27	
21	4u	27	
22	1V	105	
22	1v	105	
22	2V	105	
22	2v	105	

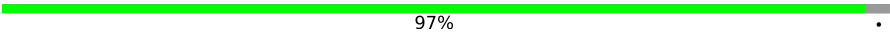
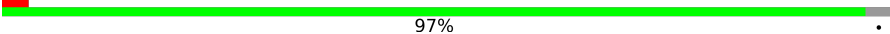
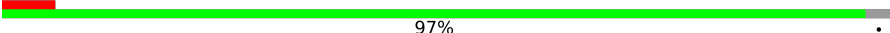
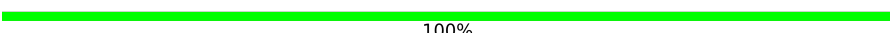
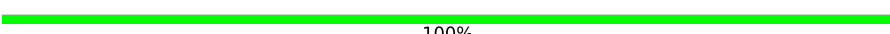
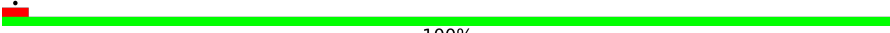
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Mol	Chain	Length	Quality of chain
22	3V	105	
22	3v	105	
22	4V	105	
22	4v	105	
23	1W	54	
23	1w	54	
23	2W	54	
23	2w	54	
23	3W	54	
23	3w	54	
23	4W	54	
23	4w	54	
24	1X	39	
24	1x	39	
24	2X	39	
24	2x	39	
24	3X	39	
24	3x	39	
24	4X	39	
24	4x	39	
25	1Y	35	
25	1y	35	
25	2Y	35	
25	2y	35	
25	3Y	35	

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Mol	Chain	Length	Quality of chain
25	3y	35	 97%
25	4Y	35	 97%
25	4y	35	 97%
26	1Z	62	 100%
26	1z	62	 100%
26	2Z	62	 100%
26	2z	62	 100%
26	3Z	62	 100%
26	3z	62	 100%
26	4Z	62	 100%
26	4z	62	 100%

2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 187864 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 Chlorophyll a-b binding protein 2, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	00	219	Total	C	N	O	0	0
			1098	660	219	219		
1	01	219	Total	C	N	O	0	0
			1097	660	219	218		
1	02	214	Total	C	N	O	0	0
			1076	648	214	214		
1	05	210	Total	C	N	O	0	0
			1052	632	210	210		
1	06	207	Total	C	N	O	0	0
			1034	620	207	207		
1	09	219	Total	C	N	O	0	0
			1098	660	219	219		
1	10	219	Total	C	N	O	0	0
			1098	660	219	219		
1	11	219	Total	C	N	O	0	0
			1097	660	219	218		
1	12	214	Total	C	N	O	0	0
			1076	648	214	214		
1	15	210	Total	C	N	O	0	0
			1052	632	210	210		
1	16	207	Total	C	N	O	0	0
			1034	620	207	207		
1	19	219	Total	C	N	O	0	0
			1098	660	219	219		
1	1G	219	Total	C	N	O	0	0
			1098	660	219	219		
1	1N	219	Total	C	N	O	0	0
			1098	660	219	219		
1	1g	219	Total	C	N	O	0	0
			1098	660	219	219		
1	1n	219	Total	C	N	O	0	0
			1098	660	219	219		
1	2G	219	Total	C	N	O	0	0
			1098	660	219	219		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	2N	219	Total	C	N	O	0	0
			1098	660	219	219		
1	2g	219	Total	C	N	O	0	0
			1098	660	219	219		
1	2n	219	Total	C	N	O	0	0
			1098	660	219	219		
1	30	219	Total	C	N	O	0	0
			1098	660	219	219		
1	31	219	Total	C	N	O	0	0
			1097	660	219	218		
1	32	214	Total	C	N	O	0	0
			1076	648	214	214		
1	35	210	Total	C	N	O	0	0
			1052	632	210	210		
1	36	207	Total	C	N	O	0	0
			1034	620	207	207		
1	39	219	Total	C	N	O	0	0
			1098	660	219	219		
1	3G	219	Total	C	N	O	0	0
			1098	660	219	219		
1	3N	219	Total	C	N	O	0	0
			1098	660	219	219		
1	3g	219	Total	C	N	O	0	0
			1098	660	219	219		
1	3n	219	Total	C	N	O	0	0
			1098	660	219	219		
1	40	219	Total	C	N	O	0	0
			1098	660	219	219		
1	41	219	Total	C	N	O	0	0
			1097	660	219	218		
1	42	214	Total	C	N	O	0	0
			1076	648	214	214		
1	45	210	Total	C	N	O	0	0
			1052	632	210	210		
1	46	207	Total	C	N	O	0	0
			1034	620	207	207		
1	49	219	Total	C	N	O	0	0
			1098	660	219	219		
1	4G	219	Total	C	N	O	0	0
			1098	660	219	219		
1	4N	219	Total	C	N	O	0	0
			1098	660	219	219		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	4g	219	Total	C	N	O	0	0
			1098	660	219	219		
1	4n	219	Total	C	N	O	0	0
			1098	660	219	219		

- Molecule 2 is a protein called Chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	03	220	Total	C	N	O	0	0
			1100	660	220	220		
2	07	220	Total	C	N	O	0	0
			1101	661	220	220		
2	13	220	Total	C	N	O	0	0
			1100	660	220	220		
2	17	220	Total	C	N	O	0	0
			1101	661	220	220		
2	33	220	Total	C	N	O	0	0
			1100	660	220	220		
2	37	220	Total	C	N	O	0	0
			1101	661	220	220		
2	43	220	Total	C	N	O	0	0
			1100	660	220	220		
2	47	220	Total	C	N	O	0	0
			1101	661	220	220		

- Molecule 3 is a protein called cDNA clone:001-040-G02, full insert sequence.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	04	200	Total	C	N	O	0	0
			1006	606	200	200		
3	08	205	Total	C	N	O	0	0
			1030	620	205	205		
3	14	200	Total	C	N	O	0	0
			1006	606	200	200		
3	18	205	Total	C	N	O	0	0
			1030	620	205	205		
3	34	200	Total	C	N	O	0	0
			1006	606	200	200		
3	38	205	Total	C	N	O	0	0
			1030	620	205	205		
3	44	200	Total	C	N	O	0	0
			1006	606	200	200		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	48	205	Total	C	N	O	0	0
			1030	620	205	205		

- Molecule 4 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	1A	334	Total	C	N	O	0	0
			1666	998	334	334		
4	1a	333	Total	C	N	O	0	0
			1661	995	333	333		
4	2A	334	Total	C	N	O	0	0
			1666	998	334	334		
4	2a	333	Total	C	N	O	0	0
			1661	995	333	333		
4	3A	334	Total	C	N	O	0	0
			1666	998	334	334		
4	3a	333	Total	C	N	O	0	0
			1661	995	333	333		
4	4A	334	Total	C	N	O	0	0
			1666	998	334	334		
4	4a	333	Total	C	N	O	0	0
			1661	995	333	333		

- Molecule 5 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	1B	503	Total	C	N	O	0	0
			2510	1504	503	503		
5	1b	503	Total	C	N	O	0	0
			2510	1504	503	503		
5	2B	503	Total	C	N	O	0	0
			2510	1504	503	503		
5	2b	503	Total	C	N	O	0	0
			2510	1504	503	503		
5	3B	503	Total	C	N	O	0	0
			2510	1504	503	503		
5	3b	503	Total	C	N	O	0	0
			2510	1504	503	503		
5	4B	503	Total	C	N	O	0	0
			2510	1504	503	503		
5	4b	503	Total	C	N	O	0	0
			2510	1504	503	503		

- Molecule 6 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	1C	450	Total	C	N	O	0	0
			2238	1338	450	450		
6	1c	450	Total	C	N	O	0	0
			2237	1337	450	450		
6	2C	450	Total	C	N	O	0	0
			2238	1338	450	450		
6	2c	450	Total	C	N	O	0	0
			2237	1337	450	450		
6	3C	450	Total	C	N	O	0	0
			2238	1338	450	450		
6	3c	450	Total	C	N	O	0	0
			2237	1337	450	450		
6	4C	450	Total	C	N	O	0	0
			2238	1338	450	450		
6	4c	450	Total	C	N	O	0	0
			2237	1337	450	450		

- Molecule 7 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	1D	340	Total	C	N	O	0	0
			1698	1018	340	340		
7	1d	341	Total	C	N	O	0	0
			1703	1021	341	341		
7	2D	340	Total	C	N	O	0	0
			1698	1018	340	340		
7	2d	341	Total	C	N	O	0	0
			1703	1021	341	341		
7	3D	340	Total	C	N	O	0	0
			1698	1018	340	340		
7	3d	341	Total	C	N	O	0	0
			1703	1021	341	341		
7	4D	340	Total	C	N	O	0	0
			1698	1018	340	340		
7	4d	341	Total	C	N	O	0	0
			1703	1021	341	341		

- Molecule 8 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	1E	75	Total	C	N	O	0	0
			379	229	75	75		

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Mol	Chain	Residues	Atoms				AltConf	Trace
8	1e	75	Total	C	N	O	0	0
			379	229	75	75		
8	2E	75	Total	C	N	O	0	0
			379	229	75	75		
8	2e	75	Total	C	N	O	0	0
			379	229	75	75		
8	3E	75	Total	C	N	O	0	0
			379	229	75	75		
8	3e	75	Total	C	N	O	0	0
			379	229	75	75		
8	4E	75	Total	C	N	O	0	0
			379	229	75	75		
8	4e	75	Total	C	N	O	0	0
			379	229	75	75		

- Molecule 9 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	1F	35	Total	C	N	O	0	0
			177	107	35	35		
9	1f	30	Total	C	N	O	0	0
			150	90	30	30		
9	2F	35	Total	C	N	O	0	0
			177	107	35	35		
9	2f	30	Total	C	N	O	0	0
			150	90	30	30		
9	3F	35	Total	C	N	O	0	0
			177	107	35	35		
9	3f	30	Total	C	N	O	0	0
			150	90	30	30		
9	4F	35	Total	C	N	O	0	0
			177	107	35	35		
9	4f	30	Total	C	N	O	0	0
			150	90	30	30		

- Molecule 10 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	1H	60	Total	C	N	O	0	0
			301	181	60	60		
10	1h	60	Total	C	N	O	0	0
			301	181	60	60		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	2H	60	Total	C	N	O	0	0
			301	181	60	60		
10	2h	60	Total	C	N	O	0	0
			301	181	60	60		
10	3H	60	Total	C	N	O	0	0
			301	181	60	60		
10	3h	60	Total	C	N	O	0	0
			301	181	60	60		
10	4H	60	Total	C	N	O	0	0
			301	181	60	60		
10	4h	60	Total	C	N	O	0	0
			301	181	60	60		

- Molecule 11 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	1I	34	Total	C	N	O	0	0
			171	103	34	34		
11	1i	34	Total	C	N	O	0	0
			171	103	34	34		
11	2I	34	Total	C	N	O	0	0
			171	103	34	34		
11	2i	34	Total	C	N	O	0	0
			171	103	34	34		
11	3I	34	Total	C	N	O	0	0
			171	103	34	34		
11	3i	34	Total	C	N	O	0	0
			171	103	34	34		
11	4I	34	Total	C	N	O	0	0
			171	103	34	34		
11	4i	34	Total	C	N	O	0	0
			171	103	34	34		

- Molecule 12 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	1J	35	Total	C	N	O	0	0
			169	99	35	35		
12	1j	35	Total	C	N	O	0	0
			169	99	35	35		
12	2J	35	Total	C	N	O	0	0
			169	99	35	35		

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Mol	Chain	Residues	Atoms				AltConf	Trace
12	2j	35	Total 169	C 99	N 35	O 35	0	0
12	3J	35	Total 169	C 99	N 35	O 35	0	0
12	3j	35	Total 169	C 99	N 35	O 35	0	0
12	4J	35	Total 169	C 99	N 35	O 35	0	0
12	4j	35	Total 169	C 99	N 35	O 35	0	0

- Molecule 13 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	1K	37	Total 193	C 119	N 37	O 37	0	0
13	1k	37	Total 193	C 119	N 37	O 37	0	0
13	2K	37	Total 193	C 119	N 37	O 37	0	0
13	2k	37	Total 193	C 119	N 37	O 37	0	0
13	3K	37	Total 193	C 119	N 37	O 37	0	0
13	3k	37	Total 193	C 119	N 37	O 37	0	0
13	4K	37	Total 193	C 119	N 37	O 37	0	0
13	4k	37	Total 193	C 119	N 37	O 37	0	0

- Molecule 14 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	1L	36	Total 181	C 109	N 36	O 36	0	0
14	1l	35	Total 176	C 106	N 35	O 35	0	0
14	2L	36	Total 181	C 109	N 36	O 36	0	0
14	2l	35	Total 176	C 106	N 35	O 35	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
14	3L	36	Total	C	N	O	0	0
			181	109	36	36		
14	3l	35	Total	C	N	O	0	0
			176	106	35	35		
14	4L	36	Total	C	N	O	0	0
			181	109	36	36		
14	4l	35	Total	C	N	O	0	0
			176	106	35	35		

- Molecule 15 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	1M	32	Total	C	N	O	0	0
			162	98	32	32		
15	1m	33	Total	C	N	O	0	0
			167	101	33	33		
15	2M	32	Total	C	N	O	0	0
			162	98	32	32		
15	2m	33	Total	C	N	O	0	0
			167	101	33	33		
15	3M	32	Total	C	N	O	0	0
			162	98	32	32		
15	3m	33	Total	C	N	O	0	0
			167	101	33	33		
15	4M	32	Total	C	N	O	0	0
			162	98	32	32		
15	4m	33	Total	C	N	O	0	0
			167	101	33	33		

- Molecule 16 is a protein called 33 kDa subunit of oxygen evolving system of photosystem II.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	1O	247	Total	C	N	O	0	0
			1239	745	247	247		
16	1o	237	Total	C	N	O	0	0
			1186	712	237	237		
16	2O	247	Total	C	N	O	0	0
			1239	745	247	247		
16	2o	237	Total	C	N	O	0	0
			1186	712	237	237		
16	3O	247	Total	C	N	O	0	0
			1239	745	247	247		

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Mol	Chain	Residues	Atoms				AltConf	Trace
16	3o	237	Total	C	N	O	0	0
			1186	712	237	237		
16	4O	247	Total	C	N	O	0	0
			1239	745	247	247		
16	4o	237	Total	C	N	O	0	0
			1186	712	237	237		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1O	248	SER	-	insertion	UNP Q943W1
1o	248	SER	-	insertion	UNP Q943W1
2O	248	SER	-	insertion	UNP Q943W1
2o	248	SER	-	insertion	UNP Q943W1
3O	248	SER	-	insertion	UNP Q943W1
3o	248	SER	-	insertion	UNP Q943W1
4O	248	SER	-	insertion	UNP Q943W1
4o	248	SER	-	insertion	UNP Q943W1

- Molecule 17 is a protein called 23 kDa subunit of oxygen evolving system of photosystem II.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	1P	186	Total	C	N	O	0	0
			926	554	186	186		
17	1p	186	Total	C	N	O	0	0
			926	554	186	186		
17	2P	186	Total	C	N	O	0	0
			926	554	186	186		
17	2p	186	Total	C	N	O	0	0
			926	554	186	186		
17	3P	186	Total	C	N	O	0	0
			926	554	186	186		
17	3p	186	Total	C	N	O	0	0
			926	554	186	186		
17	4P	186	Total	C	N	O	0	0
			926	554	186	186		
17	4p	186	Total	C	N	O	0	0
			926	554	186	186		

- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	1R	234	Total	C	N	O	0	0
			1177	709	234	234		
18	1r	234	Total	C	N	O	0	0
			1177	709	234	234		
18	2R	234	Total	C	N	O	0	0
			1177	709	234	234		
18	2r	234	Total	C	N	O	0	0
			1177	709	234	234		
18	3R	234	Total	C	N	O	0	0
			1177	709	234	234		
18	3r	234	Total	C	N	O	0	0
			1177	709	234	234		
18	4R	234	Total	C	N	O	0	0
			1177	709	234	234		
18	4r	234	Total	C	N	O	0	0
			1177	709	234	234		

- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	1S	218	Total	C	N	O	0	0
			1094	658	218	218		
19	1s	217	Total	C	N	O	0	0
			1089	655	217	217		
19	2S	218	Total	C	N	O	0	0
			1094	658	218	218		
19	2s	217	Total	C	N	O	0	0
			1089	655	217	217		
19	3S	218	Total	C	N	O	0	0
			1094	658	218	218		
19	3s	217	Total	C	N	O	0	0
			1089	655	217	217		
19	4S	218	Total	C	N	O	0	0
			1094	658	218	218		
19	4s	217	Total	C	N	O	0	0
			1089	655	217	217		

- Molecule 20 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	1T	32	Total	C	N	O	0	0
			165	101	32	32		
20	1t	31	Total	C	N	O	0	0
			160	98	31	31		

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Mol	Chain	Residues	Atoms				AltConf	Trace
20	2T	32	Total	C	N	O	0	0
			165	101	32	32		
20	2t	31	Total	C	N	O	0	0
			160	98	31	31		
20	3T	32	Total	C	N	O	0	0
			165	101	32	32		
20	3t	31	Total	C	N	O	0	0
			160	98	31	31		
20	4T	32	Total	C	N	O	0	0
			165	101	32	32		
20	4t	31	Total	C	N	O	0	0
			160	98	31	31		

- Molecule 21 is a protein called Os02g0581100 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	1U	27	Total	C	N	O	0	0
			138	84	27	27		
21	1u	27	Total	C	N	O	0	0
			138	84	27	27		
21	2U	27	Total	C	N	O	0	0
			138	84	27	27		
21	2u	27	Total	C	N	O	0	0
			138	84	27	27		
21	3U	27	Total	C	N	O	0	0
			138	84	27	27		
21	3u	27	Total	C	N	O	0	0
			138	84	27	27		
21	4U	27	Total	C	N	O	0	0
			138	84	27	27		
21	4u	27	Total	C	N	O	0	0
			138	84	27	27		

- Molecule 22 is a protein called Photosystem II 10 kDa polypeptide, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	1V	98	Total	C	N	O	0	0
			482	286	98	98		
22	1v	99	Total	C	N	O	0	0
			487	289	99	99		
22	2V	98	Total	C	N	O	0	0
			482	286	98	98		

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Mol	Chain	Residues	Atoms				AltConf	Trace
22	2v	99	Total	C	N	O	0	0
			487	289	99	99		
22	3V	98	Total	C	N	O	0	0
			482	286	98	98		
22	3v	99	Total	C	N	O	0	0
			487	289	99	99		
22	4V	98	Total	C	N	O	0	0
			482	286	98	98		
22	4v	99	Total	C	N	O	0	0
			487	289	99	99		

- Molecule 23 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	1W	54	Total	C	N	O	0	0
			262	154	54	54		
23	1w	44	Total	C	N	O	0	0
			214	126	44	44		
23	2W	54	Total	C	N	O	0	0
			262	154	54	54		
23	2w	44	Total	C	N	O	0	0
			214	126	44	44		
23	3W	54	Total	C	N	O	0	0
			262	154	54	54		
23	3w	44	Total	C	N	O	0	0
			214	126	44	44		
23	4W	54	Total	C	N	O	0	0
			262	154	54	54		
23	4w	44	Total	C	N	O	0	0
			214	126	44	44		

- Molecule 24 is a protein called Os07g0673550 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	1X	39	Total	C	N	O	0	0
			195	117	39	39		
24	1x	38	Total	C	N	O	0	0
			191	115	38	38		
24	2X	39	Total	C	N	O	0	0
			195	117	39	39		
24	2x	38	Total	C	N	O	0	0
			191	115	38	38		

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Mol	Chain	Residues	Atoms				AltConf	Trace
24	3X	39	Total	C	N	O	0	0
			195	117	39	39		
24	3x	38	Total	C	N	O	0	0
			191	115	38	38		
24	4X	39	Total	C	N	O	0	0
			195	117	39	39		
24	4x	38	Total	C	N	O	0	0
			191	115	38	38		

- Molecule 25 is a protein called cDNA clone:001-024-H10, full insert sequence.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	1Y	34	Total	C	N	O	0	0
			175	107	34	34		
25	1y	34	Total	C	N	O	0	0
			175	107	34	34		
25	2Y	34	Total	C	N	O	0	0
			175	107	34	34		
25	2y	34	Total	C	N	O	0	0
			175	107	34	34		
25	3Y	34	Total	C	N	O	0	0
			175	107	34	34		
25	3y	34	Total	C	N	O	0	0
			175	107	34	34		
25	4Y	34	Total	C	N	O	0	0
			175	107	34	34		
25	4y	34	Total	C	N	O	0	0
			175	107	34	34		

- Molecule 26 is a protein called Photosystem II reaction center protein Z.

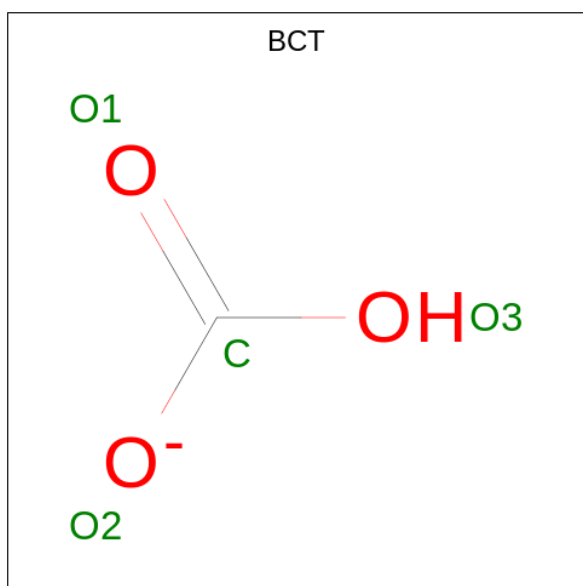
Mol	Chain	Residues	Atoms				AltConf	Trace
26	1Z	62	Total	C	N	O	0	0
			311	187	62	62		
26	1z	62	Total	C	N	O	0	0
			311	187	62	62		
26	2Z	62	Total	C	N	O	0	0
			311	187	62	62		
26	2z	62	Total	C	N	O	0	0
			311	187	62	62		
26	3Z	62	Total	C	N	O	0	0
			311	187	62	62		

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Mol	Chain	Residues	Atoms				AltConf	Trace
26	3z	62	Total	C	N	O	0	0
			311	187	62	62		
26	4Z	62	Total	C	N	O	0	0
			311	187	62	62		
26	4z	62	Total	C	N	O	0	0
			311	187	62	62		

- Molecule 27 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).

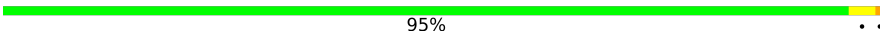


Mol	Chain	Residues	Atoms		AltConf
27	1A	1	Total	C	0
			1	1	
27	1d	1	Total	C	0
			1	1	
27	2A	1	Total	C	0
			1	1	
27	2d	1	Total	C	0
			1	1	
27	3A	1	Total	C	0
			1	1	
27	3d	1	Total	C	0
			1	1	
27	4A	1	Total	C	0
			1	1	
27	4d	1	Total	C	0
			1	1	

3 Residue-property plots [i](#)

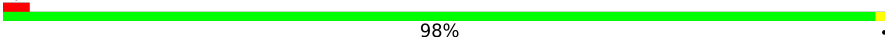
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

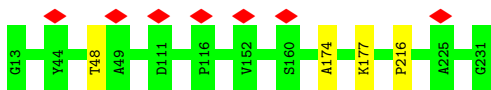
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

Chain 00:  95%

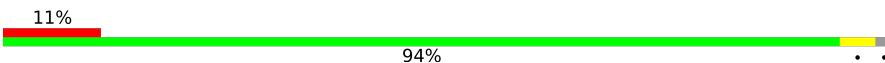


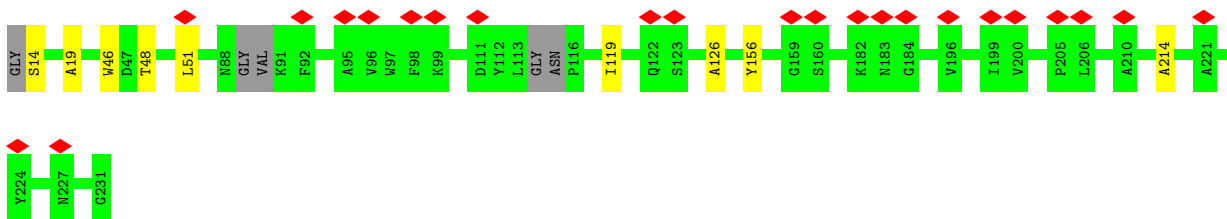
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

Chain 01:  98%



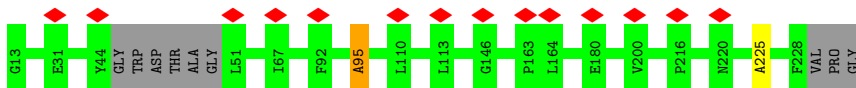
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

Chain 02:  94%



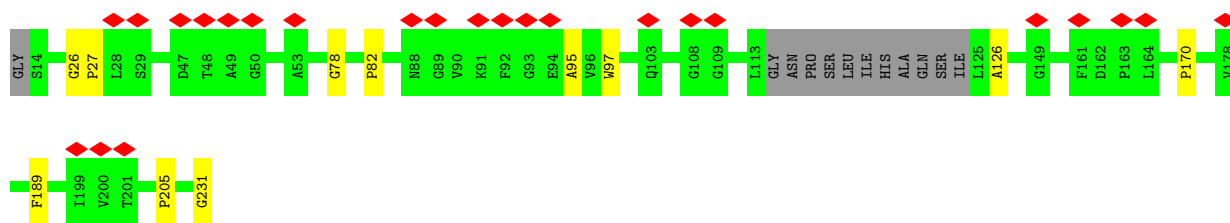
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

Chain 05:  95%



- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

Chain 06:  89%



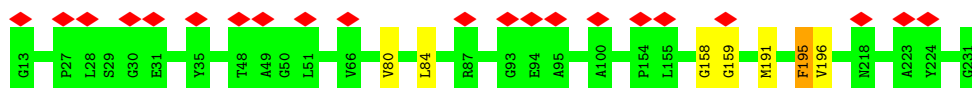
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

Chain 09: 99%



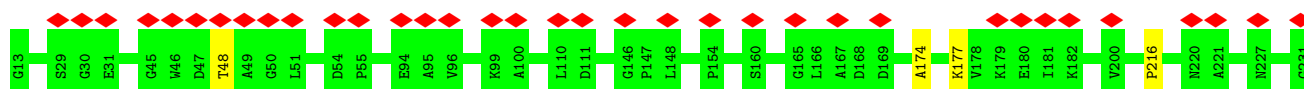
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

Chain 10: 97%



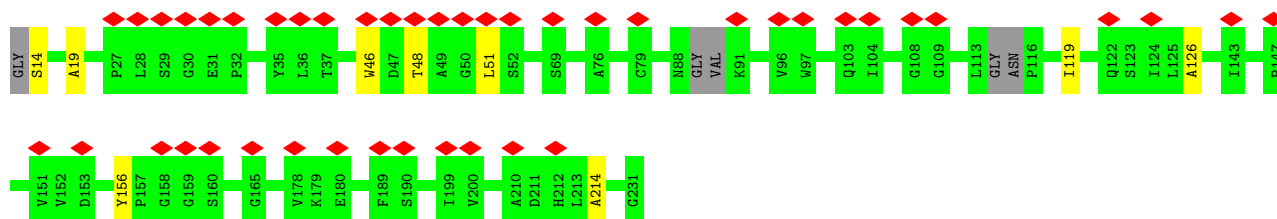
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

Chain 11: 98%



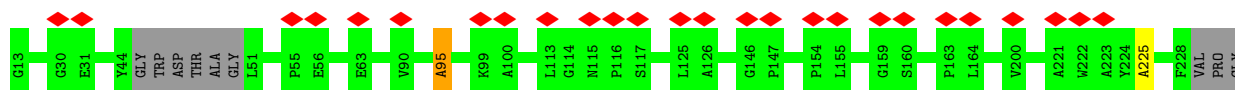
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

Chain 12: 94%

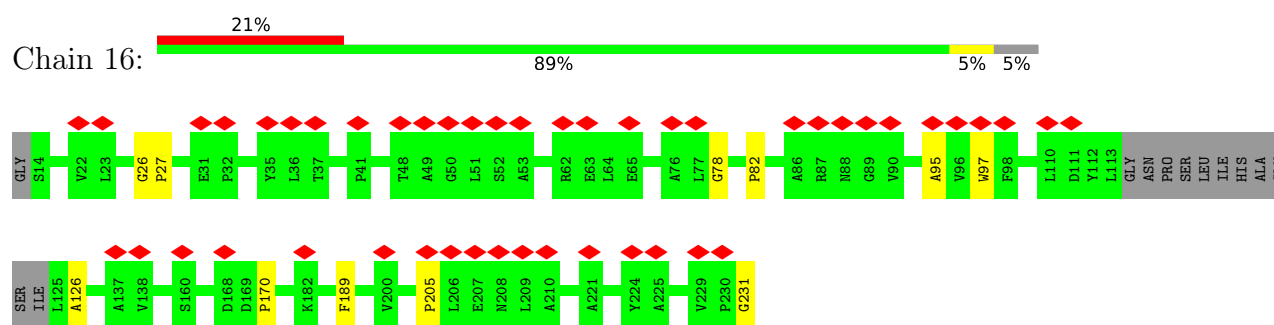


- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

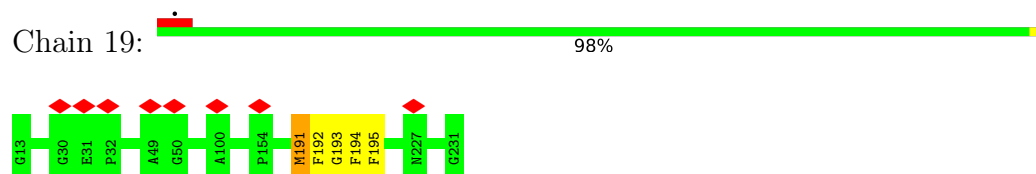
Chain 15: 95%



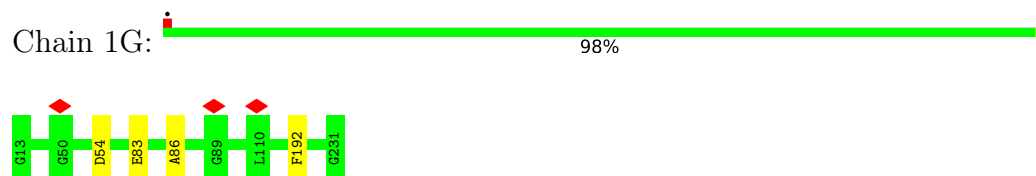
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



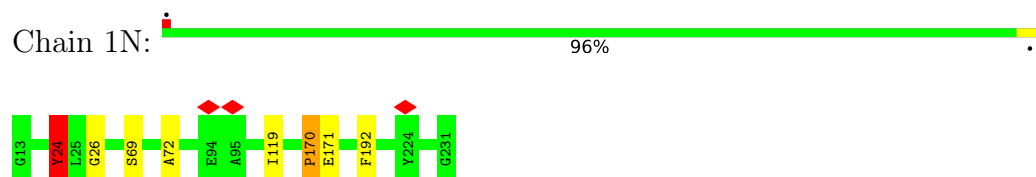
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



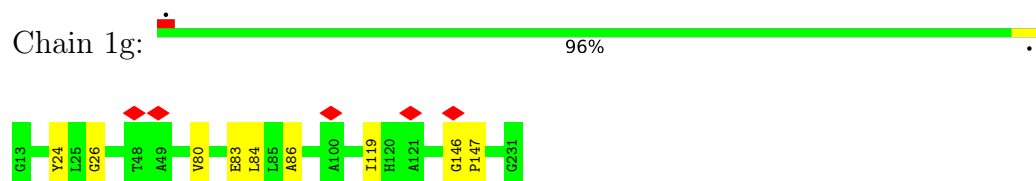
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



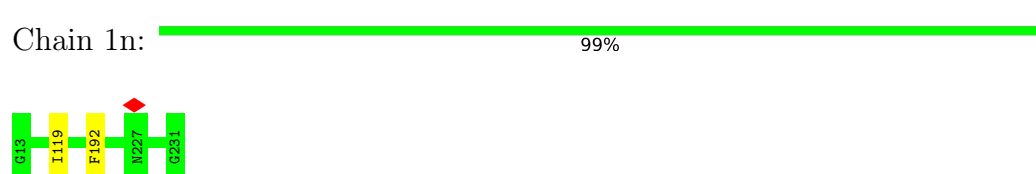
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

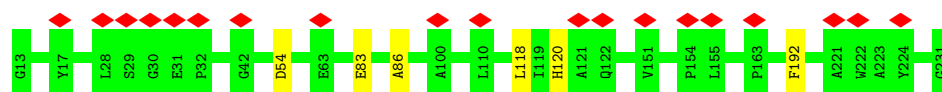


- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

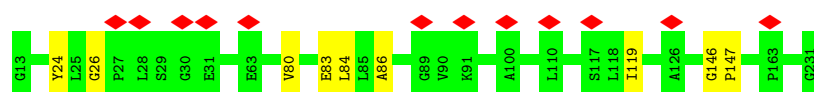




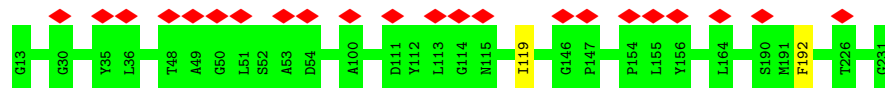
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



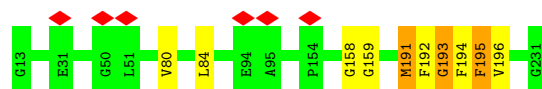
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



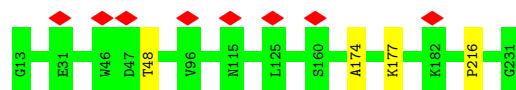
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



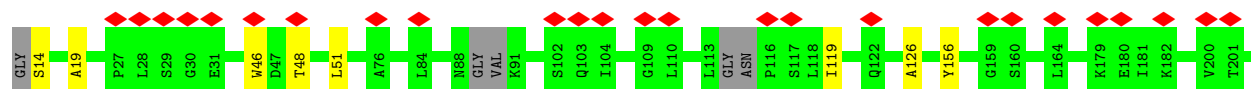
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

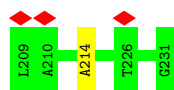


- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

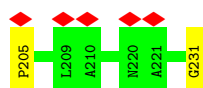
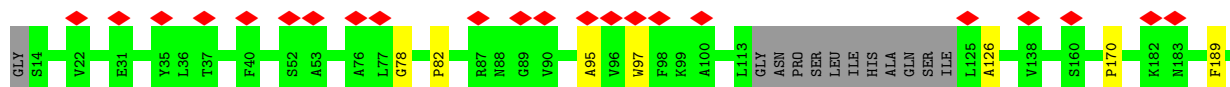




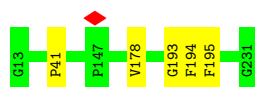
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



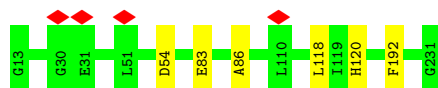
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



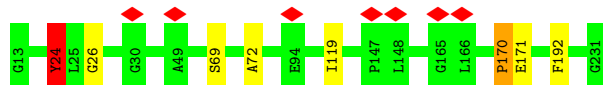
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

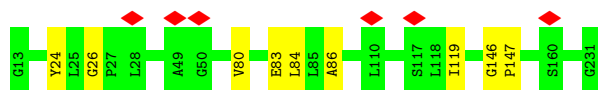


- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

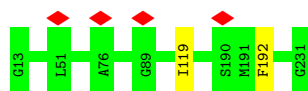


- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

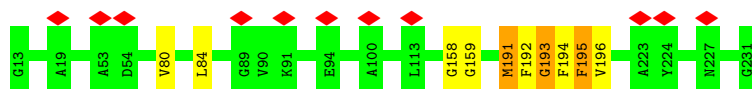




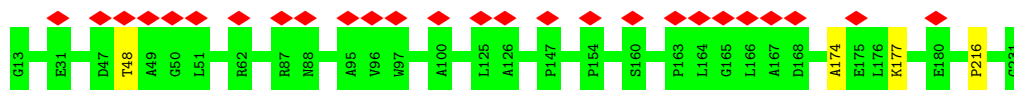
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



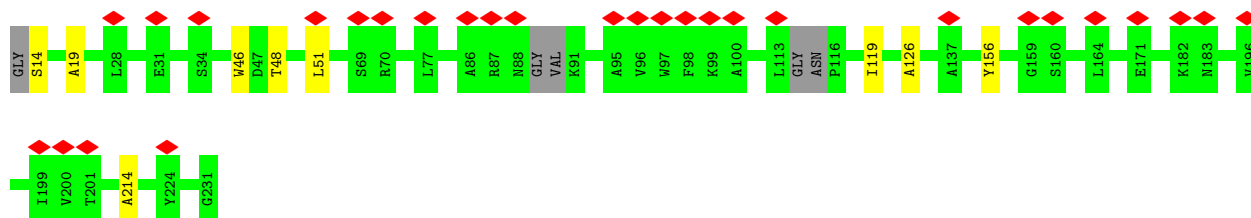
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



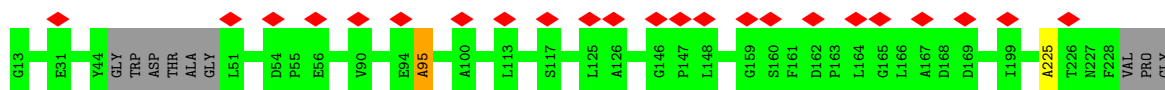
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

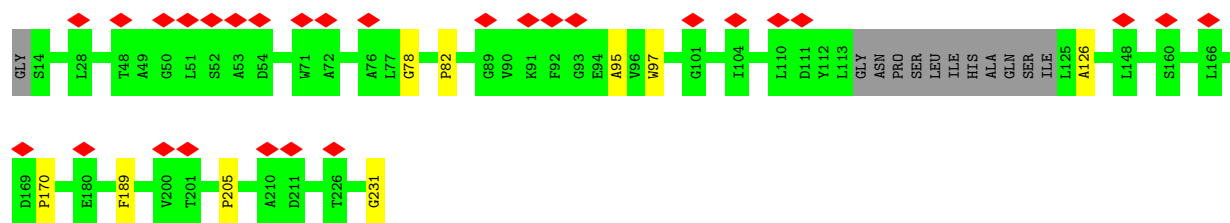


- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



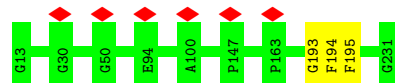
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic





- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

Chain 49: 99%



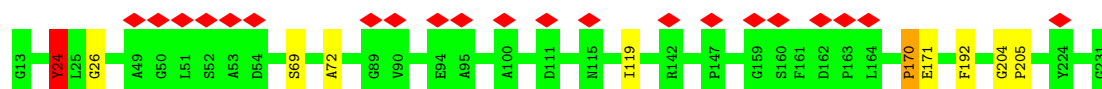
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

Chain 4G: 7% 97%



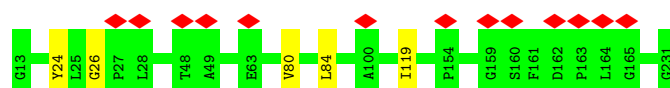
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

Chain 4N: 10% 95%



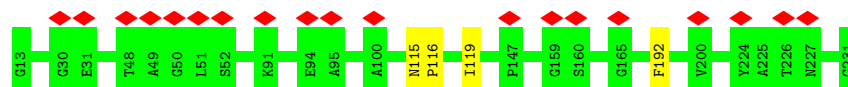
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

Chain 4g: 6% 98%



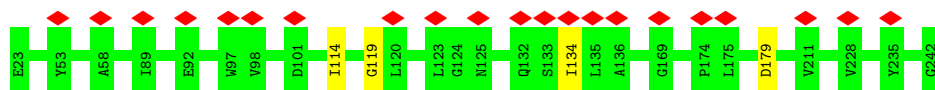
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

Chain 4n: 9% 98%

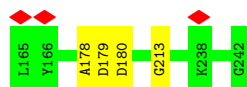
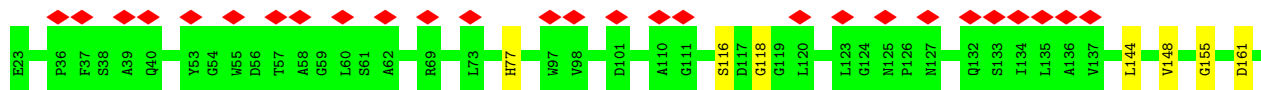


- Molecule 2: Chlorophyll a/b-binding protein

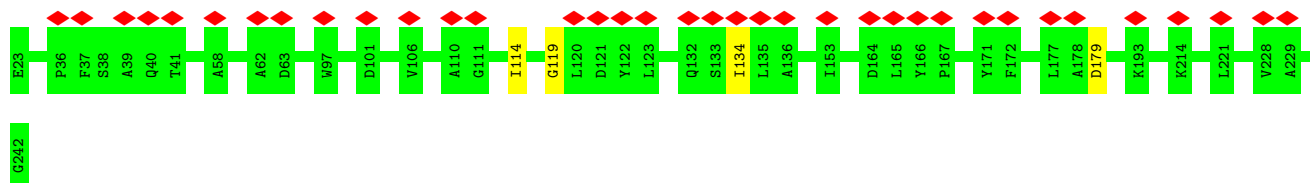
Chain 03: 10% 98%



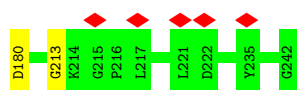
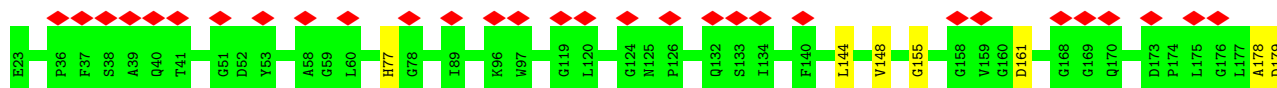
- Molecule 2: Chlorophyll a/b-binding protein



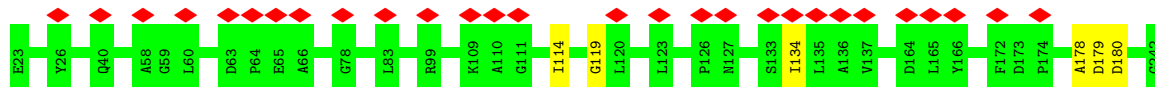
- Molecule 2: Chlorophyll a/b-binding protein



- Molecule 2: Chlorophyll a/b-binding protein



- Molecule 2: Chlorophyll a/b-binding protein

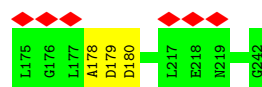
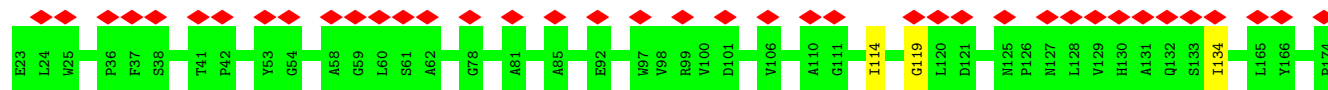


- Molecule 2: Chlorophyll a/b-binding protein





- Molecule 2: Chlorophyll a/b-binding protein



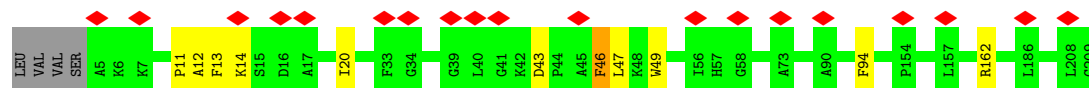
- Molecule 2: Chlorophyll a/b-binding protein



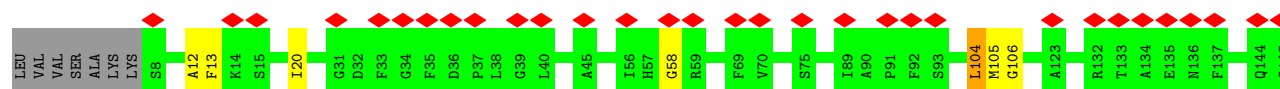
- Molecule 3: cDNA clone:001-040-G02, full insert sequence

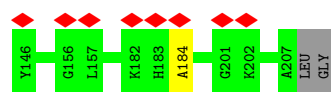


- Molecule 3: cDNA clone:001-040-G02, full insert sequence

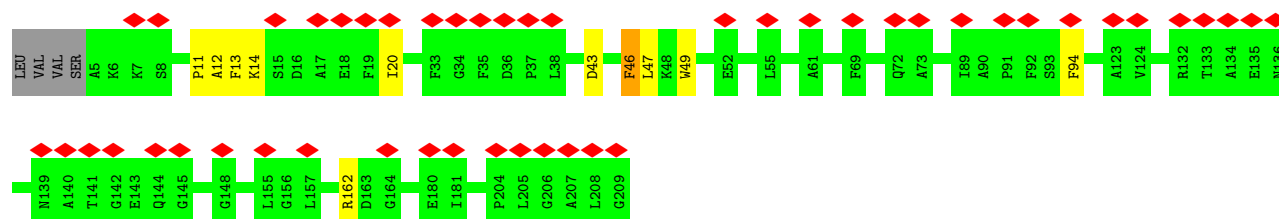


- Molecule 3: cDNA clone:001-040-G02, full insert sequence

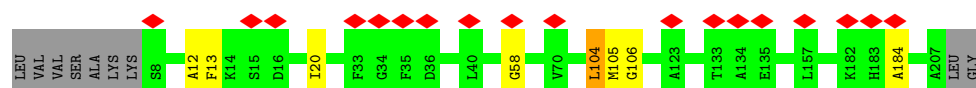




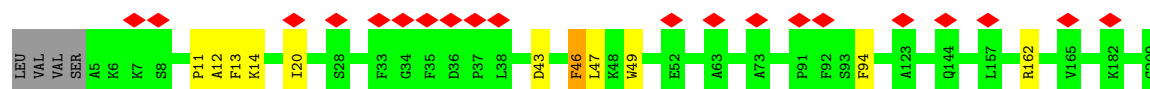
- Molecule 3: cDNA clone:001-040-G02, full insert sequence



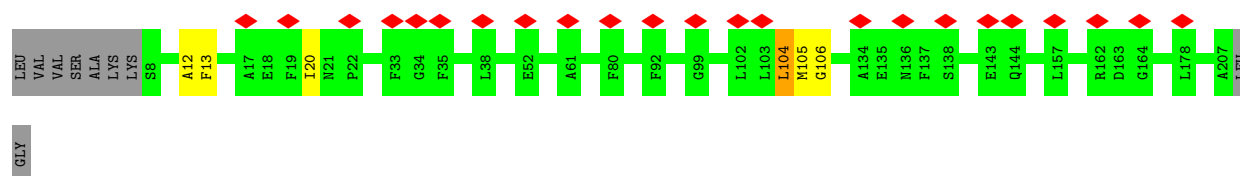
- Molecule 3: cDNA clone:001-040-G02, full insert sequence



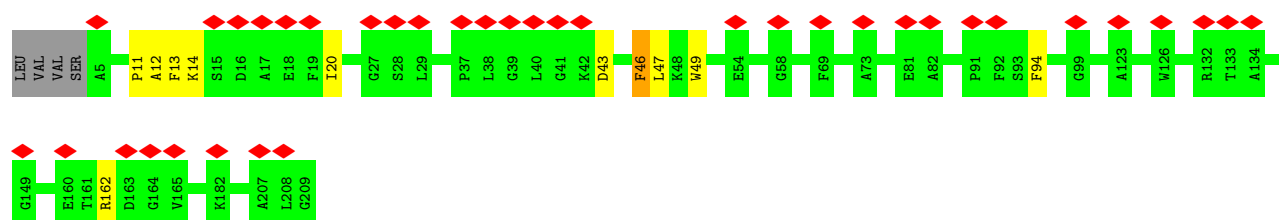
- Molecule 3: cDNA clone:001-040-G02, full insert sequence



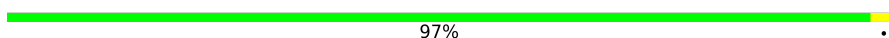
- Molecule 3: cDNA clone:001-040-G02, full insert sequence



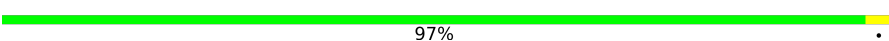
- Molecule 3: cDNA clone:001-040-G02, full insert sequence



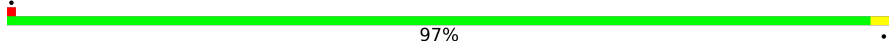
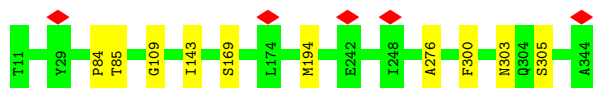
• Molecule 4: Photosystem II protein D1

Chain 1A:  97%

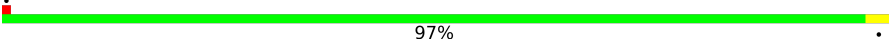
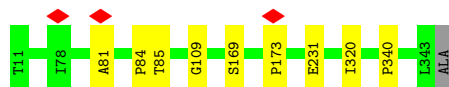
• Molecule 4: Photosystem II protein D1

Chain 1a:  97%

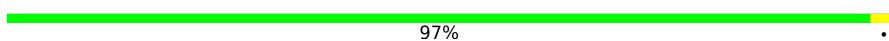
• Molecule 4: Photosystem II protein D1

Chain 2A:  97%

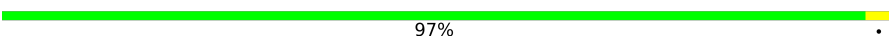
• Molecule 4: Photosystem II protein D1

Chain 2a:  97%

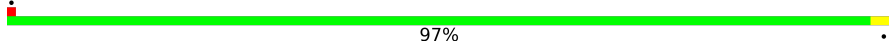
• Molecule 4: Photosystem II protein D1

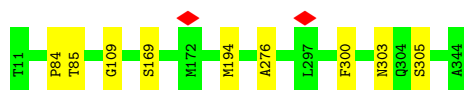
Chain 3A:  97%

• Molecule 4: Photosystem II protein D1

Chain 3a:  97%

• Molecule 4: Photosystem II protein D1

Chain 4A:  97%



- Molecule 4: Photosystem II protein D1

Chain 4a: 97%



- Molecule 5: Photosystem II CP47 reaction center protein

Chain 1B: 99%



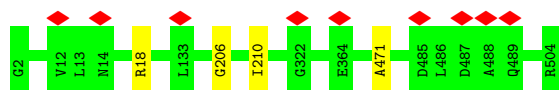
- Molecule 5: Photosystem II CP47 reaction center protein

Chain 1b: 96%



- Molecule 5: Photosystem II CP47 reaction center protein

Chain 2B: 99%



- Molecule 5: Photosystem II CP47 reaction center protein

Chain 2b: 96%

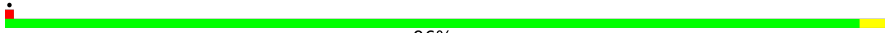


- Molecule 5: Photosystem II CP47 reaction center protein

Chain 3B: 99%

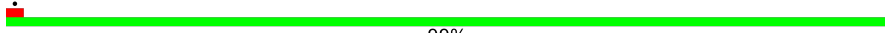


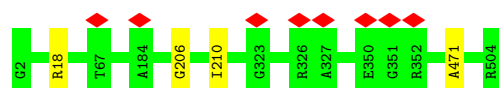
- Molecule 5: Photosystem II CP47 reaction center protein

Chain 3b:  96%



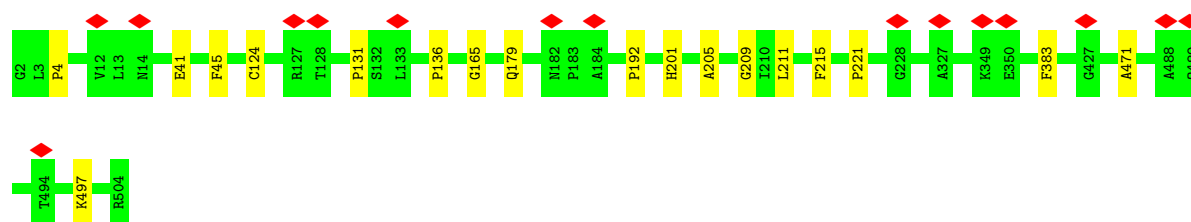
- Molecule 5: Photosystem II CP47 reaction center protein

Chain 4B:  99%

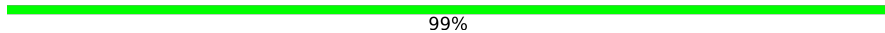


- Molecule 5: Photosystem II CP47 reaction center protein

Chain 4b:  96%

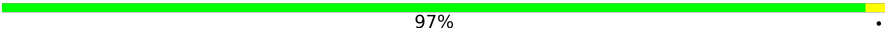


- Molecule 6: Photosystem II CP43 reaction center protein

Chain 1C:  99%



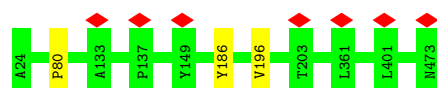
- Molecule 6: Photosystem II CP43 reaction center protein

Chain 1c:  97%



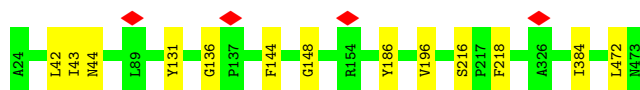
- Molecule 6: Photosystem II CP43 reaction center protein

Chain 2C:  99%



- Molecule 6: Photosystem II CP43 reaction center protein

Chain 2c:  97%



- Molecule 6: Photosystem II CP43 reaction center protein

Chain 3C: 99%



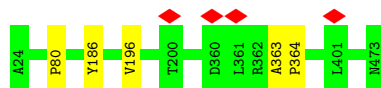
- Molecule 6: Photosystem II CP43 reaction center protein

Chain 3c: 98%



- Molecule 6: Photosystem II CP43 reaction center protein

Chain 4C: 99%



- Molecule 6: Photosystem II CP43 reaction center protein

Chain 4c: 97%



- Molecule 7: Photosystem II D2 protein

Chain 1D: 98%

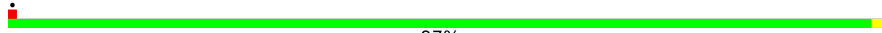


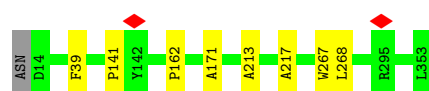
- Molecule 7: Photosystem II D2 protein

Chain 1d: 98%

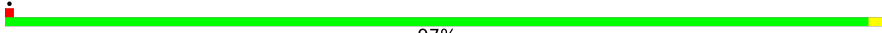


- Molecule 7: Photosystem II D2 protein

Chain 2D:  97%

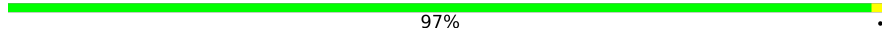


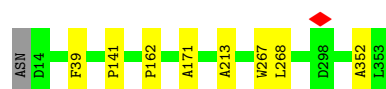
- Molecule 7: Photosystem II D2 protein

Chain 2d:  97%

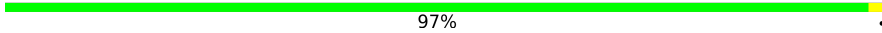


- Molecule 7: Photosystem II D2 protein

Chain 3D:  97%

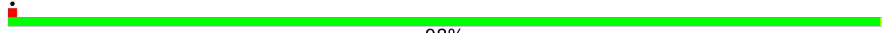


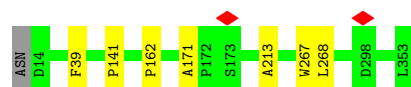
- Molecule 7: Photosystem II D2 protein

Chain 3d:  97%

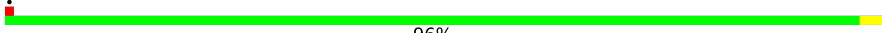


- Molecule 7: Photosystem II D2 protein

Chain 4D:  98%

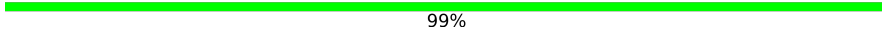


- Molecule 7: Photosystem II D2 protein

Chain 4d:  96%

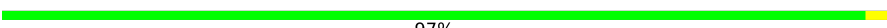


- Molecule 8: Cytochrome b559 subunit alpha

Chain 1E:  99%

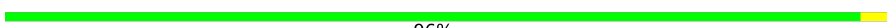


- Molecule 8: Cytochrome b559 subunit alpha

Chain 1e:  97% .

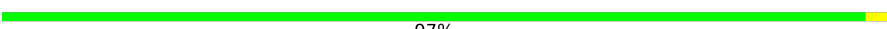


- Molecule 8: Cytochrome b559 subunit alpha

Chain 2E:  96% .

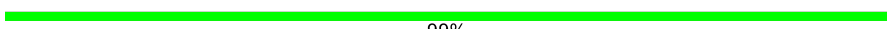


- Molecule 8: Cytochrome b559 subunit alpha

Chain 2e:  97% .

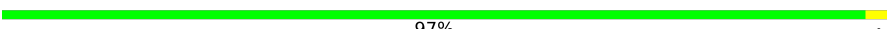


- Molecule 8: Cytochrome b559 subunit alpha

Chain 3E:  99% .

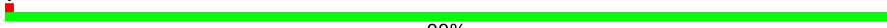


- Molecule 8: Cytochrome b559 subunit alpha

Chain 3e:  97% .

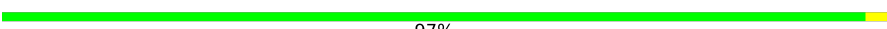


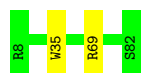
- Molecule 8: Cytochrome b559 subunit alpha

Chain 4E:  99% .

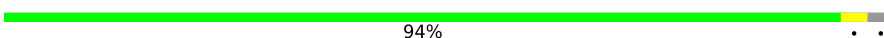


- Molecule 8: Cytochrome b559 subunit alpha

Chain 4e:  97% .



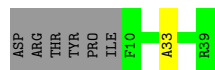
- Molecule 9: Cytochrome b559 subunit beta

Chain 1F:  94% . .

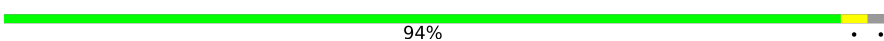


- Molecule 9: Cytochrome b559 subunit beta

Chain 1f:  81% . 17%



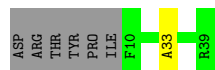
- Molecule 9: Cytochrome b559 subunit beta

Chain 2F:  94% . .

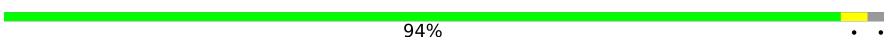


- Molecule 9: Cytochrome b559 subunit beta

Chain 2f:  81% . 17%



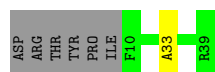
- Molecule 9: Cytochrome b559 subunit beta

Chain 3F:  94% . .

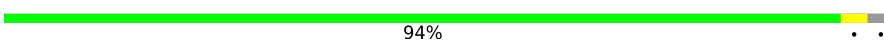


- Molecule 9: Cytochrome b559 subunit beta

Chain 3f:  81% . 17%



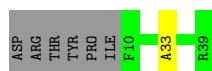
- Molecule 9: Cytochrome b559 subunit beta

Chain 4F:  94% . .

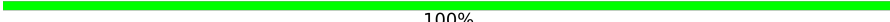


- Molecule 9: Cytochrome b559 subunit beta

Chain 4f:  81% 17%

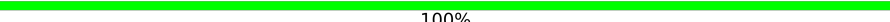


- Molecule 10: Photosystem II reaction center protein H

Chain 1H:  100%

There are no outlier residues recorded for this chain.

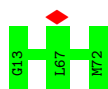
- Molecule 10: Photosystem II reaction center protein H

Chain 1h:  100%

There are no outlier residues recorded for this chain.

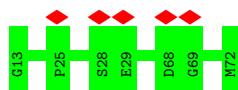
- Molecule 10: Photosystem II reaction center protein H

Chain 2H:  100%



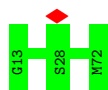
- Molecule 10: Photosystem II reaction center protein H

Chain 2h:  8% 100%



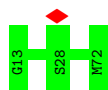
- Molecule 10: Photosystem II reaction center protein H

Chain 3H:  100%



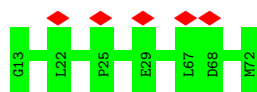
- Molecule 10: Photosystem II reaction center protein H

Chain 3h:  100%

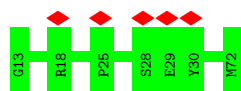


- Molecule 10: Photosystem II reaction center protein H

Chain 4H:  8% 100%



- Molecule 10: Photosystem II reaction center protein H



- Molecule 11: Photosystem II reaction center protein I

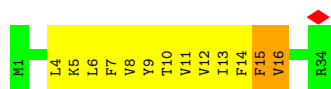


- Molecule 11: Photosystem II reaction center protein I



There are no outlier residues recorded for this chain.

- Molecule 11: Photosystem II reaction center protein I

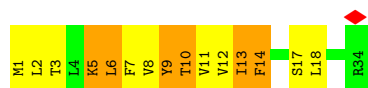


- Molecule 11: Photosystem II reaction center protein I



There are no outlier residues recorded for this chain.

- Molecule 11: Photosystem II reaction center protein I



- Molecule 11: Photosystem II reaction center protein I





- Molecule 11: Photosystem II reaction center protein I

Chain 4I: 56% 26% 18%



- Molecule 11: Photosystem II reaction center protein I

Chain 4i: 100%

There are no outlier residues recorded for this chain.

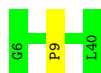
- Molecule 12: Photosystem II reaction center protein J

Chain 1J: 100%

There are no outlier residues recorded for this chain.

- Molecule 12: Photosystem II reaction center protein J

Chain 1j: 97%



- Molecule 12: Photosystem II reaction center protein J

Chain 2J: 100%

There are no outlier residues recorded for this chain.

- Molecule 12: Photosystem II reaction center protein J

Chain 2j: 97%

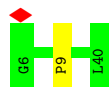


- Molecule 12: Photosystem II reaction center protein J

Chain 3J: 100%

There are no outlier residues recorded for this chain.

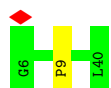
- Molecule 12: Photosystem II reaction center protein J



- Molecule 12: Photosystem II reaction center protein J



- Molecule 12: Photosystem II reaction center protein J



- Molecule 13: Photosystem II reaction center protein K

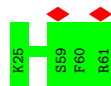


There are no outlier residues recorded for this chain.

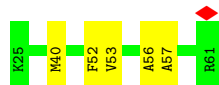
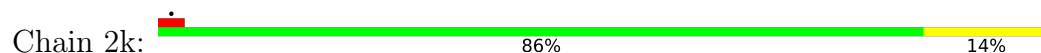
- Molecule 13: Photosystem II reaction center protein K



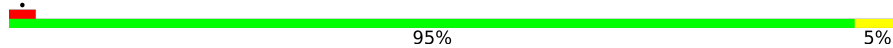
- Molecule 13: Photosystem II reaction center protein K



- Molecule 13: Photosystem II reaction center protein K



- Molecule 13: Photosystem II reaction center protein K

Chain 3K:  95% 5%

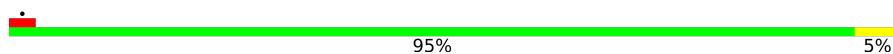


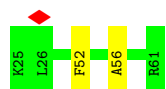
- Molecule 13: Photosystem II reaction center protein K

Chain 3k:  5% 86% 14%

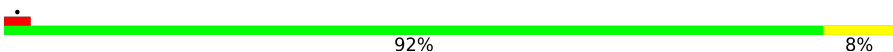


- Molecule 13: Photosystem II reaction center protein K

Chain 4K:  95% 5%

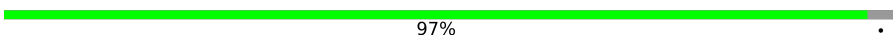


- Molecule 13: Photosystem II reaction center protein K

Chain 4k:  92% 8%



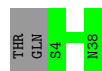
- Molecule 14: Photosystem II reaction center protein L

Chain 1L:  97% .

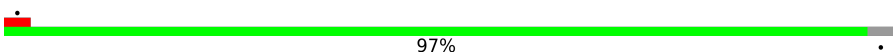


- Molecule 14: Photosystem II reaction center protein L

Chain 1l:  95% 5%



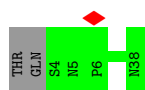
- Molecule 14: Photosystem II reaction center protein L

Chain 2L:  97% .

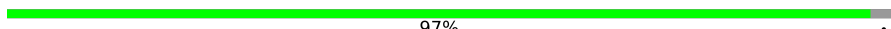


- Molecule 14: Photosystem II reaction center protein L

Chain 2l:  95% 5%



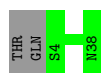
- Molecule 14: Photosystem II reaction center protein L

Chain 3L:  97% .

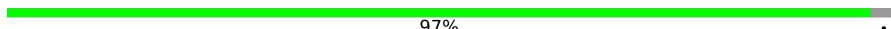


- Molecule 14: Photosystem II reaction center protein L

Chain 3l:  95% 5%



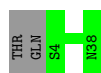
- Molecule 14: Photosystem II reaction center protein L

Chain 4L:  97% .



- Molecule 14: Photosystem II reaction center protein L

Chain 4l:  95% 5%



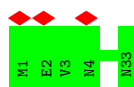
- Molecule 15: Photosystem II reaction center protein M

Chain 1M:  6% 94% . .

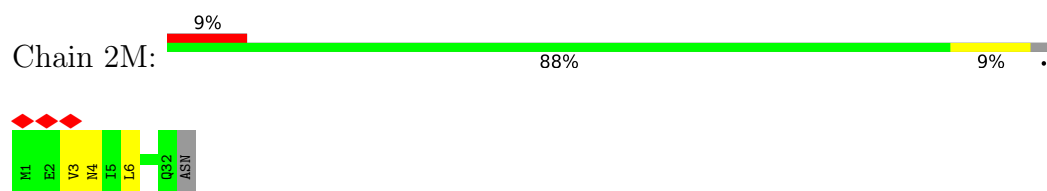


- Molecule 15: Photosystem II reaction center protein M

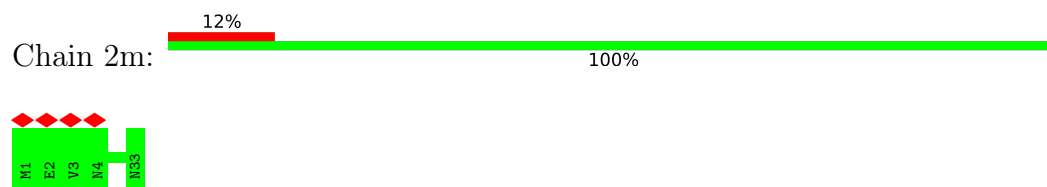
Chain 1m:  9% 100%



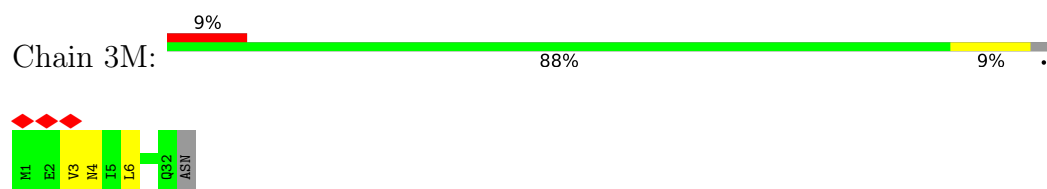
- Molecule 15: Photosystem II reaction center protein M



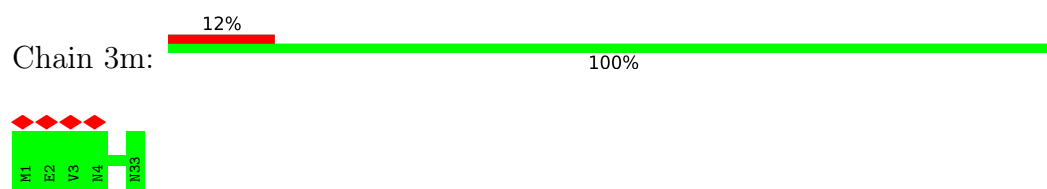
- Molecule 15: Photosystem II reaction center protein M



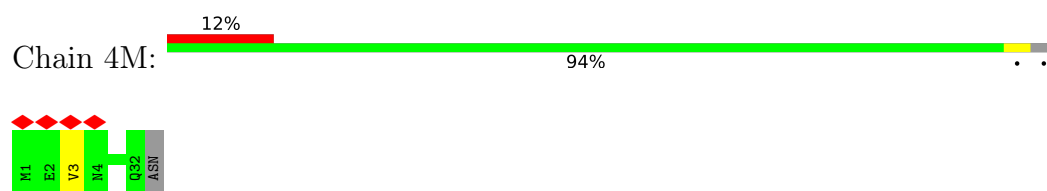
- Molecule 15: Photosystem II reaction center protein M



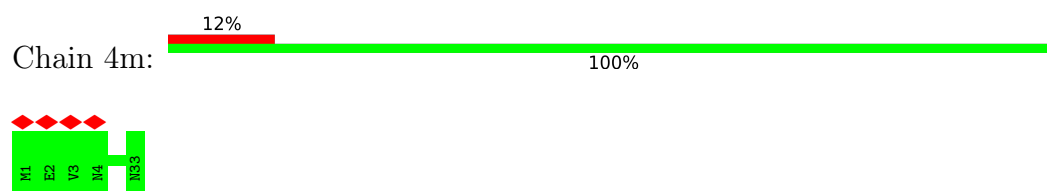
- Molecule 15: Photosystem II reaction center protein M



- Molecule 15: Photosystem II reaction center protein M



- Molecule 15: Photosystem II reaction center protein M



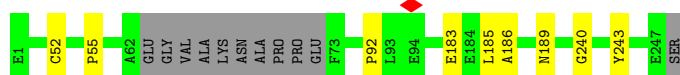
- Molecule 16: 33 kDa subunit of oxygen evolving system of photosystem II





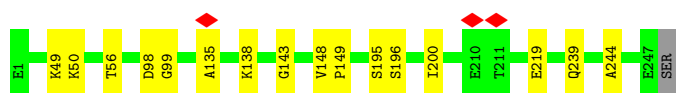
- Molecule 16: 33 kDa subunit of oxygen evolving system of photosystem II

Chain 1o: 92%



- Molecule 16: 33 kDa subunit of oxygen evolving system of photosystem II

Chain 20o: 93%



- Molecule 16: 33 kDa subunit of oxygen evolving system of photosystem II

Chain 2o: 93%



- Molecule 16: 33 kDa subunit of oxygen evolving system of photosystem II

Chain 30o: 95%



- Molecule 16: 33 kDa subunit of oxygen evolving system of photosystem II

Chain 3o: 92%

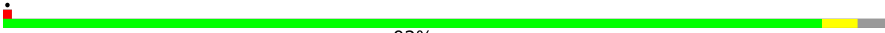


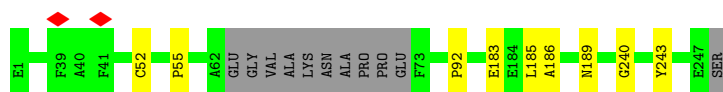
- Molecule 16: 33 kDa subunit of oxygen evolving system of photosystem II

Chain 40o: 94%

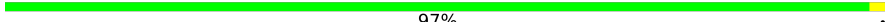


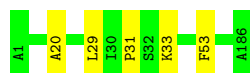
- Molecule 16: 33 kDa subunit of oxygen evolving system of photosystem II

Chain 4o:  92%

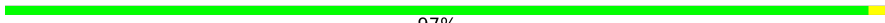


- Molecule 17: 23 kDa subunit of oxygen evolving system of photosystem II

Chain 1P:  97%



- Molecule 17: 23 kDa subunit of oxygen evolving system of photosystem II

Chain 1p:  97%



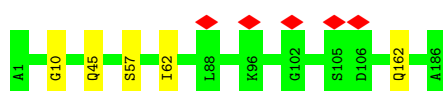
- Molecule 17: 23 kDa subunit of oxygen evolving system of photosystem II

Chain 2P:  97%

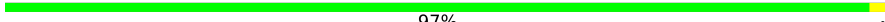


- Molecule 17: 23 kDa subunit of oxygen evolving system of photosystem II

Chain 2p:  97%



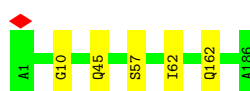
- Molecule 17: 23 kDa subunit of oxygen evolving system of photosystem II

Chain 3P:  97%

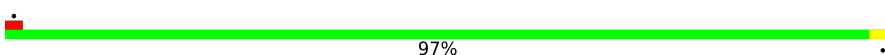


- Molecule 17: 23 kDa subunit of oxygen evolving system of photosystem II

Chain 3p:  97%

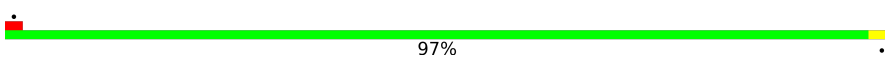


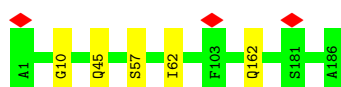
- Molecule 17: 23 kDa subunit of oxygen evolving system of photosystem II

Chain 4P:  97%

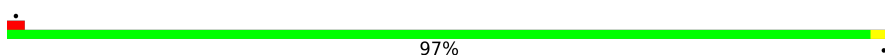


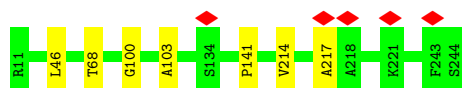
- Molecule 17: 23 kDa subunit of oxygen evolving system of photosystem II

Chain 4p:  97%

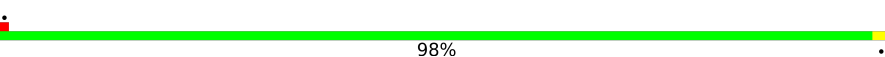


- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 1R:  97%

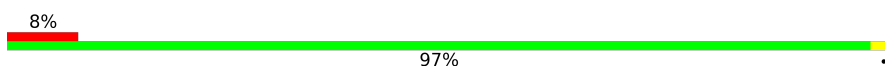


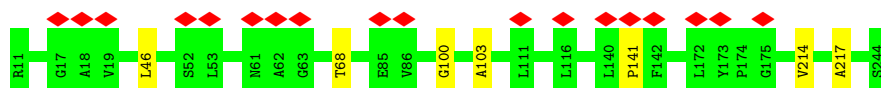
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 1r:  98%

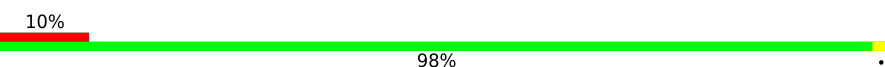


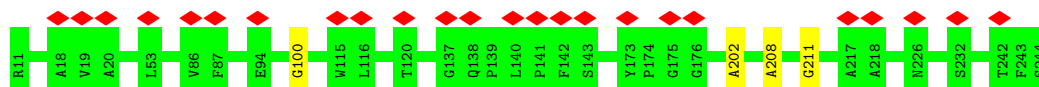
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 2R:  8% 97%

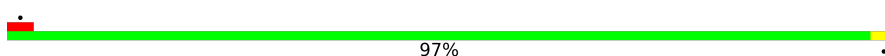


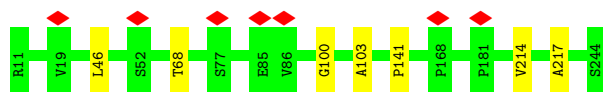
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 2r:  10% 98%

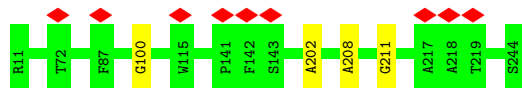


- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

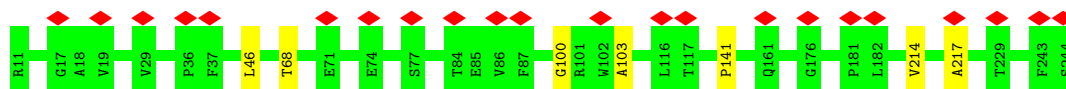
Chain 3R:  97%



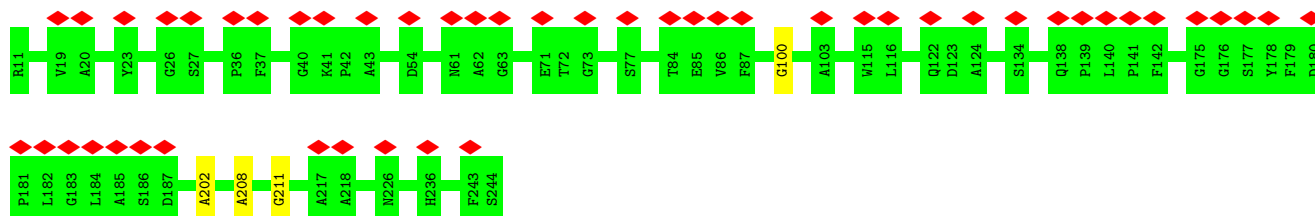
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic



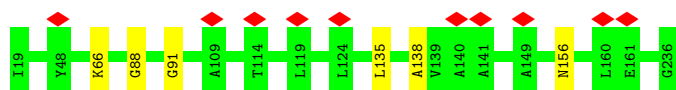
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic



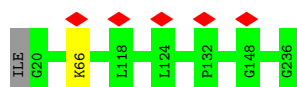
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic



- Molecule 19: Chlorophyll a-b binding protein, chloroplastic

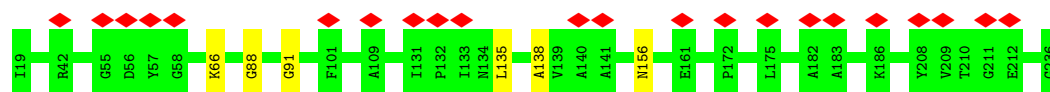


- Molecule 19: Chlorophyll a-b binding protein, chloroplastic

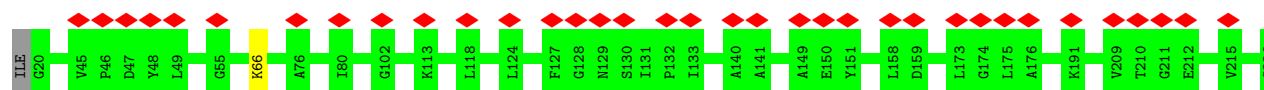


- Molecule 19: Chlorophyll a-b binding protein, chloroplastic

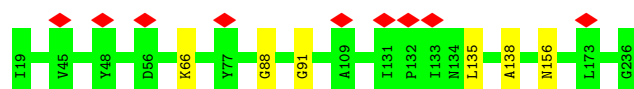




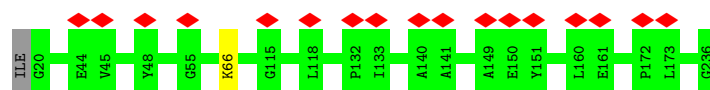
- Molecule 19: Chlorophyll a-b binding protein, chloroplastic



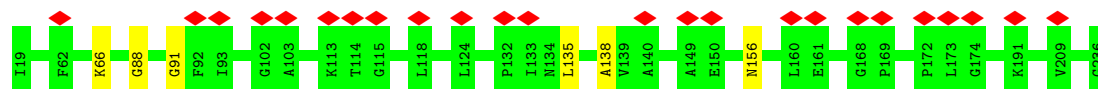
- Molecule 19: Chlorophyll a-b binding protein, chloroplastic



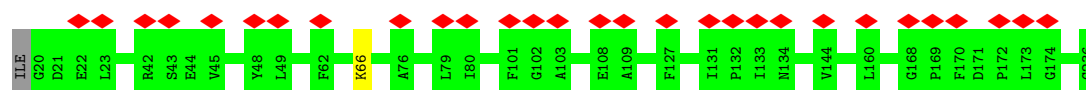
- Molecule 19: Chlorophyll a-b binding protein, chloroplastic



- Molecule 19: Chlorophyll a-b binding protein, chloroplastic



- Molecule 19: Chlorophyll a-b binding protein, chloroplastic



- Molecule 20: Photosystem II reaction center protein T



There are no outlier residues recorded for this chain.

- Molecule 20: Photosystem II reaction center protein T





- Molecule 20: Photosystem II reaction center protein T



- Molecule 20: Photosystem II reaction center protein T



- Molecule 20: Photosystem II reaction center protein T



- Molecule 20: Photosystem II reaction center protein T



- Molecule 20: Photosystem II reaction center protein T



- Molecule 20: Photosystem II reaction center protein T

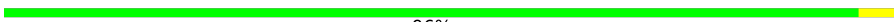


- Molecule 21: Os02g0581100 protein





- Molecule 21: Os02g0581100 protein

Chain 1u:  96%



- Molecule 21: Os02g0581100 protein

Chain 2U:  100%

There are no outlier residues recorded for this chain.

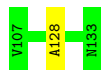
- Molecule 21: Os02g0581100 protein

Chain 2u:  96%



- Molecule 21: Os02g0581100 protein

Chain 3U:  96%



- Molecule 21: Os02g0581100 protein

Chain 3u:  96%



- Molecule 21: Os02g0581100 protein

Chain 4U:  100%

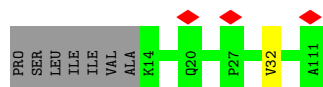
There are no outlier residues recorded for this chain.

- Molecule 21: Os02g0581100 protein

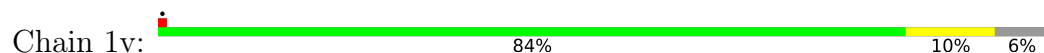
Chain 4u:  96%



- Molecule 22: Photosystem II 10 kDa polypeptide, chloroplastic



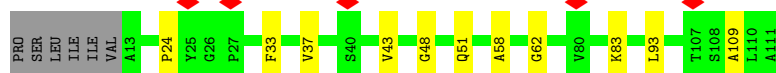
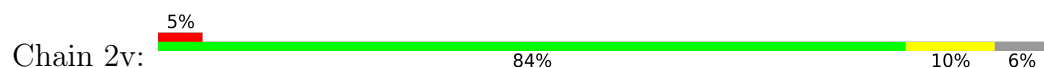
- Molecule 22: Photosystem II 10 kDa polypeptide, chloroplastic



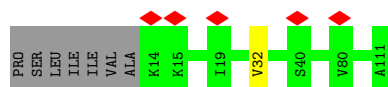
- Molecule 22: Photosystem II 10 kDa polypeptide, chloroplastic



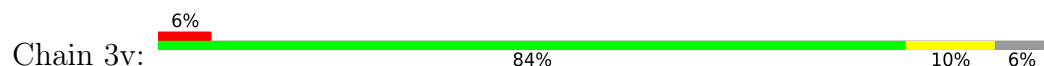
- Molecule 22: Photosystem II 10 kDa polypeptide, chloroplastic



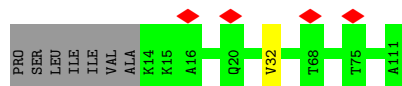
- Molecule 22: Photosystem II 10 kDa polypeptide, chloroplastic



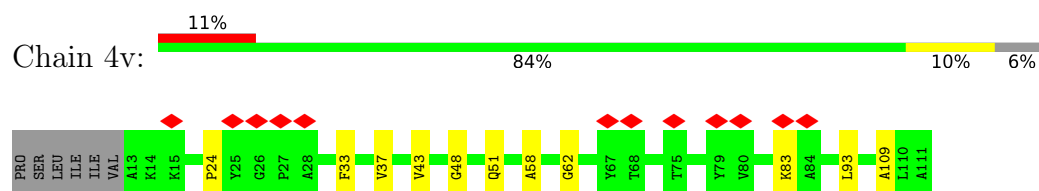
- Molecule 22: Photosystem II 10 kDa polypeptide, chloroplastic



- Molecule 22: Photosystem II 10 kDa polypeptide, chloroplastic



- Molecule 22: Photosystem II 10 kDa polypeptide, chloroplastic

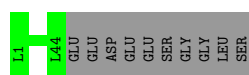
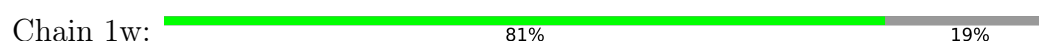


- Molecule 23: Photosystem II reaction center W protein, chloroplastic

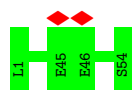


There are no outlier residues recorded for this chain.

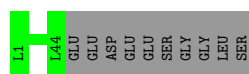
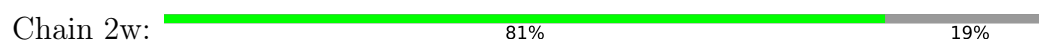
- Molecule 23: Photosystem II reaction center W protein, chloroplastic



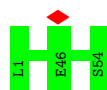
- Molecule 23: Photosystem II reaction center W protein, chloroplastic



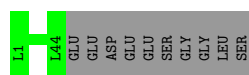
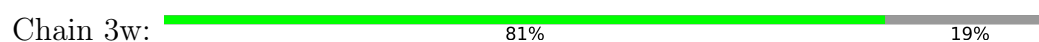
- Molecule 23: Photosystem II reaction center W protein, chloroplastic



- Molecule 23: Photosystem II reaction center W protein, chloroplastic

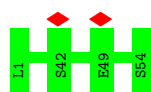


- Molecule 23: Photosystem II reaction center W protein, chloroplastic



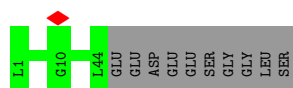
- Molecule 23: Photosystem II reaction center W protein, chloroplastic

Chain 4W:  100%

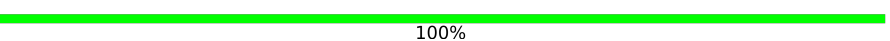


- Molecule 23: Photosystem II reaction center W protein, chloroplastic

Chain 4w:  81% 19%

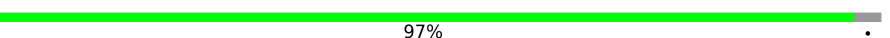


- Molecule 24: Os07g0673550 protein

Chain 1X:  100%

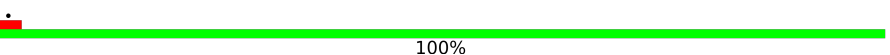
There are no outlier residues recorded for this chain.

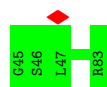
- Molecule 24: Os07g0673550 protein

Chain 1x:  97% .

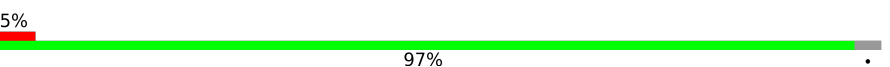


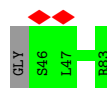
- Molecule 24: Os07g0673550 protein

Chain 2X:  100%

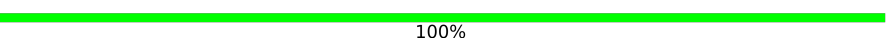


- Molecule 24: Os07g0673550 protein

Chain 2x:  5% 97% .

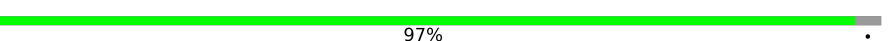


- Molecule 24: Os07g0673550 protein

Chain 3X:  100%

There are no outlier residues recorded for this chain.

- Molecule 24: Os07g0673550 protein

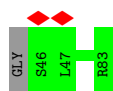
Chain 3x:  97% .



- Molecule 24: Os07g0673550 protein



- Molecule 24: Os07g0673550 protein



- Molecule 25: cDNA clone:001-024-H10, full insert sequence



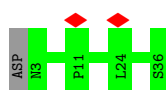
- Molecule 25: cDNA clone:001-024-H10, full insert sequence



- Molecule 25: cDNA clone:001-024-H10, full insert sequence



- Molecule 25: cDNA clone:001-024-H10, full insert sequence



- Molecule 25: cDNA clone:001-024-H10, full insert sequence





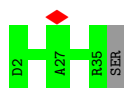
- Molecule 25: cDNA clone:001-024-H10, full insert sequence

Chain 3y: 97%



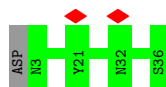
- Molecule 25: cDNA clone:001-024-H10, full insert sequence

Chain 4Y: 97%



- Molecule 25: cDNA clone:001-024-H10, full insert sequence

Chain 4y: 97%



- Molecule 26: Photosystem II reaction center protein Z

Chain 1Z: 100%

There are no outlier residues recorded for this chain.

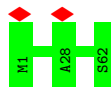
- Molecule 26: Photosystem II reaction center protein Z

Chain 1z: 100%

There are no outlier residues recorded for this chain.

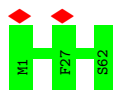
- Molecule 26: Photosystem II reaction center protein Z

Chain 2Z: 100%



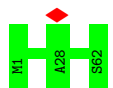
- Molecule 26: Photosystem II reaction center protein Z

Chain 2z: 100%



- Molecule 26: Photosystem II reaction center protein Z

Chain 3Z:  100%



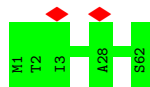
- Molecule 26: Photosystem II reaction center protein Z

Chain 3z:  100%

There are no outlier residues recorded for this chain.

- Molecule 26: Photosystem II reaction center protein Z

Chain 4Z:  100%



- Molecule 26: Photosystem II reaction center protein Z

Chain 4z:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	83210	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 ($e^-/\text{\AA}^2$)	1.375	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.715	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	737.9968, 737.9968, 737.9968	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4414, 1.4414, 1.4414	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	00	0.27	0/1113	0.62	3/1552 (0.2%)
1	01	0.28	1/1112 (0.1%)	0.69	2/1550 (0.1%)
1	02	0.27	0/1089	0.63	0/1516
1	05	0.26	0/1064	0.70	0/1482
1	06	0.58	3/1045 (0.3%)	1.12	10/1454 (0.7%)
1	09	0.25	0/1113	0.56	0/1552
1	10	0.25	0/1113	0.61	3/1552 (0.2%)
1	11	0.29	1/1112 (0.1%)	0.69	2/1550 (0.1%)
1	12	0.27	0/1089	0.63	0/1516
1	15	0.25	0/1064	0.70	0/1482
1	16	0.58	3/1045 (0.3%)	1.12	10/1454 (0.7%)
1	19	0.24	0/1113	0.55	0/1552
1	1G	0.27	0/1113	0.57	0/1552
1	1N	0.36	0/1113	0.75	3/1552 (0.2%)
1	1g	0.26	0/1113	0.59	0/1552
1	1n	0.24	0/1113	0.53	0/1552
1	2G	0.27	0/1113	0.57	0/1552
1	2N	0.36	1/1113 (0.1%)	0.75	3/1552 (0.2%)
1	2g	0.26	0/1113	0.59	0/1552
1	2n	0.23	0/1113	0.53	0/1552
1	30	0.27	0/1113	0.62	3/1552 (0.2%)
1	31	0.28	1/1112 (0.1%)	0.69	2/1550 (0.1%)
1	32	0.27	0/1089	0.63	0/1516
1	35	0.26	0/1064	0.70	0/1482
1	36	0.58	3/1045 (0.3%)	1.12	10/1454 (0.7%)
1	39	0.25	0/1113	0.59	0/1552
1	3G	0.27	0/1113	0.57	0/1552
1	3N	0.36	0/1113	0.75	3/1552 (0.2%)
1	3g	0.26	0/1113	0.59	0/1552
1	3n	0.24	0/1113	0.53	0/1552
1	40	0.27	0/1113	0.62	3/1552 (0.2%)
1	41	0.28	1/1112 (0.1%)	0.69	2/1550 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	42	0.27	0/1089	0.64	0/1516
1	45	0.26	0/1064	0.70	0/1482
1	46	0.58	3/1045 (0.3%)	1.12	10/1454 (0.7%)
1	49	0.25	0/1113	0.56	0/1552
1	4G	0.27	0/1113	0.57	0/1552
1	4N	0.36	0/1113	0.75	3/1552 (0.2%)
1	4g	0.26	0/1113	0.59	0/1552
1	4n	0.24	0/1113	0.53	0/1552
2	03	0.24	0/1113	0.67	0/1551
2	07	0.29	0/1115	0.72	1/1554 (0.1%)
2	13	0.24	0/1113	0.67	0/1551
2	17	0.29	0/1115	0.73	1/1554 (0.1%)
2	33	0.24	0/1113	0.67	0/1551
2	37	0.29	0/1115	0.73	1/1554 (0.1%)
2	43	0.24	0/1113	0.67	0/1551
2	47	0.29	0/1115	0.73	1/1554 (0.1%)
3	04	0.32	0/1020	0.82	4/1424 (0.3%)
3	08	0.32	0/1044	0.73	1/1457 (0.1%)
3	14	0.32	0/1020	0.82	4/1424 (0.3%)
3	18	0.32	0/1044	0.73	1/1457 (0.1%)
3	34	0.32	0/1020	0.82	4/1424 (0.3%)
3	38	0.32	0/1044	0.73	1/1457 (0.1%)
3	44	0.32	0/1020	0.82	4/1424 (0.3%)
3	48	0.32	0/1044	0.73	1/1457 (0.1%)
4	1A	0.28	0/1679	0.61	0/2341
4	1a	0.28	0/1674	0.61	1/2334 (0.0%)
4	2A	0.28	0/1679	0.61	0/2341
4	2a	0.27	0/1674	0.61	1/2334 (0.0%)
4	3A	0.28	0/1679	0.61	0/2341
4	3a	0.27	0/1674	0.61	1/2334 (0.0%)
4	4A	0.28	0/1679	0.61	0/2341
4	4a	0.27	0/1674	0.61	1/2334 (0.0%)
5	1B	0.24	0/2537	0.54	0/3536
5	1b	0.24	0/2537	0.55	2/3536 (0.1%)
5	2B	0.24	0/2537	0.54	0/3536
5	2b	0.24	0/2537	0.55	2/3536 (0.1%)
5	3B	0.24	0/2537	0.54	0/3536
5	3b	0.24	0/2537	0.55	4/3536 (0.1%)
5	4B	0.24	0/2537	0.54	0/3536
5	4b	0.24	0/2537	0.55	2/3536 (0.1%)
6	1C	0.36	2/2261 (0.1%)	0.79	3/3147 (0.1%)
6	1c	0.22	0/2260	0.54	0/3145
6	2C	0.36	2/2261 (0.1%)	0.79	3/3147 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	2c	0.22	0/2260	0.54	0/3145
6	3C	0.36	2/2261 (0.1%)	0.79	3/3147 (0.1%)
6	3c	0.22	0/2260	0.54	0/3145
6	4C	0.36	2/2261 (0.1%)	0.79	3/3147 (0.1%)
6	4c	0.22	0/2260	0.54	0/3145
7	1D	0.29	1/1711 (0.1%)	0.64	2/2387 (0.1%)
7	1d	0.45	2/1716 (0.1%)	0.89	6/2394 (0.3%)
7	2D	0.29	1/1711 (0.1%)	0.64	2/2387 (0.1%)
7	2d	0.45	2/1716 (0.1%)	0.89	6/2394 (0.3%)
7	3D	0.29	1/1711 (0.1%)	0.64	2/2387 (0.1%)
7	3d	0.45	2/1716 (0.1%)	0.89	6/2394 (0.3%)
7	4D	0.29	1/1711 (0.1%)	0.64	2/2387 (0.1%)
7	4d	0.45	2/1716 (0.1%)	0.89	6/2394 (0.3%)
8	1E	0.27	0/382	0.52	0/534
8	1e	0.25	0/382	0.55	0/534
8	2E	0.27	0/382	0.52	0/534
8	2e	0.25	0/382	0.55	0/534
8	3E	0.27	0/382	0.52	0/534
8	3e	0.25	0/382	0.55	0/534
8	4E	0.27	0/382	0.52	0/534
8	4e	0.25	0/382	0.55	0/534
9	1F	0.44	0/178	0.68	0/248
9	1f	0.24	0/150	0.53	0/208
9	2F	0.44	0/178	0.68	0/248
9	2f	0.25	0/150	0.54	0/208
9	3F	0.44	0/178	0.68	0/248
9	3f	0.24	0/150	0.53	0/208
9	4F	0.44	0/178	0.68	0/248
9	4f	0.24	0/150	0.53	0/208
10	1H	0.23	0/304	0.64	0/423
10	1h	0.23	0/304	0.64	0/423
10	2H	0.23	0/304	0.65	0/423
10	2h	0.23	0/304	0.64	0/423
10	3H	0.23	0/304	0.64	0/423
10	3h	0.23	0/304	0.64	0/423
10	4H	0.23	0/304	0.64	0/423
10	4h	0.23	0/304	0.64	0/423
11	1I	0.72	0/172	1.65	5/239 (2.1%)
11	1i	0.24	0/172	0.65	0/239
11	2I	0.55	0/172	0.80	0/239
11	2i	0.24	0/172	0.65	0/239
11	3I	0.72	0/172	1.65	5/239 (2.1%)
11	3i	0.24	0/172	0.65	0/239

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	4I	0.72	0/172	1.65	5/239 (2.1%)
11	4i	0.25	0/172	0.65	0/239
12	1J	0.22	0/169	0.64	0/231
12	1j	0.34	0/169	0.78	1/231 (0.4%)
12	2J	0.22	0/169	0.65	0/231
12	2j	0.34	0/169	0.78	1/231 (0.4%)
12	3J	0.22	0/169	0.64	0/231
12	3j	0.34	0/169	0.78	1/231 (0.4%)
12	4J	0.22	0/169	0.64	0/231
12	4j	0.34	0/169	0.78	1/231 (0.4%)
13	1K	0.31	0/196	0.65	0/276
13	1k	0.30	0/196	0.59	0/276
13	2K	0.31	0/196	0.65	0/276
13	2k	0.30	0/196	0.59	0/276
13	3K	0.31	0/196	0.66	0/276
13	3k	0.30	0/196	0.59	0/276
13	4K	0.31	0/196	0.65	0/276
13	4k	0.30	0/196	0.59	0/276
14	1L	0.22	0/181	0.54	0/252
14	1l	0.24	0/176	0.64	0/245
14	2L	0.21	0/181	0.54	0/252
14	2l	0.24	0/176	0.64	0/245
14	3L	0.21	0/181	0.54	0/252
14	3l	0.24	0/176	0.64	0/245
14	4L	0.22	0/181	0.54	0/252
14	4l	0.24	0/176	0.64	0/245
15	1M	0.33	0/162	0.90	0/226
15	1m	0.35	0/167	0.67	0/233
15	2M	0.34	0/162	0.90	0/226
15	2m	0.35	0/167	0.67	0/233
15	3M	0.33	0/162	0.90	0/226
15	3m	0.36	0/167	0.67	0/233
15	4M	0.34	0/162	0.90	0/226
15	4m	0.36	0/167	0.67	0/233
16	1O	0.23	0/1254	0.61	1/1750 (0.1%)
16	1o	0.22	0/1198	0.53	0/1669
16	2O	0.23	0/1254	0.61	1/1750 (0.1%)
16	2o	0.22	0/1198	0.53	0/1669
16	3O	0.23	0/1254	0.61	1/1750 (0.1%)
16	3o	0.22	0/1198	0.53	0/1669
16	4O	0.23	0/1254	0.62	1/1750 (0.1%)
16	4o	0.21	0/1198	0.53	0/1669
17	1P	0.19	0/932	0.53	0/1298

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	1p	0.17	0/932	0.45	0/1298
17	2P	0.19	0/932	0.53	0/1298
17	2p	0.17	0/932	0.45	0/1298
17	3P	0.19	0/932	0.53	0/1298
17	3p	0.17	0/932	0.45	0/1298
17	4P	0.19	0/932	0.53	0/1298
17	4p	0.17	0/932	0.45	0/1298
18	1R	0.24	0/1191	0.55	0/1664
18	1r	0.21	0/1191	0.52	0/1664
18	2R	0.24	0/1191	0.55	0/1664
18	2r	0.21	0/1191	0.52	0/1664
18	3R	0.24	0/1191	0.55	0/1664
18	3r	0.21	0/1191	0.52	0/1664
18	4R	0.24	0/1191	0.55	0/1664
18	4r	0.21	0/1191	0.52	0/1664
19	1S	0.24	0/1108	0.59	0/1546
19	1s	0.25	0/1103	0.62	0/1539
19	2S	0.24	0/1108	0.59	0/1546
19	2s	0.25	0/1103	0.62	0/1539
19	3S	0.24	0/1108	0.59	0/1546
19	3s	0.25	0/1103	0.62	0/1539
19	4S	0.24	0/1108	0.59	0/1546
19	4s	0.25	0/1103	0.62	0/1539
20	1T	0.18	0/167	0.40	0/234
20	1t	0.17	0/162	0.40	0/227
20	2T	0.19	0/167	0.40	0/234
20	2t	0.17	0/162	0.40	0/227
20	3T	0.18	0/167	0.40	0/234
20	3t	0.17	0/162	0.40	0/227
20	4T	0.18	0/167	0.40	0/234
20	4t	0.17	0/162	0.40	0/227
21	1U	0.15	0/139	0.37	0/194
21	1u	0.20	0/139	0.51	0/194
21	2U	0.14	0/139	0.37	0/194
21	2u	0.20	0/139	0.51	0/194
21	3U	0.14	0/139	0.37	0/194
21	3u	0.20	0/139	0.51	0/194
21	4U	0.14	0/139	0.37	0/194
21	4u	0.20	0/139	0.51	0/194
22	1V	0.21	0/485	0.52	0/671
22	1v	0.28	0/490	0.71	1/678 (0.1%)
22	2V	0.21	0/485	0.52	0/671
22	2v	0.28	0/490	0.70	1/678 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
22	3V	0.21	0/485	0.52	0/671
22	3v	0.28	0/490	0.71	1/678 (0.1%)
22	4V	0.22	0/485	0.52	0/671
22	4v	0.29	0/490	0.70	1/678 (0.1%)
23	1W	0.27	0/261	0.56	0/359
23	1w	0.21	0/213	0.55	0/293
23	2W	0.28	0/261	0.56	0/359
23	2w	0.21	0/213	0.55	0/293
23	3W	0.27	0/261	0.56	0/359
23	3w	0.21	0/213	0.55	0/293
23	4W	0.27	0/261	0.56	0/359
23	4w	0.21	0/213	0.56	0/293
24	1X	0.20	0/196	0.39	0/272
24	1x	0.22	0/192	0.48	0/267
24	2X	0.20	0/196	0.40	0/272
24	2x	0.23	0/192	0.48	0/267
24	3X	0.20	0/196	0.40	0/272
24	3x	0.23	0/192	0.48	0/267
24	4X	0.20	0/196	0.40	0/272
24	4x	0.22	0/192	0.48	0/267
25	1Y	0.30	0/177	0.61	0/248
25	1y	0.27	0/177	0.54	0/248
25	2Y	0.30	0/177	0.61	0/248
25	2y	0.27	0/177	0.55	0/248
25	3Y	0.30	0/177	0.60	0/248
25	3y	0.27	0/177	0.54	0/248
25	4Y	0.30	0/177	0.60	0/248
25	4y	0.27	0/177	0.54	0/248
26	1Z	0.30	0/312	0.58	0/435
26	1z	0.24	0/312	0.47	0/435
26	2Z	0.29	0/312	0.58	0/435
26	2z	0.24	0/312	0.47	0/435
26	3Z	0.30	0/312	0.58	0/435
26	3z	0.24	0/312	0.47	0/435
26	4Z	0.30	0/312	0.58	0/435
26	4z	0.24	0/312	0.47	0/435
All	All	0.29	37/189784 (0.0%)	0.65	181/264484 (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
1	02	0	1
1	05	0	1
1	06	0	1
1	12	0	1
1	15	0	1
1	16	0	1
1	1G	0	1
1	1N	0	2
1	1n	0	1
1	2G	0	1
1	2N	0	2
1	2n	0	1
1	32	0	1
1	35	0	1
1	36	0	1
1	3G	0	1
1	3N	0	2
1	3n	0	1
1	42	0	1
1	45	0	1
1	46	0	1
1	4G	0	1
1	4N	0	2
1	4n	0	1
3	04	0	1
3	14	0	1
3	34	0	1
3	44	0	1
4	1a	0	1
4	2a	0	1
4	3a	0	1
4	4a	0	1
16	1o	0	1
16	2o	0	1
16	3o	0	1
16	4o	0	1
All	All	0	40

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	4d	172	PRO	CB-CG	-11.40	0.92	1.49
7	1d	172	PRO	CB-CG	-11.40	0.92	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	3d	172	PRO	CB-CG	-11.39	0.92	1.49
7	2d	172	PRO	CB-CG	-11.39	0.92	1.49
1	36	82	PRO	CG-CD	-9.82	1.17	1.50
1	06	82	PRO	CG-CD	-9.81	1.17	1.50
1	46	82	PRO	CG-CD	-9.81	1.17	1.50
1	16	82	PRO	CG-CD	-9.78	1.17	1.50
6	3C	80	PRO	CG-CD	-9.57	1.18	1.50
6	4C	80	PRO	CG-CD	-9.56	1.18	1.50
6	1C	80	PRO	CG-CD	-9.55	1.18	1.50
6	2C	80	PRO	CG-CD	-9.54	1.18	1.50
1	36	170	PRO	CG-CD	-9.07	1.20	1.50
1	46	170	PRO	CG-CD	-9.06	1.20	1.50
1	16	170	PRO	CG-CD	-9.06	1.20	1.50
1	06	170	PRO	CG-CD	-9.05	1.20	1.50
7	2d	172	PRO	CG-CD	-9.02	1.20	1.50
7	4d	172	PRO	CG-CD	-9.01	1.20	1.50
7	3d	172	PRO	CG-CD	-9.01	1.20	1.50
7	1d	172	PRO	CG-CD	-9.00	1.20	1.50
1	06	82	PRO	CB-CG	-8.94	1.04	1.49
1	46	82	PRO	CB-CG	-8.93	1.04	1.49
1	36	82	PRO	CB-CG	-8.92	1.05	1.49
1	16	82	PRO	CB-CG	-8.92	1.05	1.49
6	1C	80	PRO	CB-CG	-8.86	1.05	1.49
6	2C	80	PRO	CB-CG	-8.85	1.05	1.49
6	3C	80	PRO	CB-CG	-8.85	1.05	1.49
6	4C	80	PRO	CB-CG	-8.85	1.05	1.49
7	1D	39	PHE	C-N	5.34	1.38	1.33
7	4D	39	PHE	C-N	5.31	1.38	1.33
7	2D	39	PHE	C-N	5.27	1.38	1.33
7	3D	39	PHE	C-N	5.24	1.38	1.33
1	11	216	PRO	CG-CD	-5.17	1.33	1.50
1	41	216	PRO	CG-CD	-5.17	1.33	1.50
1	31	216	PRO	CG-CD	-5.16	1.33	1.50
1	01	216	PRO	CG-CD	-5.16	1.33	1.50
1	2N	24	TYR	C-N	5.03	1.39	1.33

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	4C	80	PRO	CB-CG-CD	23.09	179.99	106.10
6	1C	80	PRO	CB-CG-CD	23.08	179.96	106.10
6	3C	80	PRO	CB-CG-CD	23.08	179.95	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2C	80	PRO	CB-CG-CD	23.05	179.85	106.10
1	16	82	PRO	N-CD-CG	-19.33	74.20	103.20
1	36	82	PRO	N-CD-CG	-19.31	74.23	103.20
1	06	82	PRO	N-CD-CG	-19.31	74.23	103.20
1	46	82	PRO	N-CD-CG	-19.30	74.25	103.20
1	36	82	PRO	CA-CB-CG	-18.66	69.05	104.50
1	06	82	PRO	CA-CB-CG	-18.65	69.06	104.50
1	16	82	PRO	CA-CB-CG	-18.64	69.07	104.50
1	46	82	PRO	CA-CB-CG	-18.63	69.10	104.50
6	2C	80	PRO	N-CD-CG	-18.01	76.19	103.20
6	3C	80	PRO	N-CD-CG	-18.01	76.18	103.20
6	4C	80	PRO	N-CD-CG	-17.99	76.21	103.20
6	1C	80	PRO	N-CD-CG	-17.98	76.23	103.20
7	2d	172	PRO	N-CD-CG	-17.72	76.62	103.20
7	4d	172	PRO	N-CD-CG	-17.71	76.64	103.20
7	3d	172	PRO	N-CD-CG	-17.71	76.64	103.20
7	1d	172	PRO	N-CD-CG	-17.66	76.71	103.20
7	1d	172	PRO	CB-CG-CD	17.62	162.47	106.10
7	3d	172	PRO	CB-CG-CD	17.61	162.45	106.10
7	2d	172	PRO	CB-CG-CD	17.60	162.43	106.10
7	4d	172	PRO	CB-CG-CD	17.59	162.38	106.10
7	2d	172	PRO	CA-CB-CG	-15.79	74.50	104.50
7	3d	172	PRO	CA-CB-CG	-15.78	74.52	104.50
7	1d	172	PRO	CA-CB-CG	-15.78	74.53	104.50
7	4d	172	PRO	CA-CB-CG	-15.78	74.53	104.50
6	2C	80	PRO	CA-CB-CG	-15.02	75.97	104.50
6	4C	80	PRO	CA-CB-CG	-14.97	76.06	104.50
6	3C	80	PRO	CA-CB-CG	-14.96	76.07	104.50
6	1C	80	PRO	CA-CB-CG	-14.94	76.11	104.50
11	4I	10	THR	N-CA-C	-14.79	95.24	111.36
11	3I	10	THR	N-CA-C	-14.79	95.24	111.36
11	1I	10	THR	N-CA-C	-14.71	95.33	111.36
1	36	82	PRO	CB-CG-CD	11.50	142.91	106.10
1	06	82	PRO	CB-CG-CD	11.50	142.90	106.10
1	46	82	PRO	CB-CG-CD	11.49	142.87	106.10
1	16	82	PRO	CB-CG-CD	11.48	142.83	106.10
1	06	170	PRO	N-CD-CG	-10.79	87.02	103.20
1	46	170	PRO	N-CD-CG	-10.78	87.03	103.20
11	3I	5	LYS	N-CA-C	-10.77	98.79	112.90
1	36	170	PRO	N-CD-CG	-10.77	87.05	103.20
1	16	170	PRO	N-CD-CG	-10.75	87.07	103.20
11	1I	5	LYS	N-CA-C	-10.75	98.81	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	4I	5	LYS	N-CA-C	-10.74	98.83	112.90
1	06	170	PRO	CA-N-CD	-10.42	97.42	112.00
1	46	170	PRO	CA-N-CD	-10.40	97.43	112.00
1	36	170	PRO	CA-N-CD	-10.39	97.45	112.00
1	16	170	PRO	CA-N-CD	-10.37	97.48	112.00
11	4I	6	LEU	N-CA-C	-9.19	101.21	111.14
11	3I	6	LEU	N-CA-C	-9.18	101.22	111.14
11	1I	6	LEU	N-CA-C	-9.18	101.23	111.14
1	01	216	PRO	N-CD-CG	-8.46	90.52	103.20
1	41	216	PRO	N-CD-CG	-8.45	90.52	103.20
1	11	216	PRO	N-CD-CG	-8.42	90.57	103.20
1	31	216	PRO	N-CD-CG	-8.40	90.60	103.20
1	3N	170	PRO	CA-N-CD	-8.27	100.43	112.00
1	4N	170	PRO	CA-N-CD	-8.24	100.46	112.00
1	2N	170	PRO	CA-N-CD	-8.24	100.46	112.00
1	1N	170	PRO	CA-N-CD	-8.24	100.47	112.00
1	06	82	PRO	CA-N-CD	-7.94	100.89	112.00
1	16	82	PRO	CA-N-CD	-7.93	100.89	112.00
1	36	82	PRO	CA-N-CD	-7.93	100.89	112.00
1	46	82	PRO	CA-N-CD	-7.92	100.91	112.00
5	1b	201	HIS	CB-CA-C	7.81	122.19	109.07
5	2b	201	HIS	CB-CA-C	7.79	122.16	109.07
5	4b	192	PRO	CA-N-CD	-7.58	101.39	112.00
5	1b	192	PRO	CA-N-CD	-7.54	101.44	112.00
5	3b	192	PRO	CA-N-CD	-7.54	101.44	112.00
5	2b	192	PRO	CA-N-CD	-7.54	101.44	112.00
5	4b	201	HIS	CB-CA-C	7.54	122.21	109.55
5	3b	201	HIS	CB-CA-C	7.51	122.17	109.55
1	3N	24	TYR	CA-C-N	-7.48	111.85	125.02
1	3N	24	TYR	C-N-CA	-7.48	111.85	125.02
1	4N	24	TYR	CA-C-N	-7.45	111.90	125.02
1	4N	24	TYR	C-N-CA	-7.45	111.90	125.02
1	2N	24	TYR	CA-C-N	-7.45	111.91	125.02
1	2N	24	TYR	C-N-CA	-7.45	111.91	125.02
1	1N	24	TYR	CA-C-N	-7.45	111.91	125.02
1	1N	24	TYR	C-N-CA	-7.45	111.91	125.02
1	36	170	PRO	CA-CB-CG	-6.95	91.30	104.50
1	46	170	PRO	CA-CB-CG	-6.94	91.31	104.50
1	06	170	PRO	CA-CB-CG	-6.94	91.31	104.50
1	16	170	PRO	CA-CB-CG	-6.94	91.31	104.50
1	11	216	PRO	CA-N-CD	-6.92	102.32	112.00
1	31	216	PRO	CA-N-CD	-6.91	102.33	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	01	216	PRO	CA-N-CD	-6.90	102.34	112.00
1	41	216	PRO	CA-N-CD	-6.87	102.38	112.00
4	1a	320	ILE	N-CA-C	-6.81	107.24	113.71
7	2d	172	PRO	CA-N-CD	-6.81	102.47	112.00
4	4a	320	ILE	N-CA-C	-6.78	107.27	113.71
7	3d	172	PRO	CA-N-CD	-6.78	102.51	112.00
7	1d	172	PRO	CA-N-CD	-6.77	102.52	112.00
4	3a	320	ILE	N-CA-C	-6.76	107.28	113.71
7	4d	172	PRO	CA-N-CD	-6.76	102.53	112.00
4	2a	320	ILE	N-CA-C	-6.72	107.33	113.71
3	38	46	PHE	N-CA-C	-6.66	105.29	113.41
3	08	46	PHE	N-CA-C	-6.64	105.31	113.41
3	48	46	PHE	N-CA-C	-6.63	105.32	113.41
3	18	46	PHE	N-CA-C	-6.62	105.33	113.41
11	1I	3	THR	N-CA-C	-6.12	104.61	111.28
11	4I	3	THR	N-CA-C	-6.07	104.66	111.28
11	3I	3	THR	N-CA-C	-6.06	104.67	111.28
11	1I	9	TYR	N-CA-C	-5.98	98.06	110.80
11	3I	9	TYR	N-CA-C	-5.98	98.07	110.80
11	4I	9	TYR	N-CA-C	-5.98	98.07	110.80
1	46	82	PRO	N-CA-CB	-5.87	97.05	103.39
1	06	82	PRO	N-CA-CB	-5.86	97.07	103.39
1	36	82	PRO	N-CA-CB	-5.83	97.10	103.39
1	16	82	PRO	N-CA-CB	-5.79	97.13	103.39
16	4O	49	LYS	N-CA-C	5.72	115.83	108.34
16	1O	49	LYS	N-CA-C	5.72	115.83	108.34
16	2O	49	LYS	N-CA-C	5.71	115.82	108.34
16	3O	49	LYS	N-CA-C	5.69	115.80	108.34
12	4j	9	PRO	CA-N-CD	-5.62	104.13	112.00
12	2j	9	PRO	CA-N-CD	-5.62	104.14	112.00
12	3j	9	PRO	CA-N-CD	-5.61	104.14	112.00
12	1j	9	PRO	CA-N-CD	-5.61	104.15	112.00
7	4D	267	TRP	CA-C-N	5.56	132.16	121.54
7	4D	267	TRP	C-N-CA	5.56	132.16	121.54
2	07	77	HIS	N-CA-CB	5.56	118.29	110.12
3	04	13	PHE	CA-C-N	5.55	132.13	121.54
3	04	13	PHE	C-N-CA	5.55	132.13	121.54
3	34	13	PHE	CA-C-N	5.54	132.12	121.54
3	34	13	PHE	C-N-CA	5.54	132.12	121.54
7	3D	267	TRP	CA-C-N	5.54	132.12	121.54
7	3D	267	TRP	C-N-CA	5.54	132.12	121.54
7	1D	267	TRP	CA-C-N	5.53	132.11	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	1D	267	TRP	C-N-CA	5.53	132.11	121.54
7	2D	267	TRP	CA-C-N	5.53	132.11	121.54
7	2D	267	TRP	C-N-CA	5.53	132.11	121.54
3	14	13	PHE	CA-C-N	5.53	132.11	121.54
3	14	13	PHE	C-N-CA	5.53	132.11	121.54
1	16	78	GLY	CA-C-N	5.53	129.95	120.71
1	16	78	GLY	C-N-CA	5.53	129.95	120.71
2	17	77	HIS	N-CA-CB	5.52	118.34	110.06
3	44	13	PHE	CA-C-N	5.51	132.07	121.54
3	44	13	PHE	C-N-CA	5.51	132.07	121.54
1	06	78	GLY	CA-C-N	5.50	129.90	120.71
1	06	78	GLY	C-N-CA	5.50	129.90	120.71
2	47	77	HIS	N-CA-CB	5.50	118.31	110.06
1	36	78	GLY	CA-C-N	5.50	129.89	120.71
1	36	78	GLY	C-N-CA	5.50	129.89	120.71
2	37	77	HIS	N-CA-CB	5.48	118.28	110.06
1	46	78	GLY	CA-C-N	5.47	129.85	120.71
1	46	78	GLY	C-N-CA	5.47	129.85	120.71
22	4v	93	LEU	N-CA-C	-5.39	105.30	111.07
22	2v	93	LEU	N-CA-C	-5.39	105.31	111.07
3	34	20	ILE	CA-C-N	5.38	128.31	120.51
3	34	20	ILE	C-N-CA	5.38	128.31	120.51
3	44	20	ILE	CA-C-N	5.38	128.30	120.51
3	44	20	ILE	C-N-CA	5.38	128.30	120.51
3	04	20	ILE	CA-C-N	5.37	128.29	120.51
3	04	20	ILE	C-N-CA	5.37	128.29	120.51
22	3v	93	LEU	N-CA-C	-5.37	105.33	111.07
22	1v	93	LEU	N-CA-C	-5.36	105.34	111.07
1	30	159	GLY	N-CA-C	5.35	119.35	112.83
3	14	20	ILE	CA-C-N	5.33	128.24	120.51
3	14	20	ILE	C-N-CA	5.33	128.24	120.51
1	40	159	GLY	N-CA-C	5.33	119.33	112.83
1	00	159	GLY	N-CA-C	5.33	119.33	112.83
1	10	159	GLY	N-CA-C	5.31	119.31	112.83
1	10	158	GLY	CA-C-N	5.20	125.85	120.03
1	10	158	GLY	C-N-CA	5.20	125.85	120.03
7	2d	29	VAL	CA-C-N	5.16	129.62	121.56
7	2d	29	VAL	C-N-CA	5.16	129.62	121.56
7	4d	29	VAL	CA-C-N	5.16	129.61	121.56
7	4d	29	VAL	C-N-CA	5.16	129.61	121.56
7	3d	29	VAL	CA-C-N	5.15	129.60	121.56
7	3d	29	VAL	C-N-CA	5.15	129.60	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	1d	29	VAL	CA-C-N	5.14	129.58	121.56
7	1d	29	VAL	C-N-CA	5.14	129.58	121.56
1	40	158	GLY	CA-C-N	5.12	125.77	120.03
1	40	158	GLY	C-N-CA	5.12	125.77	120.03
1	00	158	GLY	CA-C-N	5.10	125.74	120.03
1	00	158	GLY	C-N-CA	5.10	125.74	120.03
1	30	158	GLY	CA-C-N	5.10	125.74	120.03
1	30	158	GLY	C-N-CA	5.10	125.74	120.03
5	3b	200	SER	CA-C-N	-5.00	114.31	122.26
5	3b	200	SER	C-N-CA	-5.00	114.31	122.26

There are no chirality outliers.

All (40) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	02	156	TYR	Peptide
3	04	104	LEU	Peptide
1	05	95	ALA	Peptide
1	06	189	PHE	Peptide
1	12	156	TYR	Peptide
3	14	104	LEU	Peptide
1	15	95	ALA	Peptide
1	16	189	PHE	Peptide
1	1G	192	PHE	Peptide
1	1N	192	PHE	Peptide
1	1N	24	TYR	Peptide
4	1a	340	PRO	Peptide
1	1n	192	PHE	Peptide
16	1o	92	PRO	Peptide
1	2G	192	PHE	Peptide
1	2N	192	PHE	Peptide
1	2N	24	TYR	Peptide
4	2a	340	PRO	Peptide
1	2n	192	PHE	Peptide
16	2o	92	PRO	Peptide
1	32	156	TYR	Peptide
3	34	104	LEU	Peptide
1	35	95	ALA	Peptide
1	36	189	PHE	Peptide
1	3G	192	PHE	Peptide
1	3N	192	PHE	Peptide
1	3N	24	TYR	Peptide

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Mol	Chain	Res	Type	Group
4	3a	340	PRO	Peptide
1	3n	192	PHE	Peptide
16	3o	92	PRO	Peptide
1	42	156	TYR	Peptide
3	44	104	LEU	Peptide
1	45	95	ALA	Peptide
1	46	189	PHE	Peptide
1	4G	192	PHE	Peptide
1	4N	192	PHE	Peptide
1	4N	24	TYR	Peptide
4	4a	340	PRO	Peptide
1	4n	192	PHE	Peptide
16	4o	92	PRO	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	00	1098	0	618	4	0
1	01	1097	0	618	1	0
1	02	1076	0	604	2	0
1	05	1052	0	582	0	0
1	06	1034	0	571	3	0
1	09	1098	0	618	2	0
1	10	1098	0	618	2	0
1	11	1097	0	618	1	0
1	12	1076	0	604	2	0
1	15	1052	0	582	0	0
1	16	1034	0	571	3	0
1	19	1098	0	618	2	0
1	1G	1098	0	618	1	0
1	1N	1098	0	618	4	0
1	1g	1098	0	618	4	0
1	1n	1098	0	618	0	0
1	2G	1098	0	618	2	0
1	2N	1098	0	618	4	0
1	2g	1098	0	618	4	0
1	2n	1098	0	618	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	30	1098	0	618	4	0
1	31	1097	0	618	1	0
1	32	1076	0	604	2	0
1	35	1052	0	582	0	0
1	36	1034	0	571	2	0
1	39	1098	0	618	3	0
1	3G	1098	0	618	2	0
1	3N	1098	0	618	4	0
1	3g	1098	0	618	4	0
1	3n	1098	0	618	0	0
1	40	1098	0	618	4	0
1	41	1097	0	618	1	0
1	42	1076	0	604	2	0
1	45	1052	0	582	0	0
1	46	1034	0	571	2	0
1	49	1098	0	618	2	0
1	4G	1098	0	618	2	0
1	4N	1098	0	618	5	0
1	4g	1098	0	618	2	0
1	4n	1098	0	618	1	0
2	03	1100	0	596	1	0
2	07	1101	0	598	5	0
2	13	1100	0	596	1	0
2	17	1101	0	598	4	0
2	33	1100	0	596	2	0
2	37	1101	0	598	5	0
2	43	1100	0	596	2	0
2	47	1101	0	598	5	0
3	04	1006	0	564	1	0
3	08	1030	0	578	3	0
3	14	1006	0	564	2	0
3	18	1030	0	578	3	0
3	34	1006	0	564	2	0
3	38	1030	0	578	3	0
3	44	1006	0	564	1	0
3	48	1030	0	578	3	0
4	1A	1666	0	865	5	0
4	1a	1661	0	860	4	0
4	2A	1666	0	865	6	0
4	2a	1661	0	860	4	0
4	3A	1666	0	865	5	0
4	3a	1661	0	860	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	4A	1666	0	865	5	0
4	4a	1661	0	860	4	0
5	1B	2510	0	1326	3	0
5	1b	2510	0	1326	10	0
5	2B	2510	0	1326	2	0
5	2b	2510	0	1326	11	0
5	3B	2510	0	1326	3	0
5	3b	2510	0	1326	10	0
5	4B	2510	0	1326	2	0
5	4b	2510	0	1326	10	0
6	1C	2238	0	1199	1	0
6	1c	2237	0	1198	5	0
6	2C	2238	0	1199	1	0
6	2c	2237	0	1198	5	0
6	3C	2238	0	1199	1	0
6	3c	2237	0	1198	4	0
6	4C	2238	0	1199	2	0
6	4c	2237	0	1198	5	0
7	1D	1698	0	887	3	0
7	1d	1703	0	889	5	0
7	2D	1698	0	887	4	0
7	2d	1703	0	889	6	0
7	3D	1698	0	887	3	0
7	3d	1703	0	889	6	0
7	4D	1698	0	887	3	0
7	4d	1703	0	889	7	0
8	1E	379	0	182	1	0
8	1e	379	0	182	2	0
8	2E	379	0	182	2	0
8	2e	379	0	182	2	0
8	3E	379	0	182	1	0
8	3e	379	0	182	2	0
8	4E	379	0	182	1	0
8	4e	379	0	182	2	0
9	1F	177	0	90	1	0
9	1f	150	0	75	1	0
9	2F	177	0	90	1	0
9	2f	150	0	75	1	0
9	3F	177	0	90	1	0
9	3f	150	0	75	1	0
9	4F	177	0	90	1	0
9	4f	150	0	75	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	1H	301	0	158	0	0
10	1h	301	0	158	0	0
10	2H	301	0	158	0	0
10	2h	301	0	158	0	0
10	3H	301	0	158	0	0
10	3h	301	0	158	0	0
10	4H	301	0	158	0	0
10	4h	301	0	158	0	0
11	1I	171	0	83	11	0
11	1i	171	0	83	0	0
11	2I	171	0	83	6	0
11	2i	171	0	83	0	0
11	3I	171	0	83	12	0
11	3i	171	0	83	0	0
11	4I	171	0	83	11	0
11	4i	171	0	83	0	0
12	1J	169	0	85	0	0
12	1j	169	0	85	0	0
12	2J	169	0	85	0	0
12	2j	169	0	85	0	0
12	3J	169	0	85	0	0
12	3j	169	0	85	0	0
12	4J	169	0	85	0	0
12	4j	169	0	85	0	0
13	1K	193	0	108	0	0
13	1k	193	0	108	1	0
13	2K	193	0	108	0	0
13	2k	193	0	108	2	0
13	3K	193	0	108	1	0
13	3k	193	0	108	2	0
13	4K	193	0	108	1	0
13	4k	193	0	108	1	0
14	1L	181	0	80	0	0
14	1l	176	0	78	0	0
14	2L	181	0	80	0	0
14	2l	176	0	78	0	0
14	3L	181	0	80	0	0
14	3l	176	0	78	0	0
14	4L	181	0	80	0	0
14	4l	176	0	78	0	0
15	1M	162	0	83	0	0
15	1m	167	0	85	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	2M	162	0	83	1	0
15	2m	167	0	85	0	0
15	3M	162	0	83	1	0
15	3m	167	0	85	0	0
15	4M	162	0	83	0	0
15	4m	167	0	85	0	0
16	1O	1239	0	652	6	0
16	1o	1186	0	614	4	0
16	2O	1239	0	652	11	0
16	2o	1186	0	614	3	0
16	3O	1239	0	652	10	0
16	3o	1186	0	614	4	0
16	4O	1239	0	652	6	0
16	4o	1186	0	614	4	0
17	1P	926	0	484	2	0
17	1p	926	0	484	3	0
17	2P	926	0	484	2	0
17	2p	926	0	484	3	0
17	3P	926	0	484	2	0
17	3p	926	0	484	3	0
17	4P	926	0	484	2	0
17	4p	926	0	484	3	0
18	1R	1177	0	625	3	0
18	1r	1177	0	625	2	0
18	2R	1177	0	625	3	0
18	2r	1177	0	625	2	0
18	3R	1177	0	625	3	0
18	3r	1177	0	625	2	0
18	4R	1177	0	625	3	0
18	4r	1177	0	625	2	0
19	1S	1094	0	593	2	0
19	1s	1089	0	591	0	0
19	2S	1094	0	593	2	0
19	2s	1089	0	591	0	0
19	3S	1094	0	593	2	0
19	3s	1089	0	591	0	0
19	4S	1094	0	593	2	0
19	4s	1089	0	591	0	0
20	1T	165	0	88	0	0
20	1t	160	0	86	0	0
20	2T	165	0	88	0	0
20	2t	160	0	86	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	3T	165	0	88	1	0
20	3t	160	0	86	1	0
20	4T	165	0	88	0	0
20	4t	160	0	86	0	0
21	1U	138	0	73	1	0
21	1u	138	0	73	1	0
21	2U	138	0	73	0	0
21	2u	138	0	73	1	0
21	3U	138	0	73	1	0
21	3u	138	0	73	1	0
21	4U	138	0	73	0	0
21	4u	138	0	73	1	0
22	1V	482	0	264	0	0
22	1v	487	0	269	4	0
22	2V	482	0	264	0	0
22	2v	487	0	269	4	0
22	3V	482	0	264	0	0
22	3v	487	0	269	4	0
22	4V	482	0	264	0	0
22	4v	487	0	269	4	0
23	1W	262	0	118	0	0
23	1w	214	0	96	0	0
23	2W	262	0	118	0	0
23	2w	214	0	96	0	0
23	3W	262	0	118	0	0
23	3w	214	0	96	0	0
23	4W	262	0	118	0	0
23	4w	214	0	96	0	0
24	1X	195	0	100	0	0
24	1x	191	0	97	0	0
24	2X	195	0	100	0	0
24	2x	191	0	97	0	0
24	3X	195	0	100	0	0
24	3x	191	0	97	0	0
24	4X	195	0	100	0	0
24	4x	191	0	97	0	0
25	1Y	175	0	98	0	0
25	1y	175	0	98	0	0
25	2Y	175	0	98	0	0
25	2y	175	0	98	0	0
25	3Y	175	0	98	0	0
25	3y	175	0	98	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	4Y	175	0	98	0	0
25	4y	175	0	98	0	0
26	1Z	311	0	154	0	0
26	1z	311	0	154	0	0
26	2Z	311	0	154	0	0
26	2z	311	0	154	0	0
26	3Z	311	0	154	0	0
26	3z	311	0	154	0	0
26	4Z	311	0	154	0	0
26	4z	311	0	154	0	0
27	1A	1	0	0	0	0
27	1d	1	0	0	0	0
27	2A	1	0	0	0	0
27	2d	1	0	0	0	0
27	3A	1	0	0	0	0
27	3d	1	0	0	0	0
27	4A	1	0	0	0	0
27	4d	1	0	0	0	0
All	All	187864	0	100512	412	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 1.

All (412) 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)
16:2O:99:GLY:C	16:3O:98:ASP:CB	2.47	0.87
16:2O:99:GLY:O	16:3O:98:ASP:CB	2.28	0.82
16:2O:98:ASP:O	16:3O:98:ASP:C	2.25	0.78
1:06:97:TRP:H	1:06:205:PRO:HG3	1.51	0.75
1:36:97:TRP:H	1:36:205:PRO:HG3	1.51	0.75
1:16:97:TRP:H	1:16:205:PRO:HG3	1.51	0.74
1:46:97:TRP:H	1:46:205:PRO:HG3	1.51	0.73
2:07:144:LEU:O	2:07:148:VAL:N	2.26	0.68
5:1b:205:ALA:O	5:1b:209:GLY:N	2.27	0.68
5:4b:205:ALA:O	5:4b:209:GLY:N	2.27	0.67
4:1A:85:THR:HA	4:1A:109:GLY:HA3	1.76	0.67
5:4b:165:GLY:HA3	5:4b:179:GLN:O	1.95	0.66
4:3A:85:THR:HA	4:3A:109:GLY:HA3	1.76	0.66
5:3b:205:ALA:O	5:3b:209:GLY:N	2.27	0.66
2:17:144:LEU:O	2:17:148:VAL:N	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2A:85:THR:HA	4:2A:109:GLY:HA3	1.77	0.66
5:2b:165:GLY:HA3	5:2b:179:GLN:O	1.95	0.66
5:2b:205:ALA:O	5:2b:209:GLY:N	2.27	0.66
2:37:144:LEU:O	2:37:148:VAL:N	2.26	0.66
5:1b:165:GLY:HA3	5:1b:179:GLN:O	1.95	0.66
5:3b:165:GLY:HA3	5:3b:179:GLN:O	1.95	0.65
4:4A:85:THR:HA	4:4A:109:GLY:HA3	1.77	0.65
2:47:144:LEU:O	2:47:148:VAL:N	2.27	0.65
5:3b:497:LYS:HA	7:3d:25:ARG:HA	1.79	0.65
5:1b:497:LYS:HA	7:1d:25:ARG:HA	1.79	0.64
5:4b:497:LYS:HA	7:4d:25:ARG:HA	1.79	0.64
5:2b:497:LYS:HA	7:2d:25:ARG:HA	1.79	0.64
17:4p:57:SER:HA	17:4p:162:GLN:O	1.99	0.64
17:3p:57:SER:HA	17:3p:162:GLN:O	1.99	0.63
17:2p:57:SER:HA	17:2p:162:GLN:O	1.99	0.63
17:1p:57:SER:HA	17:1p:162:GLN:O	1.99	0.62
2:43:114:ILE:HA	2:43:119:GLY:HA2	1.81	0.61
2:13:114:ILE:HA	2:13:119:GLY:HA2	1.81	0.61
5:1b:124:CYS:HA	5:1b:131:PRO:HA	1.83	0.61
5:3b:124:CYS:HA	5:3b:131:PRO:HA	1.83	0.61
2:03:114:ILE:HA	2:03:119:GLY:HA2	1.81	0.61
2:33:114:ILE:HA	2:33:119:GLY:HA2	1.81	0.61
18:3R:214:VAL:HA	18:3R:217:ALA:HB3	1.83	0.61
18:4R:214:VAL:HA	18:4R:217:ALA:HB3	1.83	0.60
11:3I:7:PHE:C	11:3I:9:TYR:N	2.57	0.60
5:4b:124:CYS:HA	5:4b:131:PRO:HA	1.83	0.60
18:1R:214:VAL:HA	18:1R:217:ALA:HB3	1.83	0.60
5:2b:124:CYS:HA	5:2b:131:PRO:HA	1.82	0.59
11:4I:13:ILE:O	11:4I:14:PHE:C	2.44	0.59
18:2R:214:VAL:HA	18:2R:217:ALA:HB3	1.84	0.59
11:4I:7:PHE:C	11:4I:9:TYR:N	2.57	0.59
11:3I:13:ILE:O	11:3I:14:PHE:C	2.44	0.59
1:19:191:MET:O	1:19:192:PHE:C	2.46	0.59
1:3N:170:PRO:HD2	1:3N:171:GLU:H	1.68	0.59
3:48:46:PHE:O	3:48:49:TRP:N	2.36	0.59
11:1I:7:PHE:C	11:1I:9:TYR:N	2.57	0.58
11:1I:13:ILE:O	11:1I:14:PHE:C	2.44	0.58
3:08:46:PHE:O	3:08:49:TRP:N	2.36	0.58
1:2N:170:PRO:HD2	1:2N:171:GLU:H	1.68	0.58
11:1I:1:MET:O	11:1I:5:LYS:N	2.37	0.58
3:38:46:PHE:O	3:38:49:TRP:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:3I:1:MET:O	11:3I:5:LYS:N	2.37	0.58
1:1N:170:PRO:HD2	1:1N:171:GLU:H	1.68	0.57
1:4N:170:PRO:HD2	1:4N:171:GLU:H	1.68	0.57
11:4I:1:MET:O	11:4I:5:LYS:N	2.37	0.57
16:1O:135:ALA:HA	16:1O:143:GLY:O	2.05	0.57
3:18:46:PHE:O	3:18:49:TRP:N	2.36	0.57
5:1b:471:ALA:HB1	7:1d:141:PRO:HG2	1.87	0.57
16:4O:135:ALA:HA	16:4O:143:GLY:O	2.05	0.57
5:2b:471:ALA:HB1	7:2d:141:PRO:HG2	1.87	0.57
7:2D:162:PRO:HB3	7:2D:171:ALA:HB2	1.87	0.56
7:3D:162:PRO:HB3	7:3D:171:ALA:HB2	1.87	0.56
5:3b:471:ALA:HB1	7:3d:141:PRO:HG2	1.87	0.56
7:4D:162:PRO:HB3	7:4D:171:ALA:HB2	1.87	0.56
5:4b:471:ALA:HB1	7:4d:141:PRO:HG2	1.87	0.56
16:2O:135:ALA:HA	16:2O:143:GLY:O	2.05	0.56
4:4A:194:MET:O	4:4A:300:PHE:N	2.39	0.56
4:1A:194:MET:O	4:1A:300:PHE:N	2.39	0.55
7:1D:162:PRO:HB3	7:1D:171:ALA:HB2	1.87	0.55
16:3O:135:ALA:HA	16:3O:143:GLY:O	2.05	0.55
4:3A:194:MET:O	4:3A:300:PHE:N	2.39	0.55
1:49:193:GLY:O	1:49:194:PHE:C	2.50	0.55
1:09:193:GLY:O	1:09:194:PHE:C	2.50	0.54
13:2k:52:PHE:O	13:2k:56:ALA:N	2.40	0.54
4:3a:85:THR:HA	4:3a:109:GLY:HA3	1.90	0.54
13:4k:52:PHE:O	13:4k:56:ALA:N	2.40	0.54
4:1a:85:THR:HA	4:1a:109:GLY:HA3	1.90	0.53
11:3I:6:LEU:O	11:3I:10:THR:N	2.42	0.53
13:1k:52:PHE:O	13:1k:56:ALA:N	2.41	0.53
4:2a:85:THR:HA	4:2a:109:GLY:HA3	1.90	0.53
1:39:193:GLY:O	1:39:194:PHE:C	2.50	0.53
11:1I:6:LEU:O	11:1I:10:THR:N	2.42	0.53
4:2A:194:MET:O	4:2A:300:PHE:N	2.39	0.53
5:2b:211:LEU:O	5:2b:215:PHE:N	2.41	0.53
4:4a:85:THR:HA	4:4a:109:GLY:HA3	1.90	0.53
5:3b:211:LEU:O	5:3b:215:PHE:N	2.41	0.53
11:4I:6:LEU:O	11:4I:10:THR:N	2.42	0.52
18:4r:100:GLY:HA3	18:4r:202:ALA:HB1	1.91	0.52
11:2I:11:VAL:O	11:2I:12:VAL:C	2.52	0.52
18:2r:100:GLY:HA3	18:2r:202:ALA:HB1	1.91	0.52
18:4r:208:ALA:O	18:4r:211:GLY:N	2.43	0.52
17:2P:20:ALA:HA	17:2P:29:LEU:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1r:100:GLY:HA3	18:1r:202:ALA:HB1	1.91	0.52
11:3I:7:PHE:C	11:3I:9:TYR:H	2.18	0.51
11:4I:7:PHE:C	11:4I:9:TYR:H	2.18	0.51
18:1r:208:ALA:O	18:1r:211:GLY:N	2.43	0.51
1:19:193:GLY:O	1:19:194:PHE:C	2.54	0.51
18:2r:208:ALA:O	18:2r:211:GLY:N	2.43	0.51
18:3r:208:ALA:O	18:3r:211:GLY:N	2.43	0.51
17:1P:20:ALA:HA	17:1P:29:LEU:HA	1.92	0.51
16:1O:148:VAL:O	16:1O:196:SER:N	2.44	0.51
6:3c:186:TYR:HA	6:3c:196:VAL:HA	1.93	0.51
16:4O:148:VAL:O	16:4O:196:SER:N	2.44	0.51
13:3k:52:PHE:O	13:3k:56:ALA:N	2.40	0.51
18:3r:100:GLY:HA3	18:3r:202:ALA:HB1	1.91	0.51
7:4d:61:THR:HA	7:4d:83:ALA:HB2	1.93	0.51
7:1d:61:THR:HA	7:1d:83:ALA:HB2	1.93	0.51
6:4c:186:TYR:HA	6:4c:196:VAL:HA	1.93	0.51
1:3N:24:TYR:O	1:3N:26:GLY:N	2.45	0.51
6:1c:186:TYR:HA	6:1c:196:VAL:HA	1.93	0.50
16:1O:56:THR:N	16:1O:239:GLN:O	2.24	0.50
5:2B:206:GLY:O	5:2B:210:ILE:N	2.42	0.50
17:3P:20:ALA:HA	17:3P:29:LEU:HA	1.92	0.50
1:4N:69:SER:O	1:4N:72:ALA:N	2.44	0.50
11:1I:7:PHE:C	11:1I:9:TYR:H	2.18	0.50
1:1N:24:TYR:O	1:1N:26:GLY:N	2.45	0.50
6:2c:186:TYR:HA	6:2c:196:VAL:HA	1.93	0.50
5:4b:211:LEU:O	5:4b:215:PHE:N	2.41	0.50
16:2O:56:THR:N	16:2O:239:GLN:O	2.24	0.50
1:2N:24:TYR:O	1:2N:26:GLY:N	2.44	0.50
1:30:193:GLY:O	1:30:194:PHE:C	2.55	0.50
16:1O:200:ILE:HA	16:1O:219:GLU:O	2.12	0.50
7:2d:61:THR:HA	7:2d:83:ALA:HB2	1.93	0.50
16:4O:200:ILE:HA	16:4O:219:GLU:O	2.12	0.50
17:4P:20:ALA:HA	17:4P:29:LEU:HA	1.92	0.50
1:4N:24:TYR:O	1:4N:26:GLY:N	2.45	0.49
7:3d:61:THR:HA	7:3d:83:ALA:HB2	1.93	0.49
1:1N:69:SER:O	1:1N:72:ALA:N	2.44	0.49
6:1c:42:LEU:O	6:1c:44:ASN:N	2.46	0.49
6:2c:42:LEU:O	6:2c:44:ASN:N	2.46	0.49
16:3O:200:ILE:HA	16:3O:219:GLU:O	2.12	0.49
5:4B:206:GLY:O	5:4B:210:ILE:N	2.42	0.49
8:4E:35:TRP:HA	9:4F:33:ALA:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:48:12:ALA:O	3:48:14:LYS:N	2.46	0.49
1:2N:69:SER:O	1:2N:72:ALA:N	2.44	0.49
16:2O:200:ILE:HA	16:2O:219:GLU:O	2.12	0.49
1:00:193:GLY:O	1:00:194:PHE:C	2.55	0.49
4:3A:303:ASN:O	4:3A:305:SER:N	2.46	0.49
3:18:12:ALA:O	3:18:14:LYS:N	2.46	0.49
4:2A:303:ASN:O	4:2A:305:SER:N	2.46	0.49
8:2E:35:TRP:HA	9:2F:33:ALA:HB2	1.95	0.49
16:2O:148:VAL:O	16:2O:196:SER:N	2.44	0.49
6:3c:216:SER:O	6:3c:218:PHE:N	2.46	0.49
4:1A:303:ASN:O	4:1A:305:SER:N	2.46	0.49
16:3O:148:VAL:O	16:3O:196:SER:N	2.44	0.49
16:4O:56:THR:N	16:4O:239:GLN:O	2.24	0.49
3:08:12:ALA:O	3:08:14:LYS:N	2.46	0.48
6:1c:216:SER:O	6:1c:218:PHE:N	2.46	0.48
6:3c:42:LEU:O	6:3c:44:ASN:N	2.46	0.48
5:1b:211:LEU:O	5:1b:215:PHE:N	2.41	0.48
1:1g:80:VAL:O	1:1g:84:LEU:N	2.46	0.48
3:38:12:ALA:O	3:38:14:LYS:N	2.46	0.48
4:4A:303:ASN:O	4:4A:305:SER:N	2.46	0.48
8:1E:35:TRP:HA	9:1F:33:ALA:HB2	1.95	0.48
1:4g:80:VAL:O	1:4g:84:LEU:N	2.46	0.48
1:10:80:VAL:O	1:10:84:LEU:N	2.36	0.48
2:37:178:ALA:O	2:37:180:ASP:N	2.47	0.48
2:47:178:ALA:O	2:47:180:ASP:N	2.47	0.48
4:1a:84:PRO:HB2	4:1a:169:SER:HA	1.96	0.48
1:2g:80:VAL:O	1:2g:84:LEU:N	2.46	0.48
4:4a:84:PRO:HB2	4:4a:169:SER:HA	1.96	0.48
11:2I:13:ILE:O	11:2I:14:PHE:C	2.55	0.48
1:3g:80:VAL:O	1:3g:84:LEU:N	2.46	0.48
6:4c:216:SER:O	6:4c:218:PHE:N	2.46	0.48
6:2c:216:SER:O	6:2c:218:PHE:N	2.46	0.48
8:1e:35:TRP:HA	9:1f:33:ALA:HB2	1.96	0.47
8:3E:35:TRP:HA	9:3F:33:ALA:HB2	1.94	0.47
11:3I:7:PHE:HA	11:3I:10:THR:H	1.79	0.47
2:17:178:ALA:O	2:17:180:ASP:N	2.47	0.47
18:3R:100:GLY:O	18:3R:103:ALA:N	2.47	0.47
4:3a:84:PRO:HB2	4:3a:169:SER:HA	1.96	0.47
5:3B:206:GLY:O	5:3B:210:ILE:N	2.42	0.47
8:3e:35:TRP:HA	9:3f:33:ALA:HB2	1.96	0.47
1:40:193:GLY:O	1:40:194:PHE:C	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:4c:42:LEU:O	6:4c:44:ASN:N	2.46	0.47
1:3N:69:SER:O	1:3N:72:ALA:N	2.44	0.47
11:4I:7:PHE:HA	11:4I:10:THR:H	1.79	0.47
22:3v:33:PHE:HA	22:3v:37:VAL:HA	1.97	0.47
22:1v:33:PHE:HA	22:1v:37:VAL:HA	1.97	0.47
8:2e:35:TRP:HA	9:2f:33:ALA:HB2	1.96	0.47
1:4G:83:GLU:HA	1:4G:86:ALA:HB3	1.97	0.47
2:07:178:ALA:O	2:07:180:ASP:N	2.47	0.47
18:1R:100:GLY:O	18:1R:103:ALA:N	2.47	0.47
18:2R:100:GLY:O	18:2R:103:ALA:N	2.48	0.47
4:2a:84:PRO:HB2	4:2a:169:SER:HA	1.96	0.47
1:3G:83:GLU:HA	1:3G:86:ALA:HB3	1.97	0.47
8:4e:35:TRP:HA	9:4f:33:ALA:HB2	1.96	0.47
4:2a:81:ALA:HB1	4:2a:173:PRO:HB2	1.97	0.47
11:3I:11:VAL:C	11:3I:13:ILE:N	2.73	0.47
16:3O:56:THR:N	16:3O:239:GLN:O	2.24	0.47
18:4R:100:GLY:O	18:4R:103:ALA:N	2.47	0.47
19:4S:135:LEU:HA	19:4S:138:ALA:HB3	1.97	0.47
11:2I:4:LEU:O	11:2I:5:LYS:C	2.58	0.47
6:4c:144:PHE:O	6:4c:148:GLY:N	2.45	0.47
5:1B:206:GLY:O	5:1B:210:ILE:N	2.42	0.47
1:00:191:MET:O	1:00:192:PHE:C	2.58	0.46
5:2B:471:ALA:HB1	7:2D:141:PRO:HG2	1.98	0.46
1:30:191:MET:O	1:30:192:PHE:C	2.58	0.46
19:3S:135:LEU:HA	19:3S:138:ALA:HB3	1.97	0.46
6:2c:144:PHE:O	6:2c:148:GLY:N	2.45	0.46
11:3I:2:LEU:O	11:3I:6:LEU:N	2.40	0.46
16:4o:185:LEU:O	16:4o:189:ASN:N	2.47	0.46
1:2G:83:GLU:HA	1:2G:86:ALA:HB3	1.97	0.46
1:2g:24:TYR:O	1:2g:26:GLY:N	2.49	0.46
5:3B:471:ALA:HB1	7:3D:141:PRO:HG2	1.98	0.46
17:4p:45:GLN:HA	17:4p:62:ILE:HA	1.98	0.46
1:1G:83:GLU:HA	1:1G:86:ALA:HB3	1.97	0.46
11:1I:7:PHE:HA	11:1I:10:THR:H	1.79	0.46
3:48:43:ASP:O	3:48:47:LEU:N	2.44	0.46
1:09:194:PHE:O	1:09:195:PHE:C	2.59	0.46
4:1a:81:ALA:HB1	4:1a:173:PRO:HB2	1.97	0.46
6:1c:144:PHE:O	6:1c:148:GLY:N	2.45	0.46
1:30:195:PHE:O	1:30:196:VAL:C	2.58	0.46
16:3o:185:LEU:O	16:3o:189:ASN:N	2.47	0.46
19:1S:135:LEU:HA	19:1S:138:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4a:81:ALA:HB1	4:4a:173:PRO:HB2	1.97	0.46
16:1O:149:PRO:HA	16:1O:195:SER:HA	1.98	0.46
5:1b:41:GLU:O	5:1b:45:PHE:N	2.49	0.46
1:32:14:SER:O	1:32:19:ALA:N	2.49	0.46
19:2S:135:LEU:HA	19:2S:138:ALA:HB3	1.97	0.46
1:40:195:PHE:O	1:40:196:VAL:C	2.58	0.46
5:4b:41:GLU:O	5:4b:45:PHE:N	2.49	0.46
8:4e:69:ARG:N	21:4u:133:ASN:O	2.44	0.46
17:1p:45:GLN:HA	17:1p:62:ILE:HA	1.97	0.46
22:4v:33:PHE:HA	22:4v:37:VAL:HA	1.97	0.46
1:2N:170:PRO:HD2	1:2N:171:GLU:N	2.31	0.45
5:2b:136:PRO:HB3	5:2b:221:PRO:HG2	1.98	0.45
11:3I:7:PHE:HA	11:3I:10:THR:CB	2.46	0.45
4:3a:81:ALA:HB1	4:3a:173:PRO:HB2	1.97	0.45
1:42:14:SER:O	1:42:19:ALA:N	2.49	0.45
1:02:14:SER:O	1:02:19:ALA:N	2.49	0.45
5:1B:471:ALA:HB1	7:1D:141:PRO:HG2	1.98	0.45
11:1I:7:PHE:HA	11:1I:10:THR:CB	2.46	0.45
8:1e:69:ARG:N	21:1u:133:ASN:O	2.44	0.45
11:4I:7:PHE:HA	11:4I:10:THR:CB	2.46	0.45
1:4g:24:TYR:O	1:4g:26:GLY:N	2.49	0.45
1:12:14:SER:O	1:12:19:ALA:N	2.49	0.45
1:1N:170:PRO:HD2	1:1N:171:GLU:N	2.31	0.45
8:2e:69:ARG:N	21:2u:133:ASN:O	2.44	0.45
17:2p:45:GLN:HA	17:2p:62:ILE:HA	1.98	0.45
1:3g:24:TYR:O	1:3g:26:GLY:N	2.49	0.45
1:40:80:VAL:O	1:40:84:LEU:N	2.36	0.45
1:02:46:TRP:O	1:02:48:THR:N	2.49	0.45
16:2o:185:LEU:O	16:2o:189:ASN:N	2.47	0.45
19:3S:88:GLY:O	19:3S:91:GLY:N	2.50	0.45
1:40:191:MET:O	1:40:192:PHE:C	2.58	0.45
11:1I:11:VAL:C	11:1I:13:ILE:N	2.73	0.45
1:1g:24:TYR:O	1:1g:26:GLY:N	2.49	0.45
17:3p:45:GLN:HA	17:3p:62:ILE:HA	1.98	0.45
19:4S:88:GLY:O	19:4S:91:GLY:N	2.50	0.45
19:1S:88:GLY:O	19:1S:91:GLY:N	2.50	0.45
19:2S:88:GLY:O	19:2S:91:GLY:N	2.50	0.45
5:3b:41:GLU:O	5:3b:45:PHE:N	2.49	0.45
1:49:194:PHE:O	1:49:195:PHE:C	2.59	0.45
16:1o:55:PRO:HA	16:1o:240:GLY:HA3	1.99	0.45
5:2b:41:GLU:O	5:2b:45:PHE:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:2v:33:PHE:HA	22:2v:37:VAL:HA	1.97	0.45
16:4o:55:PRO:HA	16:4o:240:GLY:HA3	1.99	0.45
1:3N:170:PRO:HD2	1:3N:171:GLU:N	2.31	0.45
5:4B:471:ALA:HB1	7:4D:141:PRO:HG2	1.98	0.45
5:4b:136:PRO:HB3	5:4b:221:PRO:HG2	1.98	0.45
1:10:195:PHE:O	1:10:196:VAL:C	2.60	0.44
5:1b:136:PRO:HB3	5:1b:221:PRO:HG2	1.98	0.44
16:2o:55:PRO:HA	16:2o:240:GLY:HA3	1.99	0.44
5:3b:136:PRO:HB3	5:3b:221:PRO:HG2	1.98	0.44
8:3e:69:ARG:N	21:3u:133:ASN:O	2.44	0.44
16:4O:149:PRO:HA	16:4O:195:SER:HA	1.98	0.44
11:3I:2:LEU:HA	11:3I:5:LYS:CB	2.47	0.44
11:1I:2:LEU:O	11:1I:6:LEU:N	2.40	0.44
11:1I:2:LEU:HA	11:1I:5:LYS:CB	2.47	0.44
16:3O:149:PRO:HA	16:3O:195:SER:HA	1.98	0.44
4:4A:84:PRO:HB2	4:4A:169:SER:HA	2.00	0.44
4:1A:84:PRO:HB2	4:1A:169:SER:HA	2.00	0.44
7:1d:228:ASP:N	22:1v:48:GLY:O	2.51	0.44
16:1o:185:LEU:O	16:1o:189:ASN:N	2.47	0.44
22:1v:58:ALA:HB1	22:1v:62:GLY:HA3	2.00	0.44
22:3v:58:ALA:HB1	22:3v:62:GLY:HA3	2.00	0.44
22:4v:58:ALA:HB1	22:4v:62:GLY:HA3	2.00	0.44
11:4I:11:VAL:C	11:4I:13:ILE:N	2.72	0.44
1:00:195:PHE:O	1:00:196:VAL:C	2.58	0.44
16:3o:55:PRO:HA	16:3o:240:GLY:HA3	1.99	0.44
11:1I:10:THR:O	11:1I:14:PHE:N	2.51	0.43
1:36:231:GLY:HA2	2:37:213:GLY:HA3	2.00	0.43
7:3d:228:ASP:N	22:3v:48:GLY:O	2.51	0.43
18:4R:46:LEU:HA	18:4R:68:THR:HA	2.00	0.43
16:2O:149:PRO:HA	16:2O:195:SER:HA	1.98	0.43
4:3A:84:PRO:HB2	4:3A:169:SER:HA	2.00	0.43
15:3M:4:ASN:O	15:3M:6:LEU:N	2.46	0.43
11:4I:2:LEU:HA	11:4I:5:LYS:CB	2.47	0.43
4:4a:231:GLU:HA	5:4b:4:PRO:HD3	2.00	0.43
7:2d:228:ASP:N	22:2v:48:GLY:O	2.51	0.43
1:16:231:GLY:HA2	2:17:213:GLY:HA3	2.00	0.43
18:1R:46:LEU:HA	18:1R:68:THR:HA	2.01	0.43
18:2R:46:LEU:HA	18:2R:68:THR:HA	2.00	0.43
1:32:46:TRP:O	1:32:48:THR:N	2.49	0.43
7:4d:228:ASP:N	22:4v:48:GLY:O	2.51	0.43
1:06:231:GLY:HA2	2:07:213:GLY:HA3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1a:231:GLU:HA	5:1b:4:PRO:HD3	2.00	0.43
4:2A:84:PRO:HB2	4:2A:169:SER:HA	2.00	0.43
1:30:80:VAL:O	1:30:84:LEU:N	2.36	0.43
2:37:116:SER:O	2:37:118:GLY:N	2.52	0.43
1:12:46:TRP:O	1:12:48:THR:N	2.50	0.43
11:3I:10:THR:O	11:3I:14:PHE:N	2.51	0.43
16:1o:52:CYS:N	16:1o:243:TYR:O	2.50	0.43
13:2k:53:VAL:O	13:2k:57:ALA:N	2.48	0.43
22:2v:58:ALA:HB1	22:2v:62:GLY:HA3	2.00	0.43
1:39:194:PHE:O	1:39:195:PHE:C	2.59	0.43
6:3c:144:PHE:O	6:3c:148:GLY:N	2.45	0.43
1:42:46:TRP:O	1:42:48:THR:N	2.49	0.43
1:00:80:VAL:O	1:00:84:LEU:N	2.36	0.42
3:18:43:ASP:O	3:18:47:LEU:N	2.44	0.42
4:3A:276:ALA:HA	7:3D:213:ALA:HA	2.01	0.42
4:4A:276:ALA:HA	7:4D:213:ALA:HA	2.01	0.42
17:3P:31:PRO:O	17:3P:33:LYS:N	2.52	0.42
2:07:155:GLY:HA2	2:07:161:ASP:HA	2.01	0.42
6:1C:186:TYR:HA	6:1C:196:VAL:HA	2.01	0.42
4:2A:276:ALA:HA	7:2D:213:ALA:HA	2.02	0.42
1:2g:83:GLU:HA	1:2g:86:ALA:HB3	2.02	0.42
1:2g:146:GLY:HA3	1:2g:147:PRO:HD3	1.90	0.42
16:3o:183:GLU:HA	16:3o:186:ALA:HB2	2.01	0.42
2:47:116:SER:O	2:47:118:GLY:N	2.52	0.42
11:4I:10:THR:O	11:4I:14:PHE:N	2.51	0.42
3:08:43:ASP:O	3:08:47:LEU:N	2.44	0.42
1:3g:146:GLY:HA3	1:3g:147:PRO:HD3	1.90	0.42
1:46:231:GLY:HA2	2:47:213:GLY:HA3	2.00	0.42
6:4C:186:TYR:HA	6:4C:196:VAL:HA	2.02	0.42
1:1g:83:GLU:HA	1:1g:86:ALA:HB3	2.02	0.42
6:1c:131:TYR:O	6:1c:136:GLY:N	2.48	0.42
18:3R:46:LEU:HA	18:3R:68:THR:HA	2.00	0.42
1:4n:115:ASN:HA	1:4n:116:PRO:HD3	1.89	0.42
2:07:116:SER:O	2:07:118:GLY:N	2.52	0.42
17:1p:10:GLY:HA2	22:1v:109:ALA:HB3	2.02	0.42
4:2a:231:GLU:HA	5:2b:4:PRO:HD3	2.00	0.42
6:3C:186:TYR:HA	6:3C:196:VAL:HA	2.02	0.42
13:3k:53:VAL:O	13:3k:57:ALA:N	2.48	0.42
1:16:26:GLY:HA3	1:16:27:PRO:HD3	1.84	0.42
13:3K:52:PHE:O	13:3K:56:ALA:N	2.51	0.42
4:3a:231:GLU:HA	5:3b:4:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:4c:131:TYR:O	6:4c:136:GLY:N	2.48	0.42
16:4o:52:CYS:N	16:4o:243:TYR:O	2.50	0.42
4:1A:276:ALA:HA	7:1D:213:ALA:HA	2.02	0.41
15:2M:4:ASN:O	15:2M:6:LEU:N	2.46	0.41
16:2O:98:ASP:O	16:3O:98:ASP:CA	2.68	0.41
5:2b:383:PHE:H	7:2d:346:VAL:HA	1.85	0.41
11:2I:15:PHE:O	11:2I:16:VAL:C	2.62	0.41
6:2c:131:TYR:O	6:2c:136:GLY:N	2.48	0.41
1:3G:118:LEU:O	1:3G:120:HIS:N	2.53	0.41
5:4b:383:PHE:H	7:4d:346:VAL:HA	1.85	0.41
8:2E:49:SER:HA	8:2E:50:PRO:HD3	1.96	0.41
1:2G:118:LEU:O	1:2G:120:HIS:N	2.53	0.41
1:3I:174:ALA:O	1:3I:177:LYS:CB	2.69	0.41
2:47:155:GLY:HA2	2:47:161:ASP:HA	2.01	0.41
3:34:104:LEU:O	3:34:106:GLY:N	2.54	0.41
6:4C:363:ALA:HA	6:4C:364:PRO:HD3	1.93	0.41
3:04:104:LEU:O	3:04:106:GLY:N	2.54	0.41
2:17:155:GLY:HA2	2:17:161:ASP:HA	2.01	0.41
16:2o:183:GLU:HA	16:2o:186:ALA:HB2	2.01	0.41
3:38:43:ASP:O	3:38:47:LEU:N	2.44	0.41
5:3b:383:PHE:H	7:3d:346:VAL:HA	1.85	0.41
1:4G:118:LEU:O	1:4G:120:HIS:N	2.53	0.41
13:4K:52:PHE:O	13:4K:56:ALA:N	2.51	0.41
1:4N:170:PRO:HD2	1:4N:171:GLU:N	2.31	0.41
7:4d:223:LEU:HA	7:4d:245:TYR:HA	2.03	0.41
1:01:174:ALA:O	1:01:177:LYS:CB	2.69	0.41
16:1O:50:LYS:O	16:1O:244:ALA:HA	2.21	0.41
17:1P:31:PRO:O	17:1P:33:LYS:N	2.52	0.41
2:37:155:GLY:HA2	2:37:161:ASP:HA	2.01	0.41
5:3B:277:GLN:HA	21:3U:128:ALA:HA	2.03	0.41
17:4p:10:GLY:HA2	22:4v:109:ALA:HB3	2.02	0.41
1:11:174:ALA:O	1:11:177:LYS:CB	2.69	0.41
3:14:104:LEU:O	3:14:106:GLY:N	2.54	0.41
5:1B:277:GLN:HA	21:1U:128:ALA:HA	2.03	0.41
16:1o:183:GLU:HA	16:1o:186:ALA:HB2	2.02	0.41
11:2I:6:LEU:O	11:2I:7:PHE:C	2.61	0.41
16:2O:138:LYS:CB	16:3O:98:ASP:CB	2.98	0.41
17:2P:31:PRO:O	17:2P:33:LYS:N	2.52	0.41
17:2p:10:GLY:HA2	22:2v:109:ALA:HB3	2.02	0.41
7:3d:351:ASN:O	7:3d:353:LEU:N	2.54	0.41
1:3g:83:GLU:HA	1:3g:86:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:41:174:ALA:O	1:41:177:LYS:CB	2.69	0.41
1:06:26:GLY:HA3	1:06:27:PRO:HD3	1.84	0.41
6:2C:186:TYR:HA	6:2C:196:VAL:HA	2.01	0.41
11:2I:9:TYR:O	11:2I:10:THR:C	2.63	0.41
20:3t:26:PRO:HA	20:3t:27:PRO:HD3	1.91	0.41
3:44:104:LEU:O	3:44:106:GLY:N	2.54	0.41
11:4I:17:SER:O	11:4I:18:LEU:C	2.63	0.41
1:4N:204:GLY:HA2	1:4N:205:PRO:HD3	1.98	0.41
16:4o:183:GLU:HA	16:4o:186:ALA:HB2	2.02	0.41
5:1b:383:PHE:H	7:1d:346:VAL:HA	1.85	0.40
1:1g:146:GLY:HA3	1:1g:147:PRO:HD3	1.90	0.40
4:2A:143:ILE:HA	7:2D:217:ALA:HB1	2.03	0.40
7:2d:223:LEU:HA	7:2d:245:TYR:HA	2.03	0.40
20:3T:26:PRO:HA	20:3T:27:PRO:HD3	1.97	0.40
16:3o:52:CYS:N	16:3o:243:TYR:O	2.50	0.40
3:14:58:GLY:HA3	3:14:184:ALA:HB1	2.03	0.40
2:33:178:ALA:O	2:33:180:ASP:N	2.55	0.40
3:34:58:GLY:HA3	3:34:184:ALA:HB1	2.03	0.40
16:4O:50:LYS:O	16:4O:244:ALA:HA	2.21	0.40
16:2O:50:LYS:O	16:2O:244:ALA:HA	2.21	0.40
1:39:41:PRO:HB3	1:39:178:VAL:HA	2.04	0.40
2:43:178:ALA:O	2:43:180:ASP:N	2.55	0.40
17:4P:31:PRO:O	17:4P:33:LYS:N	2.52	0.40
5:2b:347:ARG:O	5:2b:397:VAL:HA	2.22	0.40
11:3I:17:SER:O	11:3I:18:LEU:C	2.63	0.40
4:3a:172:MET:HA	4:3a:173:PRO:HD3	1.86	0.40
17:3p:10:GLY:HA2	22:3v:109:ALA:HB3	2.02	0.40
7:4d:351:ASN:O	7:4d:353:LEU:N	2.54	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	00	217/219 (99%)	197 (91%)	17 (8%)	3 (1%)	9	39
1	01	217/219 (99%)	191 (88%)	25 (12%)	1 (0%)	24	62
1	02	208/219 (95%)	173 (83%)	31 (15%)	4 (2%)	6	32
1	05	206/219 (94%)	176 (85%)	28 (14%)	2 (1%)	12	47
1	06	203/219 (93%)	174 (86%)	27 (13%)	2 (1%)	12	47
1	09	217/219 (99%)	196 (90%)	21 (10%)	0	100	100
1	10	217/219 (99%)	197 (91%)	18 (8%)	2 (1%)	14	49
1	11	217/219 (99%)	191 (88%)	25 (12%)	1 (0%)	24	62
1	12	208/219 (95%)	173 (83%)	31 (15%)	4 (2%)	6	32
1	15	206/219 (94%)	175 (85%)	29 (14%)	2 (1%)	12	47
1	16	203/219 (93%)	174 (86%)	27 (13%)	2 (1%)	12	47
1	19	217/219 (99%)	193 (89%)	22 (10%)	2 (1%)	14	49
1	1G	217/219 (99%)	199 (92%)	17 (8%)	1 (0%)	24	62
1	1N	217/219 (99%)	199 (92%)	17 (8%)	1 (0%)	24	62
1	1g	217/219 (99%)	196 (90%)	20 (9%)	1 (0%)	24	62
1	1n	217/219 (99%)	199 (92%)	17 (8%)	1 (0%)	24	62
1	2G	217/219 (99%)	199 (92%)	17 (8%)	1 (0%)	24	62
1	2N	217/219 (99%)	199 (92%)	17 (8%)	1 (0%)	24	62
1	2g	217/219 (99%)	197 (91%)	19 (9%)	1 (0%)	24	62
1	2n	217/219 (99%)	199 (92%)	17 (8%)	1 (0%)	24	62
1	30	217/219 (99%)	197 (91%)	17 (8%)	3 (1%)	9	39
1	31	217/219 (99%)	191 (88%)	25 (12%)	1 (0%)	24	62
1	32	208/219 (95%)	173 (83%)	31 (15%)	4 (2%)	6	32
1	35	206/219 (94%)	175 (85%)	29 (14%)	2 (1%)	12	47
1	36	203/219 (93%)	174 (86%)	27 (13%)	2 (1%)	12	47
1	39	217/219 (99%)	196 (90%)	21 (10%)	0	100	100
1	3G	217/219 (99%)	200 (92%)	16 (7%)	1 (0%)	24	62
1	3N	217/219 (99%)	199 (92%)	17 (8%)	1 (0%)	24	62
1	3g	217/219 (99%)	197 (91%)	19 (9%)	1 (0%)	24	62
1	3n	217/219 (99%)	199 (92%)	17 (8%)	1 (0%)	24	62
1	40	217/219 (99%)	197 (91%)	17 (8%)	3 (1%)	9	39
1	41	217/219 (99%)	191 (88%)	25 (12%)	1 (0%)	24	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	42	208/219 (95%)	173 (83%)	31 (15%)	4 (2%)	6	32
1	45	206/219 (94%)	176 (85%)	28 (14%)	2 (1%)	12	47
1	46	203/219 (93%)	174 (86%)	27 (13%)	2 (1%)	12	47
1	49	217/219 (99%)	196 (90%)	21 (10%)	0	100	100
1	4G	217/219 (99%)	199 (92%)	17 (8%)	1 (0%)	24	62
1	4N	217/219 (99%)	199 (92%)	17 (8%)	1 (0%)	24	62
1	4g	217/219 (99%)	197 (91%)	19 (9%)	1 (0%)	24	62
1	4n	217/219 (99%)	199 (92%)	17 (8%)	1 (0%)	24	62
2	03	218/220 (99%)	186 (85%)	30 (14%)	2 (1%)	14	49
2	07	218/220 (99%)	188 (86%)	29 (13%)	1 (0%)	24	62
2	13	218/220 (99%)	186 (85%)	30 (14%)	2 (1%)	14	49
2	17	218/220 (99%)	188 (86%)	29 (13%)	1 (0%)	24	62
2	33	218/220 (99%)	186 (85%)	30 (14%)	2 (1%)	14	49
2	37	218/220 (99%)	188 (86%)	29 (13%)	1 (0%)	24	62
2	43	218/220 (99%)	186 (85%)	30 (14%)	2 (1%)	14	49
2	47	218/220 (99%)	188 (86%)	28 (13%)	2 (1%)	14	49
3	04	198/209 (95%)	152 (77%)	44 (22%)	2 (1%)	12	47
3	08	203/209 (97%)	170 (84%)	28 (14%)	5 (2%)	4	27
3	14	198/209 (95%)	152 (77%)	44 (22%)	2 (1%)	12	47
3	18	203/209 (97%)	170 (84%)	28 (14%)	5 (2%)	4	27
3	34	198/209 (95%)	152 (77%)	44 (22%)	2 (1%)	12	47
3	38	203/209 (97%)	170 (84%)	28 (14%)	5 (2%)	4	27
3	44	198/209 (95%)	152 (77%)	44 (22%)	2 (1%)	12	47
3	48	203/209 (97%)	170 (84%)	28 (14%)	5 (2%)	4	27
4	1A	332/334 (99%)	314 (95%)	18 (5%)	0	100	100
4	1a	331/334 (99%)	313 (95%)	18 (5%)	0	100	100
4	2A	332/334 (99%)	314 (95%)	18 (5%)	0	100	100
4	2a	331/334 (99%)	313 (95%)	18 (5%)	0	100	100
4	3A	332/334 (99%)	314 (95%)	18 (5%)	0	100	100
4	3a	331/334 (99%)	313 (95%)	18 (5%)	0	100	100
4	4A	332/334 (99%)	314 (95%)	18 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	4a	331/334 (99%)	312 (94%)	19 (6%)	0	100	100
5	1B	501/503 (100%)	476 (95%)	24 (5%)	1 (0%)	43	77
5	1b	501/503 (100%)	486 (97%)	15 (3%)	0	100	100
5	2B	501/503 (100%)	476 (95%)	24 (5%)	1 (0%)	43	77
5	2b	501/503 (100%)	486 (97%)	15 (3%)	0	100	100
5	3B	501/503 (100%)	476 (95%)	24 (5%)	1 (0%)	43	77
5	3b	501/503 (100%)	486 (97%)	15 (3%)	0	100	100
5	4B	501/503 (100%)	476 (95%)	24 (5%)	1 (0%)	43	77
5	4b	501/503 (100%)	486 (97%)	15 (3%)	0	100	100
6	1C	448/450 (100%)	430 (96%)	18 (4%)	0	100	100
6	1c	448/450 (100%)	428 (96%)	17 (4%)	3 (1%)	18	55
6	2C	448/450 (100%)	429 (96%)	19 (4%)	0	100	100
6	2c	448/450 (100%)	428 (96%)	17 (4%)	3 (1%)	18	55
6	3C	448/450 (100%)	429 (96%)	19 (4%)	0	100	100
6	3c	448/450 (100%)	428 (96%)	17 (4%)	3 (1%)	18	55
6	4C	448/450 (100%)	429 (96%)	19 (4%)	0	100	100
6	4c	448/450 (100%)	428 (96%)	17 (4%)	3 (1%)	18	55
7	1D	338/341 (99%)	319 (94%)	18 (5%)	1 (0%)	36	71
7	1d	339/341 (99%)	316 (93%)	23 (7%)	0	100	100
7	2D	338/341 (99%)	319 (94%)	18 (5%)	1 (0%)	36	71
7	2d	339/341 (99%)	316 (93%)	23 (7%)	0	100	100
7	3D	338/341 (99%)	319 (94%)	17 (5%)	2 (1%)	21	58
7	3d	339/341 (99%)	316 (93%)	23 (7%)	0	100	100
7	4D	338/341 (99%)	319 (94%)	18 (5%)	1 (0%)	36	71
7	4d	339/341 (99%)	316 (93%)	23 (7%)	0	100	100
8	1E	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
8	1e	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
8	2E	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
8	2e	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
8	3E	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
8	3e	73/75 (97%)	68 (93%)	5 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	4E	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
8	4e	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
9	1F	33/36 (92%)	33 (100%)	0	0	100	100
9	1f	28/36 (78%)	27 (96%)	1 (4%)	0	100	100
9	2F	33/36 (92%)	33 (100%)	0	0	100	100
9	2f	28/36 (78%)	27 (96%)	1 (4%)	0	100	100
9	3F	33/36 (92%)	33 (100%)	0	0	100	100
9	3f	28/36 (78%)	27 (96%)	1 (4%)	0	100	100
9	4F	33/36 (92%)	33 (100%)	0	0	100	100
9	4f	28/36 (78%)	27 (96%)	1 (4%)	0	100	100
10	1H	58/60 (97%)	53 (91%)	5 (9%)	0	100	100
10	1h	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
10	2H	58/60 (97%)	53 (91%)	5 (9%)	0	100	100
10	2h	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
10	3H	58/60 (97%)	53 (91%)	5 (9%)	0	100	100
10	3h	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
10	4H	58/60 (97%)	53 (91%)	5 (9%)	0	100	100
10	4h	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
11	1I	32/34 (94%)	23 (72%)	5 (16%)	4 (12%)	0	4
11	1i	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
11	2I	32/34 (94%)	22 (69%)	7 (22%)	3 (9%)	0	8
11	2i	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
11	3I	32/34 (94%)	23 (72%)	5 (16%)	4 (12%)	0	4
11	3i	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
11	4I	32/34 (94%)	23 (72%)	5 (16%)	4 (12%)	0	4
11	4i	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
12	1J	33/35 (94%)	33 (100%)	0	0	100	100
12	1j	33/35 (94%)	33 (100%)	0	0	100	100
12	2J	33/35 (94%)	33 (100%)	0	0	100	100
12	2j	33/35 (94%)	33 (100%)	0	0	100	100
12	3J	33/35 (94%)	33 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	3j	33/35 (94%)	33 (100%)	0	0	100	100
12	4J	33/35 (94%)	33 (100%)	0	0	100	100
12	4j	33/35 (94%)	33 (100%)	0	0	100	100
13	1K	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
13	1k	35/37 (95%)	34 (97%)	0	1 (3%)	3	24
13	2K	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
13	2k	35/37 (95%)	34 (97%)	0	1 (3%)	3	24
13	3K	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
13	3k	35/37 (95%)	34 (97%)	0	1 (3%)	3	24
13	4K	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
13	4k	35/37 (95%)	34 (97%)	0	1 (3%)	3	24
14	1L	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
14	1l	33/37 (89%)	33 (100%)	0	0	100	100
14	2L	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
14	2l	33/37 (89%)	33 (100%)	0	0	100	100
14	3L	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
14	3l	33/37 (89%)	33 (100%)	0	0	100	100
14	4L	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
14	4l	33/37 (89%)	33 (100%)	0	0	100	100
15	1M	30/33 (91%)	24 (80%)	5 (17%)	1 (3%)	3	21
15	1m	31/33 (94%)	31 (100%)	0	0	100	100
15	2M	30/33 (91%)	24 (80%)	5 (17%)	1 (3%)	3	21
15	2m	31/33 (94%)	31 (100%)	0	0	100	100
15	3M	30/33 (91%)	24 (80%)	5 (17%)	1 (3%)	3	21
15	3m	31/33 (94%)	31 (100%)	0	0	100	100
15	4M	30/33 (91%)	24 (80%)	5 (17%)	1 (3%)	3	21
15	4m	31/33 (94%)	31 (100%)	0	0	100	100
16	1O	245/248 (99%)	210 (86%)	35 (14%)	0	100	100
16	1o	233/248 (94%)	209 (90%)	24 (10%)	0	100	100
16	2O	245/248 (99%)	211 (86%)	34 (14%)	0	100	100
16	2o	233/248 (94%)	209 (90%)	24 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	3O	245/248 (99%)	211 (86%)	34 (14%)	0	100	100
16	3o	233/248 (94%)	208 (89%)	25 (11%)	0	100	100
16	4O	245/248 (99%)	210 (86%)	35 (14%)	0	100	100
16	4o	233/248 (94%)	209 (90%)	24 (10%)	0	100	100
17	1P	184/186 (99%)	164 (89%)	19 (10%)	1 (0%)	24	62
17	1p	184/186 (99%)	170 (92%)	14 (8%)	0	100	100
17	2P	184/186 (99%)	164 (89%)	19 (10%)	1 (0%)	24	62
17	2p	184/186 (99%)	170 (92%)	14 (8%)	0	100	100
17	3P	184/186 (99%)	164 (89%)	19 (10%)	1 (0%)	24	62
17	3p	184/186 (99%)	170 (92%)	14 (8%)	0	100	100
17	4P	184/186 (99%)	164 (89%)	19 (10%)	1 (0%)	24	62
17	4p	184/186 (99%)	170 (92%)	14 (8%)	0	100	100
18	1R	232/234 (99%)	209 (90%)	22 (10%)	1 (0%)	30	66
18	1r	232/234 (99%)	216 (93%)	16 (7%)	0	100	100
18	2R	232/234 (99%)	210 (90%)	21 (9%)	1 (0%)	30	66
18	2r	232/234 (99%)	216 (93%)	16 (7%)	0	100	100
18	3R	232/234 (99%)	209 (90%)	22 (10%)	1 (0%)	30	66
18	3r	232/234 (99%)	216 (93%)	16 (7%)	0	100	100
18	4R	232/234 (99%)	209 (90%)	22 (10%)	1 (0%)	30	66
18	4r	232/234 (99%)	216 (93%)	16 (7%)	0	100	100
19	1S	216/218 (99%)	186 (86%)	28 (13%)	2 (1%)	14	49
19	1s	215/218 (99%)	188 (87%)	26 (12%)	1 (0%)	24	62
19	2S	216/218 (99%)	186 (86%)	28 (13%)	2 (1%)	14	49
19	2s	215/218 (99%)	188 (87%)	26 (12%)	1 (0%)	24	62
19	3S	216/218 (99%)	186 (86%)	28 (13%)	2 (1%)	14	49
19	3s	215/218 (99%)	188 (87%)	26 (12%)	1 (0%)	24	62
19	4S	216/218 (99%)	186 (86%)	28 (13%)	2 (1%)	14	49
19	4s	215/218 (99%)	188 (87%)	26 (12%)	1 (0%)	24	62
20	1T	30/32 (94%)	30 (100%)	0	0	100	100
20	1t	29/32 (91%)	29 (100%)	0	0	100	100
20	2T	30/32 (94%)	30 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	2t	29/32 (91%)	29 (100%)	0	0	100	100
20	3T	30/32 (94%)	30 (100%)	0	0	100	100
20	3t	29/32 (91%)	29 (100%)	0	0	100	100
20	4T	30/32 (94%)	30 (100%)	0	0	100	100
20	4t	29/32 (91%)	29 (100%)	0	0	100	100
21	1U	25/27 (93%)	23 (92%)	2 (8%)	0	100	100
21	1u	25/27 (93%)	22 (88%)	3 (12%)	0	100	100
21	2U	25/27 (93%)	23 (92%)	2 (8%)	0	100	100
21	2u	25/27 (93%)	22 (88%)	3 (12%)	0	100	100
21	3U	25/27 (93%)	23 (92%)	2 (8%)	0	100	100
21	3u	25/27 (93%)	22 (88%)	3 (12%)	0	100	100
21	4U	25/27 (93%)	23 (92%)	2 (8%)	0	100	100
21	4u	25/27 (93%)	22 (88%)	3 (12%)	0	100	100
22	1V	96/105 (91%)	79 (82%)	16 (17%)	1 (1%)	12	47
22	1v	97/105 (92%)	81 (84%)	12 (12%)	4 (4%)	2	18
22	2V	96/105 (91%)	79 (82%)	16 (17%)	1 (1%)	12	47
22	2v	97/105 (92%)	81 (84%)	12 (12%)	4 (4%)	2	18
22	3V	96/105 (91%)	79 (82%)	16 (17%)	1 (1%)	12	47
22	3v	97/105 (92%)	81 (84%)	12 (12%)	4 (4%)	2	18
22	4V	96/105 (91%)	79 (82%)	16 (17%)	1 (1%)	12	47
22	4v	97/105 (92%)	81 (84%)	12 (12%)	4 (4%)	2	18
23	1W	52/54 (96%)	47 (90%)	5 (10%)	0	100	100
23	1w	42/54 (78%)	40 (95%)	2 (5%)	0	100	100
23	2W	52/54 (96%)	47 (90%)	5 (10%)	0	100	100
23	2w	42/54 (78%)	40 (95%)	2 (5%)	0	100	100
23	3W	52/54 (96%)	47 (90%)	5 (10%)	0	100	100
23	3w	42/54 (78%)	40 (95%)	2 (5%)	0	100	100
23	4W	52/54 (96%)	47 (90%)	5 (10%)	0	100	100
23	4w	42/54 (78%)	40 (95%)	2 (5%)	0	100	100
24	1X	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
24	1x	36/39 (92%)	34 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	2X	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
24	2x	36/39 (92%)	34 (94%)	2 (6%)	0	100	100
24	3X	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
24	3x	36/39 (92%)	34 (94%)	2 (6%)	0	100	100
24	4X	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
24	4x	36/39 (92%)	34 (94%)	2 (6%)	0	100	100
25	1Y	32/35 (91%)	31 (97%)	1 (3%)	0	100	100
25	1y	32/35 (91%)	32 (100%)	0	0	100	100
25	2Y	32/35 (91%)	31 (97%)	1 (3%)	0	100	100
25	2y	32/35 (91%)	32 (100%)	0	0	100	100
25	3Y	32/35 (91%)	31 (97%)	1 (3%)	0	100	100
25	3y	32/35 (91%)	32 (100%)	0	0	100	100
25	4Y	32/35 (91%)	31 (97%)	1 (3%)	0	100	100
25	4y	32/35 (91%)	32 (100%)	0	0	100	100
26	1Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
26	1z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
26	2Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
26	2z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
26	3Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
26	3z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
26	4Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
26	4z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	37024/37912 (98%)	33764 (91%)	3070 (8%)	190 (0%)	26	62

All (190) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	08	13	PHE
3	18	13	PHE
5	1B	18	ARG
7	1D	268	LEU
6	1c	43	ILE
6	1c	384	ILE
13	1k	40	MET

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Mol	Chain	Res	Type
5	2B	18	ARG
7	2D	268	LEU
6	2c	43	ILE
6	2c	384	ILE
13	2k	40	MET
3	38	13	PHE
5	3B	18	ARG
7	3D	268	LEU
6	3c	43	ILE
6	3c	384	ILE
13	3k	40	MET
3	48	13	PHE
5	4B	18	ARG
7	4D	268	LEU
6	4c	43	ILE
6	4c	384	ILE
13	4k	40	MET
1	00	191	MET
1	01	48	THR
1	02	126	ALA
1	02	214	ALA
2	03	179	ASP
1	05	95	ALA
1	06	126	ALA
2	07	179	ASP
3	08	20	ILE
1	10	191	MET
1	11	48	THR
1	12	126	ALA
1	12	214	ALA
2	13	179	ASP
1	15	95	ALA
1	16	126	ALA
2	17	179	ASP
3	18	20	ILE
1	19	191	MET
11	1I	13	ILE
15	1M	3	VAL
17	1P	53	PHE
19	1S	66	LYS
19	1s	66	LYS
22	1v	43	VAL

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Mol	Chain	Res	Type
22	1v	51	GLN
22	1v	83	LYS
15	2M	3	VAL
17	2P	53	PHE
19	2S	66	LYS
19	2s	66	LYS
22	2v	43	VAL
22	2v	51	GLN
22	2v	83	LYS
1	30	191	MET
1	31	48	THR
1	32	126	ALA
1	32	214	ALA
2	33	179	ASP
1	35	95	ALA
1	36	126	ALA
2	37	179	ASP
3	38	20	ILE
11	3I	13	ILE
15	3M	3	VAL
17	3P	53	PHE
19	3S	66	LYS
19	3s	66	LYS
22	3v	43	VAL
22	3v	51	GLN
22	3v	83	LYS
1	40	191	MET
1	41	48	THR
1	42	126	ALA
1	42	214	ALA
2	43	179	ASP
1	45	95	ALA
1	46	126	ALA
2	47	179	ASP
3	48	20	ILE
11	4I	13	ILE
15	4M	3	VAL
17	4P	53	PHE
19	4S	66	LYS
19	4s	66	LYS
22	4v	43	VAL
22	4v	51	GLN

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Mol	Chain	Res	Type
22	4v	83	LYS
1	02	51	LEU
1	05	225	ALA
3	08	94	PHE
1	10	195	PHE
1	12	51	LEU
1	15	225	ALA
3	18	94	PHE
1	19	195	PHE
1	32	51	LEU
1	35	225	ALA
1	36	95	ALA
3	38	94	PHE
1	42	51	LEU
1	45	225	ALA
3	48	94	PHE
1	00	193	GLY
3	04	105	MET
1	06	95	ALA
3	14	105	MET
1	16	95	ALA
11	2I	15	PHE
11	2I	16	VAL
1	30	193	GLY
3	34	105	MET
1	40	193	GLY
3	44	105	MET
1	46	95	ALA
1	00	195	PHE
1	02	119	ILE
1	12	119	ILE
11	1I	14	PHE
6	1c	472	LEU
1	1n	119	ILE
6	2c	472	LEU
1	2n	119	ILE
1	30	195	PHE
1	32	119	ILE
11	3I	14	PHE
6	3c	472	LEU
1	3n	119	ILE
1	40	195	PHE

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Mol	Chain	Res	Type
1	42	119	ILE
11	4I	14	PHE
6	4c	472	LEU
1	4n	119	ILE
3	04	12	ALA
3	08	11	PRO
3	08	162	ARG
3	14	12	ALA
3	18	11	PRO
3	18	162	ARG
1	1G	54	ASP
19	1S	156	ASN
22	1V	32	VAL
1	2G	54	ASP
19	2S	156	ASN
22	2V	32	VAL
3	34	12	ALA
3	38	11	PRO
3	38	162	ARG
7	3D	352	ALA
1	3G	54	ASP
19	3S	156	ASN
22	3V	32	VAL
3	44	12	ALA
3	48	11	PRO
3	48	162	ARG
1	4G	54	ASP
19	4S	156	ASN
22	4V	32	VAL
11	1I	8	VAL
11	3I	8	VAL
11	4I	8	VAL
1	1g	119	ILE
1	2g	119	ILE
1	3g	119	ILE
1	4g	119	ILE
2	03	134	ILE
2	13	134	ILE
1	1N	119	ILE
18	1R	141	PRO
22	1v	24	PRO
11	2I	8	VAL

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Mol	Chain	Res	Type
1	2N	119	ILE
18	2R	141	PRO
22	2v	24	PRO
2	33	134	ILE
1	3N	119	ILE
18	3R	141	PRO
22	3v	24	PRO
2	43	134	ILE
1	4N	119	ILE
18	4R	141	PRO
22	4v	24	PRO
11	1I	12	VAL
11	3I	12	VAL
2	47	134	ILE
11	4I	12	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	00	16/166 (10%)	16 (100%)	0	100	100
1	01	16/166 (10%)	16 (100%)	0	100	100
1	02	16/166 (10%)	16 (100%)	0	100	100
1	05	14/166 (8%)	14 (100%)	0	100	100
1	06	13/166 (8%)	13 (100%)	0	100	100
1	09	16/166 (10%)	16 (100%)	0	100	100
1	10	16/166 (10%)	16 (100%)	0	100	100
1	11	16/166 (10%)	16 (100%)	0	100	100
1	12	16/166 (10%)	16 (100%)	0	100	100
1	15	14/166 (8%)	14 (100%)	0	100	100
1	16	13/166 (8%)	13 (100%)	0	100	100
1	19	16/166 (10%)	16 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1G	16/166 (10%)	16 (100%)	0	100	100
1	1N	16/166 (10%)	16 (100%)	0	100	100
1	1g	16/166 (10%)	16 (100%)	0	100	100
1	1n	16/166 (10%)	16 (100%)	0	100	100
1	2G	16/166 (10%)	16 (100%)	0	100	100
1	2N	16/166 (10%)	16 (100%)	0	100	100
1	2g	16/166 (10%)	16 (100%)	0	100	100
1	2n	16/166 (10%)	16 (100%)	0	100	100
1	30	16/166 (10%)	16 (100%)	0	100	100
1	31	16/166 (10%)	16 (100%)	0	100	100
1	32	16/166 (10%)	16 (100%)	0	100	100
1	35	14/166 (8%)	14 (100%)	0	100	100
1	36	13/166 (8%)	13 (100%)	0	100	100
1	39	16/166 (10%)	16 (100%)	0	100	100
1	3G	16/166 (10%)	16 (100%)	0	100	100
1	3N	16/166 (10%)	16 (100%)	0	100	100
1	3g	16/166 (10%)	16 (100%)	0	100	100
1	3n	16/166 (10%)	16 (100%)	0	100	100
1	40	16/166 (10%)	16 (100%)	0	100	100
1	41	16/166 (10%)	16 (100%)	0	100	100
1	42	16/166 (10%)	16 (100%)	0	100	100
1	45	14/166 (8%)	14 (100%)	0	100	100
1	46	13/166 (8%)	13 (100%)	0	100	100
1	49	16/166 (10%)	16 (100%)	0	100	100
1	4G	16/166 (10%)	16 (100%)	0	100	100
1	4N	16/166 (10%)	16 (100%)	0	100	100
1	4g	16/166 (10%)	16 (100%)	0	100	100
1	4n	16/166 (10%)	16 (100%)	0	100	100
2	03	14/172 (8%)	14 (100%)	0	100	100
2	07	15/172 (9%)	15 (100%)	0	100	100
2	13	14/172 (8%)	14 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	17	15/172 (9%)	15 (100%)	0	100	100
2	33	14/172 (8%)	14 (100%)	0	100	100
2	37	15/172 (9%)	15 (100%)	0	100	100
2	43	14/172 (8%)	14 (100%)	0	100	100
2	47	15/172 (9%)	15 (100%)	0	100	100
3	04	15/161 (9%)	15 (100%)	0	100	100
3	08	15/161 (9%)	15 (100%)	0	100	100
3	14	15/161 (9%)	15 (100%)	0	100	100
3	18	15/161 (9%)	15 (100%)	0	100	100
3	34	15/161 (9%)	15 (100%)	0	100	100
3	38	15/161 (9%)	15 (100%)	0	100	100
3	44	15/161 (9%)	15 (100%)	0	100	100
3	48	15/161 (9%)	15 (100%)	0	100	100
4	1A	14/270 (5%)	14 (100%)	0	100	100
4	1a	14/270 (5%)	14 (100%)	0	100	100
4	2A	14/270 (5%)	14 (100%)	0	100	100
4	2a	14/270 (5%)	14 (100%)	0	100	100
4	3A	14/270 (5%)	14 (100%)	0	100	100
4	3a	14/270 (5%)	14 (100%)	0	100	100
4	4A	14/270 (5%)	14 (100%)	0	100	100
4	4a	14/270 (5%)	14 (100%)	0	100	100
5	1B	28/402 (7%)	28 (100%)	0	100	100
5	1b	28/402 (7%)	28 (100%)	0	100	100
5	2B	28/402 (7%)	28 (100%)	0	100	100
5	2b	28/402 (7%)	28 (100%)	0	100	100
5	3B	28/402 (7%)	28 (100%)	0	100	100
5	3b	28/402 (7%)	28 (100%)	0	100	100
5	4B	28/402 (7%)	28 (100%)	0	100	100
5	4b	28/402 (7%)	28 (100%)	0	100	100
6	1C	24/350 (7%)	24 (100%)	0	100	100
6	1c	24/350 (7%)	24 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	2C	24/350 (7%)	24 (100%)	0	100	100
6	2c	24/350 (7%)	24 (100%)	0	100	100
6	3C	24/350 (7%)	24 (100%)	0	100	100
6	3c	24/350 (7%)	24 (100%)	0	100	100
6	4C	24/350 (7%)	24 (100%)	0	100	100
6	4c	24/350 (7%)	24 (100%)	0	100	100
7	1D	14/275 (5%)	14 (100%)	0	100	100
7	1d	14/275 (5%)	14 (100%)	0	100	100
7	2D	14/275 (5%)	14 (100%)	0	100	100
7	2d	14/275 (5%)	14 (100%)	0	100	100
7	3D	14/275 (5%)	14 (100%)	0	100	100
7	3d	14/275 (5%)	14 (100%)	0	100	100
7	4D	14/275 (5%)	14 (100%)	0	100	100
7	4d	14/275 (5%)	14 (100%)	0	100	100
8	1E	4/68 (6%)	4 (100%)	0	100	100
8	1e	4/68 (6%)	4 (100%)	0	100	100
8	2E	4/68 (6%)	4 (100%)	0	100	100
8	2e	4/68 (6%)	4 (100%)	0	100	100
8	3E	4/68 (6%)	4 (100%)	0	100	100
8	3e	4/68 (6%)	4 (100%)	0	100	100
8	4E	4/68 (6%)	4 (100%)	0	100	100
8	4e	4/68 (6%)	4 (100%)	0	100	100
9	1F	2/31 (6%)	2 (100%)	0	100	100
9	1f	1/31 (3%)	1 (100%)	0	100	100
9	2F	2/31 (6%)	2 (100%)	0	100	100
9	2f	1/31 (3%)	1 (100%)	0	100	100
9	3F	2/31 (6%)	2 (100%)	0	100	100
9	3f	1/31 (3%)	1 (100%)	0	100	100
9	4F	2/31 (6%)	2 (100%)	0	100	100
9	4f	1/31 (3%)	1 (100%)	0	100	100
10	1H	4/49 (8%)	4 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	1h	4/49 (8%)	4 (100%)	0	100	100
10	2H	4/49 (8%)	4 (100%)	0	100	100
10	2h	4/49 (8%)	4 (100%)	0	100	100
10	3H	4/49 (8%)	4 (100%)	0	100	100
10	3h	4/49 (8%)	4 (100%)	0	100	100
10	4H	4/49 (8%)	4 (100%)	0	100	100
10	4h	4/49 (8%)	4 (100%)	0	100	100
11	1I	2/31 (6%)	2 (100%)	0	100	100
11	1i	2/31 (6%)	2 (100%)	0	100	100
11	2I	2/31 (6%)	2 (100%)	0	100	100
11	2i	2/31 (6%)	2 (100%)	0	100	100
11	3I	2/31 (6%)	2 (100%)	0	100	100
11	3i	2/31 (6%)	2 (100%)	0	100	100
11	4I	2/31 (6%)	2 (100%)	0	100	100
11	4i	2/31 (6%)	2 (100%)	0	100	100
12	1J	1/26 (4%)	1 (100%)	0	100	100
12	1j	1/26 (4%)	1 (100%)	0	100	100
12	2J	1/26 (4%)	1 (100%)	0	100	100
12	2j	1/26 (4%)	1 (100%)	0	100	100
12	3J	1/26 (4%)	1 (100%)	0	100	100
12	3j	1/26 (4%)	1 (100%)	0	100	100
12	4J	1/26 (4%)	1 (100%)	0	100	100
12	4j	1/26 (4%)	1 (100%)	0	100	100
13	1K	4/32 (12%)	4 (100%)	0	100	100
13	1k	4/32 (12%)	4 (100%)	0	100	100
13	2K	4/32 (12%)	4 (100%)	0	100	100
13	2k	4/32 (12%)	4 (100%)	0	100	100
13	3K	4/32 (12%)	4 (100%)	0	100	100
13	3k	4/32 (12%)	4 (100%)	0	100	100
13	4K	4/32 (12%)	4 (100%)	0	100	100
13	4k	4/32 (12%)	4 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	1L	1/35 (3%)	1 (100%)	0	100	100
14	1l	1/35 (3%)	1 (100%)	0	100	100
14	2L	1/35 (3%)	1 (100%)	0	100	100
14	2l	1/35 (3%)	1 (100%)	0	100	100
14	3L	1/35 (3%)	1 (100%)	0	100	100
14	3l	1/35 (3%)	1 (100%)	0	100	100
14	4L	1/35 (3%)	1 (100%)	0	100	100
14	4l	1/35 (3%)	1 (100%)	0	100	100
15	1M	1/29 (3%)	1 (100%)	0	100	100
15	1m	1/29 (3%)	1 (100%)	0	100	100
15	2M	1/29 (3%)	1 (100%)	0	100	100
15	2m	1/29 (3%)	1 (100%)	0	100	100
15	3M	1/29 (3%)	1 (100%)	0	100	100
15	3m	1/29 (3%)	1 (100%)	0	100	100
15	4M	1/29 (3%)	1 (100%)	0	100	100
15	4m	1/29 (3%)	1 (100%)	0	100	100
16	1O	16/204 (8%)	16 (100%)	0	100	100
16	1o	14/204 (7%)	14 (100%)	0	100	100
16	2O	16/204 (8%)	16 (100%)	0	100	100
16	2o	14/204 (7%)	14 (100%)	0	100	100
16	3O	16/204 (8%)	16 (100%)	0	100	100
16	3o	14/204 (7%)	14 (100%)	0	100	100
16	4O	16/204 (8%)	16 (100%)	0	100	100
16	4o	14/204 (7%)	14 (100%)	0	100	100
17	1P	7/149 (5%)	7 (100%)	0	100	100
17	1p	7/149 (5%)	7 (100%)	0	100	100
17	2P	7/149 (5%)	7 (100%)	0	100	100
17	2p	7/149 (5%)	7 (100%)	0	100	100
17	3P	7/149 (5%)	7 (100%)	0	100	100
17	3p	7/149 (5%)	7 (100%)	0	100	100
17	4P	7/149 (5%)	7 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	4p	7/149 (5%)	7 (100%)	0	100	100
18	1R	15/191 (8%)	15 (100%)	0	100	100
18	1r	15/191 (8%)	15 (100%)	0	100	100
18	2R	15/191 (8%)	15 (100%)	0	100	100
18	2r	15/191 (8%)	15 (100%)	0	100	100
18	3R	15/191 (8%)	15 (100%)	0	100	100
18	3r	15/191 (8%)	15 (100%)	0	100	100
18	4R	15/191 (8%)	15 (100%)	0	100	100
18	4r	15/191 (8%)	15 (100%)	0	100	100
19	1S	15/173 (9%)	15 (100%)	0	100	100
19	1s	15/173 (9%)	15 (100%)	0	100	100
19	2S	15/173 (9%)	15 (100%)	0	100	100
19	2s	15/173 (9%)	15 (100%)	0	100	100
19	3S	15/173 (9%)	15 (100%)	0	100	100
19	3s	15/173 (9%)	15 (100%)	0	100	100
19	4S	15/173 (9%)	15 (100%)	0	100	100
19	4s	15/173 (9%)	15 (100%)	0	100	100
20	1T	3/29 (10%)	3 (100%)	0	100	100
20	1t	3/29 (10%)	3 (100%)	0	100	100
20	2T	3/29 (10%)	3 (100%)	0	100	100
20	2t	3/29 (10%)	3 (100%)	0	100	100
20	3T	3/29 (10%)	3 (100%)	0	100	100
20	3t	3/29 (10%)	3 (100%)	0	100	100
20	4T	3/29 (10%)	3 (100%)	0	100	100
20	4t	3/29 (10%)	3 (100%)	0	100	100
21	1U	2/23 (9%)	2 (100%)	0	100	100
21	1u	2/23 (9%)	2 (100%)	0	100	100
21	2U	2/23 (9%)	2 (100%)	0	100	100
21	2u	2/23 (9%)	2 (100%)	0	100	100
21	3U	2/23 (9%)	2 (100%)	0	100	100
21	3u	2/23 (9%)	2 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	4U	2/23 (9%)	2 (100%)	0	100	100
21	4u	2/23 (9%)	2 (100%)	0	100	100
22	1V	4/77 (5%)	4 (100%)	0	100	100
22	1v	4/77 (5%)	4 (100%)	0	100	100
22	2V	4/77 (5%)	4 (100%)	0	100	100
22	2v	4/77 (5%)	4 (100%)	0	100	100
22	3V	4/77 (5%)	4 (100%)	0	100	100
22	3v	4/77 (5%)	4 (100%)	0	100	100
22	4V	4/77 (5%)	4 (100%)	0	100	100
22	4v	4/77 (5%)	4 (100%)	0	100	100
24	1X	2/32 (6%)	2 (100%)	0	100	100
24	1x	2/32 (6%)	2 (100%)	0	100	100
24	2X	2/32 (6%)	2 (100%)	0	100	100
24	2x	2/32 (6%)	2 (100%)	0	100	100
24	3X	2/32 (6%)	2 (100%)	0	100	100
24	3x	2/32 (6%)	2 (100%)	0	100	100
24	4X	2/32 (6%)	2 (100%)	0	100	100
24	4x	2/32 (6%)	2 (100%)	0	100	100
25	1Y	3/29 (10%)	3 (100%)	0	100	100
25	1y	3/29 (10%)	3 (100%)	0	100	100
25	2Y	3/29 (10%)	3 (100%)	0	100	100
25	2y	3/29 (10%)	3 (100%)	0	100	100
25	3Y	3/29 (10%)	3 (100%)	0	100	100
25	3y	3/29 (10%)	3 (100%)	0	100	100
25	4Y	3/29 (10%)	3 (100%)	0	100	100
25	4y	3/29 (10%)	3 (100%)	0	100	100
26	1Z	2/54 (4%)	2 (100%)	0	100	100
26	1z	2/54 (4%)	2 (100%)	0	100	100
26	2Z	2/54 (4%)	2 (100%)	0	100	100
26	2z	2/54 (4%)	2 (100%)	0	100	100
26	3Z	2/54 (4%)	2 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	3z	2/54 (4%)	2 (100%)	0	100	100
26	4Z	2/54 (4%)	2 (100%)	0	100	100
26	4z	2/54 (4%)	2 (100%)	0	100	100
All	All	2188/29776 (7%)	2188 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 are modelled with single atom - 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

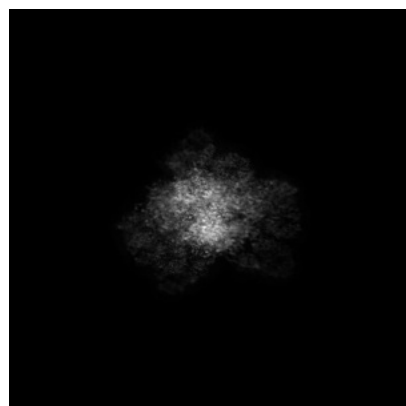
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-68043. These allow visual inspection of the internal detail of the map and identification of artifacts.

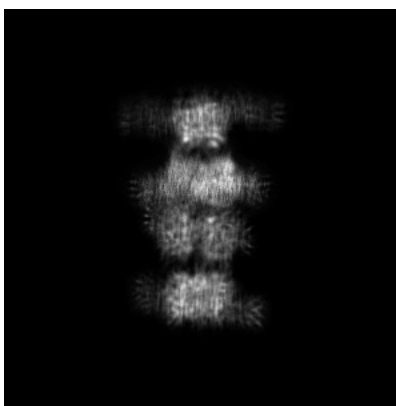
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

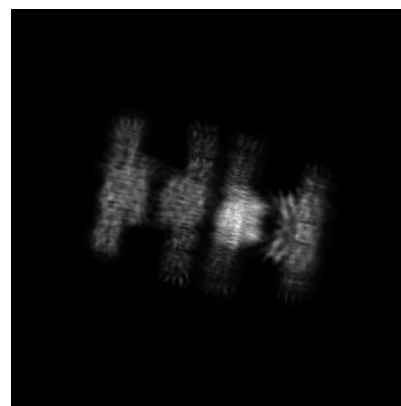
6.1.1 Primary map



X

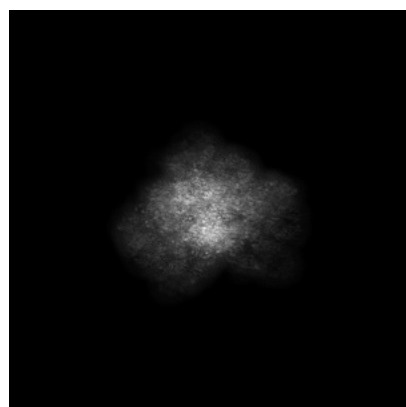


Y

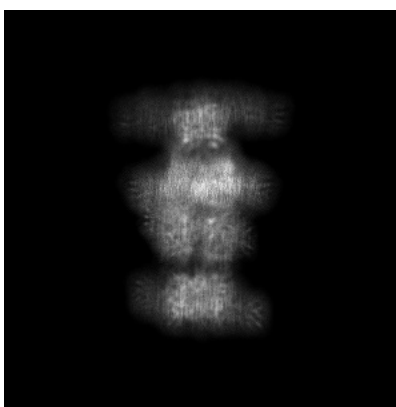


Z

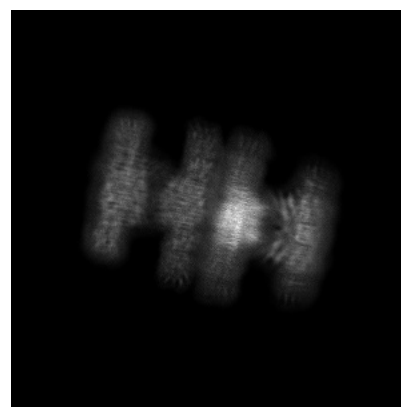
6.1.2 Raw map



X



Y



Z

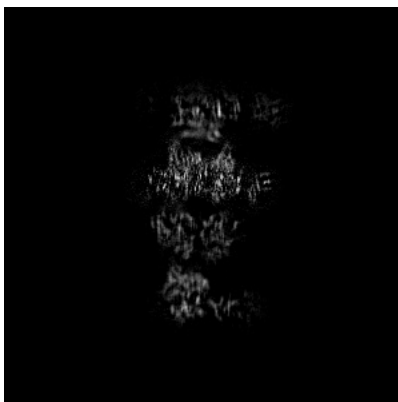
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

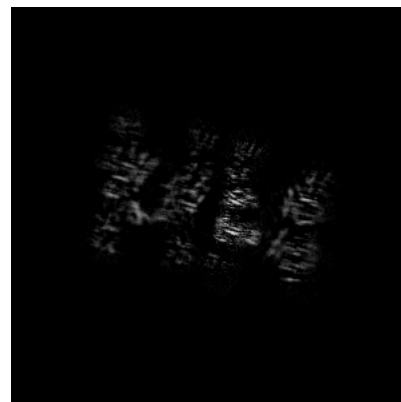
6.2.1 Primary map



X Index: 256

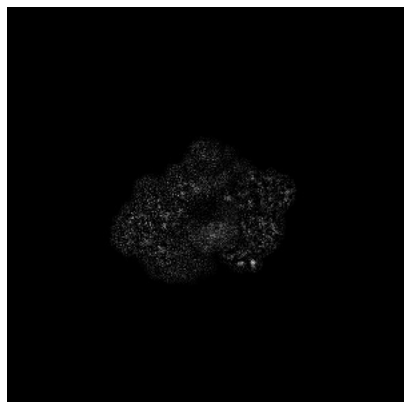


Y Index: 256

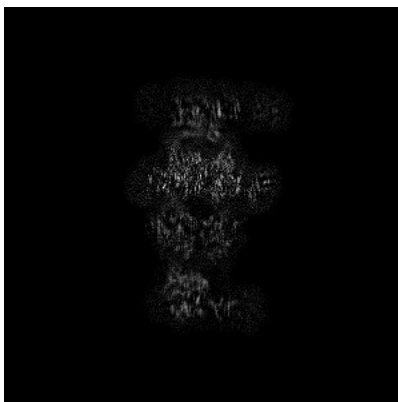


Z Index: 256

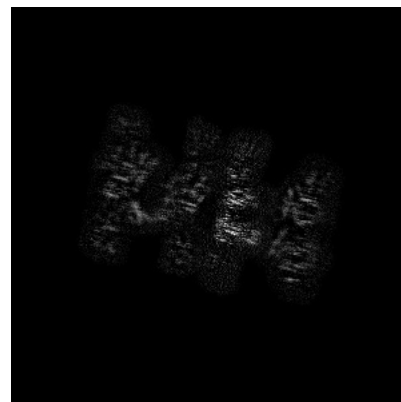
6.2.2 Raw map



X Index: 256



Y Index: 256

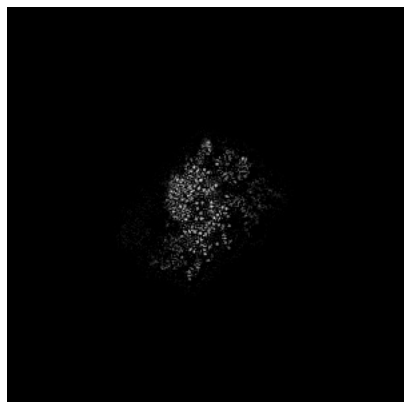


Z Index: 256

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

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 288

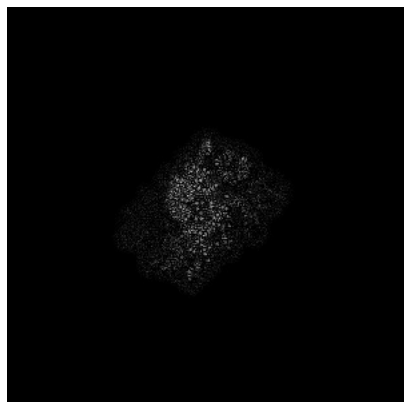


Y Index: 252

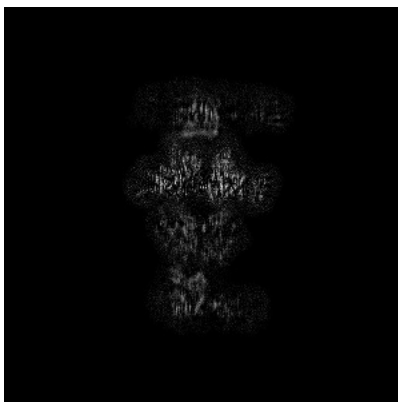


Z Index: 269

6.3.2 Raw map



X Index: 288



Y Index: 252

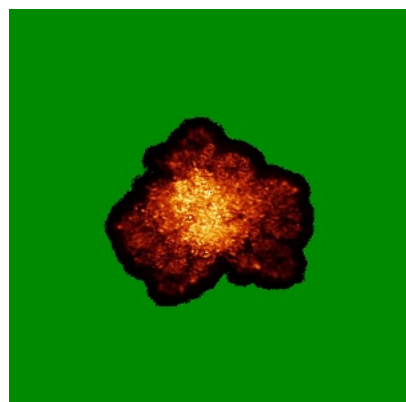


Z Index: 267

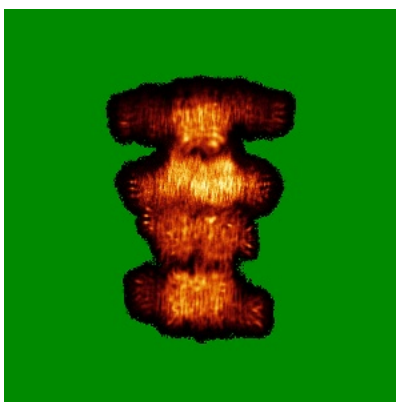
The images above show the largest variance slices of the map in three orthogonal directions.

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

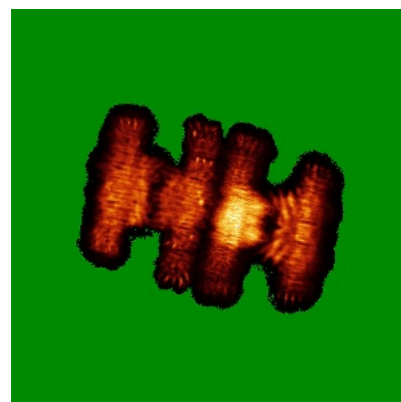
6.4.1 Primary map



X

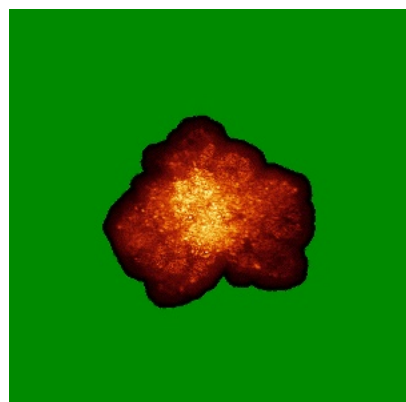


Y

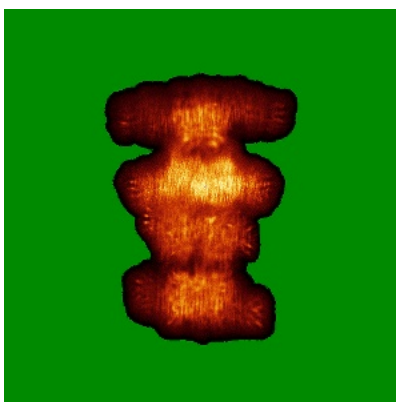


Z

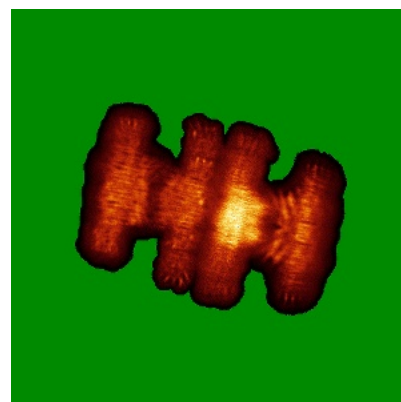
6.4.2 Raw map



X



Y



Z

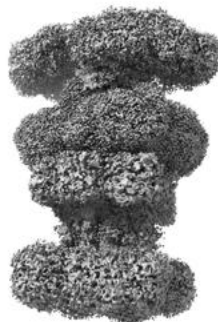
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

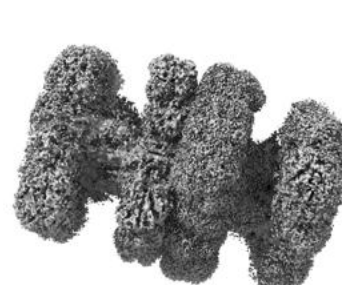
6.5.1 Primary map



X



Y



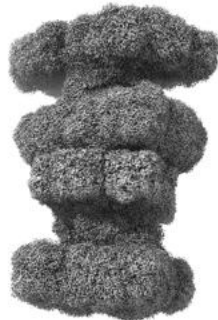
Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

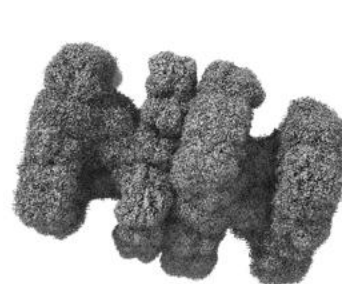
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

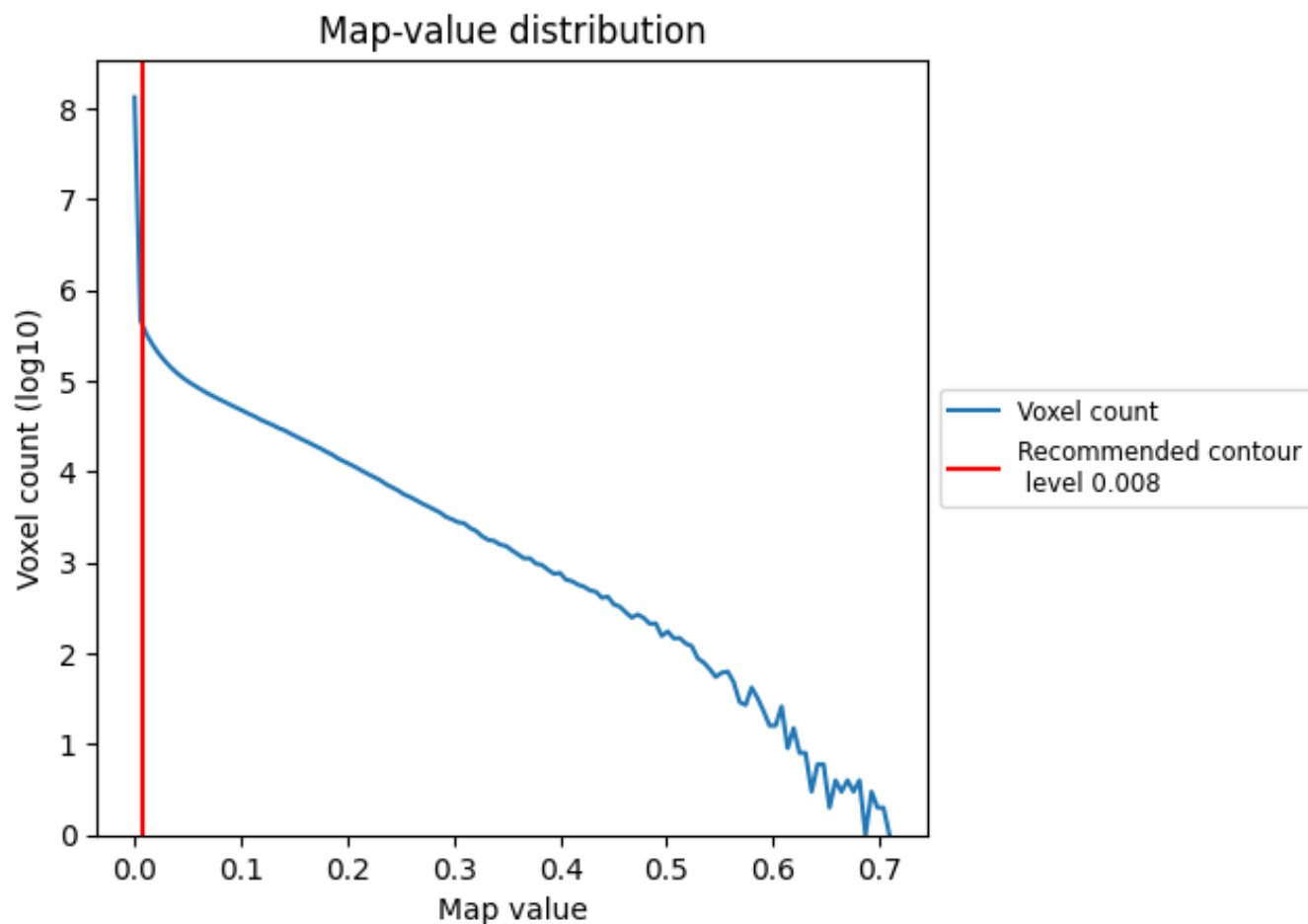
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

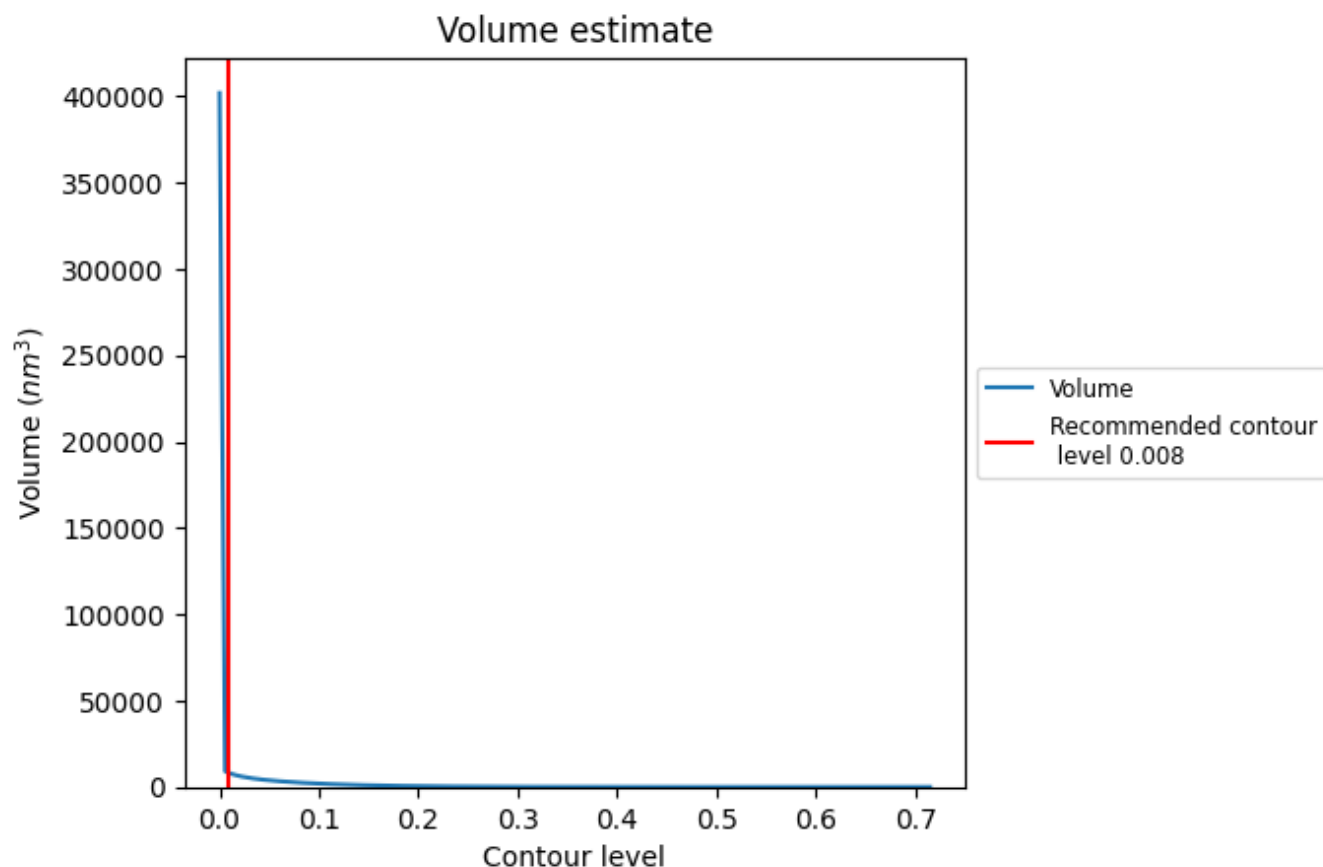
This section contains the results of statistical analysis of the map.

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.

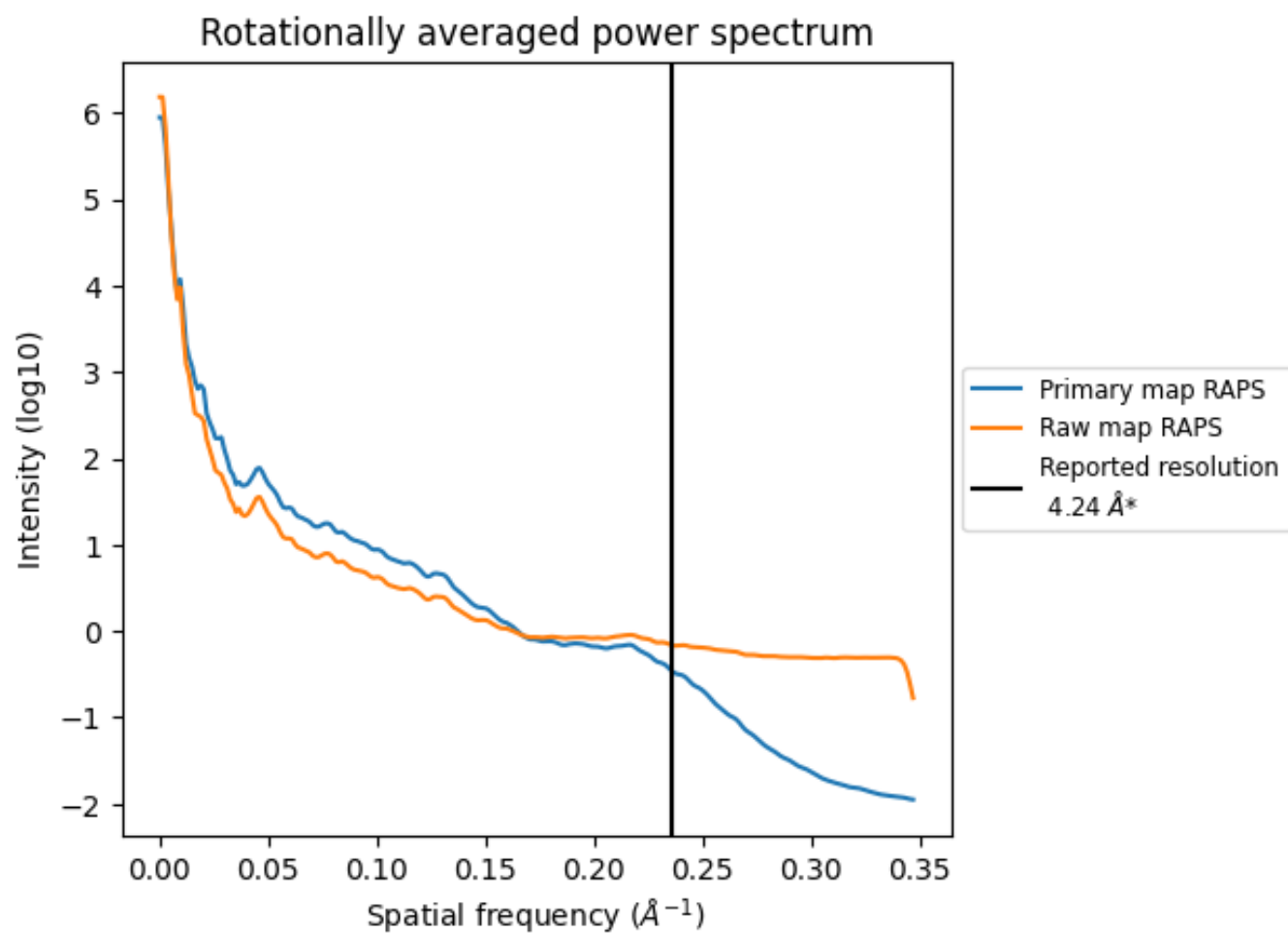
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 8524 nm^3 ; this corresponds to an approximate mass of 7700 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 [i](#)

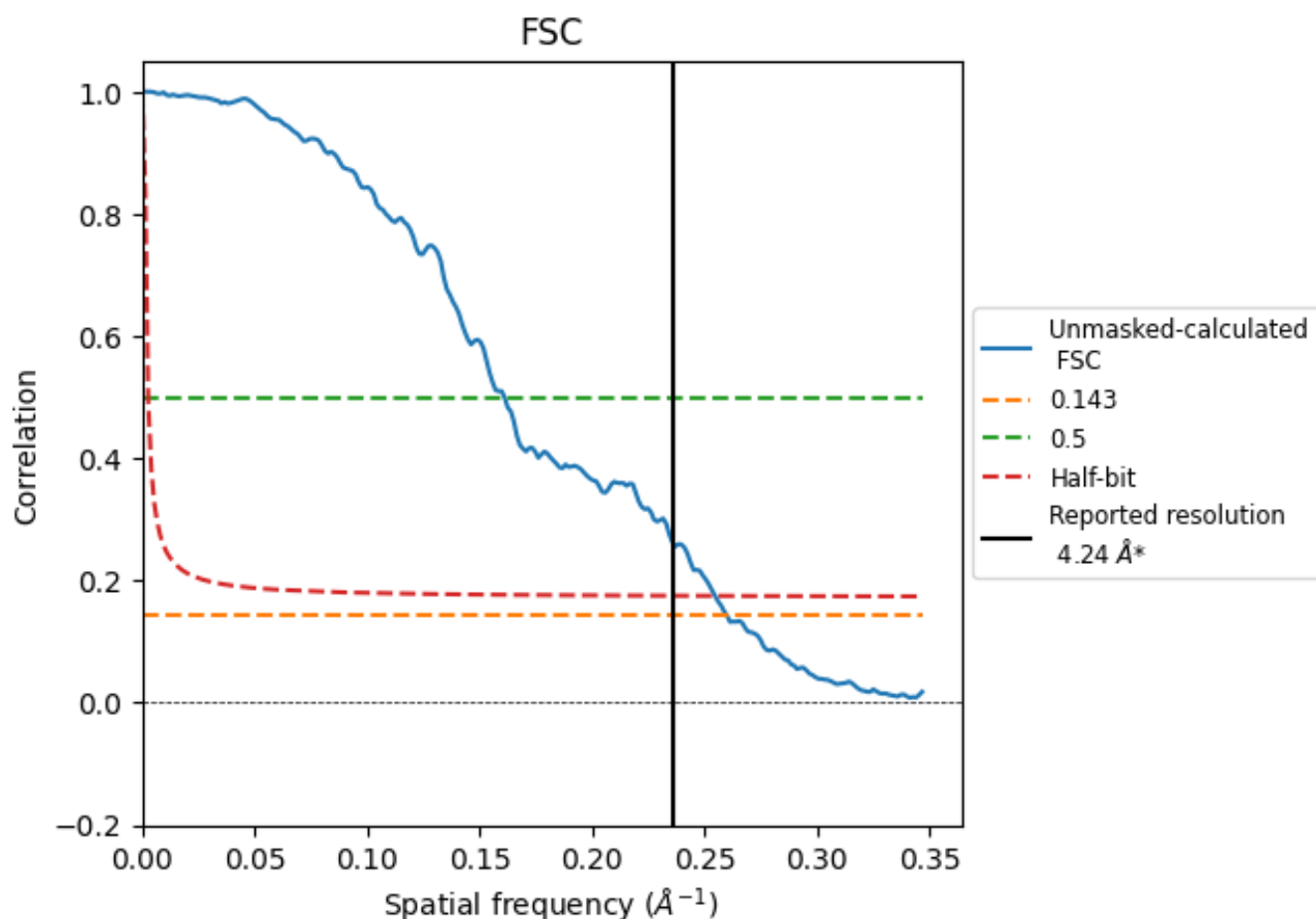


*Reported resolution corresponds to spatial frequency of $0.236 \text{ \AA}^{-1}$

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 0.236 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

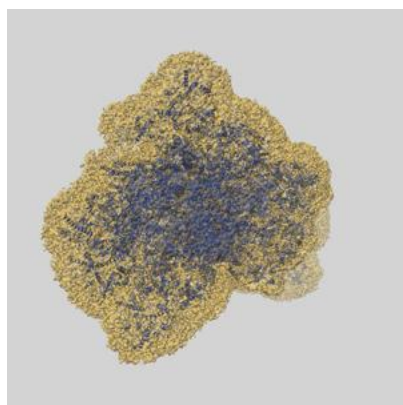
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.24	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.85	6.21	3.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

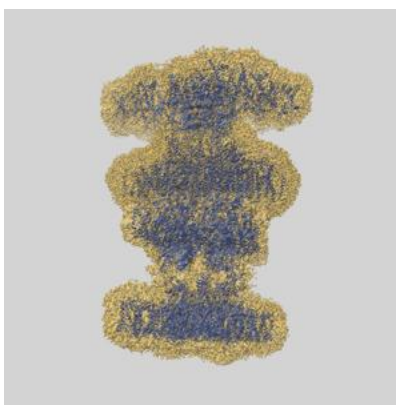
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-68043 and PDB model 21WD. Per-residue inclusion information can be found in [section 3](#) on [page 28](#).

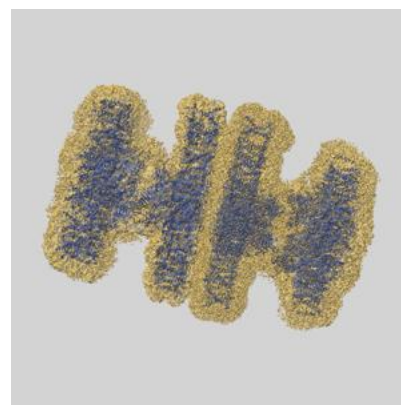
9.1 Map-model overlay [i](#)



X



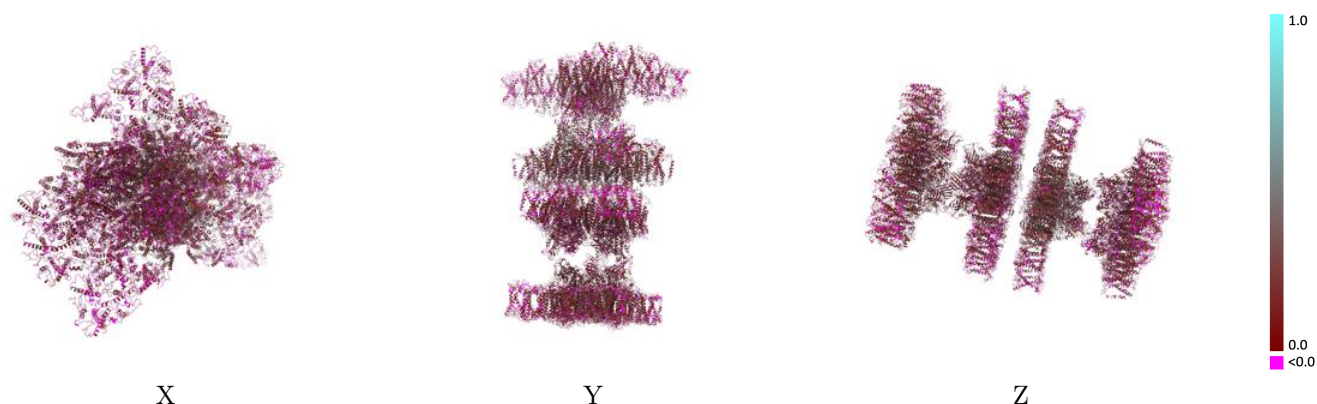
Y



Z

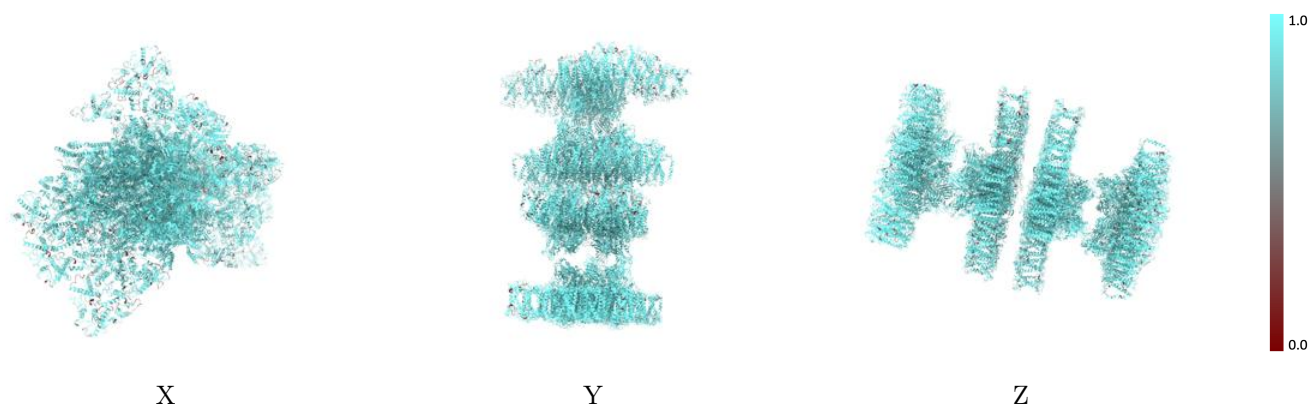
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



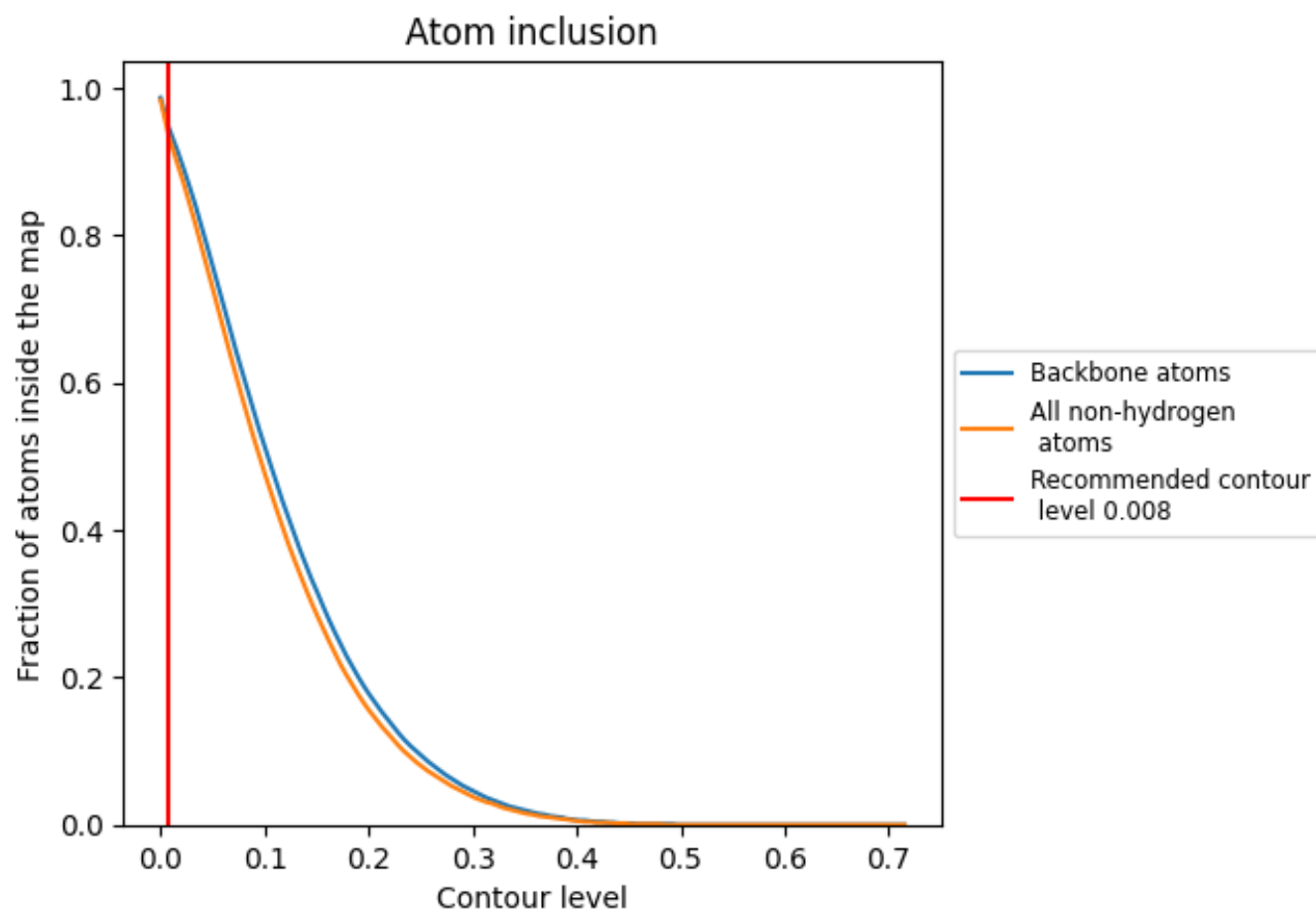
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 93% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9340	 0.1780
00	 0.9750	 0.2700
01	 0.8980	 0.1610
02	 0.8390	 0.0950
03	 0.8500	 0.1150
04	 0.8900	 0.1350
05	 0.8630	 0.1400
06	 0.8480	 0.0860
07	 0.8410	 0.1500
08	 0.8540	 0.1350
09	 0.9650	 0.2750
10	 0.8570	 0.1360
11	 0.8090	 0.0940
12	 0.7730	 0.0550
13	 0.7930	 0.0780
14	 0.7680	 0.0850
15	 0.8230	 0.0830
16	 0.7470	 0.0400
17	 0.7820	 0.0900
18	 0.7380	 0.0860
19	 0.9190	 0.1800
1A	 0.9950	 0.2970
1B	 0.9950	 0.2870
1C	 0.9950	 0.2830
1D	 0.9920	 0.2850
1E	 1.0000	 0.3070
1F	 0.9940	 0.2760
1G	 0.9410	 0.2210
1H	 0.9570	 0.2250
1I	 0.9940	 0.3230
1J	 0.9820	 0.2350
1K	 0.9590	 0.2740
1L	 0.9950	 0.2930
1M	 0.9440	 0.2760
1N	 0.9520	 0.2260



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Chain	Atom inclusion	Q-score
1O	 0.9980	 0.2610
1P	 0.9950	 0.2590
1R	 0.9300	 0.2400
1S	 0.9120	 0.2100
1T	 0.9940	 0.3050
1U	 1.0000	 0.2220
1V	 0.9420	 0.1730
1W	 0.9920	 0.2760
1X	 0.9800	 0.2610
1Y	 0.9600	 0.2190
1Z	 0.9610	 0.2140
1a	 0.9990	 0.2960
1b	 0.9960	 0.2760
1c	 0.9990	 0.2970
1d	 0.9980	 0.3020
1e	 0.9970	 0.2950
1f	 1.0000	 0.2690
1g	 0.9370	 0.2210
1h	 0.9730	 0.2720
1i	 0.9880	 0.3050
1j	 1.0000	 0.2760
1k	 0.9850	 0.2830
1l	 0.9890	 0.2740
1m	 0.9160	 0.2600
1n	 0.9570	 0.2500
1o	 0.9970	 0.2830
1p	 0.9970	 0.2530
1r	 0.9590	 0.2400
1s	 0.9320	 0.2230
1t	 1.0000	 0.3170
1u	 1.0000	 0.2840
1v	 0.9630	 0.2020
1w	 1.0000	 0.2900
1x	 0.9950	 0.2860
1y	 0.9660	 0.2630
1z	 0.9870	 0.2470
2A	 0.9750	 0.1780
2B	 0.9760	 0.1800
2C	 0.9670	 0.1930
2D	 0.9810	 0.1860
2E	 0.9950	 0.2170
2F	 0.9830	 0.2090

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Chain	Atom inclusion	Q-score
2G	 0.8590	 0.1220
2H	 0.9570	 0.1680
2I	 0.9420	 0.2460
2J	 0.9940	 0.2570
2K	 0.9220	 0.1820
2L	 0.9720	 0.1990
2M	 0.9070	 0.2020
2N	 0.8630	 0.1220
2O	 0.9770	 0.1830
2P	 0.9870	 0.2040
2R	 0.8880	 0.1490
2S	 0.8570	 0.1380
2T	 0.9640	 0.2470
2U	 1.0000	 0.1880
2V	 0.8780	 0.1250
2W	 0.9200	 0.2070
2X	 0.9440	 0.1880
2Y	 0.9540	 0.1620
2Z	 0.9360	 0.1770
2a	 0.9800	 0.1750
2b	 0.9800	 0.1800
2c	 0.9760	 0.1990
2d	 0.9830	 0.1780
2e	 0.9970	 0.2260
2f	 0.9870	 0.1610
2g	 0.9020	 0.1360
2h	 0.8770	 0.1480
2i	 1.0000	 0.2020
2j	 0.9820	 0.2130
2k	 0.9330	 0.2210
2l	 0.9550	 0.1680
2m	 0.8860	 0.1930
2n	 0.8680	 0.1260
2o	 0.9770	 0.1640
2p	 0.9510	 0.1630
2r	 0.8580	 0.1280
2s	 0.8150	 0.1160
2t	 0.9750	 0.2390
2u	 1.0000	 0.1320
2v	 0.9100	 0.1150
2w	 0.9950	 0.2570
2x	 0.9420	 0.2230

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Chain	Atom inclusion	Q-score
2y	 0.8800	 0.1560
2z	 0.9450	 0.2000
30	 0.9540	 0.1930
31	 0.9140	 0.1300
32	 0.8340	 0.0770
33	 0.8600	 0.1000
34	 0.8680	 0.1190
35	 0.9210	 0.1180
36	 0.8450	 0.0730
37	 0.9170	 0.1200
38	 0.8540	 0.1290
39	 0.9660	 0.2050
3A	 0.9960	 0.2130
3B	 0.9940	 0.2070
3C	 0.9950	 0.2240
3D	 0.9970	 0.2170
3E	 0.9970	 0.2400
3F	 0.9890	 0.2240
3G	 0.9650	 0.1720
3H	 0.9640	 0.2010
3I	 0.9770	 0.2430
3J	 0.9940	 0.2230
3K	 0.9640	 0.1960
3L	 0.9950	 0.2180
3M	 0.8950	 0.2110
3N	 0.9470	 0.1620
3O	 0.9900	 0.1880
3P	 0.9980	 0.2060
3R	 0.9340	 0.1790
3S	 0.9270	 0.1630
3T	 0.9820	 0.2730
3U	 1.0000	 0.1790
3V	 0.9210	 0.1630
3W	 0.9620	 0.2010
3X	 0.9850	 0.2500
3Y	 0.9430	 0.1940
3Z	 0.9740	 0.2140
3a	 0.9870	 0.1940
3b	 0.9920	 0.2100
3c	 0.9910	 0.2160
3d	 0.9880	 0.2060
3e	 0.9920	 0.2240

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Chain	Atom inclusion	Q-score
3f	 1.0000	 0.2000
3g	 0.9510	 0.1680
3h	 0.9470	 0.2020
3i	 0.9770	 0.2200
3j	 0.9700	 0.2090
3k	 0.9330	 0.1910
3l	 0.9770	 0.2440
3m	 0.8860	 0.1970
3n	 0.9420	 0.1760
3o	 0.9960	 0.2020
3p	 0.9940	 0.1900
3r	 0.9170	 0.1710
3s	 0.8800	 0.1360
3t	 0.9880	 0.2360
3u	 1.0000	 0.2060
3v	 0.8910	 0.1440
3w	 0.9950	 0.2440
3x	 0.9840	 0.2390
3y	 0.9260	 0.2140
3z	 0.9840	 0.2160
40	 0.8950	 0.1400
41	 0.8390	 0.0990
42	 0.8190	 0.0810
43	 0.7830	 0.0740
44	 0.8340	 0.0920
45	 0.8430	 0.0810
46	 0.8070	 0.0500
47	 0.8000	 0.0840
48	 0.7820	 0.0820
49	 0.9250	 0.1670
4A	 0.9740	 0.1420
4B	 0.9770	 0.1550
4C	 0.9820	 0.1720
4D	 0.9820	 0.1610
4E	 0.9760	 0.1730
4F	 0.9720	 0.1800
4G	 0.8950	 0.1310
4H	 0.8470	 0.1340
4I	 1.0000	 0.2320
4J	 0.9230	 0.1510
4K	 0.9170	 0.1830
4L	 0.9830	 0.1550

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Chain	Atom inclusion	Q-score
4M	 0.8830	 0.1700
4N	 0.8730	 0.1250
4O	 0.9890	 0.1130
4P	 0.9590	 0.1140
4R	 0.8560	 0.1210
4S	 0.8610	 0.1320
4T	 0.9640	 0.1990
4U	 1.0000	 0.1420
4V	 0.9290	 0.0990
4W	 0.9390	 0.1520
4X	 0.9230	 0.1820
4Y	 0.8910	 0.1420
4Z	 0.9390	 0.1960
4a	 0.9860	 0.1650
4b	 0.9600	 0.1460
4c	 0.9690	 0.1660
4d	 0.9790	 0.1610
4e	 0.9920	 0.1960
4f	 0.9870	 0.1660
4g	 0.8930	 0.1270
4h	 0.8470	 0.1120
4i	 1.0000	 0.2020
4j	 0.9230	 0.1590
4k	 0.9430	 0.2060
4l	 0.9770	 0.1870
4m	 0.8800	 0.1570
4n	 0.8900	 0.1440
4o	 0.9880	 0.1420
4p	 0.9720	 0.1310
4r	 0.7590	 0.0800
4s	 0.8440	 0.1190
4t	 0.9440	 0.1790
4u	 1.0000	 0.1710
4v	 0.8460	 0.0610
4w	 0.9770	 0.2120
4x	 0.9110	 0.1730
4y	 0.8460	 0.1300
4z	 0.9520	 0.2000