



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 06:22 PM UTC

PDB ID : 7AH9 / pdb_00007ah9
EMDB ID : EMD-11781
Title : Substrate-engaged type 3 secretion system needle complex from *Salmonella enterica typhimurium* - SpaR state 1
Authors : Fahrenkamp, D.; Goessweiner-Mohr, N.; Miletic, S.; Wald, J.; Marlovits, T.
Deposited on : 2020-09-24
Resolution : 3.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

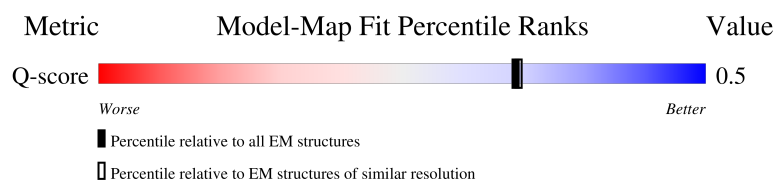
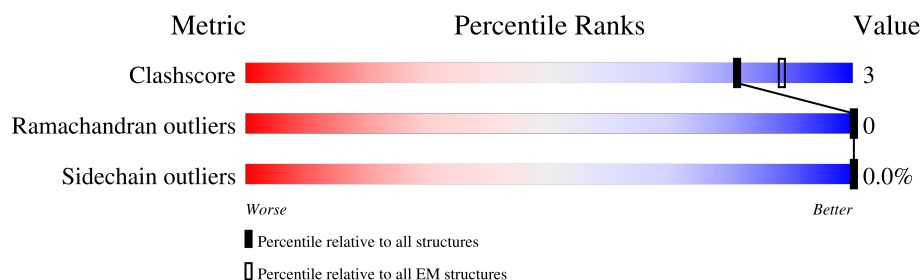
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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.



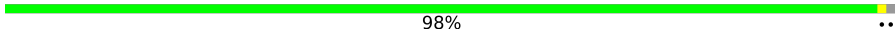
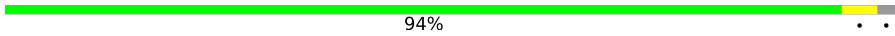
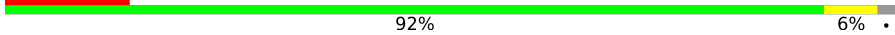
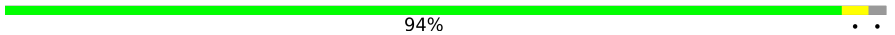
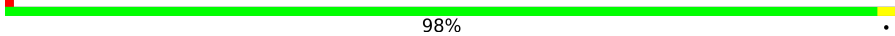
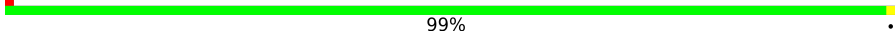
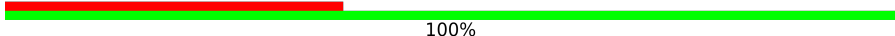
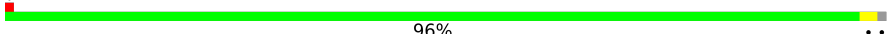
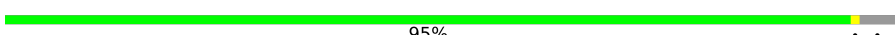
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	1A	224	6% 92% 8%
1	1B	224	93% 6%
1	1C	224	96% .
1	1D	224	96% ..

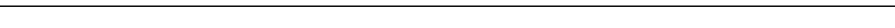
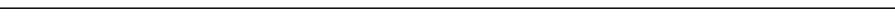
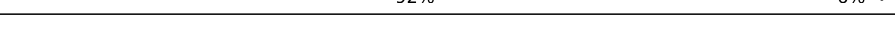
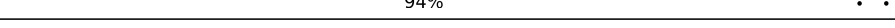
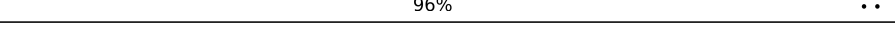
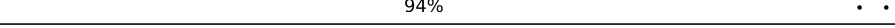
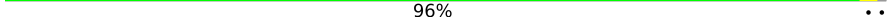
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Mol	Chain	Length	Quality of chain
1	1E	224	
2	1F	263	
3	1G	86	
3	1H	86	
3	1I	86	
3	1J	86	
4	1K	101	
4	1L	101	
4	1M	101	
4	1N	101	
4	1O	101	
4	1P	101	
5	1Z	141	
6	2A	80	
6	2B	80	
6	2C	80	
6	2D	80	
6	2E	80	
6	2F	80	
6	2G	80	
6	2H	80	
6	2I	80	
6	2J	80	
6	2K	80	
6	2L	80	

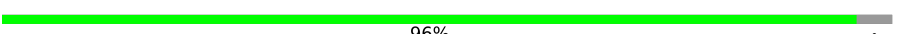
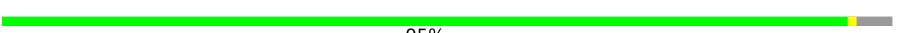
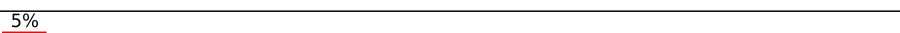
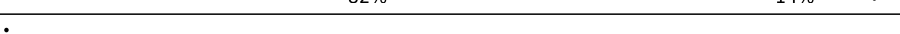
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Mol	Chain	Length	Quality of chain
6	2M	80	 90% 8% .
6	2N	80	 90% 8% .
6	2O	80	 86% 11% .
6	2P	80	 92% . .
6	2Q	80	 91% 6% .
6	2R	80	 94% 5% .
6	2S	80	 92% 5% .
6	2T	80	 95% . .
6	2U	80	 95% . .
6	2V	80	 94% 5% .
6	2W	80	 94% 5% .
6	2X	80	 90% 8% .
6	2Y	80	 89% 9% .
6	2Z	80	 92% 5% .
6	3A	80	 92% 6% .
6	3B	80	 90% 9% .
6	3C	80	 94% . .
6	3D	80	 96% . .
6	3E	80	 94% . .
6	3F	80	 89% 9% .
6	3G	80	 96% . .
6	3H	80	 92% 5% .
6	3I	80	 89% 9% .
6	3J	80	 91% 6% .
6	3K	80	 95% . .

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Mol	Chain	Length	Quality of chain
6	3L	80	 92% . .
6	3M	80	 92% 5% .
6	3N	80	 91% 6% .
6	3O	80	 91% 5% .
6	3P	80	 96% .
6	3Q	80	 95% . .
6	3R	80	 95% . .
6	3S	80	 90% 6% .
6	3T	80	 85% 11% .
6	3U	80	 91% 5% .
6	3V	80	 89% 8% .
6	3W	80	 86% 10% .
6	3X	80	 85% 11% .
6	3Y	80	 78% 19% .
6	3Z	80	 5% 82% 14% .
6	4A	80	 90% 6% .
6	4B	80	 86% 10% .
6	4C	80	 85% 11% .
6	4D	80	 88% 9% .
6	4E	80	 6% 89% 8% .
6	4F	80	 88% 9% .
6	4G	80	 6% 91% 5% .
6	4H	80	 90% 6% .
6	4I	80	 9% 84% 12% .
6	4J	80	 10% 81% 15% .

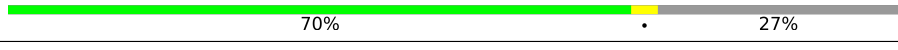
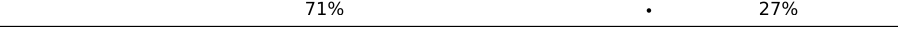
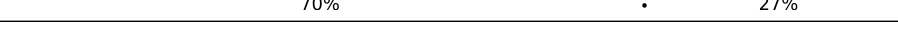
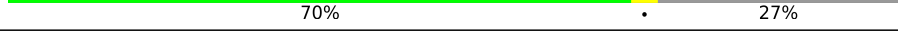
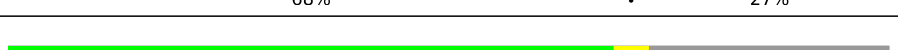
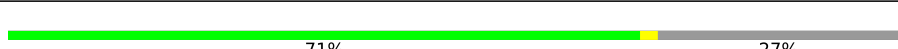
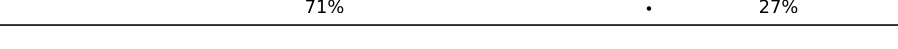
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Mol	Chain	Length	Quality of chain
6	4K	80	
6	4L	80	
6	4M	80	
6	4N	80	
6	4O	80	
6	4P	80	
6	4Q	80	
6	4R	80	
6	4S	80	
6	4T	80	
7	5A	562	
7	5B	562	
7	5C	562	
7	5D	562	
7	5E	562	
7	5F	562	
7	5G	562	
7	5H	562	
7	5I	562	
7	5J	562	
7	5K	562	
7	5L	562	
7	5M	562	
7	5N	562	
7	5O	562	

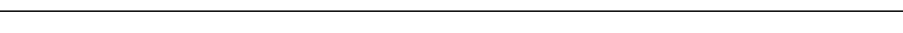
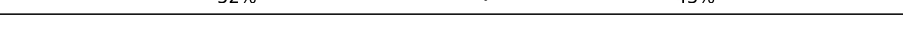
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Mol	Chain	Length	Quality of chain
7	5P	562	
8	6A	252	
8	6B	252	
8	6C	252	
8	6D	252	
8	6E	252	
8	6F	252	
8	6G	252	
8	6H	252	
8	6I	252	
8	6J	252	
8	6K	252	
8	6L	252	
8	6M	252	
8	6N	252	
8	6O	252	
8	6P	252	
8	6Q	252	
8	6R	252	
8	6S	252	
8	6T	252	
8	6U	252	
8	6V	252	
8	6W	252	
8	6X	252	

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Mol	Chain	Length	Quality of chain
9	7A	392	 53% . 44%
9	7B	392	 54% . 43%
9	7C	392	 54% . 43%
9	7D	392	 54% . 44%
9	7E	392	 55% . 43%
9	7F	392	 53% . 43%
9	7G	392	 52% . 44%
9	7H	392	 54% . 43%
9	7I	392	 52% 5% 43%
9	7J	392	 54% . 44%
9	7K	392	 54% . 43%
9	7L	392	 54% . 43%
9	7M	392	 54% . 44%
9	7N	392	 55% . 43%
9	7O	392	 52% . 43%
9	7P	392	 53% . 44%
9	7Q	392	 52% . 43%
9	7R	392	 54% . 43%
9	7S	392	 53% . 44%
9	7T	392	 55% . 43%
9	7U	392	 53% . 43%
9	7V	392	 52% . 44%
9	7W	392	 53% . 43%
9	7X	392	 53% . 43%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 399559 atoms, of which 199567 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 Surface presentation of antigens protein SpaP.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	1A	223	Total	C	H	N	O	S	0	0
			3573	1166	1806	267	322	12		
1	1B	223	Total	C	H	N	O	S	0	0
			3551	1166	1784	267	322	12		
1	1C	223	Total	C	H	N	O	S	0	0
			3577	1166	1810	267	322	12		
1	1D	220	Total	C	H	N	O	S	0	0
			3536	1153	1790	264	317	12		
1	1E	221	Total	C	H	N	O	S	0	0
			3545	1157	1791	265	320	12		

- Molecule 2 is a protein called Surface presentation of antigens protein SpaR.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	1F	257	Total	C	H	N	O	S	0	0
			3967	1297	2007	311	338	14		

- Molecule 3 is a protein called Surface presentation of antigens protein SpaQ.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	1G	84	Total	C	H	N	O	S	0	0
			1339	438	692	97	109	3		
3	1H	84	Total	C	H	N	O	S	0	0
			1339	438	692	97	109	3		
3	1I	86	Total	C	H	N	O	S	0	0
			1369	446	708	100	112	3		
3	1J	86	Total	C	H	N	O	S	0	0
			1369	446	708	100	112	3		

- Molecule 4 is a protein called Protein PrgJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1K	90	Total	C	H	N	O	S	
			1386	424	701	116	142	3	0
4	1L	94	Total	C	H	N	O	S	
			1440	441	726	121	149	3	0
4	1M	90	Total	C	H	N	O	S	
			1386	424	701	116	142	3	0
4	1N	89	Total	C	H	N	O	S	
			1370	419	692	115	141	3	0
4	1O	90	Total	C	H	N	O	S	
			1386	424	701	116	142	3	0
4	1P	90	Total	C	H	N	O	S	
			1387	424	702	116	142	3	0

- Molecule 5 is a protein called SptP3x-GFP-FLAG.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1Z	141	Total	C	H	N	O		
			1413	423	707	141	142	0	0

- Molecule 6 is a protein called Protein PrgI.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	2A	68	Total	C	H	N	O		
			1062	336	528	89	109	0	0
6	2B	60	Total	C	H	N	O		
			948	298	474	81	95	0	0
6	2C	59	Total	C	H	N	O		
			936	294	470	80	92	0	0
6	2D	79	Total	C	H	N	O		
			1220	390	603	102	125	0	0
6	2E	68	Total	C	H	N	O		
			1070	342	530	90	108	0	0
6	2F	75	Total	C	H	N	O		
			1158	367	574	97	120	0	0
6	2G	76	Total	C	H	N	O		
			1182	378	584	99	121	0	0
6	2H	75	Total	C	H	N	O		
			1158	367	574	97	120	0	0
6	2I	75	Total	C	H	N	O		
			1158	367	574	97	120	0	0
6	2J	75	Total	C	H	N	O		
			1158	367	574	97	120	0	0
6	2K	77	Total	C	H	N	O		
			1197	383	592	100	122	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	2L	78	Total	C	H	N	O	0	0
			1210	387	598	101	124		
6	2M	78	Total	C	H	N	O	0	0
			1210	387	598	101	124		
6	2N	78	Total	C	H	N	O	0	0
			1210	387	598	101	124		
6	2O	78	Total	C	H	N	O	0	0
			1210	387	598	101	124		
6	2P	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	2Q	78	Total	C	H	N	O	0	0
			1210	387	598	101	124		
6	2R	79	Total	C	H	N	O	0	0
			1220	390	603	102	125		
6	2S	78	Total	C	H	N	O	0	0
			1210	387	598	101	124		
6	2T	79	Total	C	H	N	O	0	0
			1220	390	603	102	125		
6	2U	78	Total	C	H	N	O	0	0
			1210	387	598	101	124		
6	2V	79	Total	C	H	N	O	0	0
			1220	390	603	102	125		
6	2W	79	Total	C	H	N	O	0	0
			1220	390	603	102	125		
6	2X	78	Total	C	H	N	O	0	0
			1210	387	598	101	124		
6	2Y	78	Total	C	H	N	O	0	0
			1210	387	598	101	124		
6	2Z	78	Total	C	H	N	O	0	0
			1210	387	598	101	124		
6	3A	79	Total	C	H	N	O	0	0
			1220	390	603	102	125		
6	3B	79	Total	C	H	N	O	0	0
			1220	390	603	102	125		
6	3C	78	Total	C	H	N	O	0	0
			1210	387	598	101	124		
6	3D	78	Total	C	H	N	O	0	0
			1210	387	598	101	124		
6	3E	78	Total	C	H	N	O	0	0
			1210	387	598	101	124		
6	3F	78	Total	C	H	N	O	0	0
			1210	387	598	101	124		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	3G	79	Total	C	H	N	O	0	0
			1220	390	603	102	125		
6	3H	78	Total	C	H	N	O	0	0
			1210	387	598	101	124		
6	3I	78	Total	C	H	N	O	0	0
			1210	387	598	101	124		
6	3J	78	Total	C	H	N	O	0	0
			1210	387	598	101	124		
6	3K	78	Total	C	H	N	O	0	0
			1210	387	598	101	124		
6	3L	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	3M	78	Total	C	H	N	O	0	0
			1210	387	598	101	124		
6	3N	78	Total	C	H	N	O	0	0
			1210	387	598	101	124		
6	3O	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	3P	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	3Q	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	3R	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	3S	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	3T	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	3U	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	3V	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	3W	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	3X	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	3Y	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	3Z	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	4A	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	4B	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	4C	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	4D	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	4E	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	4F	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	4G	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	4H	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	4I	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	4J	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	4K	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	4L	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	4M	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	4N	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	4O	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	4P	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	4Q	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	4R	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	4S	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		
6	4T	77	Total	C	H	N	O	0	0
			1197	383	592	100	122		

- Molecule 7 is a protein called Type 3 secretion system secretin.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	5A	141	Total	C	H	N	O	S	0	0
			2241	719	1119	191	206	6		
7	5B	502	Total	C	H	N	O	S	0	0
			7884	2474	3971	680	747	12		
7	5C	501	Total	C	H	N	O	S	0	0
			7862	2468	3959	678	745	12		
7	5D	506	Total	C	H	N	O	S	0	0
			7953	2496	4007	685	753	12		
7	5E	503	Total	C	H	N	O	S	0	0
			7898	2479	3978	681	748	12		
7	5F	506	Total	C	H	N	O	S	0	0
			7953	2496	4007	685	753	12		
7	5G	504	Total	C	H	N	O	S	0	0
			7909	2482	3983	682	750	12		
7	5H	506	Total	C	H	N	O	S	0	0
			7952	2496	4006	685	753	12		
7	5I	503	Total	C	H	N	O	S	0	0
			7898	2479	3978	681	748	12		
7	5J	508	Total	C	H	N	O	S	0	0
			7981	2504	4021	687	756	13		
7	5K	502	Total	C	H	N	O	S	0	0
			7879	2473	3967	680	747	12		
7	5L	506	Total	C	H	N	O	S	0	0
			7954	2496	4008	685	753	12		
7	5M	500	Total	C	H	N	O	S	0	0
			7847	2463	3951	677	744	12		
7	5N	501	Total	C	H	N	O	S	0	0
			7873	2471	3966	679	745	12		
7	5O	498	Total	C	H	N	O	S	0	0
			7817	2454	3936	675	740	12		
7	5P	500	Total	C	H	N	O	S	0	0
			7851	2465	3953	677	744	12		

- Molecule 8 is a protein called Lipoprotein PrgK.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	6A	183	Total	C	H	N	O	S	0	0
			2849	899	1421	248	278	3		
8	6B	183	Total	C	H	N	O	S	0	0
			2849	899	1421	248	278	3		
8	6C	183	Total	C	H	N	O	S	0	0
			2849	899	1421	248	278	3		
8	6D	183	Total	C	H	N	O	S	0	0
			2849	899	1421	248	278	3		

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Mol	Chain	Residues	Atoms						AltConf	Trace
8	6E	183	Total 2849	C 899	H 1421	N 248	O 278	S 3	0	0
8	6F	183	Total 2849	C 899	H 1421	N 248	O 278	S 3	0	0
8	6G	183	Total 2849	C 899	H 1421	N 248	O 278	S 3	0	0
8	6H	183	Total 2849	C 899	H 1421	N 248	O 278	S 3	0	0
8	6I	183	Total 2849	C 899	H 1421	N 248	O 278	S 3	0	0
8	6J	183	Total 2849	C 899	H 1421	N 248	O 278	S 3	0	0
8	6K	183	Total 2849	C 899	H 1421	N 248	O 278	S 3	0	0
8	6L	183	Total 2849	C 899	H 1421	N 248	O 278	S 3	0	0
8	6M	183	Total 2849	C 899	H 1421	N 248	O 278	S 3	0	0
8	6N	183	Total 2849	C 899	H 1421	N 248	O 278	S 3	0	0
8	6O	183	Total 2849	C 899	H 1421	N 248	O 278	S 3	0	0
8	6P	183	Total 2849	C 899	H 1421	N 248	O 278	S 3	0	0
8	6Q	183	Total 2849	C 899	H 1421	N 248	O 278	S 3	0	0
8	6R	183	Total 2849	C 899	H 1421	N 248	O 278	S 3	0	0
8	6S	183	Total 2848	C 899	H 1420	N 248	O 278	S 3	0	0
8	6T	183	Total 2849	C 899	H 1421	N 248	O 278	S 3	0	0
8	6U	183	Total 2849	C 899	H 1421	N 248	O 278	S 3	0	0
8	6V	183	Total 2848	C 899	H 1420	N 248	O 278	S 3	0	0
8	6W	183	Total 2849	C 899	H 1421	N 248	O 278	S 3	0	0
8	6X	183	Total 2849	C 899	H 1421	N 248	O 278	S 3	0	0

- Molecule 9 is a protein called Protein PrgH.

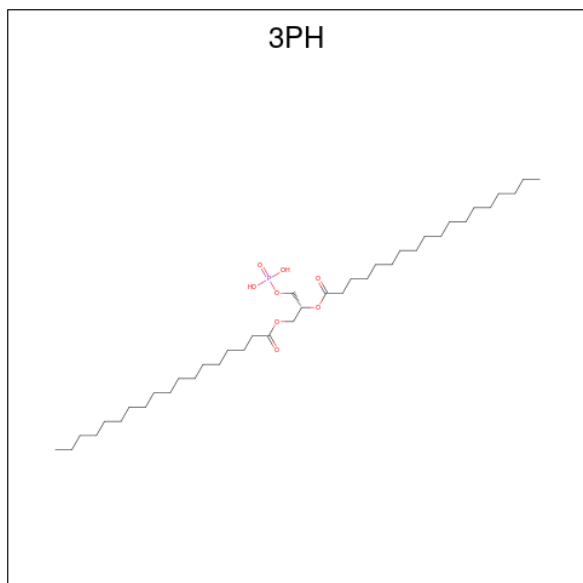
Mol	Chain	Residues	Atoms						AltConf	Trace
9	7A	220	Total	C	H	N	O	S	0	0
			3602	1159	1782	324	332	5		
9	7B	222	Total	C	H	N	O	S	0	0
			3636	1170	1800	326	335	5		
9	7C	222	Total	C	H	N	O	S	0	0
			3636	1170	1800	326	335	5		
9	7D	220	Total	C	H	N	O	S	0	0
			3602	1159	1782	324	332	5		
9	7E	222	Total	C	H	N	O	S	0	0
			3636	1170	1800	326	335	5		
9	7F	222	Total	C	H	N	O	S	0	0
			3636	1170	1800	326	335	5		
9	7G	220	Total	C	H	N	O	S	0	0
			3602	1159	1782	324	332	5		
9	7H	222	Total	C	H	N	O	S	0	0
			3636	1170	1800	326	335	5		
9	7I	222	Total	C	H	N	O	S	0	0
			3636	1170	1800	326	335	5		
9	7J	220	Total	C	H	N	O	S	0	0
			3602	1159	1782	324	332	5		
9	7K	222	Total	C	H	N	O	S	0	0
			3636	1170	1800	326	335	5		
9	7L	222	Total	C	H	N	O	S	0	0
			3636	1170	1800	326	335	5		
9	7M	220	Total	C	H	N	O	S	0	0
			3602	1159	1782	324	332	5		
9	7N	222	Total	C	H	N	O	S	0	0
			3636	1170	1800	326	335	5		
9	7O	222	Total	C	H	N	O	S	0	0
			3636	1170	1800	326	335	5		
9	7P	220	Total	C	H	N	O	S	0	0
			3602	1159	1782	324	332	5		
9	7Q	222	Total	C	H	N	O	S	0	0
			3636	1170	1800	326	335	5		
9	7R	222	Total	C	H	N	O	S	0	0
			3636	1170	1800	326	335	5		
9	7S	220	Total	C	H	N	O	S	0	0
			3602	1159	1782	324	332	5		
9	7T	222	Total	C	H	N	O	S	0	0
			3636	1170	1800	326	335	5		
9	7U	222	Total	C	H	N	O	S	0	0
			3636	1170	1800	326	335	5		
9	7V	220	Total	C	H	N	O	S	0	0
			3602	1159	1782	324	332	5		

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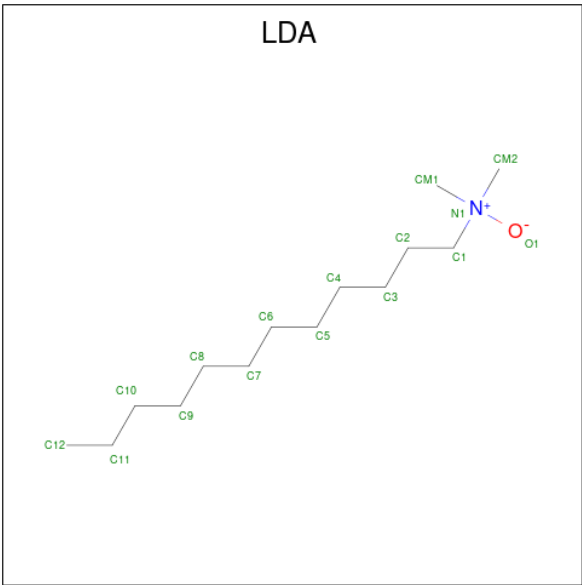
Mol	Chain	Residues	Atoms						AltConf	Trace
9	7W	222	Total	C	H	N	O	S	0	0
			3636	1170	1800	326	335	5		
9	7X	222	Total	C	H	N	O	S	0	0
			3636	1170	1800	326	335	5		

- Molecule 10 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



Mol	Chain	Residues	Atoms					AltConf
10	1A	1	Total	C	H	O	P	0
			81	27	45	8	1	
10	1L	1	Total	C	H	O	P	0
			69	25	35	8	1	
10	1M	1	Total	C	H	O	P	0
			67	25	33	8	1	
10	1N	1	Total	C	H	O	P	0
			67	25	33	8	1	
10	1P	1	Total	C	H	O	P	0
			116	37	70	8	1	

- Molecule 11 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).

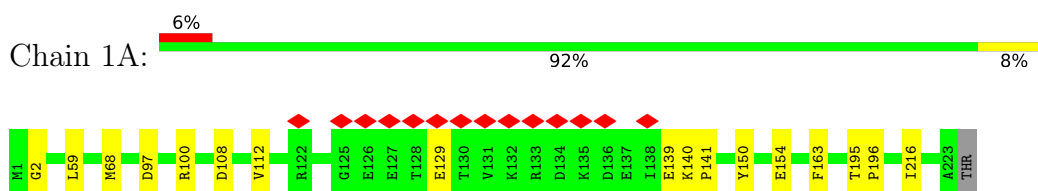


Mol	Chain	Residues	Atoms					AltConf
11	1A	1	Total	C	H	N	O	0
			47	14	31	1	1	
11	1D	1	Total	C	H	N	O	0
			47	14	31	1	1	
11	1G	1	Total	C	H	N	O	0
			47	14	31	1	1	
11	1H	1	Total	C	H	N	O	0
			47	14	31	1	1	
11	1I	1	Total	C	H	N	O	0
			47	14	31	1	1	
11	1I	1	Total	C	H	N	O	0
			47	14	31	1	1	
11	1I	1	Total	C	H	N	O	0
			47	14	31	1	1	
11	1J	1	Total	C	H	N	O	0
			47	14	31	1	1	
11	1J	1	Total	C	H	N	O	0
			47	14	31	1	1	

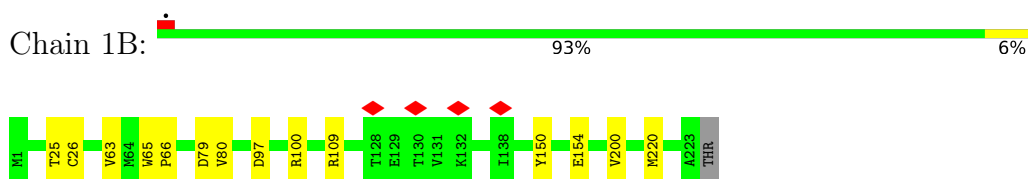
3 Residue-property plots [i](#)

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.

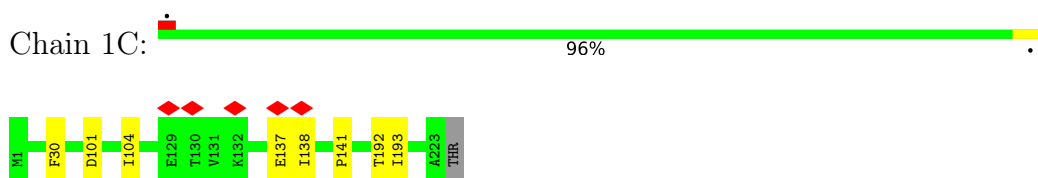
- Molecule 1: Surface presentation of antigens protein SpaP



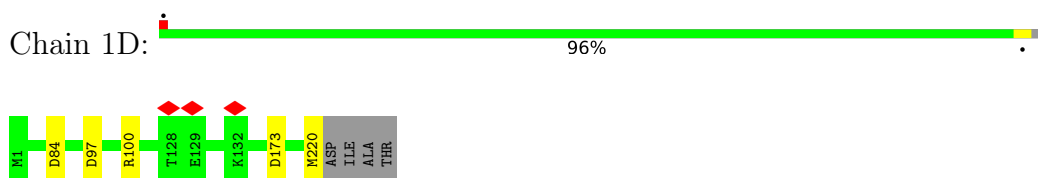
- Molecule 1: Surface presentation of antigens protein SpaP



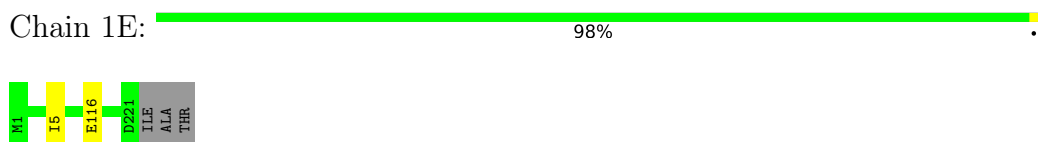
- Molecule 1: Surface presentation of antigens protein SpaP



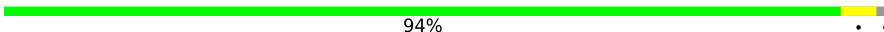
- Molecule 1: Surface presentation of antigens protein SpaP



- Molecule 1: Surface presentation of antigens protein SpaP

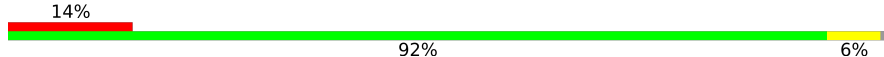


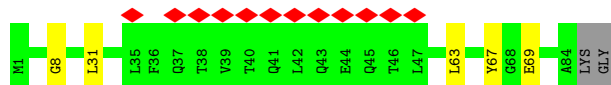
- Molecule 2: Surface presentation of antigens protein SpaR

Chain 1F:  94%

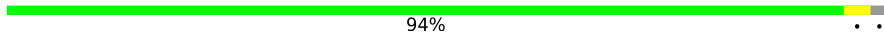


- Molecule 3: Surface presentation of antigens protein SpaQ

Chain 1G:  92% 6%

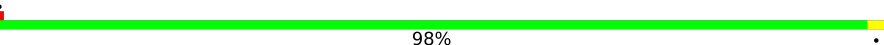


- Molecule 3: Surface presentation of antigens protein SpaQ

Chain 1H:  94%

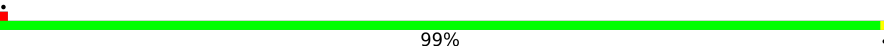


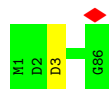
- Molecule 3: Surface presentation of antigens protein SpaQ

Chain 1I:  98%



- Molecule 3: Surface presentation of antigens protein SpaQ

Chain 1J:  99%



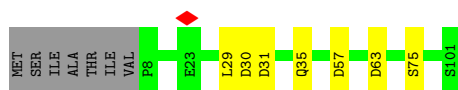
- Molecule 4: Protein PrgJ

Chain 1K:  83% 6% 11%

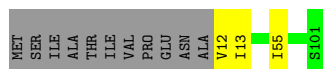
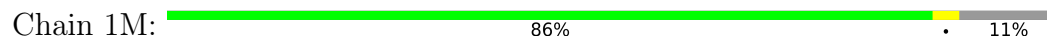


- Molecule 4: Protein PrgJ

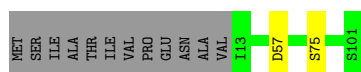
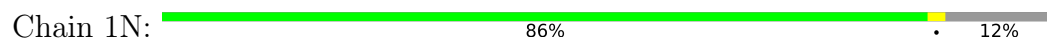
Chain 1L:  86% 7% 7%



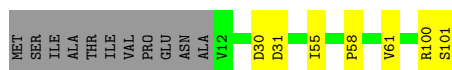
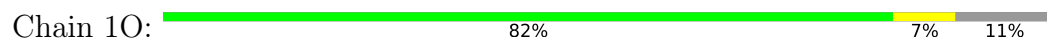
• Molecule 4: Protein PrgJ



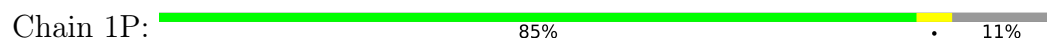
• Molecule 4: Protein PrgJ



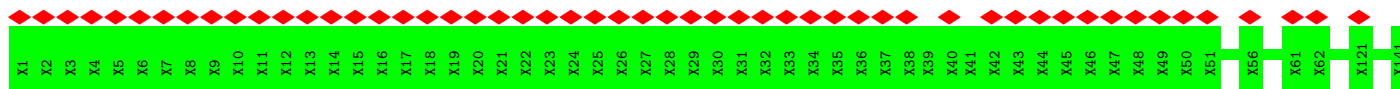
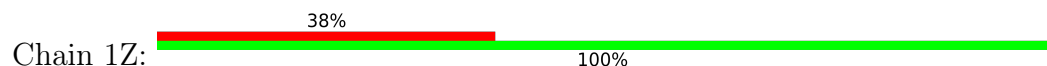
• Molecule 4: Protein PrgJ



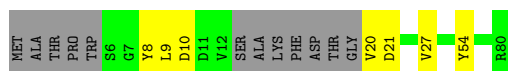
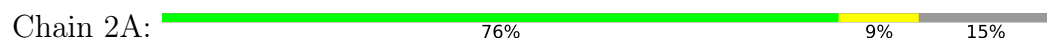
• Molecule 4: Protein PrgJ



• Molecule 5: SptP3x-GFP-FLAG

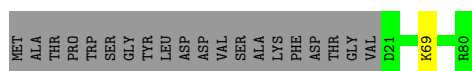


• Molecule 6: Protein PrgI

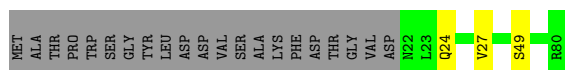


• Molecule 6: Protein PrgI

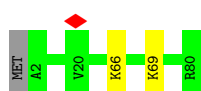




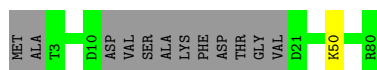
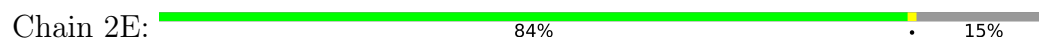
● Molecule 6: Protein PrgI



● Molecule 6: Protein PrgI



● Molecule 6: Protein PrgI



● Molecule 6: Protein PrgI



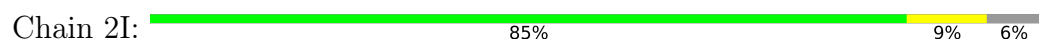
● Molecule 6: Protein PrgI

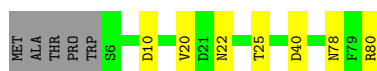


● Molecule 6: Protein PrgI



● Molecule 6: Protein PrgI

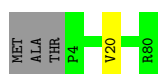




• Molecule 6: Protein PrgI



• Molecule 6: Protein PrgI



• Molecule 6: Protein PrgI



• Molecule 6: Protein PrgI



• Molecule 6: Protein PrgI



• Molecule 6: Protein PrgI



• Molecule 6: Protein PrgI





- Molecule 6: Protein PrgI



- Molecule 6: Protein PrgI



- Molecule 6: Protein PrgI



- Molecule 6: Protein PrgI



- Molecule 6: Protein PrgI

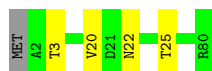


- Molecule 6: Protein PrgI



- Molecule 6: Protein PrgI





- Molecule 6: Protein PrgI

Chain 2X: 90% 8% .



- Molecule 6: Protein PrgI

Chain 2Y: 89% 9% .



- Molecule 6: Protein PrgI

Chain 2Z: 92% 5% .



- Molecule 6: Protein PrgI

Chain 3A: 92% 6% .



- Molecule 6: Protein PrgI

Chain 3B: 90% 9% .



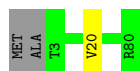
- Molecule 6: Protein PrgI

Chain 3C: 94% . .

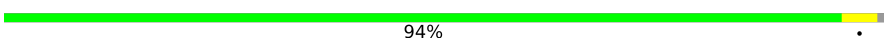


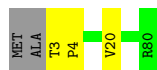
- Molecule 6: Protein PrgI

Chain 3D: 96% . .



- Molecule 6: Protein PrgI

Chain 3E:  94% . .

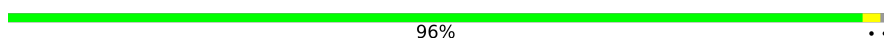


- Molecule 6: Protein PrgI

Chain 3F:  89% 9% .

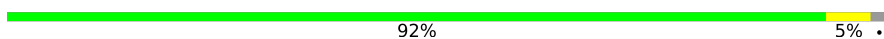


- Molecule 6: Protein PrgI

Chain 3G:  96% . .



- Molecule 6: Protein PrgI

Chain 3H:  92% 5% .



- Molecule 6: Protein PrgI

Chain 3I:  89% 9% .

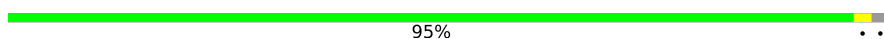


- Molecule 6: Protein PrgI

Chain 3J:  91% 6% .



- Molecule 6: Protein PrgI

Chain 3K:  95% . .



- Molecule 6: Protein PrgI

Chain 3L: 92% . .



- Molecule 6: Protein PrgI

Chain 3M: 92% 5% .



- Molecule 6: Protein PrgI

Chain 3N: 91% 6% .



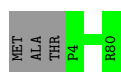
- Molecule 6: Protein PrgI

Chain 3O: 91% 5% .



- Molecule 6: Protein PrgI

Chain 3P: 96% .



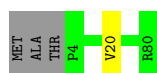
- Molecule 6: Protein PrgI

Chain 3Q: 95% . .

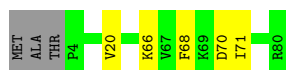


- Molecule 6: Protein PrgI

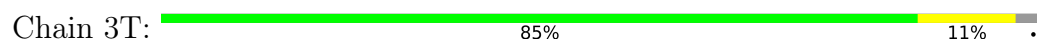
Chain 3R: 95% . .



• Molecule 6: Protein PrgI



• Molecule 6: Protein PrgI



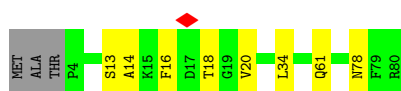
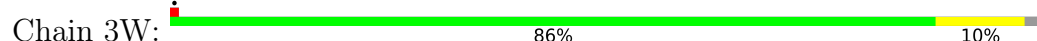
• Molecule 6: Protein PrgI



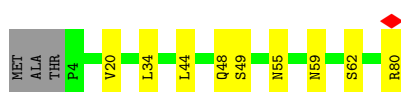
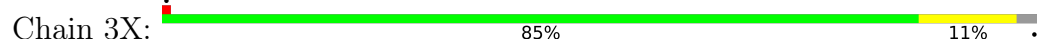
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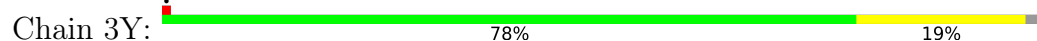
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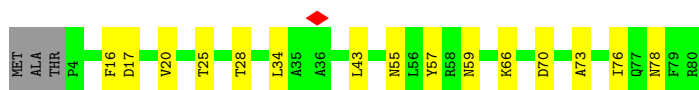


• Molecule 6: Protein PrgI

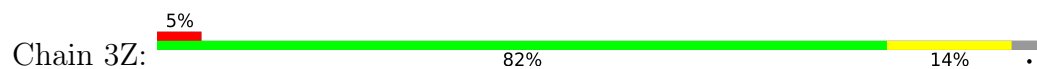


• Molecule 6: Protein PrgI

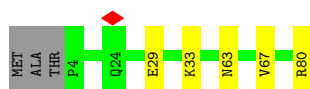
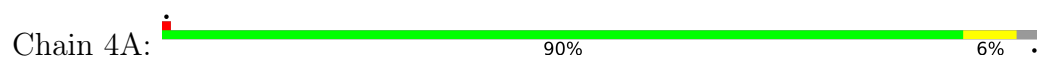




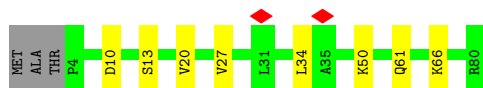
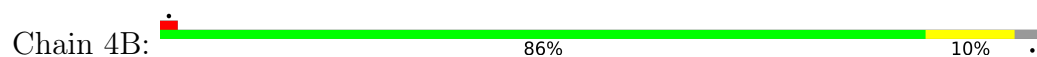
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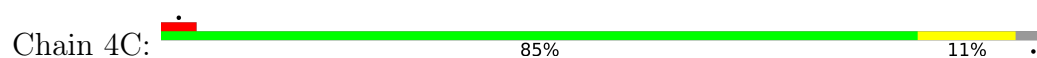
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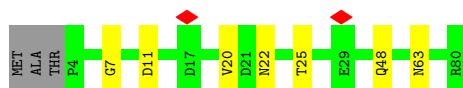
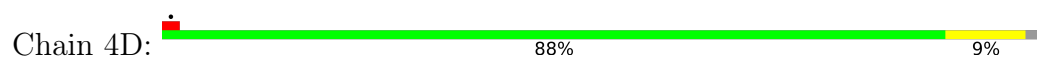
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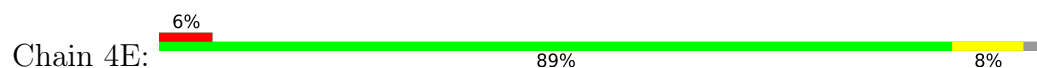
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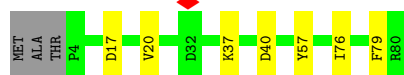
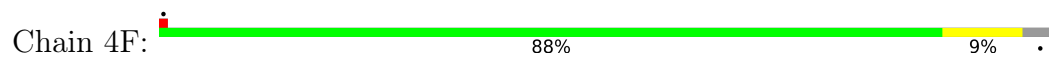
• Molecule 6: Protein PrgI



• Molecule 6: Protein PrgI



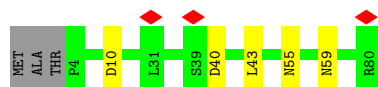
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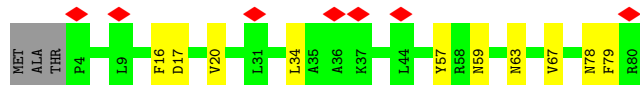
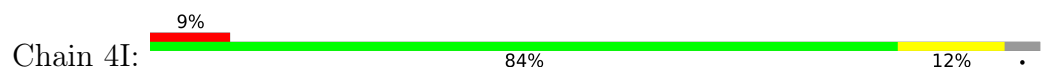
- Molecule 6: Protein PrgI



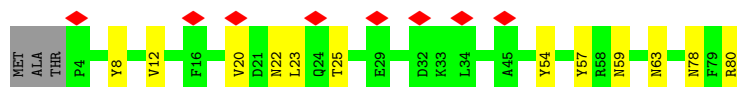
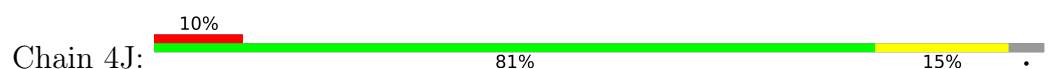
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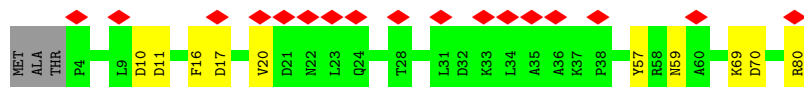
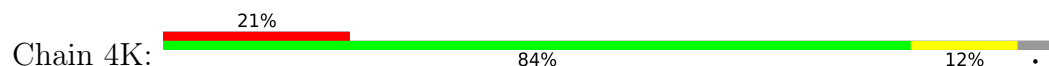
- Molecule 6: Protein PrgI



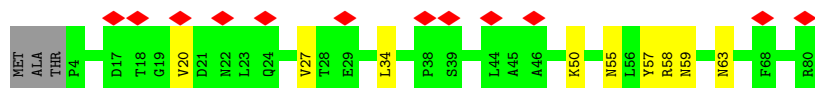
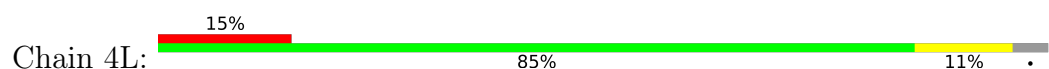
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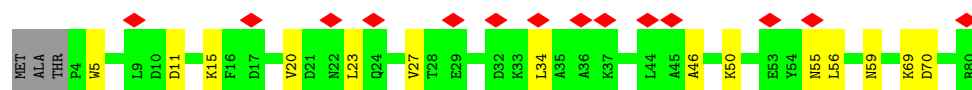
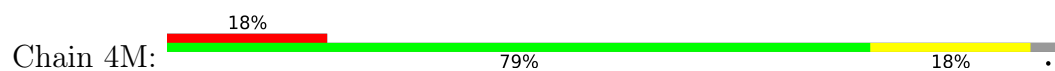
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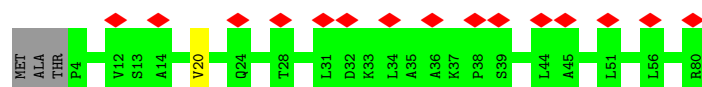
- Molecule 6: Protein PrgI



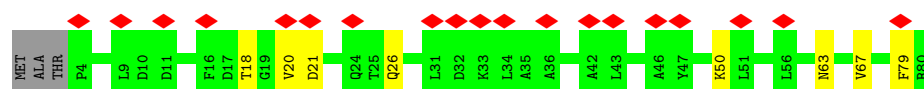
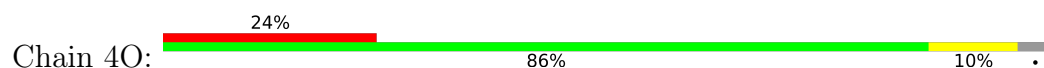
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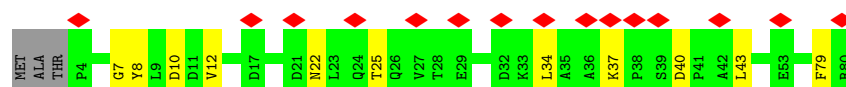
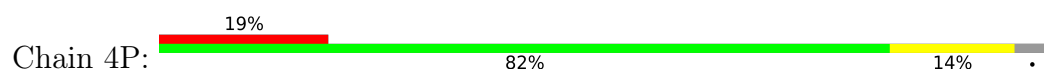
• Molecule 6: Protein PrgI



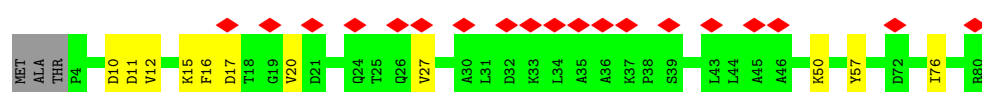
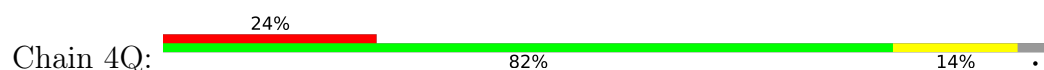
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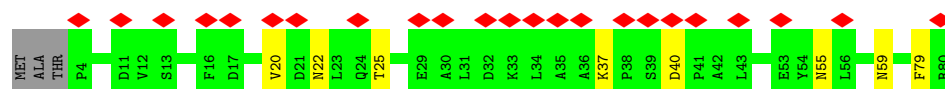
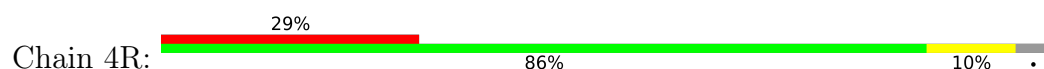
• Molecule 6: Protein PrgI



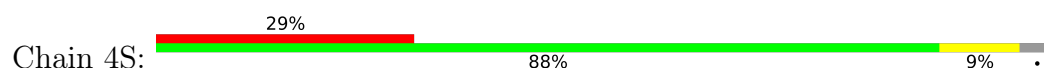
• Molecule 6: Protein PrgI



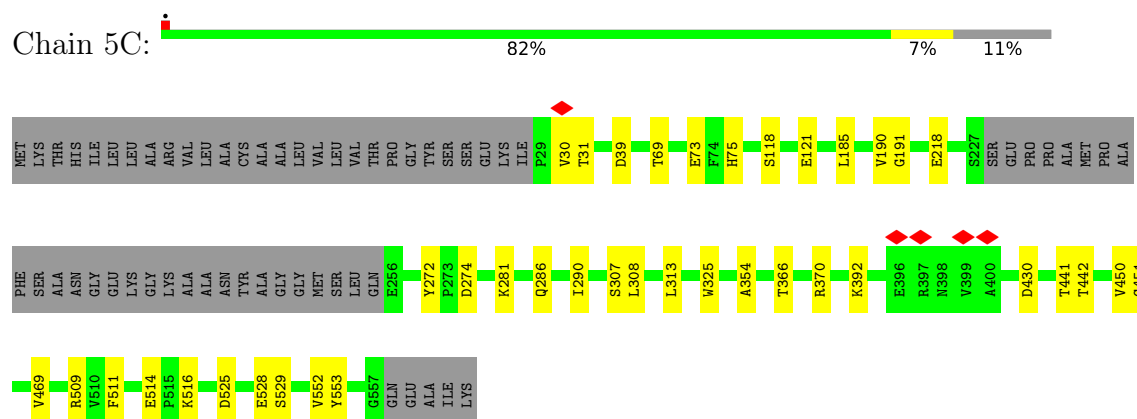
• Molecule 6: Protein PrgI



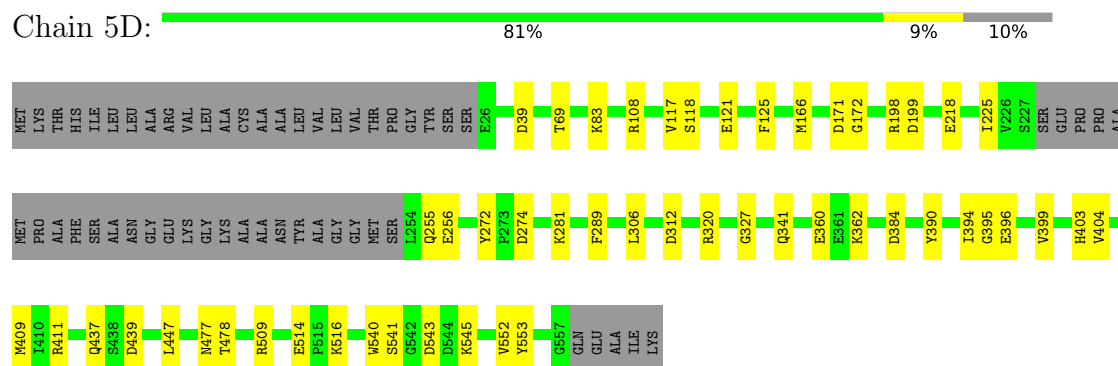
• Molecule 6: Protein PrgI



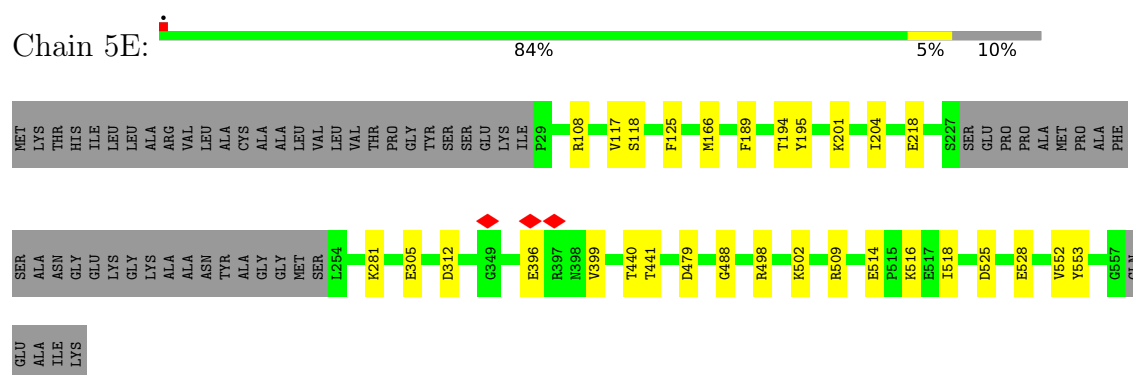
• Molecule 7: Type 3 secretion system secretin



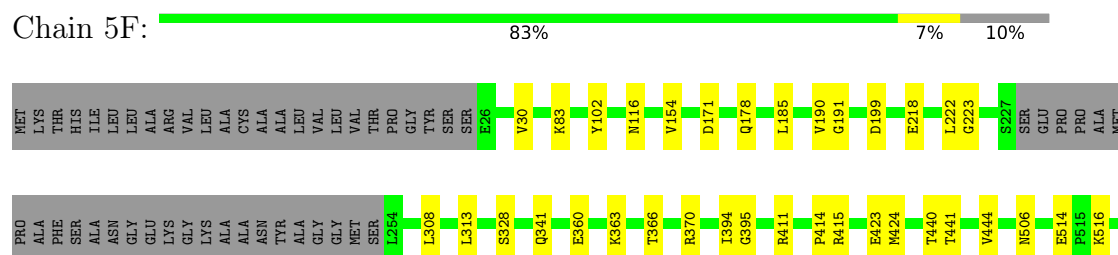
• Molecule 7: Type 3 secretion system secretin

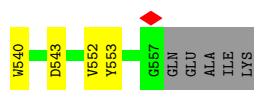


• Molecule 7: Type 3 secretion system secretin



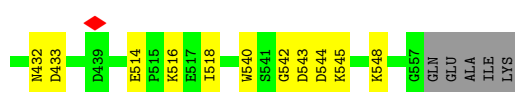
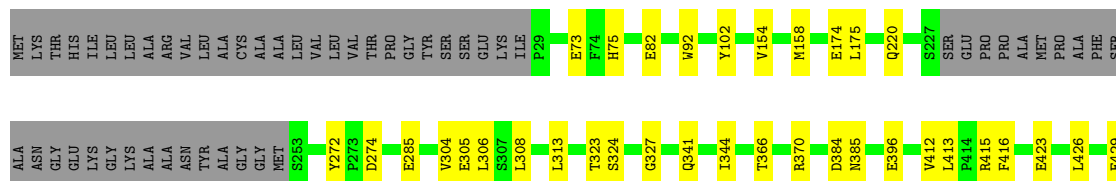
• Molecule 7: Type 3 secretion system secretin





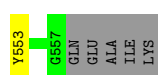
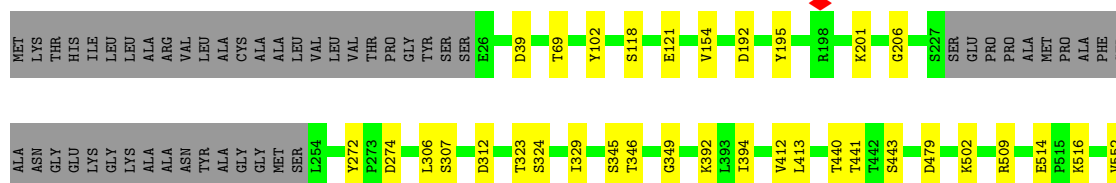
- Molecule 7: Type 3 secretion system secretin

Chain 5G: 81% 8% 10%



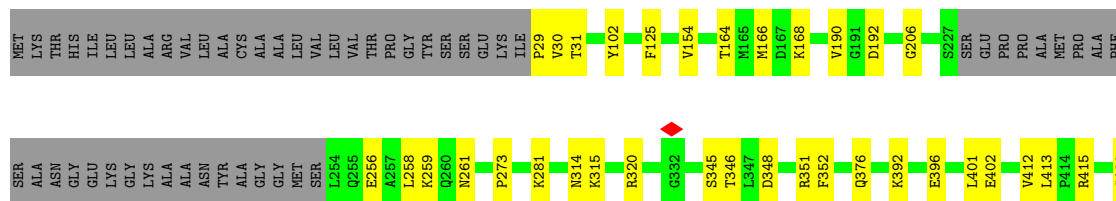
- Molecule 7: Type 3 secretion system secretin

Chain 5H: 84% 6% 10%



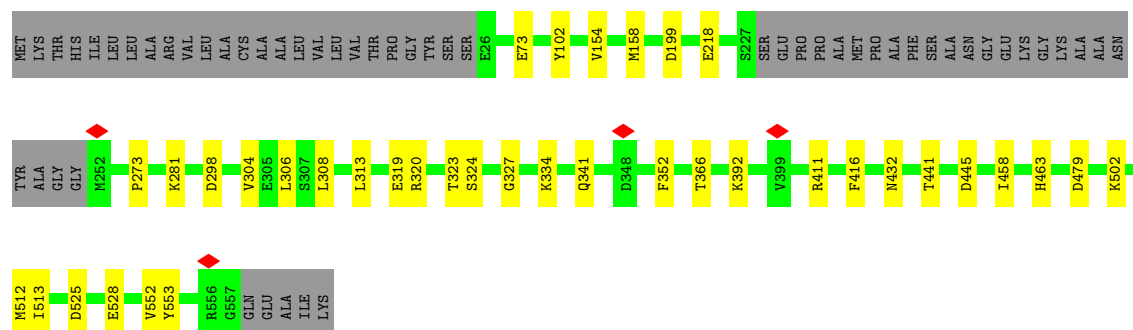
- Molecule 7: Type 3 secretion system secretin

Chain 5I: 81% 8% 10%



- Molecule 7: Type 3 secretion system secretin

Chain 5J: 84% 7% 10%



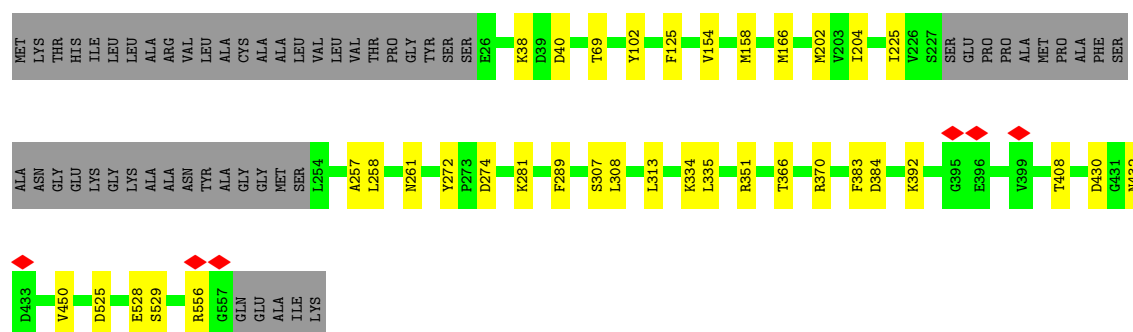
- Molecule 7: Type 3 secretion system secretin

Chain 5K: 83% 6% 11%



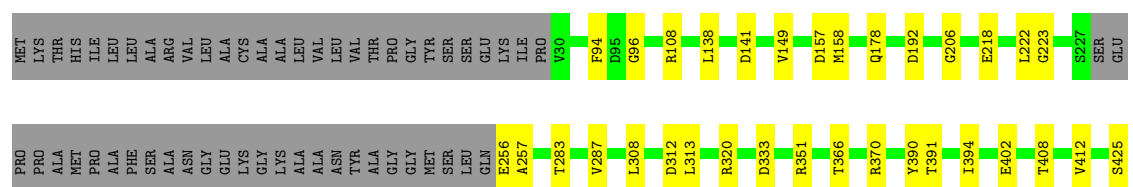
- Molecule 7: Type 3 secretion system secretin

Chain 5L: 83% 7% 10%



- Molecule 7: Type 3 secretion system secretin

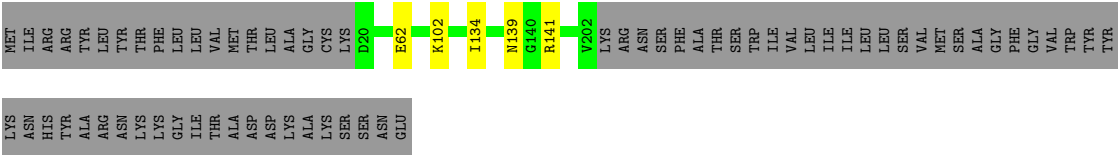
Chain 5M: 81% 8% 11%



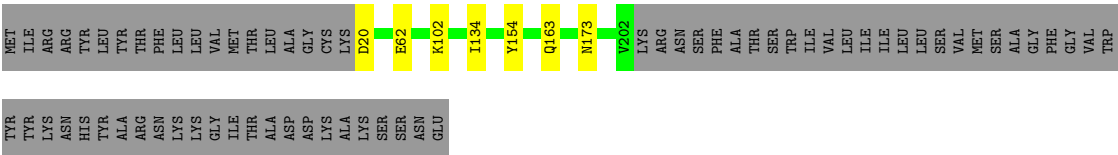




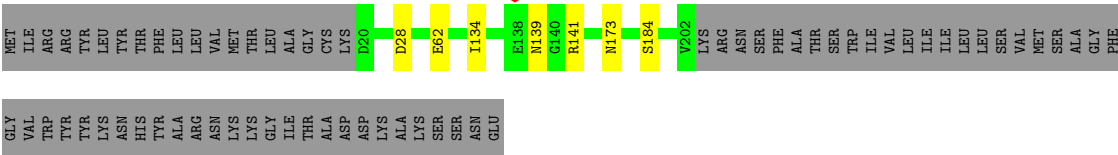
• Molecule 8: Lipoprotein PrgK



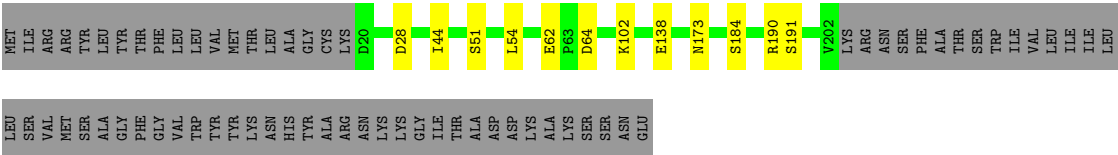
• Molecule 8: Lipoprotein PrgK



• Molecule 8: Lipoprotein PrgK



• Molecule 8: Lipoprotein PrgK



• Molecule 8: Lipoprotein PrgK



VAL MET ILE ARG SER ARG ALA ALA PHE GLY VAL TRP TRP TYR LYS ASN HIS TYR ALA TYR ARG ASN LYS LYS GLY THR ILE THR ALA ASP ASP LYS LYS ALA LYS SER SER SER ASN GLU

• Molecule 8: Lipoprotein PrgK

Chain 6G:  70% 27%

MET ILE ARG ARG TYR LEU TYR TRP PHE LEU TYR THR ASN THR MET THR LEU ALA TYR LYS GLY CYS LYS D20 E62 K102 I134 D135 A136 G137 E138 N139 P143 N173 Q194 V202 LYS ARG ASN SER PHE THR TRP ILE VAL LEU ILE ILE LEU LEU SER VAL MET SER ALA GLY ASN GLU

• Molecule 8: Lipoprotein PrgK

Chain 6H:  70% 27%

MET ILE ARG ARG TYR LEU TYR TRP PHE LEU TYR THR ASN THR MET THR LEU ALA TYR LYS GLY CYS LYS D20 Q28 Q29 E62 K102 I134 N173 S184 V202 LYS ARG ASN SER PHE THR TRP ILE VAL LEU ILE ILE LEU LEU SER VAL MET SER ALA GLY PHE GLY VAL TRP TYR LYS ASN GLU

• Molecule 8: Lipoprotein PrgK

Chain 6I:  67% 6% 27%

MET ILE ARG ARG TYR LEU TYR TRP PHE LEU TYR THR ASN THR MET THR LEU ALA TYR LYS GLY CYS LYS D20 D28 S51 L54 E62 I134 E110 I130 E138 N139 G140 R141 P142 P143 K172 N173 V178 S184 V202 LYS ARG ASN SER PHE THR TRP ILE VAL LEU ILE ILE LEU LEU SER VAL MET SER ALA GLY PHE GLY VAL TRP TYR LYS ASN GLU

• Molecule 8: Lipoprotein PrgK

Chain 6J:  70% 27%

MET ILE ARG ARG TYR LEU TYR TRP PHE LEU TYR THR ASN THR MET THR LEU ALA TYR LYS GLY CYS LYS D20 Q29 E62 K102 I134 D135 M173 S184 V202 LYS ARG ASN SER PHE THR TRP ILE VAL LEU ILE ILE LEU LEU SER VAL MET SER ALA GLY PHE GLY VAL TRP TYR LYS ASN GLU

• Molecule 8: Lipoprotein PrgK

Chain 6K:  69% 27%

MET ILE ARG ARG TYR LEU TYR TRP PHE LEU TYR THR ASN THR MET THR LEU ALA TYR LYS GLY CYS LYS D20 D28 E62 K102 I134 D135 D166 M173 S184 R190 S191 V202 LYS ARG ASN SER PHE THR TRP ILE VAL LEU ILE ILE LEU LEU SER VAL MET SER ALA GLY PHE GLY VAL TRP TYR LYS ASN GLU

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• Molecule 8: Lipoprotein PrgK



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E62
K102
I134
N139
G140
R141
N173
S184
Q194
V202
LYS
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ASN
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• Molecule 8: Lipoprotein PrgK



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R80
K102
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D177
S184
V202
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ARG
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• Molecule 8: Lipoprotein PrgK



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• Molecule 8: Lipoprotein PrgK



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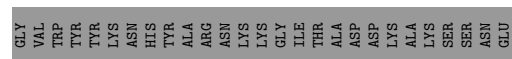
• Molecule 8: Lipoprotein PrgK



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Response	Percentage
Doing a good job	69%
Doing a bad job	27%



- Molecule 8: Lipoprotein PrgK

69% 27%



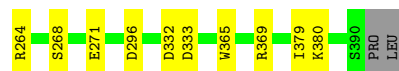
- Molecule 8: Lipoprotein PrgK

Response	Percentage
Doing a good job	68%
Doing a bad job	27%



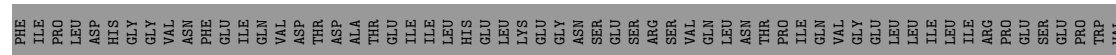
- Molecule 9: Protein PrgH

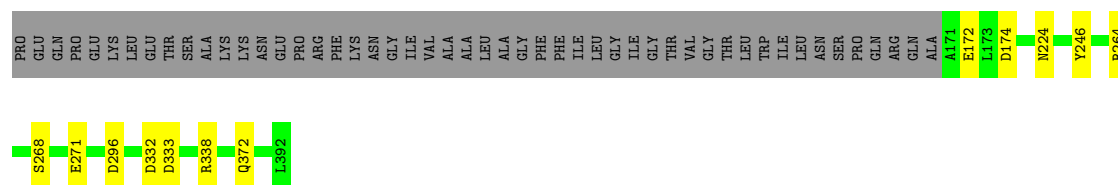
Satisfaction Level	Percentage
Very satisfied	53%
Satisfied	44%



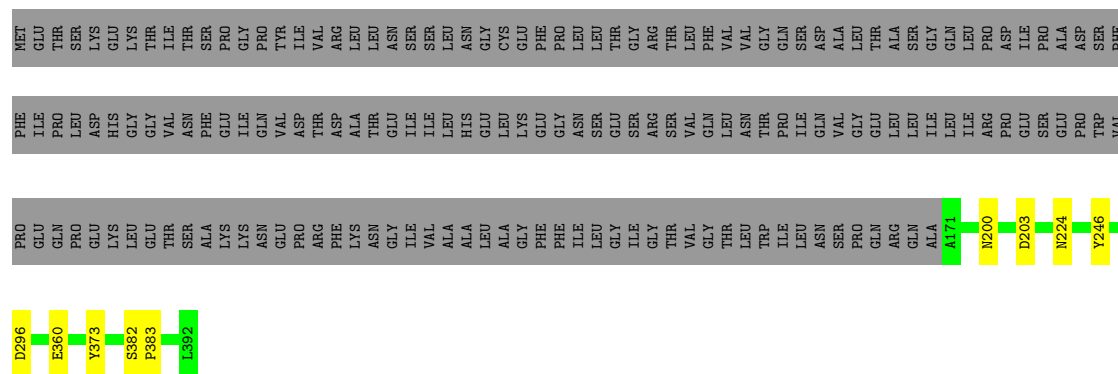
- Molecule 9: Protein PrgH

Opinion	Percentage
Doing a good job	54%
Doing a bad job	43%

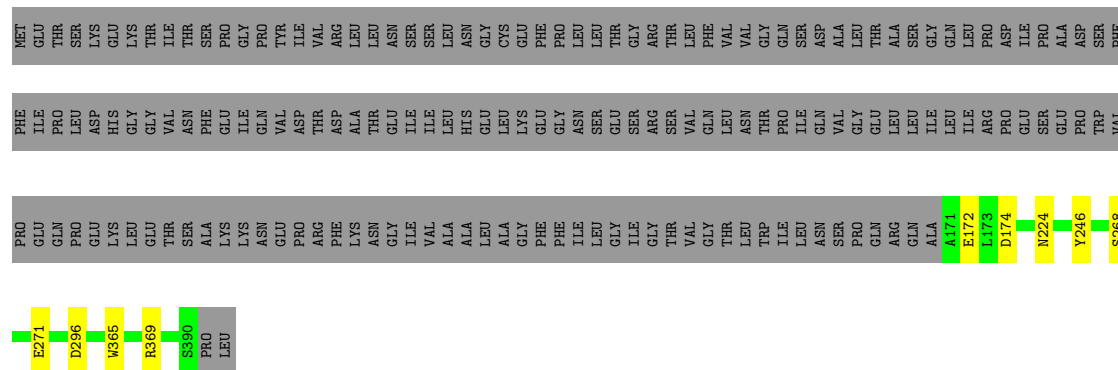




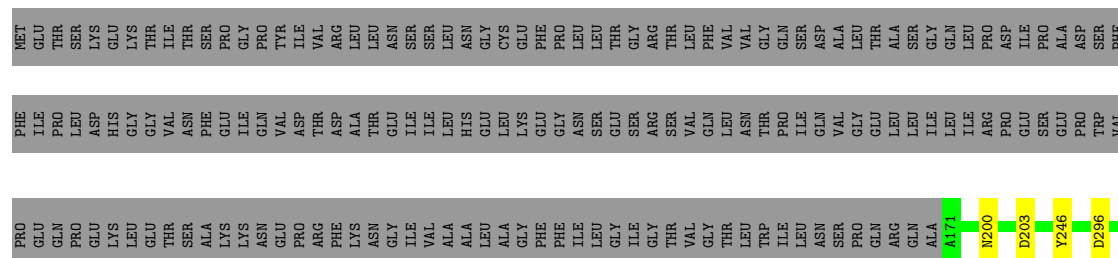
- Molecule 9: Protein PrgH

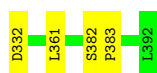


- Molecule 9: Protein PrgH



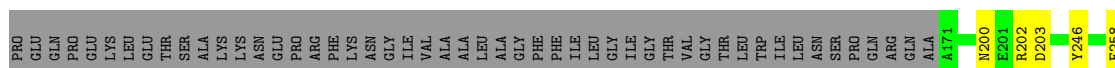
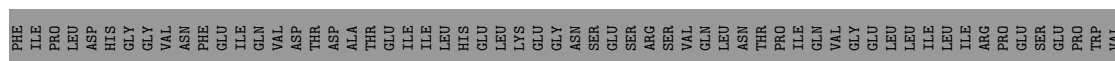
- Molecule 9: Protein PrgH





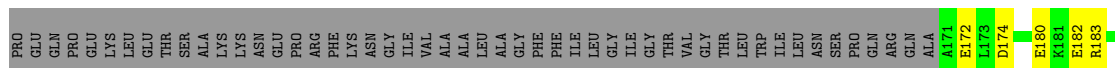
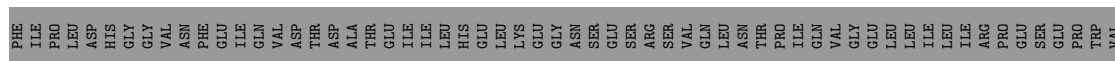
- Molecule 9: Protein PrgH

Chain 7F: 53% . 43%



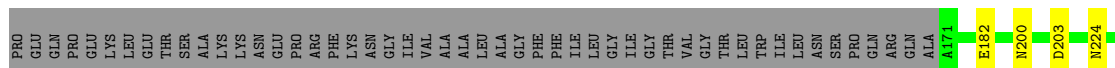
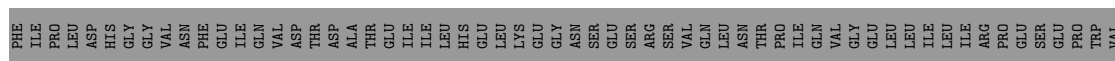
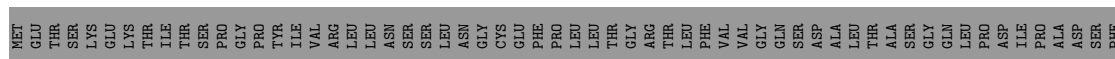
- Molecule 9: Protein PrgH

Chain 7G: 52% . 44%



- Molecule 9: Protein PrgH

Chain 7H: 54% . 43%

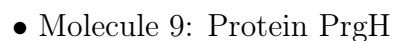


- Molecule 9: Protein PrgH

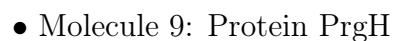
Usage Category	Percentage
Used	52%
Used a little	5%
Never used	43%



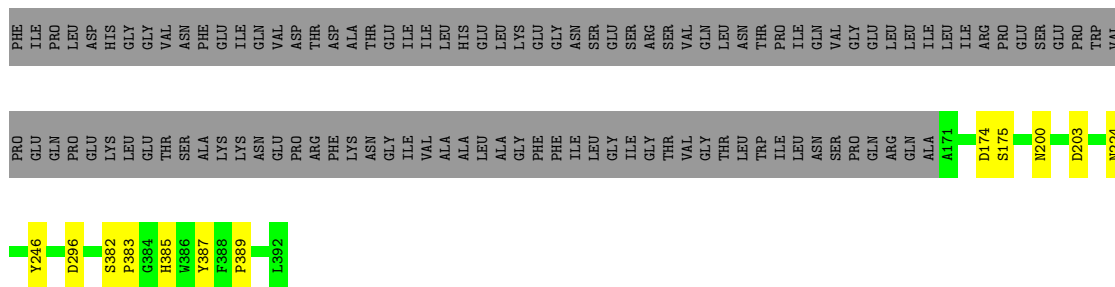
Response	Percentage
Yes, the U.S. is a democracy	54%
No, the U.S. is not a democracy	44%



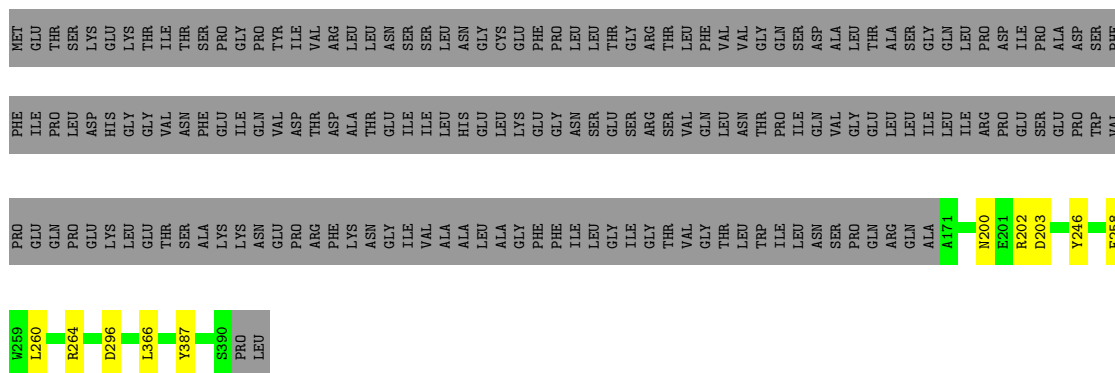
:
 54% 43%



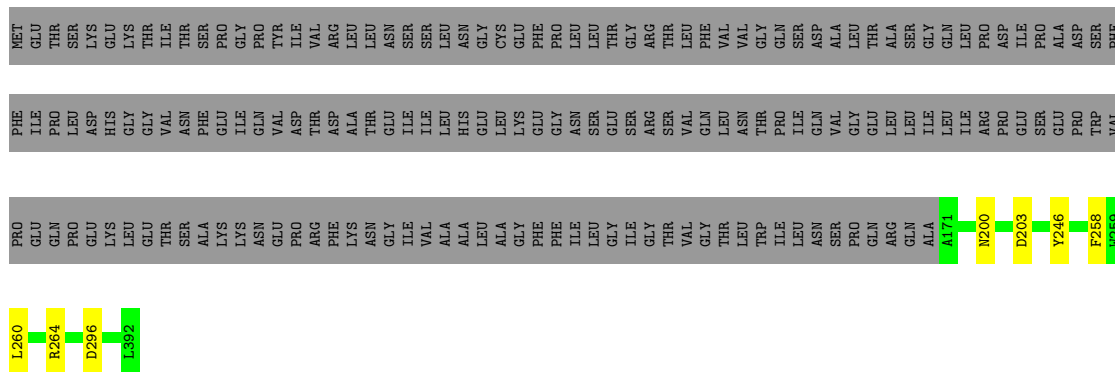
54% . 43%



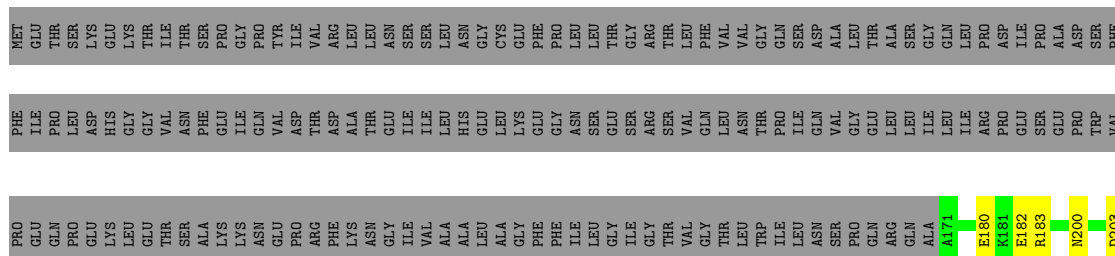
- Molecule 9: Protein PrgH



- Molecule 9: Protein PrgH

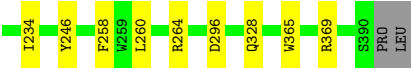
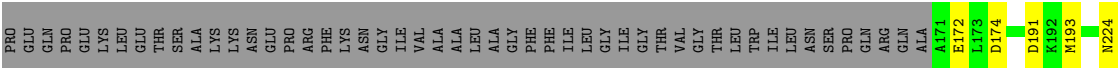
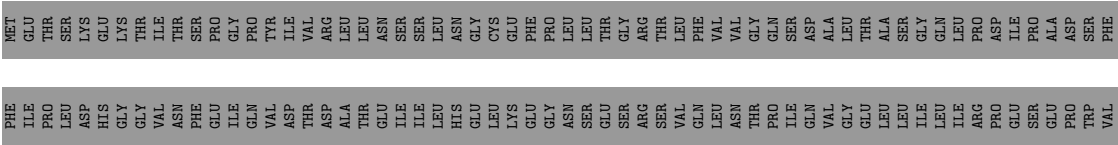


- Molecule 9: Protein PrgH

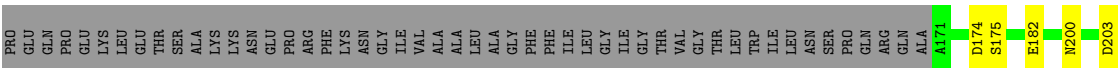
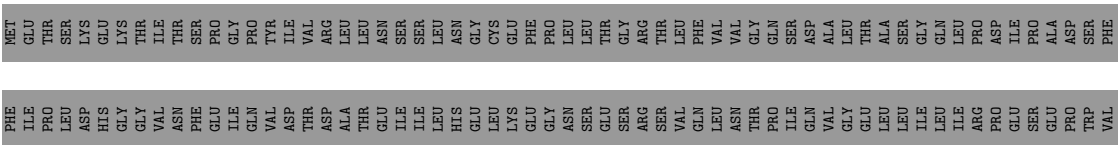




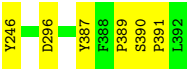
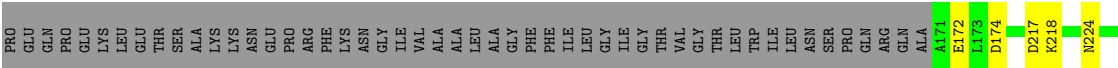
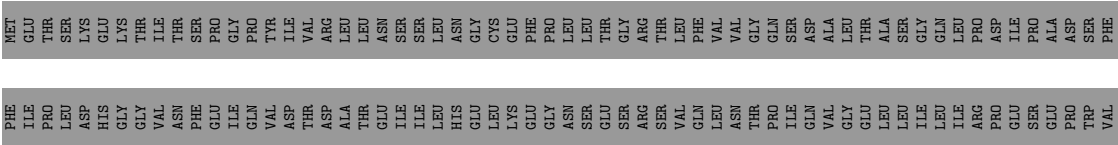
• Molecule 9: Protein PrgH



• Molecule 9: Protein PrgH



• Molecule 9: Protein PrgH

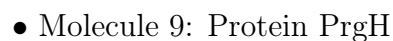


• Molecule 9: Protein PrgH

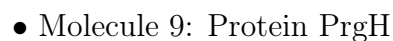
Opinion	Percentage
Doing a good job	53%
Doing a bad job	44%



Response	Percentage
Yes, it is a crisis	55%
No, it is not a crisis	43%



Opinion	Percentage
Doing a good job	53%
Doing a bad job	43%



Opinion	Percentage
Doing a good job	52%
Doing a bad job	44%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77411	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 ($e^-/\text{\AA}^2$)	53.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.067	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	Depositor
Map size ($\text{\AA}$)	660.0, 660.0, 660.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, 3PH

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	1A	0.45	0/1805	0.60	0/2448
1	1B	0.46	0/1805	0.62	0/2448
1	1C	0.45	0/1805	0.64	0/2448
1	1D	0.48	0/1784	0.65	0/2419
1	1E	0.48	0/1792	0.62	0/2430
2	1F	0.47	0/2012	0.63	0/2754
3	1G	0.34	0/660	0.53	0/900
3	1H	0.39	0/660	0.56	0/900
3	1I	0.40	0/674	0.62	0/916
3	1J	0.41	0/674	0.62	0/916
4	1K	0.40	0/689	0.64	0/933
4	1L	0.46	0/719	0.63	0/974
4	1M	0.48	0/689	0.56	0/933
4	1N	0.47	0/682	0.67	0/923
4	1O	0.47	0/689	0.59	0/933
4	1P	0.47	0/689	0.61	0/933
6	2A	0.55	0/540	0.69	0/730
6	2B	0.55	0/480	0.65	0/649
6	2C	0.54	0/472	0.65	0/638
6	2D	0.50	0/628	0.64	0/853
6	2E	0.50	0/549	0.61	0/744
6	2F	0.54	0/592	0.65	0/801
6	2G	0.54	0/608	0.67	0/824
6	2H	0.55	0/592	0.63	0/801
6	2I	0.53	0/592	0.63	0/801
6	2J	0.55	0/592	0.67	0/801
6	2K	0.52	0/616	0.67	0/835
6	2L	0.53	0/623	0.68	0/846
6	2M	0.54	0/623	0.64	0/846
6	2N	0.53	0/623	0.62	0/846
6	2O	0.51	0/623	0.63	0/846
6	2P	0.51	0/616	0.70	0/835

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	2Q	0.51	0/623	0.65	0/846
6	2R	0.50	0/628	0.66	0/853
6	2S	0.50	0/623	0.66	0/846
6	2T	0.47	0/628	0.62	0/853
6	2U	0.47	0/623	0.59	0/846
6	2V	0.45	0/628	0.63	0/853
6	2W	0.46	0/628	0.66	0/853
6	2X	0.47	0/623	0.64	0/846
6	2Y	0.46	0/623	0.63	0/846
6	2Z	0.44	0/623	0.63	0/846
6	3A	0.42	0/628	0.63	0/853
6	3B	0.41	0/628	0.59	0/853
6	3C	0.40	0/623	0.62	0/846
6	3D	0.42	0/623	0.59	0/846
6	3E	0.40	0/623	0.58	0/846
6	3F	0.40	0/623	0.58	0/846
6	3G	0.38	0/628	0.56	0/853
6	3H	0.36	0/623	0.59	0/846
6	3I	0.37	0/623	0.58	0/846
6	3J	0.37	0/623	0.60	0/846
6	3K	0.35	0/623	0.58	0/846
6	3L	0.35	0/616	0.56	0/835
6	3M	0.31	0/623	0.56	0/846
6	3N	0.32	0/623	0.56	0/846
6	3O	0.32	0/616	0.61	0/835
6	3P	0.33	0/616	0.52	0/835
6	3Q	0.30	0/616	0.50	0/835
6	3R	0.29	0/616	0.56	0/835
6	3S	0.29	0/616	0.57	0/835
6	3T	0.28	0/616	0.54	0/835
6	3U	0.28	0/616	0.53	0/835
6	3V	0.28	0/616	0.52	0/835
6	3W	0.27	0/616	0.51	0/835
6	3X	0.26	0/616	0.57	0/835
6	3Y	0.25	0/616	0.51	0/835
6	3Z	0.26	0/616	0.53	0/835
6	4A	0.26	0/616	0.54	0/835
6	4B	0.24	0/616	0.48	0/835
6	4C	0.24	0/616	0.52	0/835
6	4D	0.24	0/616	0.53	0/835
6	4E	0.22	0/616	0.53	0/835
6	4F	0.25	0/616	0.56	0/835
6	4G	0.21	0/616	0.44	0/835

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	4H	0.22	0/616	0.51	0/835
6	4I	0.20	0/616	0.49	0/835
6	4J	0.22	0/616	0.52	0/835
6	4K	0.22	0/616	0.50	0/835
6	4L	0.22	0/616	0.49	0/835
6	4M	0.20	0/616	0.50	0/835
6	4N	0.19	0/616	0.45	0/835
6	4O	0.21	0/616	0.53	0/835
6	4P	0.21	0/616	0.53	0/835
6	4Q	0.19	0/616	0.49	0/835
6	4R	0.19	0/616	0.52	0/835
6	4S	0.19	0/616	0.45	0/835
6	4T	0.20	0/616	0.50	0/835
7	5A	0.46	0/1145	0.63	0/1545
7	5B	0.35	0/3978	0.63	0/5385
7	5C	0.35	0/3968	0.62	0/5372
7	5D	0.37	0/4011	0.64	0/5430
7	5E	0.38	0/3985	0.64	0/5395
7	5F	0.39	0/4011	0.65	0/5430
7	5G	0.38	0/3991	0.64	0/5403
7	5H	0.39	0/4011	0.68	0/5430
7	5I	0.38	0/3985	0.65	0/5395
7	5J	0.38	0/4025	0.65	0/5448
7	5K	0.37	0/3977	0.65	0/5384
7	5L	0.36	0/4011	0.64	0/5430
7	5M	0.35	0/3960	0.59	0/5361
7	5N	0.35	0/3972	0.60	0/5377
7	5O	0.34	0/3946	0.60	0/5342
7	5P	0.34	0/3963	0.59	0/5366
8	6A	0.45	0/1456	0.62	0/1978
8	6B	0.45	0/1456	0.63	0/1978
8	6C	0.46	0/1456	0.60	0/1978
8	6D	0.46	0/1456	0.63	0/1978
8	6E	0.45	0/1456	0.61	0/1978
8	6F	0.45	0/1456	0.61	0/1978
8	6G	0.44	0/1456	0.61	0/1978
8	6H	0.45	0/1456	0.63	0/1978
8	6I	0.44	0/1456	0.62	0/1978
8	6J	0.44	0/1456	0.64	0/1978
8	6K	0.44	0/1456	0.65	0/1978
8	6L	0.44	0/1456	0.62	0/1978
8	6M	0.44	0/1456	0.63	0/1978
8	6N	0.44	0/1456	0.64	0/1978

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	6O	0.44	0/1456	0.62	0/1978
8	6P	0.43	0/1456	0.65	0/1978
8	6Q	0.45	0/1456	0.62	0/1978
8	6R	0.45	0/1456	0.66	0/1978
8	6S	0.45	0/1456	0.65	0/1978
8	6T	0.44	0/1456	0.63	0/1978
8	6U	0.44	0/1456	0.57	0/1978
8	6V	0.44	0/1456	0.60	0/1978
8	6W	0.46	0/1456	0.64	0/1978
8	6X	0.45	0/1456	0.62	0/1978
9	7A	0.44	0/1864	0.57	0/2518
9	7B	0.41	0/1881	0.57	0/2541
9	7C	0.44	0/1881	0.59	0/2541
9	7D	0.44	0/1864	0.59	0/2518
9	7E	0.42	0/1881	0.60	0/2541
9	7F	0.44	0/1881	0.60	0/2541
9	7G	0.43	0/1864	0.60	0/2518
9	7H	0.41	0/1881	0.58	0/2541
9	7I	0.43	0/1881	0.59	0/2541
9	7J	0.43	0/1864	0.60	0/2518
9	7K	0.41	0/1881	0.57	0/2541
9	7L	0.43	0/1881	0.59	0/2541
9	7M	0.42	0/1864	0.60	0/2518
9	7N	0.41	0/1881	0.60	0/2541
9	7O	0.42	0/1881	0.60	0/2541
9	7P	0.42	0/1864	0.57	0/2518
9	7Q	0.40	0/1881	0.62	0/2541
9	7R	0.42	0/1881	0.58	0/2541
9	7S	0.42	0/1864	0.59	0/2518
9	7T	0.40	0/1881	0.53	0/2541
9	7U	0.42	0/1881	0.55	1/2541 (0.0%)
9	7V	0.43	0/1864	0.58	0/2518
9	7W	0.42	0/1881	0.61	1/2541 (0.0%)
9	7X	0.44	0/1881	0.63	1/2541 (0.0%)
All	All	0.41	0/202780	0.61	3/274731 (0.0%)

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
7	5B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	6M	0	1
9	7S	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	7W	329	GLY	N-CA-C	6.58	118.21	111.56
9	7U	178	GLY	N-CA-C	6.20	118.34	110.96
9	7X	388	PHE	CB-CA-C	-5.15	105.87	110.71

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	5B	115	ARG	Sidechain
8	6M	80	ARG	Sidechain
9	7S	348	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	1767	1806	1810	11	0
1	1B	1767	1784	1810	9	0
1	1C	1767	1810	1810	5	0
1	1D	1746	1790	1790	4	0
1	1E	1754	1791	1794	2	0
2	1F	1960	2007	2008	7	0
3	1G	647	692	692	4	0
3	1H	647	692	692	2	0
3	1I	661	708	708	2	0
3	1J	661	708	708	1	0
4	1K	685	701	701	7	0
4	1L	714	726	726	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	1M	685	701	701	5	0
4	1N	678	692	692	2	0
4	1O	685	701	701	5	0
4	1P	685	702	701	4	0
5	1Z	706	707	167	0	0
6	2A	534	528	527	4	0
6	2B	474	474	474	1	0
6	2C	466	470	470	2	0
6	2D	617	603	603	2	0
6	2E	540	530	529	1	0
6	2F	584	574	574	2	0
6	2G	598	584	584	3	0
6	2H	584	574	574	2	0
6	2I	584	574	574	6	0
6	2J	584	574	574	4	0
6	2K	605	592	592	1	0
6	2L	612	598	598	2	0
6	2M	612	598	598	5	0
6	2N	612	598	598	5	0
6	2O	612	598	598	7	0
6	2P	605	592	592	2	0
6	2Q	612	598	598	4	0
6	2R	617	603	603	3	0
6	2S	612	598	598	4	0
6	2T	617	603	603	2	0
6	2U	612	598	598	2	0
6	2V	617	603	603	4	0
6	2W	617	603	603	3	0
6	2X	612	598	598	5	0
6	2Y	612	598	598	5	0
6	2Z	612	598	598	4	0
6	3A	617	603	603	4	0
6	3B	617	603	603	4	0
6	3C	612	598	598	4	0
6	3D	612	598	598	1	0
6	3E	612	598	598	3	0
6	3F	612	598	598	5	0
6	3G	617	603	603	3	0
6	3H	612	598	598	5	0
6	3I	612	598	598	6	0
6	3J	612	598	598	5	0
6	3K	612	598	598	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	3L	605	592	592	2	0
6	3M	612	598	598	2	0
6	3N	612	598	598	4	0
6	3O	605	592	592	3	0
6	3P	605	592	592	0	0
6	3Q	605	592	592	1	0
6	3R	605	592	592	1	0
6	3S	605	592	592	3	0
6	3T	605	592	592	8	0
6	3U	605	592	592	3	0
6	3V	605	592	592	5	0
6	3W	605	592	592	6	0
6	3X	605	592	592	9	0
6	3Y	605	592	592	10	0
6	3Z	605	592	592	8	0
6	4A	605	592	592	4	0
6	4B	605	592	592	7	0
6	4C	605	592	592	7	0
6	4D	605	592	592	7	0
6	4E	605	592	592	4	0
6	4F	605	592	592	5	0
6	4G	605	592	592	5	0
6	4H	605	592	592	3	0
6	4I	605	592	592	8	0
6	4J	605	592	592	8	0
6	4K	605	592	592	6	0
6	4L	605	592	592	6	0
6	4M	605	592	592	9	0
6	4N	605	592	592	1	0
6	4O	605	592	592	5	0
6	4P	605	592	592	6	0
6	4Q	605	592	592	7	0
6	4R	605	592	592	6	0
6	4S	605	592	592	5	0
6	4T	605	592	592	8	0
7	5A	1122	1119	1119	5	0
7	5B	3913	3971	3970	35	0
7	5C	3903	3959	3958	25	0
7	5D	3946	4007	4006	40	0
7	5E	3920	3978	3977	21	0
7	5F	3946	4007	4006	26	0
7	5G	3926	3983	3982	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	5H	3946	4006	4006	21	0
7	5I	3920	3978	3977	31	0
7	5J	3960	4021	4020	26	0
7	5K	3912	3967	3966	25	0
7	5L	3946	4008	4006	25	0
7	5M	3896	3951	3950	29	0
7	5N	3907	3966	3965	33	0
7	5O	3881	3936	3936	29	0
7	5P	3898	3953	3952	18	0
8	6A	1428	1421	1421	5	0
8	6B	1428	1421	1421	5	0
8	6C	1428	1421	1421	5	0
8	6D	1428	1421	1421	6	0
8	6E	1428	1421	1421	8	0
8	6F	1428	1421	1421	7	0
8	6G	1428	1421	1421	6	0
8	6H	1428	1421	1421	5	0
8	6I	1428	1421	1421	10	0
8	6J	1428	1421	1421	6	0
8	6K	1428	1421	1421	7	0
8	6L	1428	1421	1421	8	0
8	6M	1428	1421	1421	6	0
8	6N	1428	1421	1421	9	0
8	6O	1428	1421	1421	7	0
8	6P	1428	1421	1421	5	0
8	6Q	1428	1421	1421	8	0
8	6R	1428	1421	1421	8	0
8	6S	1428	1420	1421	5	0
8	6T	1428	1421	1421	6	0
8	6U	1428	1421	1421	6	0
8	6V	1428	1420	1421	5	0
8	6W	1428	1421	1421	7	0
8	6X	1428	1421	1421	10	0
9	7A	1820	1782	1782	8	0
9	7B	1836	1800	1800	8	0
9	7C	1836	1800	1800	6	0
9	7D	1820	1782	1782	5	0
9	7E	1836	1800	1800	5	0
9	7F	1836	1800	1800	11	0
9	7G	1820	1782	1782	10	0
9	7H	1836	1800	1800	8	0
9	7I	1836	1800	1800	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	7J	1820	1782	1782	7	0
9	7K	1836	1800	1800	8	0
9	7L	1836	1800	1800	9	0
9	7M	1820	1782	1782	7	0
9	7N	1836	1800	1800	4	0
9	7O	1836	1800	1800	13	0
9	7P	1820	1782	1782	9	0
9	7Q	1836	1800	1800	11	0
9	7R	1836	1800	1800	7	0
9	7S	1820	1782	1782	7	0
9	7T	1836	1800	1800	5	0
9	7U	1836	1800	1800	10	0
9	7V	1820	1782	1782	9	0
9	7W	1836	1800	1800	7	0
9	7X	1836	1800	1800	9	0
10	1A	36	45	45	1	0
10	1L	34	35	41	0	0
10	1M	34	33	41	0	0
10	1N	34	33	41	1	0
10	1P	46	70	68	0	0
11	1A	16	31	31	0	0
11	1D	16	31	31	0	0
11	1G	16	31	31	1	0
11	1H	16	31	31	0	0
11	1I	48	93	93	1	0
11	1J	32	62	62	0	0
All	All	199992	199567	199066	1030	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 3.

All (1030) 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)
8:6P:173:ASN:OD1	8:6Q:184:SER:OG	1.82	0.98
8:6R:173:ASN:OD1	8:6S:184:SER:OG	1.84	0.92
8:6N:173:ASN:OD1	8:6O:184:SER:OG	1.87	0.92
8:6K:173:ASN:OD1	8:6L:184:SER:OG	1.88	0.92
7:5C:514:GLU:OE2	7:5C:516:LYS:NZ	2.02	0.91
8:6V:173:ASN:OD1	8:6W:184:SER:OG	1.88	0.91
8:6G:173:ASN:OD1	8:6H:184:SER:OG	1.90	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5B:553:TYR:HH	7:5C:529:SER:HG	1.17	0.88
9:7Q:246:TYR:OH	9:7Q:296:ASP:OD1	1.92	0.87
7:5F:199:ASP:OD2	7:5F:411:ARG:NH1	2.08	0.87
8:6J:173:ASN:OD1	8:6K:184:SER:OG	1.92	0.86
8:6Q:173:ASN:OD1	8:6R:184:SER:OG	1.94	0.86
7:5D:198:ARG:NH1	7:5D:384:ASP:OD2	2.08	0.86
8:6I:173:ASN:OD1	8:6J:184:SER:OG	1.94	0.86
7:5E:312:ASP:OD1	7:5E:509:ARG:NH1	2.09	0.85
8:6W:173:ASN:OD1	8:6X:184:SER:OG	1.94	0.85
8:6M:173:ASN:OD1	8:6N:184:SER:OG	1.95	0.84
8:6O:173:ASN:OD1	8:6P:184:SER:OG	1.94	0.84
8:6D:173:ASN:OD1	8:6E:184:SER:OG	1.94	0.84
8:6E:173:ASN:OD1	8:6F:184:SER:OG	1.95	0.83
8:6B:139:ASN:O	8:6B:141:ARG:NH1	2.11	0.83
7:5D:39:ASP:H	7:5D:69:THR:HG22	1.43	0.83
7:5O:514:GLU:OE2	7:5O:516:LYS:NZ	2.11	0.82
8:6C:173:ASN:OD1	8:6D:184:SER:OG	1.95	0.82
6:3Z:78:ASN:OD1	6:4A:80:ARG:NH2	2.13	0.81
8:6H:173:ASN:OD1	8:6I:184:SER:OG	1.99	0.81
7:5B:39:ASP:H	7:5B:69:THR:HG22	1.44	0.81
8:6L:173:ASN:OD1	8:6M:184:SER:OG	1.98	0.80
7:5G:514:GLU:OE2	7:5G:516:LYS:NZ	2.15	0.80
7:5N:312:ASP:OD1	7:5N:509:ARG:NH1	2.13	0.80
9:7N:246:TYR:OH	9:7N:296:ASP:OD1	2.00	0.80
7:5I:348:ASP:OD2	7:5I:351:ARG:NH1	2.16	0.79
6:3W:13:SER:OG	6:3W:61:GLN:NE2	2.14	0.78
1:1A:97:ASP:OD1	1:1A:100:ARG:NH1	2.17	0.78
9:7P:246:TYR:OH	9:7P:296:ASP:OD1	2.01	0.77
7:5L:432:ASN:ND2	7:5L:450:VAL:O	2.16	0.75
9:7M:246:TYR:OH	9:7M:296:ASP:OD1	2.04	0.74
7:5I:392:LYS:O	7:5J:320:ARG:NH2	2.21	0.74
9:7J:246:TYR:OH	9:7J:296:ASP:OD1	2.05	0.74
7:5M:312:ASP:OD1	7:5M:509:ARG:NH1	2.20	0.73
7:5N:351:ARG:NH1	7:5O:333:ASP:O	2.20	0.73
6:4Q:17:ASP:OD2	6:4Q:57:TYR:OH	2.06	0.73
9:7G:246:TYR:OH	9:7G:296:ASP:OD1	2.06	0.73
4:1K:45:ALA:HB1	4:1K:73:MET:HE3	1.70	0.73
7:5C:39:ASP:H	7:5C:69:THR:HG22	1.54	0.72
9:7I:246:TYR:OH	9:7I:296:ASP:OD1	2.06	0.72
9:7V:246:TYR:OH	9:7V:296:ASP:OD1	2.07	0.72
9:7U:264:ARG:NH1	9:7U:296:ASP:OD2	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:7O:246:TYR:OH	9:7O:296:ASP:OD1	2.07	0.71
9:7H:246:TYR:OH	9:7H:296:ASP:OD1	2.07	0.71
6:3Z:22:ASN:CG	6:3Z:25:THR:HG1	1.98	0.71
9:7L:246:TYR:OH	9:7L:296:ASP:OD1	2.08	0.70
9:7C:246:TYR:OH	9:7C:296:ASP:OD1	2.09	0.70
2:1F:191:VAL:HG21	2:1F:226:ILE:CD1	2.21	0.70
9:7B:246:TYR:OH	9:7B:296:ASP:OD1	2.09	0.69
4:1M:12:VAL:HG13	4:1M:13:ILE:H	1.56	0.69
7:5I:432:ASN:ND2	7:5I:450:VAL:O	2.25	0.69
8:6W:194:GLN:OE1	9:7V:202:ARG:NH2	2.24	0.69
6:4D:22:ASN:CG	6:4D:25:THR:HG1	2.01	0.69
7:5D:312:ASP:OD1	7:5D:509:ARG:NH1	2.26	0.69
7:5B:73:GLU:OE1	7:5B:75:HIS:ND1	2.23	0.69
7:5N:178:GLN:NE2	7:5O:218:GLU:OE2	2.25	0.68
1:1A:68:MET:HE1	2:1F:75:LEU:HD12	1.75	0.68
8:6T:166:ASP:OD2	9:7T:340:ARG:NH1	2.26	0.68
7:5O:314:ASN:OD1	7:5O:315:LYS:N	2.26	0.68
6:4T:59:ASN:O	6:4T:63:ASN:ND2	2.26	0.68
8:6S:173:ASN:OD1	8:6T:184:SER:OG	2.12	0.68
6:2O:77:GLN:OE1	6:2O:80:ARG:NH2	2.27	0.68
9:7K:246:TYR:OH	9:7K:296:ASP:OD1	2.11	0.68
9:7J:365:TRP:O	9:7J:369:ARG:NH1	2.26	0.67
8:6B:134:ILE:HD12	8:6B:134:ILE:H	1.57	0.67
6:3C:20:VAL:O	6:3C:20:VAL:HG23	1.94	0.67
7:5M:514:GLU:OE2	7:5M:516:LYS:NZ	2.23	0.67
6:2M:22:ASN:OD1	6:2M:25:THR:OG1	2.13	0.67
8:6A:139:ASN:O	8:6A:141:ARG:NH1	2.24	0.67
6:4E:22:ASN:CG	6:4E:25:THR:HG1	2.02	0.67
2:1F:191:VAL:HG21	2:1F:226:ILE:HD13	1.76	0.67
7:5H:39:ASP:H	7:5H:69:THR:HG22	1.59	0.66
6:4K:69:LYS:NZ	6:4K:70:ASP:OD1	2.28	0.66
7:5M:108:ARG:NH2	7:5M:157:ASP:OD1	2.29	0.66
6:2M:20:VAL:HG23	6:2M:20:VAL:O	1.96	0.65
6:3N:22:ASN:CG	6:3N:25:THR:HG1	2.03	0.65
7:5D:541:SER:OG	7:5F:506:ASN:OD1	2.14	0.65
6:2H:21:ASP:OD1	7:5O:216:GLN:NE2	2.30	0.65
6:4B:20:VAL:HG23	6:4B:20:VAL:O	1.94	0.65
7:5L:257:ALA:O	7:5L:261:ASN:ND2	2.28	0.65
9:7O:264:ARG:NH1	9:7O:296:ASP:OD2	2.28	0.65
6:2R:20:VAL:HG23	6:2R:20:VAL:O	1.96	0.65
9:7R:246:TYR:OH	9:7R:296:ASP:OD1	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5H:312:ASP:OD1	7:5H:509:ARG:NH1	2.27	0.65
6:4D:20:VAL:HG23	6:4D:20:VAL:O	1.97	0.65
9:7P:264:ARG:NH1	9:7P:296:ASP:OD2	2.30	0.64
6:4R:22:ASN:CG	6:4R:25:THR:HG1	2.04	0.64
7:5J:102:TYR:OH	7:5J:154:VAL:HG23	1.98	0.64
7:5F:514:GLU:OE2	7:5F:516:LYS:NZ	2.30	0.64
6:2Z:20:VAL:HG23	6:2Z:20:VAL:O	1.97	0.64
7:5I:102:TYR:OH	7:5I:154:VAL:HG23	1.97	0.64
7:5F:363:LYS:NZ	7:5F:444:VAL:O	2.29	0.64
7:5M:351:ARG:NH1	7:5N:333:ASP:O	2.31	0.64
6:3Y:20:VAL:HG23	6:3Y:20:VAL:O	1.98	0.64
6:3R:20:VAL:HG23	6:3R:20:VAL:O	1.97	0.63
9:7T:264:ARG:NH1	9:7T:296:ASP:OD2	2.30	0.63
6:3W:20:VAL:O	6:3W:20:VAL:HG23	1.98	0.63
6:4J:59:ASN:O	6:4J:63:ASN:ND2	2.30	0.63
6:3O:20:VAL:O	6:3O:20:VAL:HG23	1.97	0.63
7:5C:430:ASP:OD1	7:5C:509:ARG:NH2	2.28	0.63
6:3B:20:VAL:HG23	6:3B:20:VAL:O	1.97	0.63
9:7A:246:TYR:OH	9:7A:296:ASP:OD1	2.17	0.63
1:1D:97:ASP:OD1	1:1D:100:ARG:NH2	2.32	0.62
9:7L:200:ASN:ND2	9:7L:203:ASP:OD2	2.32	0.62
9:7S:246:TYR:OH	9:7S:296:ASP:OD1	2.16	0.62
6:2A:20:VAL:HG22	6:2A:21:ASP:H	1.64	0.62
6:4F:20:VAL:HG23	6:4F:20:VAL:O	1.99	0.62
6:3H:20:VAL:HG23	6:3H:20:VAL:O	1.98	0.62
6:4I:20:VAL:O	6:4I:20:VAL:HG23	1.97	0.62
6:4D:63:ASN:OD1	6:4I:78:ASN:ND2	2.32	0.62
6:4N:20:VAL:HG23	6:4N:20:VAL:O	1.98	0.62
8:6T:173:ASN:OD1	8:6U:184:SER:OG	2.17	0.62
6:3S:20:VAL:O	6:3S:20:VAL:HG23	1.97	0.62
7:5C:281:LYS:NZ	7:5D:218:GLU:OE1	2.30	0.61
7:5D:171:ASP:OD1	7:5D:172:GLY:N	2.32	0.61
7:5F:83:LYS:NZ	9:7H:375:ALA:O	2.33	0.61
7:5F:102:TYR:OH	7:5F:154:VAL:HG23	2.00	0.61
6:3G:20:VAL:HG23	6:3G:20:VAL:O	2.00	0.61
7:5B:281:LYS:NZ	7:5C:218:GLU:OE1	2.30	0.61
7:5F:178:GLN:NE2	7:5G:220:GLN:OE1	2.34	0.61
9:7Q:264:ARG:NH1	9:7Q:296:ASP:OD2	2.32	0.61
7:5O:450:VAL:HG23	7:5O:450:VAL:O	2.00	0.61
6:2A:8:TYR:C	6:2A:9:LEU:HD22	2.26	0.61
6:2X:20:VAL:O	6:2X:20:VAL:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2V:20:VAL:HG23	6:2V:20:VAL:O	2.01	0.60
6:2Y:20:VAL:HG23	6:2Y:20:VAL:O	2.00	0.60
7:5F:415:ARG:NE	7:5F:423:GLU:OE1	2.31	0.60
9:7U:268:SER:N	9:7U:271:GLU:OE1	2.27	0.60
9:7S:328:GLN:NE2	9:7S:360:GLU:OE1	2.32	0.60
6:3E:20:VAL:HG23	6:3E:20:VAL:O	2.00	0.60
6:3L:20:VAL:HG23	6:3L:20:VAL:O	2.02	0.60
9:7W:246:TYR:OH	9:7W:296:ASP:OD1	2.18	0.60
6:2S:20:VAL:HG23	6:2S:20:VAL:O	2.01	0.60
7:5D:83:LYS:NZ	9:7K:375:ALA:O	2.25	0.60
6:3A:20:VAL:HG23	6:3A:20:VAL:O	2.02	0.60
6:3Y:55:ASN:OD1	6:3Y:59:ASN:ND2	2.34	0.60
7:5D:327:GLY:O	7:5D:341:GLN:NE2	2.35	0.59
6:4L:20:VAL:HG23	6:4L:20:VAL:O	2.02	0.59
7:5B:412:VAL:HG23	7:5B:426:LEU:HD23	1.84	0.59
7:5D:281:LYS:NZ	7:5E:218:GLU:OE1	2.29	0.59
7:5O:392:LYS:NZ	7:5P:361:GLU:OE2	2.34	0.59
6:3W:78:ASN:OD1	6:3X:80:ARG:NH2	2.35	0.59
6:3Z:20:VAL:HG23	6:3Z:20:VAL:O	2.01	0.59
6:4P:7:GLY:N	6:4P:10:ASP:OD2	2.35	0.59
6:2L:20:VAL:O	6:2L:20:VAL:HG23	2.02	0.59
7:5J:73:GLU:OE2	9:7B:372:GLN:NE2	2.36	0.59
9:7F:246:TYR:OH	9:7F:296:ASP:OD1	2.21	0.59
7:5K:514:GLU:OE2	7:5K:516:LYS:NZ	2.27	0.59
9:7V:268:SER:N	9:7V:271:GLU:OE1	2.33	0.59
6:2Q:20:VAL:HG23	6:2Q:20:VAL:O	2.03	0.58
6:4B:66:LYS:NZ	6:4G:80:ARG:O	2.26	0.58
9:7X:246:TYR:OH	9:7X:296:ASP:OD1	2.20	0.58
6:4Q:20:VAL:O	6:4Q:20:VAL:HG23	2.03	0.58
7:5B:408:THR:OG1	7:5B:430:ASP:OD2	2.20	0.58
7:5M:391:THR:HG22	7:5M:402:GLU:HB2	1.85	0.58
9:7Q:200:ASN:ND2	9:7Q:203:ASP:OD2	2.35	0.58
7:5G:102:TYR:OH	7:5G:154:VAL:HG23	2.03	0.58
6:2O:32:ASP:OD1	6:2O:33:LYS:N	2.36	0.58
7:5E:281:LYS:NZ	7:5F:218:GLU:OE1	2.30	0.58
6:3D:20:VAL:HG23	6:3D:20:VAL:O	2.04	0.58
9:7A:365:TRP:O	9:7A:369:ARG:NH1	2.32	0.58
6:4B:13:SER:OG	6:4B:61:GLN:NE2	2.38	0.57
7:5B:102:TYR:OH	7:5B:154:VAL:HG23	2.05	0.57
6:2R:17:ASP:OD1	6:2R:57:TYR:OH	2.19	0.57
7:5E:125:PHE:CG	7:5E:166:MET:HE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5O:102:TYR:OH	7:5O:154:VAL:HG23	2.04	0.57
7:5H:345:SER:O	7:5H:346:THR:HG22	2.03	0.57
7:5H:514:GLU:OE2	7:5H:516:LYS:NZ	2.34	0.57
9:7A:332:ASP:OD1	9:7A:333:ASP:N	2.38	0.57
6:3V:49:SER:OG	6:4B:10:ASP:OD2	2.11	0.57
6:4G:20:VAL:HG23	6:4G:20:VAL:O	2.04	0.57
9:7G:338:ARG:NH2	9:7H:360:GLU:OE2	2.36	0.57
9:7O:200:ASN:ND2	9:7O:203:ASP:OD2	2.37	0.57
6:4J:22:ASN:CG	6:4J:25:THR:HG1	2.13	0.57
9:7J:332:ASP:OD2	9:7K:362:LYS:NZ	2.35	0.57
6:2G:20:VAL:HG23	6:2G:20:VAL:O	2.03	0.57
8:6L:134:ILE:H	8:6L:134:ILE:HD12	1.70	0.57
9:7X:200:ASN:ND2	9:7X:203:ASP:OD2	2.38	0.57
3:1G:69:GLU:CD	3:1G:69:GLU:H	2.13	0.56
6:4J:20:VAL:HG23	6:4J:20:VAL:O	2.03	0.56
7:5D:514:GLU:OE2	7:5D:516:LYS:NZ	2.37	0.56
6:4K:10:ASP:OD1	6:4K:11:ASP:N	2.37	0.56
9:7E:200:ASN:ND2	9:7E:203:ASP:OD2	2.37	0.56
6:3H:3:THR:HB	6:3H:4:PRO:HD2	1.88	0.56
6:4M:55:ASN:OD1	6:4M:59:ASN:ND2	2.39	0.56
6:2T:20:VAL:HG23	6:2T:20:VAL:O	2.06	0.56
6:2I:78:ASN:OD1	6:2J:80:ARG:NH2	2.39	0.56
6:3K:20:VAL:HG23	6:3K:20:VAL:O	2.05	0.56
7:5I:125:PHE:CG	7:5I:166:MET:HE1	2.41	0.56
7:5B:320:ARG:NH2	7:5P:392:LYS:O	2.35	0.55
8:6Q:190:ARG:NH1	8:6Q:191:SER:O	2.39	0.55
9:7G:268:SER:N	9:7G:271:GLU:OE1	2.34	0.55
6:2J:20:VAL:HG23	6:2J:20:VAL:O	2.05	0.55
9:7Q:258:PHE:CE2	9:7Q:260:LEU:HD21	2.41	0.55
6:4O:26:GLN:OE1	6:4O:50:LYS:NZ	2.32	0.55
7:5L:281:LYS:NZ	7:5M:218:GLU:OE1	2.31	0.55
8:6I:139:ASN:O	8:6I:141:ARG:NH1	2.33	0.55
7:5I:420:GLY:O	7:5I:463:HIS:ND1	2.34	0.55
6:3I:22:ASN:OD1	6:3I:25:THR:OG1	2.13	0.55
6:4I:63:ASN:O	6:4I:67:VAL:HG23	2.07	0.55
7:5J:392:LYS:O	7:5K:320:ARG:NH2	2.38	0.55
6:3V:20:VAL:HG23	6:3V:20:VAL:O	2.05	0.55
7:5O:477:ASN:ND2	7:5O:503:ASN:O	2.38	0.55
6:2N:77:GLN:OE1	6:2N:80:ARG:NH2	2.39	0.55
6:2W:20:VAL:HG23	6:2W:20:VAL:O	2.05	0.55
7:5G:415:ARG:NE	7:5G:423:GLU:OE1	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:7I:387:TYR:CE2	9:7I:389:PRO:HB3	2.41	0.55
6:4B:34:LEU:C	6:4B:34:LEU:HD13	2.32	0.55
9:7W:200:ASN:ND2	9:7W:203:ASP:OD2	2.39	0.55
7:5D:39:ASP:N	7:5D:69:THR:HG22	2.19	0.55
8:6P:141:ARG:CD	8:6P:141:ARG:H	2.20	0.55
7:5L:225:ILE:HD11	7:5L:289:PHE:HB3	1.90	0.54
8:6J:134:ILE:HD12	8:6J:134:ILE:H	1.72	0.54
6:3T:77:GLN:OE1	6:3U:80:ARG:NH2	2.35	0.54
9:7O:364:ASP:OD2	9:7O:368:GLY:N	2.40	0.54
6:3I:20:VAL:HG23	6:3I:20:VAL:O	2.07	0.54
7:5E:488:GLY:O	7:5E:498:ARG:NH2	2.36	0.54
9:7F:387:TYR:CD1	9:7F:387:TYR:O	2.60	0.54
6:2O:17:ASP:OD2	6:2O:57:TYR:OH	2.26	0.54
7:5C:73:GLU:OE1	7:5C:75:HIS:NE2	2.38	0.54
6:2H:20:VAL:O	6:2H:20:VAL:HG23	2.06	0.54
6:4S:13:SER:OG	6:4S:61:GLN:OE1	2.23	0.54
7:5H:392:LYS:O	7:5I:320:ARG:NH2	2.40	0.54
9:7Q:310:GLN:OE1	9:7Q:338:ARG:NH1	2.39	0.54
6:3N:34:LEU:HD13	6:3N:34:LEU:C	2.32	0.54
1:1B:79:ASP:OD2	1:1B:80:VAL:N	2.40	0.54
6:3F:3:THR:HB	6:3F:4:PRO:HD3	1.90	0.54
7:5F:116:ASN:ND2	7:5F:171:ASP:OD2	2.41	0.54
6:4R:20:VAL:HG23	6:4R:20:VAL:O	2.08	0.54
7:5D:199:ASP:OD2	7:5D:411:ARG:NH2	2.39	0.54
6:2Y:17:ASP:OD2	6:2Y:57:TYR:OH	2.25	0.54
6:3N:20:VAL:HG23	6:3N:20:VAL:O	2.06	0.54
6:3S:66:LYS:NZ	6:3S:70:ASP:OD2	2.35	0.54
4:1K:49:GLN:HG3	4:1K:73:MET:HE1	1.89	0.53
6:3T:10:ASP:OD2	6:3T:11:ASP:N	2.41	0.53
6:3X:55:ASN:OD1	6:3X:59:ASN:ND2	2.40	0.53
6:4L:34:LEU:HD13	6:4L:34:LEU:C	2.33	0.53
6:3X:34:LEU:HD11	6:3X:44:LEU:HD23	1.90	0.53
8:6V:62:GLU:H	8:6V:62:GLU:CD	2.16	0.53
9:7C:200:ASN:ND2	9:7C:203:ASP:OD2	2.41	0.53
9:7U:387:TYR:O	9:7U:387:TYR:CD1	2.61	0.53
6:3A:34:LEU:HD13	6:3A:34:LEU:C	2.33	0.53
7:5L:313:LEU:HD23	7:5L:366:THR:HG23	1.91	0.53
6:3Q:20:VAL:HG23	6:3Q:20:VAL:O	2.08	0.53
8:6K:166:ASP:OD2	9:7K:340:ARG:NH2	2.40	0.53
9:7E:332:ASP:OD2	9:7F:362:LYS:NZ	2.41	0.53
6:3F:3:THR:HB	6:3F:4:PRO:CD	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:4T:10:ASP:OD1	6:4T:11:ASP:N	2.42	0.53
6:4O:20:VAL:HG23	6:4O:20:VAL:O	2.08	0.53
8:6E:62:GLU:H	8:6E:62:GLU:CD	2.17	0.53
8:6F:28:ASP:OD2	8:6F:29:GLN:N	2.42	0.53
8:6G:62:GLU:CD	8:6G:62:GLU:H	2.16	0.53
6:3Y:17:ASP:OD1	6:3Y:57:TYR:OH	2.24	0.53
7:5B:514:GLU:OE2	7:5B:516:LYS:NZ	2.42	0.53
1:1C:192:THR:HG23	1:1C:193:ILE:HG13	1.89	0.53
6:3Y:73:ALA:O	6:3Y:76:ILE:HG12	2.09	0.53
8:6P:62:GLU:CD	8:6P:62:GLU:H	2.16	0.53
1:1A:195:THR:OG1	1:1A:196:PRO:HD3	2.10	0.52
4:1N:75:SER:HB3	6:2D:69:LYS:HD3	1.91	0.52
6:2Q:31:LEU:C	6:2Q:31:LEU:HD23	2.34	0.52
8:6W:28:ASP:OD1	8:6W:29:GLN:N	2.41	0.52
9:7I:390:SER:OG	9:7I:391:PRO:HD2	2.09	0.52
6:4J:8:TYR:O	6:4J:12:VAL:HG23	2.10	0.52
7:5F:414:PRO:HB3	7:5F:424:MET:HE1	1.92	0.52
7:5F:540:TRP:NE1	7:5F:543:ASP:OD1	2.40	0.52
8:6X:62:GLU:CD	8:6X:62:GLU:H	2.18	0.52
9:7S:264:ARG:NH1	9:7S:296:ASP:OD2	2.43	0.52
4:1M:55:ILE:O	4:1M:55:ILE:HG22	2.09	0.52
9:7A:200:ASN:ND2	9:7A:203:ASP:OD2	2.43	0.52
3:1I:64:SER:HB3	11:1I:501:LDA:HM11	1.91	0.52
7:5O:329:ILE:HA	7:5O:349:GLY:HA2	1.90	0.52
6:4P:8:TYR:O	6:4P:12:VAL:HG23	2.10	0.52
9:7D:365:TRP:O	9:7D:369:ARG:NH1	2.43	0.52
7:5D:477:ASN:OD1	7:5D:478:THR:N	2.43	0.52
7:5L:38:LYS:N	7:5L:40:ASP:OD2	2.42	0.52
7:5N:225:ILE:HD11	7:5N:289:PHE:HB3	1.90	0.52
6:3U:20:VAL:HG23	6:3U:20:VAL:O	2.10	0.52
6:3Z:34:LEU:HD13	6:3Z:34:LEU:C	2.34	0.52
8:6P:141:ARG:H	8:6P:141:ARG:HD2	1.75	0.52
8:6N:62:GLU:CD	8:6N:62:GLU:H	2.17	0.52
8:6F:62:GLU:CD	8:6F:62:GLU:H	2.17	0.51
9:7R:172:GLU:HB2	9:7R:174:ASP:OD1	2.10	0.51
7:5D:552:VAL:HG13	7:5D:553:TYR:N	2.25	0.51
7:5N:192:ASP:OD1	7:5N:206:GLY:N	2.29	0.51
7:5M:540:TRP:NE1	7:5M:543:ASP:OD1	2.44	0.51
7:5O:344:ILE:HG23	7:5O:346:THR:H	1.76	0.51
8:6A:62:GLU:H	8:6A:62:GLU:CD	2.19	0.51
4:1O:30:ASP:OD2	4:1O:31:ASP:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:4Q:16:PHE:HB3	6:4Q:57:TYR:HE1	1.76	0.51
9:7O:387:TYR:O	9:7O:387:TYR:CD1	2.63	0.51
4:1O:55:ILE:HG22	4:1O:55:ILE:O	2.10	0.51
6:2I:20:VAL:HG23	6:2I:20:VAL:O	2.09	0.51
6:2O:20:VAL:HG23	6:2O:20:VAL:O	2.11	0.51
6:4C:34:LEU:HD13	6:4C:34:LEU:C	2.35	0.51
7:5E:514:GLU:OE2	7:5E:516:LYS:NZ	2.42	0.51
7:5K:408:THR:OG1	7:5K:430:ASP:OD2	2.28	0.51
6:4F:17:ASP:OD2	6:4F:57:TYR:OH	2.25	0.51
8:6M:62:GLU:H	8:6M:62:GLU:CD	2.19	0.51
8:6R:134:ILE:HD12	8:6R:134:ILE:H	1.76	0.51
8:6X:134:ILE:H	8:6X:134:ILE:HD12	1.74	0.51
9:7A:268:SER:N	9:7A:271:GLU:OE1	2.35	0.51
9:7J:264:ARG:NH1	9:7J:296:ASP:OD2	2.42	0.51
6:3T:20:VAL:HG23	6:3T:20:VAL:O	2.11	0.51
7:5O:185:LEU:CD1	7:5O:190:VAL:HG12	2.41	0.51
9:7N:200:ASN:ND2	9:7N:203:ASP:OD2	2.43	0.51
7:5L:125:PHE:CG	7:5L:166:MET:HE1	2.46	0.51
1:1A:59:LEU:HD22	1:1A:216:ILE:HD11	1.93	0.51
3:1G:63:LEU:HD11	3:1G:67:TYR:CZ	2.47	0.51
7:5L:272:TYR:CE2	7:5L:274:ASP:HB3	2.46	0.51
6:3F:20:VAL:HG23	6:3F:20:VAL:O	2.11	0.50
8:6I:62:GLU:H	8:6I:62:GLU:CD	2.19	0.50
8:6S:190:ARG:NH1	8:6S:191:SER:O	2.44	0.50
9:7U:364:ASP:N	9:7U:364:ASP:OD1	2.44	0.50
7:5M:394:ILE:HG21	7:5O:341:GLN:HB2	1.93	0.50
7:5G:412:VAL:HG23	7:5G:426:LEU:HD23	1.93	0.50
9:7D:268:SER:N	9:7D:271:GLU:OE1	2.36	0.50
9:7H:200:ASN:ND2	9:7H:203:ASP:OD2	2.44	0.50
4:1O:30:ASP:OD2	4:1O:30:ASP:C	2.55	0.50
6:4O:63:ASN:O	6:4O:67:VAL:HG23	2.11	0.50
7:5G:73:GLU:OE2	7:5G:75:HIS:NE2	2.45	0.50
8:6V:102:LYS:HD2	8:6V:134:ILE:HG13	1.93	0.50
6:4I:17:ASP:OD2	6:4I:57:TYR:OH	2.30	0.50
8:6H:62:GLU:CD	8:6H:62:GLU:H	2.19	0.50
7:5B:552:VAL:HG13	7:5B:553:TYR:N	2.27	0.50
7:5D:541:SER:HG	7:5F:506:ASN:CG	2.20	0.50
8:6W:190:ARG:NH1	8:6W:191:SER:O	2.45	0.50
6:4K:17:ASP:OD2	6:4K:57:TYR:OH	2.30	0.50
6:4T:20:VAL:HG12	6:4T:20:VAL:O	2.12	0.50
8:6K:102:LYS:HD2	8:6K:134:ILE:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:7M:258:PHE:CE2	9:7M:260:LEU:HD21	2.46	0.50
9:7R:390:SER:OG	9:7R:391:PRO:HD2	2.11	0.50
1:1D:173:ASP:C	1:1D:173:ASP:OD1	2.54	0.50
7:5E:195:TYR:HE1	7:5E:204:ILE:HD12	1.77	0.50
9:7H:258:PHE:CE2	9:7H:260:LEU:HD21	2.47	0.50
9:7S:258:PHE:CE2	9:7S:260:LEU:HD21	2.46	0.50
6:2M:63:ASN:OD1	6:2S:80:ARG:NH2	2.44	0.49
7:5B:396:GLU:HB3	7:5C:442:THR:HA	1.94	0.49
7:5C:469:VAL:HG22	7:5C:511:PHE:O	2.12	0.49
7:5K:118:SER:N	7:5K:121:GLU:OE1	2.40	0.49
3:1H:21:TRP:HB2	3:1H:22:PRO:HD3	1.94	0.49
8:6U:62:GLU:H	8:6U:62:GLU:CD	2.21	0.49
8:6T:62:GLU:CD	8:6T:62:GLU:H	2.20	0.49
1:1A:97:ASP:OD1	1:1A:140:LYS:NZ	2.44	0.49
7:5N:272:TYR:CE2	7:5N:274:ASP:HB3	2.47	0.49
1:1D:220:MET:HE2	1:1D:220:MET:HA	1.94	0.49
7:5K:102:TYR:OH	7:5K:154:VAL:HG23	2.12	0.49
7:5O:313:LEU:CD2	7:5O:366:THR:HG23	2.43	0.49
8:6L:62:GLU:CD	8:6L:62:GLU:H	2.19	0.49
8:6S:62:GLU:CD	8:6S:62:GLU:H	2.21	0.49
9:7N:264:ARG:NH1	9:7N:296:ASP:OD2	2.46	0.49
6:2K:20:VAL:HG23	6:2K:20:VAL:O	2.12	0.49
7:5G:272:TYR:CE2	7:5G:274:ASP:HB3	2.47	0.49
7:5G:544:ASP:OD1	7:5I:315:LYS:NZ	2.33	0.49
7:5L:202:MET:HE1	7:5L:204:ILE:HG12	1.94	0.49
6:4S:34:LEU:HD13	6:4S:34:LEU:C	2.38	0.49
7:5E:396:GLU:OE1	7:5F:441:THR:OG1	2.21	0.49
7:5I:190:VAL:HG21	7:5I:273:PRO:HA	1.93	0.49
7:5J:327:GLY:CA	7:5J:341:GLN:HE21	2.25	0.49
7:5O:82:GLU:OE2	7:5O:92:TRP:NE1	2.44	0.49
8:6X:102:LYS:HD2	8:6X:134:ILE:HG13	1.94	0.49
6:2X:3:THR:HG22	6:2X:4:PRO:HD3	1.94	0.49
7:5B:313:LEU:CD2	7:5B:366:THR:HG23	2.43	0.49
7:5L:313:LEU:CD2	7:5L:366:THR:HG23	2.43	0.49
7:5P:322:GLY:HA3	7:5P:499:TYR:HA	1.95	0.49
3:1H:3:ASP:OD1	3:1H:3:ASP:N	2.44	0.49
6:3Y:25:THR:O	6:3Y:28:THR:HG22	2.12	0.49
7:5B:28:ILE:HA	9:7M:366:LEU:HD21	1.94	0.49
7:5P:351:ARG:HD3	7:5P:352:PHE:N	2.28	0.49
8:6H:102:LYS:HD2	8:6H:134:ILE:HG12	1.95	0.49
8:6M:102:LYS:HD2	8:6M:134:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1P:19:ILE:HG22	4:1P:20:ARG:N	2.28	0.48
6:2Z:34:LEU:C	6:2Z:34:LEU:HD23	2.38	0.48
7:5D:404:VAL:HG22	7:5D:447:LEU:HD13	1.95	0.48
8:6E:28:ASP:C	8:6E:28:ASP:OD1	2.56	0.48
9:7O:180:GLU:OE1	9:7O:183:ARG:NH1	2.46	0.48
2:1F:186:SER:HB3	2:1F:187:PRO:HD3	1.94	0.48
7:5L:102:TYR:OH	7:5L:154:VAL:HG23	2.12	0.48
8:6N:99:ARG:HG3	8:6N:134:ILE:HG22	1.95	0.48
9:7V:200:ASN:ND2	9:7V:203:ASP:OD2	2.47	0.48
1:1B:97:ASP:OD1	1:1B:100:ARG:NH1	2.46	0.48
1:1E:5:ILE:N	1:1E:5:ILE:HD12	2.28	0.48
6:4C:20:VAL:HG23	6:4C:20:VAL:O	2.13	0.48
7:5D:117:VAL:HG12	7:5D:118:SER:N	2.28	0.48
8:6M:102:LYS:C	8:6M:134:ILE:HD13	2.38	0.48
8:6X:134:ILE:HD12	8:6X:134:ILE:N	2.28	0.48
4:1O:58:PRO:HA	4:1O:61:VAL:HG12	1.96	0.48
7:5B:327:GLY:C	7:5B:341:GLN:HE21	2.21	0.48
8:6B:62:GLU:CD	8:6B:62:GLU:H	2.21	0.48
1:1C:137:GLU:O	1:1C:141:PRO:HD3	2.13	0.48
7:5H:440:THR:HG23	7:5H:443:SER:H	1.77	0.48
7:5N:412:VAL:HG23	7:5N:426:LEU:CD2	2.44	0.48
4:1K:45:ALA:HB1	4:1K:73:MET:CE	2.42	0.48
6:3F:7:GLY:O	6:3F:10:ASP:OD1	2.31	0.48
6:3K:34:LEU:HD23	6:3K:34:LEU:C	2.38	0.48
7:5K:550:VAL:CG1	7:5M:510:VAL:HG11	2.44	0.48
8:6G:194:GLN:OE1	9:7F:202:ARG:NH2	2.33	0.48
9:7U:246:TYR:OH	9:7U:296:ASP:OD1	2.29	0.48
6:3W:34:LEU:C	6:3W:34:LEU:HD13	2.39	0.48
8:6K:62:GLU:CD	8:6K:62:GLU:H	2.21	0.48
9:7I:180:GLU:OE1	9:7I:183:ARG:NH1	2.47	0.48
9:7K:200:ASN:ND2	9:7K:203:ASP:OD2	2.47	0.48
7:5D:255:GLN:NE2	7:5D:256:GLU:OE1	2.41	0.48
7:5M:138:LEU:HD22	7:5M:149:VAL:HG22	1.96	0.48
7:5M:390:TYR:OH	7:5N:435:THR:HG21	2.12	0.48
7:5M:552:VAL:HG13	7:5M:553:TYR:N	2.29	0.48
8:6N:102:LYS:HD2	8:6N:134:ILE:HG12	1.96	0.48
8:6O:62:GLU:H	8:6O:62:GLU:CD	2.22	0.48
8:6R:62:GLU:H	8:6R:62:GLU:CD	2.21	0.48
9:7F:387:TYR:CE2	9:7F:389:PRO:HB3	2.49	0.48
9:7G:258:PHE:CE2	9:7G:260:LEU:HD21	2.49	0.48
6:3X:80:ARG:HG2	6:3X:80:ARG:OXT	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5B:218:GLU:OE1	7:5P:281:LYS:NZ	2.47	0.48
7:5L:408:THR:OG1	7:5L:430:ASP:OD2	2.25	0.48
8:6D:62:GLU:CD	8:6D:62:GLU:H	2.22	0.48
9:7A:379:ILE:HG22	9:7A:380:LYS:N	2.28	0.48
7:5I:352:PHE:N	7:5J:334:LYS:O	2.44	0.47
7:5M:432:ASN:OD1	7:5M:432:ASN:C	2.57	0.47
6:4R:55:ASN:O	6:4R:59:ASN:ND2	2.37	0.47
8:6J:62:GLU:CD	8:6J:62:GLU:H	2.20	0.47
7:5A:118:SER:HB2	7:5A:121:GLU:HG2	1.96	0.47
6:3Z:23:LEU:O	6:3Z:27:VAL:HG23	2.14	0.47
7:5F:552:VAL:HG13	7:5F:553:TYR:N	2.30	0.47
7:5G:327:GLY:C	7:5G:341:GLN:HE21	2.22	0.47
7:5O:30:VAL:HG23	7:5O:31:THR:HG23	1.97	0.47
8:6W:62:GLU:CD	8:6W:62:GLU:H	2.21	0.47
9:7X:390:SER:OG	9:7X:391:PRO:HD2	2.15	0.47
1:1C:138:ILE:O	1:1C:141:PRO:CD	2.63	0.47
7:5J:313:LEU:CD2	7:5J:366:THR:HG23	2.45	0.47
7:5O:195:TYR:HE1	7:5O:204:ILE:HD12	1.79	0.47
8:6N:102:LYS:NZ	8:6N:138:GLU:OE1	2.43	0.47
9:7Q:182:GLU:OE1	9:7Q:182:GLU:N	2.40	0.47
4:1M:12:VAL:O	7:5N:169:GLN:NE2	2.38	0.47
6:3M:34:LEU:HD11	6:3M:44:LEU:HD23	1.97	0.47
7:5K:272:TYR:CE2	7:5K:274:ASP:HB3	2.50	0.47
8:6F:179:ASP:OD2	9:7F:367:LYS:NZ	2.41	0.47
9:7A:234:ILE:HG23	9:7X:348:ARG:HH22	1.79	0.47
9:7H:182:GLU:OE1	9:7H:182:GLU:N	2.37	0.47
9:7U:387:TYR:CE2	9:7U:389:PRO:HB3	2.49	0.47
6:2A:10:ASP:OD2	7:5D:108:ARG:NH1	2.41	0.47
6:3T:34:LEU:HD13	6:3T:34:LEU:C	2.40	0.47
6:4E:20:VAL:O	6:4E:20:VAL:HG23	2.15	0.47
7:5G:540:TRP:NE1	7:5G:543:ASP:OD1	2.39	0.47
7:5I:434:LYS:NZ	7:5I:438:SER:OG	2.41	0.47
7:5N:440:THR:HG22	7:5N:441:THR:H	1.80	0.47
7:5P:408:THR:OG1	7:5P:430:ASP:OD2	2.32	0.47
9:7B:264:ARG:NH1	9:7B:296:ASP:OD2	2.47	0.47
9:7U:201:GLU:CD	9:7U:201:GLU:H	2.21	0.47
9:7W:310:GLN:OE1	9:7W:338:ARG:NH1	2.44	0.47
6:4G:37:LYS:NZ	6:4G:40:ASP:OD2	2.35	0.47
6:4H:55:ASN:O	6:4H:59:ASN:ND2	2.35	0.47
6:4Q:27:VAL:HG22	6:4Q:50:LYS:HB3	1.97	0.47
8:6T:139:ASN:O	8:6T:141:ARG:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:7B:332:ASP:OD2	9:7B:333:ASP:N	2.48	0.47
6:2P:20:VAL:HG23	6:2P:20:VAL:O	2.14	0.47
6:4I:34:LEU:C	6:4I:34:LEU:HD13	2.40	0.47
7:5D:545:LYS:HD2	7:5D:545:LYS:N	2.30	0.47
7:5E:488:GLY:O	7:5E:498:ARG:NE	2.48	0.47
7:5I:415:ARG:NE	7:5I:423:GLU:OE1	2.40	0.47
1:1B:65:TRP:CD2	4:1L:29:LEU:HD21	2.50	0.47
1:1B:150:TYR:OH	1:1B:154:GLU:OE1	2.28	0.47
7:5N:526:ALA:O	7:5N:530:VAL:HG23	2.15	0.47
6:4C:7:GLY:O	6:4C:10:ASP:OD1	2.33	0.46
6:4Q:10:ASP:OD1	6:4Q:11:ASP:N	2.48	0.46
7:5G:432:ASN:OD1	7:5G:433:ASP:N	2.48	0.46
7:5H:329:ILE:HA	7:5H:349:GLY:H	1.79	0.46
7:5J:479:ASP:OD1	7:5J:502:LYS:NZ	2.48	0.46
7:5K:116:ASN:ND2	7:5K:171:ASP:OD2	2.47	0.46
7:5N:552:VAL:HG13	7:5N:553:TYR:N	2.30	0.46
8:6A:190:ARG:NH1	8:6A:191:SER:O	2.47	0.46
8:6C:62:GLU:H	8:6C:62:GLU:CD	2.23	0.46
9:7F:200:ASN:ND2	9:7F:203:ASP:OD2	2.48	0.46
6:4I:59:ASN:O	6:4I:63:ASN:ND2	2.48	0.46
7:5J:552:VAL:HG13	7:5J:553:TYR:N	2.30	0.46
8:6L:139:ASN:O	8:6L:141:ARG:NH1	2.33	0.46
9:7S:387:TYR:C	9:7S:387:TYR:CD2	2.93	0.46
4:1M:12:VAL:HG13	4:1M:13:ILE:N	2.28	0.46
6:3G:34:LEU:HD23	6:3G:34:LEU:C	2.41	0.46
6:3X:48:GLN:OE1	6:3X:49:SER:N	2.48	0.46
8:6H:28:ASP:OD1	8:6H:29:GLN:N	2.46	0.46
9:7B:338:ARG:NH2	9:7C:360:GLU:OE2	2.46	0.46
6:4A:63:ASN:O	6:4A:67:VAL:HG23	2.15	0.46
6:4S:37:LYS:HE3	6:4S:40:ASP:HB2	1.96	0.46
7:5C:308:LEU:O	7:5C:370:ARG:HA	2.16	0.46
7:5H:306:LEU:HD23	7:5H:306:LEU:C	2.40	0.46
7:5I:30:VAL:HG23	7:5I:31:THR:HG23	1.97	0.46
8:6O:110:GLU:HG3	8:6O:130:ILE:HD12	1.97	0.46
8:6V:110:GLU:HG3	8:6V:130:ILE:HD12	1.97	0.46
7:5G:384:ASP:OD1	7:5G:384:ASP:C	2.57	0.46
7:5K:305:GLU:HB2	7:5K:518:ILE:HG13	1.98	0.46
7:5N:525:ASP:HB3	7:5N:528:GLU:HG3	1.98	0.46
7:5O:192:ASP:OD1	7:5O:206:GLY:N	2.39	0.46
8:6Q:102:LYS:HD2	8:6Q:134:ILE:HG12	1.97	0.46
6:4J:23:LEU:HD21	6:4J:54:TYR:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:4P:22:ASN:OD1	6:4P:25:THR:CG2	2.64	0.46
7:5D:540:TRP:NE1	7:5D:543:ASP:OD1	2.47	0.46
7:5I:192:ASP:OD1	7:5I:206:GLY:N	2.47	0.46
8:6Q:62:GLU:H	8:6Q:62:GLU:CD	2.24	0.46
9:7I:268:SER:N	9:7I:271:GLU:OE1	2.38	0.46
9:7P:172:GLU:HB2	9:7P:174:ASP:OD1	2.16	0.46
1:1A:150:TYR:OH	1:1A:154:GLU:OE1	2.22	0.46
6:2M:34:LEU:C	6:2M:34:LEU:HD13	2.41	0.46
6:3X:20:VAL:HG23	6:3X:20:VAL:O	2.15	0.46
6:4T:63:ASN:O	6:4T:67:VAL:HG23	2.16	0.46
7:5C:272:TYR:CE2	7:5C:274:ASP:HB3	2.51	0.46
7:5K:432:ASN:ND2	7:5K:450:VAL:O	2.48	0.46
6:2Y:34:LEU:HD11	6:2Y:44:LEU:HD23	1.98	0.46
6:3X:34:LEU:C	6:3X:34:LEU:HD23	2.41	0.46
7:5M:192:ASP:OD1	7:5M:206:GLY:N	2.38	0.46
7:5N:556:ARG:NH2	7:5O:523:THR:O	2.47	0.46
9:7U:174:ASP:OD1	9:7U:175:SER:N	2.49	0.46
6:2I:22:ASN:OD1	6:2I:25:THR:OG1	2.34	0.46
6:3V:34:LEU:HD13	6:3V:34:LEU:C	2.40	0.46
7:5F:185:LEU:HD12	7:5F:190:VAL:HG12	1.98	0.46
8:6R:190:ARG:NH1	8:6R:191:SER:O	2.49	0.46
9:7T:174:ASP:OD1	9:7T:175:SER:N	2.49	0.46
4:1K:45:ALA:CB	4:1K:73:MET:HE3	2.41	0.45
6:2G:79:PHE:O	6:2G:80:ARG:OXT	2.34	0.45
6:3V:10:ASP:OD1	6:3V:10:ASP:N	2.46	0.45
6:4C:76:ILE:HA	6:4C:79:PHE:CD1	2.50	0.45
7:5G:285:GLU:CD	7:5G:285:GLU:H	2.24	0.45
7:5H:118:SER:HB2	7:5H:121:GLU:HG2	1.97	0.45
7:5H:552:VAL:HG13	7:5H:553:TYR:N	2.29	0.45
7:5K:477:ASN:OD1	7:5K:478:THR:N	2.49	0.45
9:7T:172:GLU:HB2	9:7T:174:ASP:OD1	2.17	0.45
9:7X:387:TYR:CE2	9:7X:389:PRO:HB3	2.50	0.45
6:3I:3:THR:N	6:3I:4:PRO:CD	2.78	0.45
7:5E:189:PHE:CE2	7:5F:415:ARG:HD3	2.51	0.45
8:6Q:102:LYS:C	8:6Q:134:ILE:HD13	2.41	0.45
8:6X:44:ILE:HG23	8:6X:64:ASP:HB3	1.98	0.45
9:7V:258:PHE:CE2	9:7V:260:LEU:HD21	2.51	0.45
6:2C:24:GLN:O	6:2C:27:VAL:HG12	2.16	0.45
7:5B:398:ASN:O	7:5C:441:THR:OG1	2.27	0.45
7:5N:306:LEU:C	7:5N:306:LEU:HD23	2.41	0.45
7:5N:401:LEU:HD21	7:5O:441:THR:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:7O:348:ARG:HH22	9:7P:234:ILE:HG23	1.80	0.45
9:7W:258:PHE:CE2	9:7W:260:LEU:HD21	2.52	0.45
6:2W:22:ASN:OD1	6:2W:25:THR:HG22	2.16	0.45
6:3T:55:ASN:OD1	6:3T:59:ASN:ND2	2.50	0.45
7:5B:192:ASP:OD1	7:5B:206:GLY:N	2.36	0.45
9:7M:200:ASN:ND2	9:7M:203:ASP:OD2	2.50	0.45
9:7W:172:GLU:HB2	9:7W:174:ASP:OD1	2.16	0.45
6:3Z:7:GLY:N	6:3Z:10:ASP:OD1	2.43	0.45
7:5B:327:GLY:HA3	7:5B:352:PHE:CD1	2.52	0.45
7:5J:199:ASP:OD2	7:5J:411:ARG:NH1	2.43	0.45
9:7O:182:GLU:OE1	9:7O:182:GLU:N	2.38	0.45
6:2U:20:VAL:HG23	6:2U:20:VAL:O	2.17	0.45
6:3I:34:LEU:C	6:3I:34:LEU:HD23	2.42	0.45
9:7O:387:TYR:CE2	9:7O:389:PRO:HB3	2.52	0.45
4:1L:30:ASP:OD1	4:1L:31:ASP:N	2.50	0.45
6:3I:48:GLN:OE1	6:3T:78:ASN:ND2	2.50	0.45
6:4A:29:GLU:OE1	6:4A:33:LYS:NZ	2.50	0.45
6:4M:23:LEU:O	6:4M:27:VAL:HG23	2.16	0.45
6:4S:10:ASP:N	6:4S:10:ASP:OD1	2.43	0.45
6:4T:54:TYR:O	6:4T:57:TYR:HB3	2.17	0.45
7:5B:272:TYR:CE2	7:5B:274:ASP:HB3	2.51	0.45
7:5N:141:ASP:C	7:5N:141:ASP:OD1	2.59	0.45
8:6D:134:ILE:H	8:6D:134:ILE:HD12	1.81	0.45
8:6E:102:LYS:NZ	8:6E:138:GLU:OE1	2.27	0.45
9:7U:182:GLU:CD	9:7U:182:GLU:H	2.25	0.45
6:2Y:22:ASN:OD1	6:2Y:25:THR:HG22	2.17	0.45
6:4H:10:ASP:OD2	6:4H:10:ASP:N	2.49	0.45
6:4M:34:LEU:C	6:4M:34:LEU:HD13	2.42	0.45
8:6B:102:LYS:HB3	8:6B:134:ILE:HG12	1.99	0.45
9:7V:182:GLU:OE1	9:7V:182:GLU:N	2.46	0.45
7:5E:194:THR:HG21	7:5E:201:LYS:NZ	2.32	0.45
7:5N:411:ARG:HB2	7:5N:427:ASP:OD1	2.17	0.45
9:7I:264:ARG:NH1	9:7I:296:ASP:OD2	2.49	0.45
9:7L:387:TYR:CE2	9:7L:389:PRO:HB3	2.52	0.45
7:5A:125:PHE:CD1	7:5A:166:MET:HE1	2.52	0.45
7:5N:440:THR:HG22	7:5N:441:THR:N	2.32	0.45
7:5N:553:TYR:CD1	7:5O:522:LEU:HD22	2.52	0.45
9:7B:172:GLU:HB2	9:7B:174:ASP:OD1	2.17	0.45
9:7M:264:ARG:NH1	9:7M:296:ASP:OD2	2.50	0.45
1:1C:30:PHE:N	1:1C:30:PHE:CD1	2.85	0.44
6:2N:20:VAL:HG23	6:2N:20:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:4J:78:ASN:OD1	6:4K:80:ARG:NH2	2.50	0.44
7:5F:30:VAL:HG22	9:7H:386:TRP:CG	2.53	0.44
7:5P:432:ASN:OD1	7:5P:432:ASN:C	2.60	0.44
9:7G:172:GLU:HB2	9:7G:174:ASP:OD1	2.17	0.44
9:7G:328:GLN:HA	9:7G:360:GLU:O	2.17	0.44
6:2N:72:ASP:OD1	6:2N:72:ASP:C	2.58	0.44
6:2O:3:THR:HB	6:2O:4:PRO:HD3	2.00	0.44
6:4K:59:ASN:HB3	6:4Q:76:ILE:HG21	1.99	0.44
7:5B:204:ILE:HG23	7:5B:205:PRO:HD2	2.00	0.44
7:5G:174:GLU:OE2	7:5G:175:LEU:N	2.46	0.44
7:5L:351:ARG:NH1	7:5M:333:ASP:OD2	2.50	0.44
9:7L:387:TYR:O	9:7L:387:TYR:CD1	2.70	0.44
9:7O:304:GLU:OE2	9:7O:314:TYR:OH	2.24	0.44
9:7X:372:GLN:O	9:7X:377:GLY:CA	2.66	0.44
6:2A:27:VAL:HG21	6:2A:54:TYR:HB2	1.99	0.44
6:3J:20:VAL:HG23	6:3J:20:VAL:O	2.18	0.44
6:4D:63:ASN:OD1	6:4J:80:ARG:HD3	2.18	0.44
7:5E:479:ASP:OD2	7:5E:502:LYS:NZ	2.47	0.44
7:5H:195:TYR:O	7:5H:201:LYS:HA	2.18	0.44
7:5L:308:LEU:O	7:5L:370:ARG:HA	2.18	0.44
7:5N:402:GLU:HB3	7:5N:444:VAL:HG11	1.99	0.44
8:6G:102:LYS:HD2	8:6G:134:ILE:HG12	1.99	0.44
8:6I:138:GLU:OE2	8:6I:143:PRO:HA	2.16	0.44
6:3F:27:VAL:HG22	6:3F:50:LYS:HB3	2.00	0.44
6:3I:3:THR:N	6:3I:4:PRO:HD2	2.32	0.44
6:3U:14:ALA:O	6:3U:18:THR:HG23	2.17	0.44
7:5H:102:TYR:OH	7:5H:154:VAL:HG23	2.17	0.44
7:5L:158:MET:SD	7:5L:158:MET:C	3.00	0.44
7:5L:525:ASP:N	7:5L:528:GLU:OE1	2.45	0.44
7:5N:412:VAL:HG23	7:5N:426:LEU:HD23	2.00	0.44
7:5P:552:VAL:HG13	7:5P:553:TYR:N	2.32	0.44
9:7P:258:PHE:CE2	9:7P:260:LEU:HD21	2.52	0.44
6:2O:32:ASP:OD1	6:2O:32:ASP:C	2.58	0.44
6:2U:40:ASP:C	6:2U:40:ASP:OD1	2.60	0.44
6:4P:37:LYS:HE3	6:4P:40:ASP:HB2	1.99	0.44
6:4R:79:PHE:CD1	6:4R:79:PHE:C	2.95	0.44
7:5B:118:SER:HB2	7:5B:121:GLU:HG2	2.00	0.44
7:5C:450:VAL:HG12	7:5C:451:GLY:N	2.31	0.44
7:5C:525:ASP:N	7:5C:528:GLU:OE1	2.40	0.44
7:5D:272:TYR:CE2	7:5D:274:ASP:HB3	2.53	0.44
7:5D:396:GLU:OE1	7:5E:441:THR:OG1	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5E:125:PHE:CD1	7:5E:166:MET:HE1	2.52	0.44
7:5G:396:GLU:OE2	7:5H:441:THR:OG1	2.22	0.44
7:5I:402:GLU:HA	7:5I:402:GLU:OE1	2.16	0.44
7:5I:412:VAL:HG22	7:5I:413:LEU:N	2.32	0.44
7:5M:408:THR:OG1	7:5M:430:ASP:OD2	2.19	0.44
8:6O:190:ARG:NH1	8:6O:191:SER:O	2.50	0.44
9:7S:263:GLN:NE2	9:7S:295:ASP:OD1	2.40	0.44
6:3W:14:ALA:O	6:3W:18:THR:HG23	2.18	0.44
7:5B:333:ASP:O	7:5P:351:ARG:HG2	2.18	0.44
7:5E:117:VAL:HG12	7:5E:118:SER:N	2.33	0.44
8:6A:134:ILE:O	8:6A:134:ILE:HG22	2.17	0.44
8:6X:99:ARG:HG3	8:6X:134:ILE:CG2	2.48	0.44
1:1B:65:TRP:HB3	1:1B:66:PRO:HD3	1.99	0.44
4:1O:100:ARG:O	4:1O:101:SER:OXT	2.36	0.44
6:2S:34:LEU:HD13	6:2S:34:LEU:C	2.42	0.44
6:3H:3:THR:CB	6:3H:4:PRO:HD2	2.47	0.44
6:3H:34:LEU:HD13	6:3H:34:LEU:C	2.43	0.44
6:4D:7:GLY:O	6:4D:11:ASP:CG	2.61	0.44
7:5G:545:LYS:H	7:5G:545:LYS:HD2	1.83	0.44
7:5N:525:ASP:OD2	7:5N:527:SER:OG	2.32	0.44
8:6I:28:ASP:C	8:6I:28:ASP:OD1	2.60	0.44
8:6I:172:LYS:NZ	8:6I:178:VAL:O	2.46	0.44
8:6O:44:ILE:HG23	8:6O:64:ASP:HB3	1.99	0.44
6:4B:20:VAL:O	6:4B:20:VAL:CG2	2.63	0.44
7:5N:512:MET:SD	7:5N:512:MET:N	2.91	0.44
7:5N:540:TRP:NE1	7:5N:543:ASP:OD1	2.45	0.44
9:7F:382:SER:HB2	9:7F:383:PRO:HD2	2.00	0.44
2:1F:146:MET:O	2:1F:149:VAL:HG12	2.17	0.44
3:1J:3:ASP:OD1	3:1J:3:ASP:N	2.50	0.44
7:5H:394:ILE:HD11	7:5I:320:ARG:HD2	2.00	0.44
7:5J:298:ASP:O	7:5J:298:ASP:CG	2.61	0.44
7:5M:141:ASP:OD1	7:5M:141:ASP:C	2.61	0.44
8:6L:102:LYS:HB3	8:6L:134:ILE:HG12	2.00	0.44
9:7C:382:SER:HB2	9:7C:383:PRO:HD2	2.00	0.44
9:7J:348:ARG:HH22	9:7K:234:ILE:HG23	1.83	0.44
6:2X:3:THR:N	6:2X:4:PRO:HD2	2.33	0.43
6:3C:34:LEU:HD23	6:3C:34:LEU:C	2.42	0.43
6:4G:20:VAL:HG12	6:4M:5:TRP:CZ2	2.52	0.43
7:5J:308:LEU:HD12	7:5J:512:MET:O	2.18	0.43
8:6D:139:ASN:O	8:6D:141:ARG:NH1	2.49	0.43
8:6K:190:ARG:NH1	8:6K:191:SER:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1F:65:PHE:HB3	2:1F:160:MET:HE1	2.00	0.43
3:1G:31:LEU:HD23	3:1G:31:LEU:C	2.43	0.43
7:5D:306:LEU:HD23	7:5D:306:LEU:C	2.42	0.43
7:5K:330:THR:OG1	7:5K:346:THR:OG1	2.22	0.43
7:5K:553:TYR:OH	7:5L:529:SER:OG	2.30	0.43
7:5P:272:TYR:CE2	7:5P:274:ASP:HB3	2.52	0.43
6:4T:24:GLN:O	6:4T:28:THR:HG23	2.18	0.43
7:5D:545:LYS:N	7:5D:545:LYS:CD	2.81	0.43
7:5I:281:LYS:NZ	7:5J:218:GLU:OE1	2.43	0.43
7:5I:441:THR:HG22	7:5I:443:SER:H	1.83	0.43
7:5J:463:HIS:ND1	7:5J:463:HIS:C	2.76	0.43
7:5M:222:LEU:HG	7:5M:223:GLY:H	1.83	0.43
9:7Q:376:GLU:CD	9:7Q:376:GLU:N	2.76	0.43
1:1A:163:PHE:CE1	1:1B:200:VAL:CG2	3.01	0.43
1:1B:63:VAL:HA	1:1B:220:MET:HE2	2.00	0.43
4:1M:55:ILE:O	4:1M:55:ILE:CG2	2.65	0.43
6:2M:10:ASP:OD1	6:2M:10:ASP:N	2.51	0.43
6:2R:34:LEU:HD13	6:2R:34:LEU:C	2.43	0.43
6:3V:8:TYR:O	6:3V:12:VAL:HG23	2.18	0.43
7:5B:409:MET:SD	7:5B:410:ILE:N	2.91	0.43
7:5F:308:LEU:O	7:5F:370:ARG:HA	2.18	0.43
7:5N:308:LEU:O	7:5N:371:PRO:HD2	2.17	0.43
7:5O:552:VAL:HG13	7:5O:553:TYR:N	2.33	0.43
9:7B:268:SER:N	9:7B:271:GLU:OE1	2.45	0.43
9:7Q:174:ASP:OD1	9:7Q:175:SER:N	2.52	0.43
4:1L:63:ASP:OD1	4:1L:63:ASP:C	2.61	0.43
4:1P:90:LYS:NZ	6:2F:80:ARG:OXT	2.51	0.43
6:4F:76:ILE:O	6:4F:79:PHE:HD1	2.01	0.43
6:4L:57:TYR:CE2	6:4L:58:ARG:HD3	2.53	0.43
7:5B:197:LEU:N	7:5B:200:GLN:O	2.50	0.43
7:5C:313:LEU:CD2	7:5C:366:THR:HG23	2.48	0.43
7:5E:399:VAL:HB	7:5F:440:THR:HA	1.99	0.43
7:5H:345:SER:O	7:5H:346:THR:CG2	2.66	0.43
7:5I:29:PRO:HB3	9:7C:373:TYR:CE1	2.53	0.43
7:5I:545:LYS:HA	7:5I:548:LYS:HE3	2.01	0.43
7:5L:258:LEU:HA	7:5L:261:ASN:ND2	2.33	0.43
7:5L:307:SER:OG	7:5L:370:ARG:HD3	2.19	0.43
7:5L:334:LYS:HG3	7:5L:335:LEU:HG	2.00	0.43
7:5M:308:LEU:O	7:5M:370:ARG:HA	2.18	0.43
7:5M:412:VAL:HA	7:5M:425:SER:O	2.19	0.43
8:6G:138:GLU:OE2	8:6G:143:PRO:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:7I:364:ASP:OD2	9:7I:367:LYS:N	2.52	0.43
3:1G:8:GLY:HA3	11:1G:201:LDA:H21	2.00	0.43
6:4M:20:VAL:O	6:4M:20:VAL:HG23	2.18	0.43
7:5E:525:ASP:HB2	7:5E:528:GLU:HG3	2.01	0.43
7:5F:394:ILE:HG13	7:5F:395:GLY:H	1.83	0.43
7:5J:306:LEU:HD11	7:5J:513:ILE:HD11	2.01	0.43
7:5L:383:PHE:C	7:5L:383:PHE:CD2	2.96	0.43
8:6C:102:LYS:HD2	8:6C:134:ILE:HG12	1.99	0.43
9:7R:217:ASP:OD1	9:7R:218:LYS:N	2.51	0.43
1:1A:108:ASP:O	1:1A:112:VAL:HG23	2.19	0.43
6:4L:55:ASN:OD1	6:4L:59:ASN:ND2	2.52	0.43
6:4T:17:ASP:OD2	6:4T:57:TYR:OH	2.32	0.43
7:5B:197:LEU:O	7:5B:198:ARG:C	2.61	0.43
7:5H:272:TYR:CE2	7:5H:274:ASP:HB3	2.53	0.43
7:5H:479:ASP:OD1	7:5H:502:LYS:NZ	2.44	0.43
7:5L:556:ARG:NH2	7:5M:523:THR:O	2.50	0.43
9:7D:246:TYR:OH	9:7D:296:ASP:OD1	2.36	0.43
6:3O:62:SER:O	6:3T:78:ASN:ND2	2.47	0.43
6:4C:27:VAL:HG22	6:4C:50:LYS:HB3	2.01	0.43
7:5I:256:GLU:O	7:5I:259:LYS:HG2	2.19	0.43
7:5L:69:THR:HG23	9:7X:387:TYR:HD1	1.84	0.43
8:6R:173:ASN:CG	8:6S:184:SER:HG	2.16	0.43
9:7I:200:ASN:ND2	9:7I:203:ASP:OD2	2.51	0.43
9:7N:258:PHE:CE2	9:7N:260:LEU:HD21	2.54	0.43
1:1A:2:GLY:HA3	4:1K:36:ALA:O	2.18	0.43
6:2E:50:LYS:HD2	6:2E:50:LYS:N	2.34	0.43
6:4B:27:VAL:HG22	6:4B:50:LYS:HB3	2.00	0.43
6:4H:40:ASP:OD1	6:4H:43:LEU:HD12	2.19	0.43
7:5I:396:GLU:HA	7:5K:342:SER:HB2	2.00	0.43
7:5J:158:MET:SD	7:5J:158:MET:C	3.02	0.43
7:5K:552:VAL:HG13	7:5K:553:TYR:N	2.32	0.43
7:5O:308:LEU:O	7:5O:370:ARG:HA	2.19	0.43
7:5P:441:THR:O	7:5P:444:VAL:HG12	2.19	0.43
8:6L:194:GLN:OE1	9:7K:202:ARG:NH2	2.35	0.43
9:7X:332:ASP:OD1	9:7X:333:ASP:N	2.52	0.43
6:2Z:47:TYR:O	6:2Z:48:GLN:C	2.60	0.43
7:5B:458:ILE:HG22	7:5P:376:GLN:OE1	2.18	0.43
7:5G:412:VAL:HG22	7:5G:413:LEU:N	2.34	0.43
8:6U:190:ARG:NH1	8:6U:191:SER:O	2.52	0.43
9:7R:387:TYR:CE2	9:7R:389:PRO:HB3	2.53	0.43
1:1B:109:ARG:CD	1:1B:109:ARG:H	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2V:37:LYS:HE3	6:2V:40:ASP:HB2	2.00	0.42
7:5C:30:VAL:HG12	7:5C:31:THR:N	2.34	0.42
7:5G:158:MET:SD	7:5G:158:MET:C	3.02	0.42
8:6K:28:ASP:OD1	8:6K:28:ASP:C	2.62	0.42
9:7I:224:ASN:C	9:7I:224:ASN:OD1	2.62	0.42
6:2V:40:ASP:OD1	6:2V:40:ASP:C	2.62	0.42
6:4I:16:PHE:HB3	6:4I:57:TYR:HE1	1.84	0.42
7:5B:190:VAL:HG23	7:5B:191:GLY:N	2.34	0.42
7:5E:552:VAL:HG13	7:5E:553:TYR:N	2.34	0.42
7:5F:313:LEU:CD2	7:5F:366:THR:HG23	2.50	0.42
8:6E:51:SER:HB2	8:6E:54:LEU:HB2	2.02	0.42
8:6G:102:LYS:C	8:6G:134:ILE:HD13	2.44	0.42
8:6Q:166:ASP:OD2	9:7Q:340:ARG:NH1	2.52	0.42
9:7F:258:PHE:CE2	9:7F:260:LEU:HD21	2.54	0.42
9:7J:361:LEU:HD12	9:7J:361:LEU:N	2.34	0.42
3:1I:44:GLU:CD	3:1I:44:GLU:N	2.77	0.42
7:5D:255:GLN:CD	7:5D:255:GLN:H	2.28	0.42
7:5D:399:VAL:HG11	7:5E:440:THR:HG23	2.02	0.42
7:5F:222:LEU:HG	7:5F:223:GLY:H	1.84	0.42
7:5I:258:LEU:O	7:5I:261:ASN:ND2	2.44	0.42
8:6D:28:ASP:OD1	8:6D:28:ASP:C	2.61	0.42
6:2F:27:VAL:HG23	6:2F:28:THR:N	2.34	0.42
6:3Z:55:ASN:OD1	6:3Z:59:ASN:ND2	2.52	0.42
6:4T:10:ASP:OD1	6:4T:10:ASP:C	2.62	0.42
7:5A:109:ASN:HB3	7:5A:150:SER:HB3	2.01	0.42
7:5B:28:ILE:HG23	7:5B:28:ILE:O	2.20	0.42
7:5C:325:TRP:CZ3	7:5C:354:ALA:HB2	2.54	0.42
7:5H:192:ASP:OD1	7:5H:206:GLY:N	2.48	0.42
7:5P:26:GLU:HA	7:5P:26:GLU:OE1	2.20	0.42
8:6F:44:ILE:HG23	8:6F:64:ASP:HB3	2.01	0.42
9:7H:224:ASN:OD1	9:7H:224:ASN:C	2.62	0.42
6:4C:10:ASP:OD1	6:4C:10:ASP:N	2.52	0.42
6:4J:20:VAL:HG21	6:4J:57:TYR:CZ	2.54	0.42
6:4L:27:VAL:HG22	6:4L:50:LYS:HB3	2.01	0.42
6:4M:11:ASP:OD1	6:4M:15:LYS:NZ	2.53	0.42
7:5B:409:MET:SD	7:5B:409:MET:C	3.02	0.42
7:5C:552:VAL:HG13	7:5C:553:TYR:N	2.35	0.42
7:5D:69:THR:HG23	9:7L:385:HIS:NE2	2.34	0.42
7:5D:394:ILE:HG22	7:5D:395:GLY:N	2.35	0.42
9:7G:180:GLU:OE1	9:7G:183:ARG:NH1	2.48	0.42
9:7J:172:GLU:HB2	9:7J:174:ASP:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:7R:224:ASN:OD1	9:7R:224:ASN:C	2.63	0.42
6:2W:3:THR:HG23	7:5G:429:GLU:OE2	2.20	0.42
6:3C:20:VAL:O	6:3C:20:VAL:CG2	2.66	0.42
6:3E:3:THR:HB	6:3E:4:PRO:CD	2.50	0.42
6:4M:69:LYS:NZ	6:4M:70:ASP:OD1	2.42	0.42
7:5A:93:TYR:CG	7:5A:94:PHE:N	2.88	0.42
7:5B:193:ARG:HG3	7:5B:195:TYR:CE2	2.55	0.42
7:5B:306:LEU:HD23	7:5B:307:SER:N	2.35	0.42
7:5I:449:GLU:OE1	7:5I:449:GLU:HA	2.19	0.42
7:5L:392:LYS:O	7:5M:320:ARG:NH2	2.36	0.42
8:6E:190:ARG:NH1	8:6E:191:SER:O	2.53	0.42
9:7G:182:GLU:H	9:7G:182:GLU:CD	2.28	0.42
6:2T:17:ASP:OD2	6:2T:57:TYR:OH	2.31	0.42
6:3X:34:LEU:HD23	6:3X:34:LEU:O	2.20	0.42
6:4P:34:LEU:HA	6:4P:43:LEU:HD13	2.01	0.42
7:5O:108:ARG:NH2	7:5O:157:ASP:OD1	2.50	0.42
7:5O:432:ASN:C	7:5O:432:ASN:OD1	2.63	0.42
8:6I:140:GLY:C	8:6I:141:ARG:HD2	2.44	0.42
9:7E:361:LEU:N	9:7E:361:LEU:HD12	2.35	0.42
9:7Q:361:LEU:N	9:7Q:361:LEU:HD12	2.35	0.42
10:1A:401:3PH:H31	10:1A:401:3PH:H222	2.02	0.42
4:1K:63:ASP:OD2	4:1K:63:ASP:C	2.62	0.42
6:4E:16:PHE:HB3	6:4E:57:TYR:HE1	1.84	0.42
6:4M:56:LEU:HD22	6:4S:76:ILE:HD12	2.02	0.42
7:5G:323:THR:HG22	7:5G:324:SER:N	2.34	0.42
7:5I:401:LEU:HD12	7:5I:401:LEU:O	2.20	0.42
8:6V:28:ASP:OD2	8:6V:29:GLN:N	2.50	0.42
9:7G:224:ASN:OD1	9:7G:224:ASN:C	2.63	0.42
9:7R:387:TYR:O	9:7R:387:TYR:CD1	2.73	0.42
9:7V:332:ASP:OD1	9:7V:333:ASP:N	2.49	0.42
9:7W:268:SER:N	9:7W:271:GLU:OE1	2.39	0.42
6:3M:37:LYS:HE3	6:3M:40:ASP:HB2	2.02	0.42
6:3X:62:SER:O	6:4C:78:ASN:ND2	2.53	0.42
6:4A:63:ASN:OD1	6:4G:80:ARG:NH1	2.53	0.42
6:4F:20:VAL:O	6:4F:20:VAL:CG2	2.68	0.42
7:5D:199:ASP:OD2	7:5D:411:ARG:NH1	2.50	0.42
8:6I:110:GLU:HG3	8:6I:130:ILE:HD12	2.02	0.42
8:6R:172:LYS:NZ	8:6R:178:VAL:O	2.49	0.42
9:7F:264:ARG:NH1	9:7F:296:ASP:OD2	2.51	0.42
9:7O:367:LYS:N	9:7O:367:LYS:HD2	2.35	0.42
4:1L:75:SER:HB3	6:2B:69:LYS:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:4F:37:LYS:HE3	6:4F:40:ASP:HB2	2.02	0.42
7:5G:308:LEU:O	7:5G:370:ARG:HA	2.19	0.42
7:5K:450:VAL:O	7:5K:450:VAL:HG23	2.19	0.42
9:7K:224:ASN:OD1	9:7K:224:ASN:C	2.63	0.42
1:1E:116:GLU:HA	1:1E:116:GLU:OE1	2.19	0.41
6:2Y:34:LEU:HD23	6:2Y:34:LEU:C	2.45	0.41
6:3J:59:ASN:O	6:3J:63:ASN:ND2	2.42	0.41
7:5D:118:SER:O	7:5D:121:GLU:N	2.52	0.41
7:5G:306:LEU:C	7:5G:306:LEU:HD23	2.45	0.41
7:5G:384:ASP:OD1	7:5G:385:ASN:N	2.53	0.41
7:5G:415:ARG:NH2	7:5G:423:GLU:OE1	2.52	0.41
7:5H:412:VAL:HG22	7:5H:413:LEU:N	2.34	0.41
7:5K:215:LEU:O	7:5K:216:GLN:C	2.63	0.41
7:5M:158:MET:SD	7:5M:158:MET:C	3.03	0.41
8:6C:154:TYR:CZ	8:6C:163:GLN:OE1	2.73	0.41
8:6R:138:GLU:OE2	8:6R:143:PRO:HA	2.20	0.41
9:7B:224:ASN:OD1	9:7B:224:ASN:C	2.62	0.41
9:7X:258:PHE:CE2	9:7X:260:LEU:HD21	2.55	0.41
4:1N:57:ASP:OD2	4:1N:57:ASP:C	2.63	0.41
6:3J:3:THR:HG22	6:3J:4:PRO:HD3	2.02	0.41
6:3Y:16:PHE:O	6:3Y:20:VAL:HG22	2.19	0.41
7:5B:304:VAL:HG22	7:5B:416:PHE:CZ	2.56	0.41
7:5B:328:SER:HB3	7:5B:341:GLN:NE2	2.35	0.41
7:5I:541:SER:OG	7:5K:506:ASN:ND2	2.47	0.41
7:5O:185:LEU:HD12	7:5O:190:VAL:HG12	2.02	0.41
7:5P:479:ASP:OD1	7:5P:502:LYS:HG2	2.20	0.41
8:6X:28:ASP:OD1	8:6X:29:GLN:N	2.54	0.41
9:7L:382:SER:HB2	9:7L:383:PRO:HD2	2.03	0.41
4:1K:61:VAL:O	4:1K:61:VAL:HG12	2.20	0.41
4:1P:57:ASP:OD1	4:1P:57:ASP:C	2.63	0.41
6:4M:46:ALA:O	6:4M:50:LYS:HG2	2.21	0.41
7:5C:185:LEU:HD12	7:5C:190:VAL:HG12	2.02	0.41
7:5D:409:MET:SD	7:5D:409:MET:C	3.03	0.41
7:5E:305:GLU:HB2	7:5E:518:ILE:HG13	2.02	0.41
7:5G:82:GLU:OE2	7:5G:92:TRP:NE1	2.46	0.41
6:2V:24:GLN:O	6:2V:24:GLN:NE2	2.42	0.41
6:3T:39:SER:OG	6:4E:8:TYR:HB3	2.21	0.41
7:5D:125:PHE:CD1	7:5D:166:MET:HE1	2.56	0.41
7:5H:306:LEU:HD23	7:5H:307:SER:N	2.36	0.41
7:5M:526:ALA:O	7:5M:530:VAL:HG23	2.21	0.41
7:5P:141:ASP:OD1	7:5P:141:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:6Q:138:GLU:OE2	8:6Q:143:PRO:HA	2.19	0.41
9:7G:365:TRP:O	9:7G:369:ARG:NH1	2.47	0.41
9:7I:217:ASP:OD1	9:7I:217:ASP:N	2.53	0.41
1:1A:139:GLU:O	1:1A:141:PRO:HD2	2.20	0.41
6:2G:79:PHE:O	6:2G:80:ARG:C	2.62	0.41
6:3B:3:THR:O	6:3B:4:PRO:C	2.63	0.41
6:3E:3:THR:HB	6:3E:4:PRO:HD3	2.01	0.41
6:4Q:12:VAL:O	6:4Q:15:LYS:HB2	2.20	0.41
7:5C:190:VAL:HG23	7:5C:191:GLY:N	2.34	0.41
7:5F:190:VAL:HG23	7:5F:191:GLY:N	2.35	0.41
7:5J:432:ASN:OD1	7:5J:432:ASN:C	2.63	0.41
7:5P:175:LEU:HD13	7:5P:262:ALA:HB2	2.03	0.41
9:7L:224:ASN:OD1	9:7L:224:ASN:C	2.63	0.41
1:1A:129:GLU:OE2	1:1A:129:GLU:N	2.46	0.41
4:1L:57:ASP:C	4:1L:57:ASP:OD2	2.62	0.41
6:3B:8:TYR:O	6:3B:12:VAL:HG23	2.20	0.41
6:3Y:34:LEU:HA	6:3Y:43:LEU:HD13	2.02	0.41
7:5B:158:MET:SD	7:5B:158:MET:C	3.03	0.41
7:5C:313:LEU:HD23	7:5C:366:THR:HG23	2.02	0.41
7:5H:323:THR:HG22	7:5H:324:SER:N	2.35	0.41
7:5K:116:ASN:O	7:5K:255:GLN:NE2	2.51	0.41
8:6L:102:LYS:HD2	8:6L:134:ILE:HG13	2.02	0.41
9:7E:246:TYR:OH	9:7E:296:ASP:OD1	2.38	0.41
9:7V:174:ASP:OD1	9:7V:175:SER:N	2.54	0.41
6:3J:3:THR:N	6:3J:4:PRO:HD2	2.36	0.41
6:3Y:66:LYS:NZ	6:3Y:70:ASP:OD2	2.40	0.41
6:4O:18:THR:O	6:4O:21:ASP:OD2	2.39	0.41
6:4P:79:PHE:N	6:4P:79:PHE:CD2	2.88	0.41
7:5O:409:MET:C	7:5O:409:MET:SD	3.04	0.41
8:6A:102:LYS:HB3	8:6A:134:ILE:CD1	2.50	0.41
8:6N:110:GLU:HG3	8:6N:130:ILE:HD12	2.03	0.41
9:7P:224:ASN:OD1	9:7P:224:ASN:C	2.64	0.41
6:2C:49:SER:OG	6:2I:10:ASP:OD1	2.36	0.41
6:2D:66:LYS:NZ	6:2I:80:ARG:OXT	2.45	0.41
6:3C:34:LEU:HD11	6:3C:44:LEU:HD23	2.03	0.41
7:5G:305:GLU:HB2	7:5G:518:ILE:HG13	2.03	0.41
7:5G:542:GLY:O	7:5G:548:LYS:HE2	2.20	0.41
7:5I:376:GLN:HE21	7:5J:458:ILE:HG22	1.85	0.41
7:5J:319:GLU:CD	7:5J:319:GLU:C	2.89	0.41
7:5N:27:LYS:HG2	9:7S:365:TRP:CE3	2.55	0.41
7:5N:334:LYS:HG3	7:5N:335:LEU:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5N:374:LEU:HD23	7:5N:374:LEU:C	2.46	0.41
7:5O:158:MET:SD	7:5O:158:MET:C	3.04	0.41
8:6J:102:LYS:HD2	8:6J:134:ILE:CG1	2.50	0.41
9:7I:258:PHE:CE2	9:7I:260:LEU:HD21	2.55	0.41
9:7O:367:LYS:N	9:7O:367:LYS:CD	2.83	0.41
4:1P:19:ILE:CG2	4:1P:20:ARG:N	2.84	0.41
6:2P:66:LYS:NZ	6:2P:70:ASP:OD2	2.46	0.41
6:2Z:20:VAL:O	6:2Z:20:VAL:CG2	2.68	0.41
6:3A:40:ASP:OD1	6:3A:40:ASP:C	2.64	0.41
6:3L:34:LEU:HD11	6:3L:44:LEU:HD23	2.03	0.41
6:3Y:20:VAL:O	6:3Y:20:VAL:CG2	2.68	0.41
6:3Z:55:ASN:O	6:3Z:59:ASN:ND2	2.51	0.41
7:5A:94:PHE:CE2	7:5A:96:GLY:HA2	2.56	0.41
7:5C:118:SER:HB2	7:5C:121:GLU:HG2	2.02	0.41
7:5C:286:GLN:O	7:5C:290:ILE:HG12	2.21	0.41
7:5D:69:THR:OG1	9:7L:387:TYR:HD1	2.04	0.41
7:5D:360:GLU:OE2	7:5D:362:LYS:NZ	2.51	0.41
7:5E:108:ARG:HG2	7:5E:108:ARG:HH11	1.85	0.41
7:5G:313:LEU:HD23	7:5G:366:THR:HG23	2.02	0.41
7:5K:283:THR:O	7:5K:287:VAL:HG23	2.21	0.41
7:5M:94:PHE:CZ	7:5M:96:GLY:HA2	2.56	0.41
7:5N:170:ASN:HA	7:5N:173:ILE:HG12	2.03	0.41
7:5P:219:GLU:N	7:5P:219:GLU:CD	2.79	0.41
8:6F:99:ARG:HG3	8:6F:134:ILE:CG2	2.51	0.41
8:6M:177:ASP:OD1	8:6N:144:LYS:NZ	2.46	0.41
8:6T:102:LYS:HD2	8:6T:134:ILE:HG12	2.03	0.41
8:6U:102:LYS:HD2	8:6U:134:ILE:HG12	2.02	0.41
9:7C:224:ASN:OD1	9:7C:224:ASN:C	2.62	0.41
9:7D:172:GLU:HB2	9:7D:174:ASP:OD1	2.21	0.41
9:7D:224:ASN:OD1	9:7D:224:ASN:C	2.64	0.41
9:7P:191:ASP:OD2	9:7P:193:MET:HE2	2.21	0.41
9:7P:365:TRP:O	9:7P:369:ARG:NH1	2.51	0.41
4:1L:31:ASP:O	4:1L:35:GLN:HG2	2.21	0.41
10:1N:601:3PH:H361	10:1N:601:3PH:H391	1.68	0.41
6:2Q:17:ASP:OD1	6:2Q:57:TYR:OH	2.37	0.41
6:2S:24:GLN:H	6:2S:24:GLN:CD	2.28	0.41
6:3B:34:LEU:HD11	6:3B:44:LEU:HD23	2.02	0.41
6:4D:20:VAL:O	6:4D:20:VAL:CG2	2.68	0.41
6:4K:16:PHE:O	6:4K:20:VAL:HG22	2.21	0.41
6:4R:37:LYS:HE3	6:4R:40:ASP:HB2	2.01	0.41
7:5C:307:SER:OG	7:5C:370:ARG:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5J:304:VAL:HG22	7:5J:416:PHE:CZ	2.56	0.41
7:5N:479:ASP:OD1	7:5N:502:LYS:NZ	2.49	0.41
8:6F:51:SER:HB2	8:6F:54:LEU:HB2	2.03	0.41
1:1D:84:ASP:OD1	1:1D:84:ASP:C	2.64	0.40
6:2J:24:GLN:CD	6:2J:24:GLN:H	2.27	0.40
6:2X:79:PHE:O	6:2X:80:ARG:C	2.64	0.40
6:4D:48:GLN:HB2	6:4O:79:PHE:CE2	2.56	0.40
7:5C:392:LYS:O	7:5D:320:ARG:NH2	2.40	0.40
7:5D:225:ILE:HD12	7:5D:289:PHE:HB3	2.03	0.40
7:5I:314:ASN:OD1	7:5I:314:ASN:C	2.64	0.40
7:5J:281:LYS:NZ	7:5K:218:GLU:OE1	2.46	0.40
7:5M:178:GLN:CG	7:5N:220:GLN:HB2	2.51	0.40
7:5M:256:GLU:CD	7:5M:257:ALA:N	2.79	0.40
7:5O:73:GLU:OE1	7:5O:75:HIS:NE2	2.44	0.40
7:5P:185:LEU:HD12	7:5P:190:VAL:HG12	2.03	0.40
8:6E:44:ILE:HG23	8:6E:64:ASP:HB3	2.04	0.40
8:6N:194:GLN:OE1	9:7M:202:ARG:NH2	2.37	0.40
8:6X:134:ILE:HG22	8:6X:134:ILE:O	2.21	0.40
9:7U:201:GLU:CD	9:7U:201:GLU:N	2.79	0.40
1:1C:101:ASP:O	1:1C:104:ILE:HG22	2.21	0.40
6:2I:40:ASP:OD1	6:2I:40:ASP:C	2.64	0.40
6:2L:22:ASN:O	6:2L:23:LEU:C	2.64	0.40
6:2X:40:ASP:OD1	6:2X:40:ASP:C	2.64	0.40
6:3J:3:THR:CG2	6:3J:4:PRO:HD3	2.50	0.40
6:3S:68:PHE:HA	6:3S:71:ILE:HD12	2.04	0.40
7:5G:344:ILE:H	7:5G:344:ILE:HD12	1.85	0.40
7:5I:345:SER:C	7:5I:346:THR:HG23	2.46	0.40
7:5J:273:PRO:O	7:5K:378:ASN:ND2	2.48	0.40
7:5J:323:THR:HG22	7:5J:324:SER:N	2.37	0.40
7:5J:327:GLY:HA3	7:5J:352:PHE:CD1	2.57	0.40
7:5J:525:ASP:HB2	7:5J:528:GLU:HG3	2.02	0.40
8:6B:102:LYS:HD2	8:6B:134:ILE:HG13	2.03	0.40
8:6J:28:ASP:OD1	8:6J:29:GLN:N	2.52	0.40
8:6O:131:SER:OG	8:6O:147:HIS:HB2	2.22	0.40
8:6W:44:ILE:HG23	8:6W:64:ASP:HB3	2.03	0.40
9:7P:328:GLN:C	9:7P:328:GLN:CD	2.89	0.40
9:7V:348:ARG:HH22	9:7W:234:ILE:HG23	1.86	0.40
1:1B:25:THR:HG22	1:1B:26:CYS:N	2.36	0.40
2:1F:90:TRP:CD1	2:1F:90:TRP:C	2.99	0.40
6:2O:3:THR:N	6:2O:4:PRO:CD	2.85	0.40
6:3G:20:VAL:O	6:3G:20:VAL:CG2	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3H:3:THR:HB	6:3H:4:PRO:CD	2.52	0.40
8:6C:20:ASP:OD1	8:6C:20:ASP:N	2.53	0.40
8:6I:51:SER:HB2	8:6I:54:LEU:HB2	2.04	0.40
8:6U:154:TYR:CE2	8:6U:163:GLN:OE1	2.74	0.40
9:7F:390:SER:OG	9:7F:391:PRO:HD2	2.21	0.40
9:7L:174:ASP:OD1	9:7L:175:SER:N	2.54	0.40
9:7M:387:TYR:CD2	9:7M:387:TYR:C	2.99	0.40
6:2N:34:LEU:HD13	6:2N:34:LEU:C	2.46	0.40
6:2Q:34:LEU:C	6:2Q:34:LEU:HD13	2.46	0.40
6:3W:16:PHE:O	6:3W:20:VAL:HG22	2.22	0.40
6:4I:79:PHE:CD2	6:4I:79:PHE:C	2.99	0.40
7:5B:27:LYS:O	7:5B:28:ILE:HG22	2.21	0.40
7:5D:225:ILE:CD1	7:5D:289:PHE:HB3	2.51	0.40
7:5D:390:TYR:CD2	7:5D:403:HIS:HB3	2.56	0.40
7:5K:118:SER:HB2	7:5K:121:GLU:OE2	2.22	0.40
7:5K:192:ASP:HB3	7:5K:206:GLY:H	1.87	0.40
7:5L:384:ASP:OD1	7:5L:384:ASP:C	2.63	0.40
8:6U:134:ILE:O	8:6U:134:ILE:HG22	2.21	0.40
8:6X:190:ARG:NH1	8:6X:191:SER:O	2.55	0.40
9:7Q:268:SER:N	9:7Q:271:GLU:OE1	2.43	0.40
9:7T:270:LYS:O	9:7T:274:VAL:HG23	2.21	0.40
6:2J:37:LYS:O	6:2J:39:SER:N	2.55	0.40
6:2N:24:GLN:O	6:2N:24:GLN:NE2	2.53	0.40
6:3A:27:VAL:HG22	6:3A:50:LYS:HB3	2.04	0.40
6:3N:48:GLN:NE2	6:3Y:78:ASN:O	2.52	0.40
6:3O:6:SER:HA	6:3O:10:ASP:OD2	2.22	0.40
6:4L:63:ASN:HB3	6:4R:79:PHE:CE1	2.56	0.40
7:5D:437:GLN:O	7:5D:439:ASP:N	2.51	0.40
7:5F:328:SER:OG	7:5F:341:GLN:OE1	2.30	0.40
7:5F:360:GLU:CD	7:5F:360:GLU:C	2.89	0.40
7:5G:304:VAL:HG22	7:5G:416:PHE:CZ	2.56	0.40
7:5I:164:THR:HG22	7:5I:168:LYS:HE3	2.03	0.40
7:5J:441:THR:O	7:5J:445:ASP:CG	2.64	0.40
7:5K:97:GLN:N	7:5K:97:GLN:CD	2.80	0.40
7:5M:283:THR:O	7:5M:287:VAL:HG23	2.22	0.40
7:5M:313:LEU:CD2	7:5M:366:THR:HG23	2.52	0.40
9:7A:264:ARG:NH1	9:7A:296:ASP:OD2	2.53	0.40
9:7E:382:SER:HB2	9:7E:383:PRO:HD2	2.03	0.40
9:7O:224:ASN:OD1	9:7O:224:ASN:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	221/224 (99%)	217 (98%)	4 (2%)	0	100	100
1	1B	221/224 (99%)	218 (99%)	3 (1%)	0	100	100
1	1C	221/224 (99%)	214 (97%)	7 (3%)	0	100	100
1	1D	218/224 (97%)	213 (98%)	5 (2%)	0	100	100
1	1E	219/224 (98%)	215 (98%)	4 (2%)	0	100	100
2	1F	255/263 (97%)	251 (98%)	4 (2%)	0	100	100
3	1G	82/86 (95%)	81 (99%)	1 (1%)	0	100	100
3	1H	82/86 (95%)	82 (100%)	0	0	100	100
3	1I	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
3	1J	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
4	1K	88/101 (87%)	86 (98%)	2 (2%)	0	100	100
4	1L	92/101 (91%)	91 (99%)	1 (1%)	0	100	100
4	1M	88/101 (87%)	88 (100%)	0	0	100	100
4	1N	87/101 (86%)	85 (98%)	2 (2%)	0	100	100
4	1O	88/101 (87%)	88 (100%)	0	0	100	100
4	1P	88/101 (87%)	87 (99%)	1 (1%)	0	100	100
6	2A	64/80 (80%)	63 (98%)	1 (2%)	0	100	100
6	2B	58/80 (72%)	57 (98%)	1 (2%)	0	100	100
6	2C	57/80 (71%)	56 (98%)	1 (2%)	0	100	100
6	2D	77/80 (96%)	76 (99%)	1 (1%)	0	100	100
6	2E	64/80 (80%)	64 (100%)	0	0	100	100
6	2F	73/80 (91%)	72 (99%)	1 (1%)	0	100	100
6	2G	74/80 (92%)	74 (100%)	0	0	100	100
6	2H	73/80 (91%)	72 (99%)	1 (1%)	0	100	100
6	2I	73/80 (91%)	71 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	2J	73/80 (91%)	72 (99%)	1 (1%)	0	100	100
6	2K	75/80 (94%)	73 (97%)	2 (3%)	0	100	100
6	2L	76/80 (95%)	72 (95%)	4 (5%)	0	100	100
6	2M	76/80 (95%)	75 (99%)	1 (1%)	0	100	100
6	2N	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
6	2O	76/80 (95%)	75 (99%)	1 (1%)	0	100	100
6	2P	75/80 (94%)	75 (100%)	0	0	100	100
6	2Q	76/80 (95%)	73 (96%)	3 (4%)	0	100	100
6	2R	77/80 (96%)	73 (95%)	4 (5%)	0	100	100
6	2S	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
6	2T	77/80 (96%)	76 (99%)	1 (1%)	0	100	100
6	2U	76/80 (95%)	75 (99%)	1 (1%)	0	100	100
6	2V	77/80 (96%)	77 (100%)	0	0	100	100
6	2W	77/80 (96%)	76 (99%)	1 (1%)	0	100	100
6	2X	76/80 (95%)	75 (99%)	1 (1%)	0	100	100
6	2Y	76/80 (95%)	75 (99%)	1 (1%)	0	100	100
6	2Z	76/80 (95%)	75 (99%)	1 (1%)	0	100	100
6	3A	77/80 (96%)	76 (99%)	1 (1%)	0	100	100
6	3B	77/80 (96%)	74 (96%)	3 (4%)	0	100	100
6	3C	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
6	3D	76/80 (95%)	76 (100%)	0	0	100	100
6	3E	76/80 (95%)	75 (99%)	1 (1%)	0	100	100
6	3F	76/80 (95%)	75 (99%)	1 (1%)	0	100	100
6	3G	77/80 (96%)	77 (100%)	0	0	100	100
6	3H	76/80 (95%)	72 (95%)	4 (5%)	0	100	100
6	3I	76/80 (95%)	75 (99%)	1 (1%)	0	100	100
6	3J	76/80 (95%)	75 (99%)	1 (1%)	0	100	100
6	3K	76/80 (95%)	76 (100%)	0	0	100	100
6	3L	75/80 (94%)	74 (99%)	1 (1%)	0	100	100
6	3M	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
6	3N	76/80 (95%)	74 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	3O	75/80 (94%)	72 (96%)	3 (4%)	0	100	100
6	3P	75/80 (94%)	74 (99%)	1 (1%)	0	100	100
6	3Q	75/80 (94%)	74 (99%)	1 (1%)	0	100	100
6	3R	75/80 (94%)	72 (96%)	3 (4%)	0	100	100
6	3S	75/80 (94%)	73 (97%)	2 (3%)	0	100	100
6	3T	75/80 (94%)	72 (96%)	3 (4%)	0	100	100
6	3U	75/80 (94%)	74 (99%)	1 (1%)	0	100	100
6	3V	75/80 (94%)	74 (99%)	1 (1%)	0	100	100
6	3W	75/80 (94%)	73 (97%)	2 (3%)	0	100	100
6	3X	75/80 (94%)	73 (97%)	2 (3%)	0	100	100
6	3Y	75/80 (94%)	73 (97%)	2 (3%)	0	100	100
6	3Z	75/80 (94%)	74 (99%)	1 (1%)	0	100	100
6	4A	75/80 (94%)	73 (97%)	2 (3%)	0	100	100
6	4B	75/80 (94%)	71 (95%)	4 (5%)	0	100	100
6	4C	75/80 (94%)	73 (97%)	2 (3%)	0	100	100
6	4D	75/80 (94%)	73 (97%)	2 (3%)	0	100	100
6	4E	75/80 (94%)	72 (96%)	3 (4%)	0	100	100
6	4F	75/80 (94%)	73 (97%)	2 (3%)	0	100	100
6	4G	75/80 (94%)	73 (97%)	2 (3%)	0	100	100
6	4H	75/80 (94%)	73 (97%)	2 (3%)	0	100	100
6	4I	75/80 (94%)	74 (99%)	1 (1%)	0	100	100
6	4J	75/80 (94%)	74 (99%)	1 (1%)	0	100	100
6	4K	75/80 (94%)	74 (99%)	1 (1%)	0	100	100
6	4L	75/80 (94%)	75 (100%)	0	0	100	100
6	4M	75/80 (94%)	72 (96%)	3 (4%)	0	100	100
6	4N	75/80 (94%)	72 (96%)	3 (4%)	0	100	100
6	4O	75/80 (94%)	74 (99%)	1 (1%)	0	100	100
6	4P	75/80 (94%)	74 (99%)	1 (1%)	0	100	100
6	4Q	75/80 (94%)	75 (100%)	0	0	100	100
6	4R	75/80 (94%)	74 (99%)	1 (1%)	0	100	100
6	4S	75/80 (94%)	75 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	4T	75/80 (94%)	73 (97%)	2 (3%)	0	100	100
7	5A	139/562 (25%)	133 (96%)	6 (4%)	0	100	100
7	5B	498/562 (89%)	489 (98%)	9 (2%)	0	100	100
7	5C	497/562 (88%)	487 (98%)	10 (2%)	0	100	100
7	5D	502/562 (89%)	492 (98%)	10 (2%)	0	100	100
7	5E	499/562 (89%)	490 (98%)	9 (2%)	0	100	100
7	5F	502/562 (89%)	494 (98%)	8 (2%)	0	100	100
7	5G	500/562 (89%)	489 (98%)	11 (2%)	0	100	100
7	5H	502/562 (89%)	486 (97%)	16 (3%)	0	100	100
7	5I	499/562 (89%)	489 (98%)	10 (2%)	0	100	100
7	5J	504/562 (90%)	491 (97%)	13 (3%)	0	100	100
7	5K	498/562 (89%)	492 (99%)	6 (1%)	0	100	100
7	5L	502/562 (89%)	490 (98%)	12 (2%)	0	100	100
7	5M	496/562 (88%)	489 (99%)	7 (1%)	0	100	100
7	5N	497/562 (88%)	486 (98%)	11 (2%)	0	100	100
7	5O	494/562 (88%)	485 (98%)	9 (2%)	0	100	100
7	5P	496/562 (88%)	485 (98%)	11 (2%)	0	100	100
8	6A	181/252 (72%)	177 (98%)	4 (2%)	0	100	100
8	6B	181/252 (72%)	179 (99%)	2 (1%)	0	100	100
8	6C	181/252 (72%)	180 (99%)	1 (1%)	0	100	100
8	6D	181/252 (72%)	180 (99%)	1 (1%)	0	100	100
8	6E	181/252 (72%)	179 (99%)	2 (1%)	0	100	100
8	6F	181/252 (72%)	180 (99%)	1 (1%)	0	100	100
8	6G	181/252 (72%)	179 (99%)	2 (1%)	0	100	100
8	6H	181/252 (72%)	178 (98%)	3 (2%)	0	100	100
8	6I	181/252 (72%)	178 (98%)	3 (2%)	0	100	100
8	6J	181/252 (72%)	179 (99%)	2 (1%)	0	100	100
8	6K	181/252 (72%)	179 (99%)	2 (1%)	0	100	100
8	6L	181/252 (72%)	179 (99%)	2 (1%)	0	100	100
8	6M	181/252 (72%)	177 (98%)	4 (2%)	0	100	100
8	6N	181/252 (72%)	179 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	6O	181/252 (72%)	177 (98%)	4 (2%)	0	100	100
8	6P	181/252 (72%)	179 (99%)	2 (1%)	0	100	100
8	6Q	181/252 (72%)	177 (98%)	4 (2%)	0	100	100
8	6R	181/252 (72%)	179 (99%)	2 (1%)	0	100	100
8	6S	181/252 (72%)	180 (99%)	1 (1%)	0	100	100
8	6T	181/252 (72%)	178 (98%)	3 (2%)	0	100	100
8	6U	181/252 (72%)	179 (99%)	2 (1%)	0	100	100
8	6V	181/252 (72%)	180 (99%)	1 (1%)	0	100	100
8	6W	181/252 (72%)	177 (98%)	4 (2%)	0	100	100
8	6X	181/252 (72%)	180 (99%)	1 (1%)	0	100	100
9	7A	218/392 (56%)	217 (100%)	1 (0%)	0	100	100
9	7B	220/392 (56%)	217 (99%)	3 (1%)	0	100	100
9	7C	220/392 (56%)	216 (98%)	4 (2%)	0	100	100
9	7D	218/392 (56%)	212 (97%)	6 (3%)	0	100	100
9	7E	220/392 (56%)	217 (99%)	3 (1%)	0	100	100
9	7F	220/392 (56%)	217 (99%)	3 (1%)	0	100	100
9	7G	218/392 (56%)	216 (99%)	2 (1%)	0	100	100
9	7H	220/392 (56%)	216 (98%)	4 (2%)	0	100	100
9	7I	220/392 (56%)	215 (98%)	5 (2%)	0	100	100
9	7J	218/392 (56%)	216 (99%)	2 (1%)	0	100	100
9	7K	220/392 (56%)	219 (100%)	1 (0%)	0	100	100
9	7L	220/392 (56%)	216 (98%)	4 (2%)	0	100	100
9	7M	218/392 (56%)	214 (98%)	4 (2%)	0	100	100
9	7N	220/392 (56%)	217 (99%)	3 (1%)	0	100	100
9	7O	220/392 (56%)	216 (98%)	4 (2%)	0	100	100
9	7P	218/392 (56%)	216 (99%)	2 (1%)	0	100	100
9	7Q	220/392 (56%)	217 (99%)	3 (1%)	0	100	100
9	7R	220/392 (56%)	216 (98%)	4 (2%)	0	100	100
9	7S	218/392 (56%)	214 (98%)	4 (2%)	0	100	100
9	7T	220/392 (56%)	215 (98%)	5 (2%)	0	100	100
9	7U	220/392 (56%)	210 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	7V	218/392 (56%)	212 (97%)	6 (3%)	0	100	100
9	7W	220/392 (56%)	215 (98%)	5 (2%)	0	100	100
9	7X	220/392 (56%)	218 (99%)	2 (1%)	0	100	100
All	All	24821/32541 (76%)	24373 (98%)	448 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	1A	198/199 (100%)	198 (100%)	0	100	100
1	1B	198/199 (100%)	198 (100%)	0	100	100
1	1C	198/199 (100%)	198 (100%)	0	100	100
1	1D	196/199 (98%)	196 (100%)	0	100	100
1	1E	197/199 (99%)	197 (100%)	0	100	100
2	1F	214/219 (98%)	213 (100%)	1 (0%)	81	83
3	1G	70/71 (99%)	70 (100%)	0	100	100
3	1H	70/71 (99%)	70 (100%)	0	100	100
3	1I	71/71 (100%)	71 (100%)	0	100	100
3	1J	71/71 (100%)	71 (100%)	0	100	100
4	1K	79/88 (90%)	79 (100%)	0	100	100
4	1L	82/88 (93%)	82 (100%)	0	100	100
4	1M	79/88 (90%)	79 (100%)	0	100	100
4	1N	78/88 (89%)	78 (100%)	0	100	100
4	1O	79/88 (90%)	79 (100%)	0	100	100
4	1P	79/88 (90%)	79 (100%)	0	100	100
6	2A	58/67 (87%)	58 (100%)	0	100	100
6	2B	51/67 (76%)	51 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	2C	50/67 (75%)	50 (100%)	0	100	100
6	2D	66/67 (98%)	66 (100%)	0	100	100
6	2E	58/67 (87%)	58 (100%)	0	100	100
6	2F	63/67 (94%)	63 (100%)	0	100	100
6	2G	64/67 (96%)	64 (100%)	0	100	100
6	2H	63/67 (94%)	63 (100%)	0	100	100
6	2I	63/67 (94%)	63 (100%)	0	100	100
6	2J	63/67 (94%)	63 (100%)	0	100	100
6	2K	65/67 (97%)	65 (100%)	0	100	100
6	2L	66/67 (98%)	66 (100%)	0	100	100
6	2M	66/67 (98%)	66 (100%)	0	100	100
6	2N	66/67 (98%)	66 (100%)	0	100	100
6	2O	66/67 (98%)	66 (100%)	0	100	100
6	2P	65/67 (97%)	65 (100%)	0	100	100
6	2Q	66/67 (98%)	66 (100%)	0	100	100
6	2R	66/67 (98%)	66 (100%)	0	100	100
6	2S	66/67 (98%)	66 (100%)	0	100	100
6	2T	66/67 (98%)	66 (100%)	0	100	100
6	2U	66/67 (98%)	66 (100%)	0	100	100
6	2V	66/67 (98%)	66 (100%)	0	100	100
6	2W	66/67 (98%)	66 (100%)	0	100	100
6	2X	66/67 (98%)	66 (100%)	0	100	100
6	2Y	66/67 (98%)	66 (100%)	0	100	100
6	2Z	66/67 (98%)	66 (100%)	0	100	100
6	3A	66/67 (98%)	66 (100%)	0	100	100
6	3B	66/67 (98%)	66 (100%)	0	100	100
6	3C	66/67 (98%)	66 (100%)	0	100	100
6	3D	66/67 (98%)	66 (100%)	0	100	100
6	3E	66/67 (98%)	66 (100%)	0	100	100
6	3F	66/67 (98%)	66 (100%)	0	100	100
6	3G	66/67 (98%)	66 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	3H	66/67 (98%)	66 (100%)	0	100	100
6	3I	66/67 (98%)	66 (100%)	0	100	100
6	3J	66/67 (98%)	66 (100%)	0	100	100
6	3K	66/67 (98%)	66 (100%)	0	100	100
6	3L	65/67 (97%)	65 (100%)	0	100	100
6	3M	66/67 (98%)	66 (100%)	0	100	100
6	3N	66/67 (98%)	66 (100%)	0	100	100
6	3O	65/67 (97%)	65 (100%)	0	100	100
6	3P	65/67 (97%)	65 (100%)	0	100	100
6	3Q	65/67 (97%)	65 (100%)	0	100	100
6	3R	65/67 (97%)	65 (100%)	0	100	100
6	3S	65/67 (97%)	65 (100%)	0	100	100
6	3T	65/67 (97%)	65 (100%)	0	100	100
6	3U	65/67 (97%)	65 (100%)	0	100	100
6	3V	65/67 (97%)	65 (100%)	0	100	100
6	3W	65/67 (97%)	65 (100%)	0	100	100
6	3X	65/67 (97%)	65 (100%)	0	100	100
6	3Y	65/67 (97%)	65 (100%)	0	100	100
6	3Z	65/67 (97%)	65 (100%)	0	100	100
6	4A	65/67 (97%)	65 (100%)	0	100	100
6	4B	65/67 (97%)	65 (100%)	0	100	100
6	4C	65/67 (97%)	65 (100%)	0	100	100
6	4D	65/67 (97%)	65 (100%)	0	100	100
6	4E	65/67 (97%)	65 (100%)	0	100	100
6	4F	65/67 (97%)	65 (100%)	0	100	100
6	4G	65/67 (97%)	65 (100%)	0	100	100
6	4H	65/67 (97%)	65 (100%)	0	100	100
6	4I	65/67 (97%)	65 (100%)	0	100	100
6	4J	65/67 (97%)	65 (100%)	0	100	100
6	4K	65/67 (97%)	65 (100%)	0	100	100
6	4L	65/67 (97%)	65 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	4M	65/67 (97%)	65 (100%)	0	100	100
6	4N	65/67 (97%)	65 (100%)	0	100	100
6	4O	65/67 (97%)	65 (100%)	0	100	100
6	4P	65/67 (97%)	65 (100%)	0	100	100
6	4Q	65/67 (97%)	65 (100%)	0	100	100
6	4R	65/67 (97%)	65 (100%)	0	100	100
6	4S	65/67 (97%)	65 (100%)	0	100	100
6	4T	65/67 (97%)	65 (100%)	0	100	100
7	5A	121/477 (25%)	121 (100%)	0	100	100
7	5B	434/477 (91%)	434 (100%)	0	100	100
7	5C	432/477 (91%)	432 (100%)	0	100	100
7	5D	437/477 (92%)	437 (100%)	0	100	100
7	5E	434/477 (91%)	434 (100%)	0	100	100
7	5F	437/477 (92%)	437 (100%)	0	100	100
7	5G	435/477 (91%)	435 (100%)	0	100	100
7	5H	437/477 (92%)	437 (100%)	0	100	100
7	5I	434/477 (91%)	434 (100%)	0	100	100
7	5J	439/477 (92%)	439 (100%)	0	100	100
7	5K	433/477 (91%)	433 (100%)	0	100	100
7	5L	437/477 (92%)	437 (100%)	0	100	100
7	5M	431/477 (90%)	431 (100%)	0	100	100
7	5N	433/477 (91%)	433 (100%)	0	100	100
7	5O	430/477 (90%)	430 (100%)	0	100	100
7	5P	432/477 (91%)	432 (100%)	0	100	100
8	6A	156/215 (73%)	156 (100%)	0	100	100
8	6B	156/215 (73%)	156 (100%)	0	100	100
8	6C	156/215 (73%)	156 (100%)	0	100	100
8	6D	156/215 (73%)	156 (100%)	0	100	100
8	6E	156/215 (73%)	156 (100%)	0	100	100
8	6F	156/215 (73%)	156 (100%)	0	100	100
8	6G	156/215 (73%)	156 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	6H	156/215 (73%)	156 (100%)	0	100	100
8	6I	156/215 (73%)	156 (100%)	0	100	100
8	6J	156/215 (73%)	156 (100%)	0	100	100
8	6K	156/215 (73%)	156 (100%)	0	100	100
8	6L	156/215 (73%)	156 (100%)	0	100	100
8	6M	156/215 (73%)	156 (100%)	0	100	100
8	6N	156/215 (73%)	156 (100%)	0	100	100
8	6O	156/215 (73%)	156 (100%)	0	100	100
8	6P	156/215 (73%)	156 (100%)	0	100	100
8	6Q	156/215 (73%)	156 (100%)	0	100	100
8	6R	156/215 (73%)	156 (100%)	0	100	100
8	6S	156/215 (73%)	156 (100%)	0	100	100
8	6T	156/215 (73%)	156 (100%)	0	100	100
8	6U	156/215 (73%)	156 (100%)	0	100	100
8	6V	156/215 (73%)	156 (100%)	0	100	100
8	6W	156/215 (73%)	156 (100%)	0	100	100
8	6X	156/215 (73%)	156 (100%)	0	100	100
9	7A	188/337 (56%)	188 (100%)	0	100	100
9	7B	190/337 (56%)	190 (100%)	0	100	100
9	7C	190/337 (56%)	190 (100%)	0	100	100
9	7D	188/337 (56%)	188 (100%)	0	100	100
9	7E	190/337 (56%)	190 (100%)	0	100	100
9	7F	190/337 (56%)	190 (100%)	0	100	100
9	7G	188/337 (56%)	188 (100%)	0	100	100
9	7H	190/337 (56%)	190 (100%)	0	100	100
9	7I	190/337 (56%)	190 (100%)	0	100	100
9	7J	188/337 (56%)	188 (100%)	0	100	100
9	7K	190/337 (56%)	190 (100%)	0	100	100
9	7L	190/337 (56%)	190 (100%)	0	100	100
9	7M	188/337 (56%)	188 (100%)	0	100	100
9	7N	190/337 (56%)	190 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	7O	190/337 (56%)	190 (100%)	0	100	100
9	7P	188/337 (56%)	188 (100%)	0	100	100
9	7Q	190/337 (56%)	190 (100%)	0	100	100
9	7R	190/337 (56%)	190 (100%)	0	100	100
9	7S	188/337 (56%)	188 (100%)	0	100	100
9	7T	190/337 (56%)	190 (100%)	0	100	100
9	7U	190/337 (56%)	190 (100%)	0	100	100
9	7V	188/337 (56%)	188 (100%)	0	100	100
9	7W	190/337 (56%)	190 (100%)	0	100	100
9	7X	190/337 (56%)	190 (100%)	0	100	100
All	All	21539/27730 (78%)	21538 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
2	1F	238	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (162) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	113	GLN
1	1A	117	ASN
1	1D	44	GLN
1	1E	119	GLN
2	1F	130	ASN
2	1F	175	ASN
2	1F	208	GLN
3	1I	43	GLN
3	1I	77	GLN
4	1L	10	ASN
4	1L	35	GLN
4	1L	49	GLN
6	2A	59	ASN
6	2B	61	GLN
6	2D	61	GLN
6	2E	59	ASN
6	2E	61	GLN

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Mol	Chain	Res	Type
6	2F	59	ASN
6	2G	59	ASN
6	2H	24	GLN
6	2I	59	ASN
6	2J	48	GLN
6	2J	59	ASN
6	2K	77	GLN
6	2L	24	GLN
6	2L	77	GLN
6	2M	24	GLN
6	2M	59	ASN
6	2R	24	GLN
6	2T	24	GLN
6	2X	59	ASN
6	2Y	24	GLN
6	2Z	59	ASN
6	3B	24	GLN
6	3D	48	GLN
6	3F	59	ASN
6	3G	77	GLN
6	3G	78	ASN
6	3H	24	GLN
6	3H	78	ASN
6	3K	61	GLN
6	3K	78	ASN
6	3M	24	GLN
6	3N	24	GLN
6	3P	59	ASN
6	3T	59	ASN
6	3T	61	GLN
6	3W	61	GLN
6	3X	26	GLN
6	3X	59	ASN
6	3Y	59	ASN
6	3Y	61	GLN
6	3Y	78	ASN
6	3Z	59	ASN
6	3Z	61	GLN
6	4A	59	ASN
6	4B	61	GLN
6	4D	59	ASN
6	4D	61	GLN

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Mol	Chain	Res	Type
6	4E	59	ASN
6	4F	24	GLN
6	4I	24	GLN
6	4I	61	GLN
6	4I	78	ASN
6	4J	61	GLN
6	4K	61	GLN
6	4L	59	ASN
6	4M	26	GLN
6	4M	59	ASN
6	4O	63	ASN
6	4P	63	ASN
6	4T	24	GLN
7	5B	187	ASN
7	5B	288	HIS
7	5B	357	ASN
7	5C	288	HIS
7	5C	385	ASN
7	5D	266	ASN
7	5D	403	HIS
7	5E	116	ASN
7	5E	170	ASN
7	5E	288	HIS
7	5F	87	GLN
7	5G	161	ASN
7	5G	341	GLN
7	5H	178	GLN
7	5H	341	GLN
7	5H	357	ASN
7	5H	463	HIS
7	5H	506	ASN
7	5I	532	ASN
7	5J	87	GLN
7	5J	341	GLN
7	5J	357	ASN
7	5K	87	GLN
7	5K	200	GLN
7	5K	357	ASN
7	5L	87	GLN
7	5M	116	ASN
7	5M	142	ASN
7	5M	196	ASN

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Mol	Chain	Res	Type
7	5M	260	GLN
7	5M	261	ASN
7	5N	386	ASN
7	5N	482	GLN
7	5O	109	ASN
7	5O	341	GLN
7	5O	403	HIS
7	5O	503	ASN
7	5O	506	ASN
8	6K	47	ASN
8	6K	76	GLN
8	6O	47	ASN
8	6P	162	HIS
8	6Q	163	GLN
8	6S	76	GLN
8	6U	47	ASN
8	6U	76	GLN
8	6U	162	HIS
8	6U	173	ASN
9	7A	179	GLN
9	7A	249	HIS
9	7A	319	HIS
9	7B	249	HIS
9	7B	310	GLN
9	7B	319	HIS
9	7C	356	GLN
9	7D	219	ASN
9	7D	226	ASN
9	7D	249	HIS
9	7D	319	HIS
9	7E	319	HIS
9	7E	341	GLN
9	7E	372	GLN
9	7G	385	HIS
9	7H	341	GLN
9	7H	372	GLN
9	7I	341	GLN
9	7K	226	ASN
9	7K	249	HIS
9	7K	319	HIS
9	7L	179	GLN
9	7L	319	HIS

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Mol	Chain	Res	Type
9	7M	226	ASN
9	7M	310	GLN
9	7M	319	HIS
9	7N	319	HIS
9	7O	226	ASN
9	7O	319	HIS
9	7O	341	GLN
9	7P	219	ASN
9	7P	319	HIS
9	7Q	249	HIS
9	7S	185	GLN
9	7T	226	ASN
9	7T	249	HIS
9	7T	319	HIS
9	7U	229	ASN
9	7U	319	HIS
9	7V	385	HIS
9	7W	249	HIS
9	7X	328	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	3PH	1P	201	-	45,45,47	0.92	4 (8%)	48,50,52	1.06	3 (6%)
11	LDA	1A	402	-	13,15,15	2.44	2 (15%)	14,17,17	0.83	0
10	3PH	1L	201	-	33,33,47	1.04	4 (12%)	36,38,52	1.25	2 (5%)
11	LDA	1J	401	-	13,15,15	2.50	2 (15%)	14,17,17	1.03	1 (7%)
10	3PH	1N	601	-	33,33,47	1.04	3 (9%)	36,38,52	1.25	2 (5%)
10	3PH	1M	201	-	33,33,47	1.00	3 (9%)	36,38,52	1.18	2 (5%)
11	LDA	1I	502	-	13,15,15	2.53	2 (15%)	14,17,17	0.67	0
11	LDA	1D	301	-	13,15,15	2.41	2 (15%)	14,17,17	0.53	0
11	LDA	1J	402	-	13,15,15	2.55	2 (15%)	14,17,17	0.67	0
11	LDA	1I	503	-	13,15,15	2.51	2 (15%)	14,17,17	0.69	0
11	LDA	1I	501	-	13,15,15	2.42	2 (15%)	14,17,17	0.66	0
11	LDA	1H	101	-	13,15,15	2.61	2 (15%)	14,17,17	0.64	0
11	LDA	1G	201	-	13,15,15	2.50	2 (15%)	14,17,17	0.82	0
10	3PH	1A	401	-	35,35,47	0.99	4 (11%)	38,40,52	1.27	2 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	3PH	1P	201	-	-	29/47/47/49	-
11	LDA	1A	402	-	-	2/13/13/13	-
10	3PH	1L	201	-	-	11/35/35/49	-
11	LDA	1J	401	-	-	0/13/13/13	-
10	3PH	1N	601	-	-	23/35/35/49	-
10	3PH	1M	201	-	-	15/35/35/49	-
11	LDA	1I	502	-	-	2/13/13/13	-
11	LDA	1D	301	-	-	5/13/13/13	-
11	LDA	1J	402	-	-	4/13/13/13	-
11	LDA	1I	503	-	-	0/13/13/13	-
11	LDA	1I	501	-	-	0/13/13/13	-
11	LDA	1H	101	-	-	1/13/13/13	-
11	LDA	1G	201	-	-	3/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	3PH	1A	401	-	-	16/37/37/49	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1J	401	LDA	O1-N1	-7.12	1.24	1.42
11	1J	402	LDA	O1-N1	-7.08	1.24	1.42
11	1I	501	LDA	O1-N1	-7.05	1.24	1.42
11	1H	101	LDA	O1-N1	-7.04	1.24	1.42
11	1G	201	LDA	O1-N1	-7.00	1.25	1.42
11	1I	503	LDA	O1-N1	-6.98	1.25	1.42
11	1I	502	LDA	O1-N1	-6.97	1.25	1.42
11	1D	301	LDA	O1-N1	-6.88	1.25	1.42
11	1A	402	LDA	O1-N1	-6.87	1.25	1.42
11	1H	101	LDA	C1-N1	-6.24	1.45	1.51
11	1I	502	LDA	C1-N1	-5.84	1.45	1.51
11	1J	402	LDA	C1-N1	-5.80	1.45	1.51
11	1I	503	LDA	C1-N1	-5.71	1.45	1.51
11	1G	201	LDA	C1-N1	-5.63	1.45	1.51
11	1A	402	LDA	C1-N1	-5.49	1.45	1.51
11	1J	401	LDA	C1-N1	-5.45	1.45	1.51
11	1D	301	LDA	C1-N1	-5.27	1.46	1.51
11	1I	501	LDA	C1-N1	-5.06	1.46	1.51
10	1P	201	3PH	O21-C2	-3.04	1.39	1.46
10	1N	601	3PH	O21-C2	-2.98	1.39	1.46
10	1L	201	3PH	O21-C2	-2.85	1.39	1.46
10	1M	201	3PH	O21-C2	-2.67	1.40	1.46
10	1A	401	3PH	O31-C3	-2.67	1.39	1.45
10	1P	201	3PH	O31-C3	-2.52	1.39	1.45
10	1L	201	3PH	O31-C3	-2.40	1.39	1.45
10	1N	601	3PH	O31-C3	-2.39	1.39	1.45
10	1M	201	3PH	O31-C3	-2.37	1.39	1.45
10	1A	401	3PH	O21-C21	2.32	1.40	1.34
10	1L	201	3PH	O31-C31	2.26	1.39	1.33
10	1M	201	3PH	O31-C31	2.23	1.39	1.33
10	1N	601	3PH	O31-C31	2.18	1.39	1.33
10	1L	201	3PH	O21-C21	2.17	1.40	1.34
10	1A	401	3PH	O31-C31	2.13	1.39	1.33
10	1A	401	3PH	O21-C2	-2.12	1.41	1.46
10	1P	201	3PH	O21-C21	2.05	1.40	1.34
10	1P	201	3PH	O31-C31	2.03	1.39	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	1A	401	3PH	O21-C21-C22	5.10	122.52	111.48
10	1N	601	3PH	O21-C21-C22	4.50	121.22	111.48
10	1P	201	3PH	O21-C21-C22	4.36	120.91	111.48
10	1M	201	3PH	O21-C21-C22	4.33	120.84	111.48
10	1L	201	3PH	O21-C21-C22	4.28	120.74	111.48
11	1J	401	LDA	CM1-N1-C1	2.81	116.14	110.23
10	1N	601	3PH	O31-C31-C32	2.51	119.50	111.83
10	1A	401	3PH	O31-C31-C32	2.49	119.42	111.83
10	1P	201	3PH	O31-C31-C32	2.28	118.79	111.83
10	1L	201	3PH	O31-C31-C32	2.25	118.69	111.83
10	1M	201	3PH	O21-C21-O22	-2.19	118.58	123.70
10	1P	201	3PH	O21-C21-O22	-2.00	119.02	123.70

There are no chirality outliers.

All (111) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	1A	401	3PH	O22-C21-O21-C2
10	1A	401	3PH	C22-C21-O21-C2
10	1L	201	3PH	C22-C21-O21-C2
10	1M	201	3PH	C1-O11-P-O13
10	1M	201	3PH	C1-O11-P-O14
10	1M	201	3PH	C22-C21-O21-C2
10	1N	601	3PH	C1-O11-P-O13
10	1N	601	3PH	C1-O11-P-O14
10	1N	601	3PH	C22-C21-O21-C2
10	1P	201	3PH	C1-O11-P-O13
10	1P	201	3PH	C1-O11-P-O14
10	1P	201	3PH	C1-O11-P-O12
10	1P	201	3PH	C22-C21-O21-C2
11	1D	301	LDA	N1-C1-C2-C3
10	1A	401	3PH	O32-C31-O31-C3
10	1M	201	3PH	O32-C31-O31-C3
10	1N	601	3PH	O32-C31-O31-C3
10	1L	201	3PH	O22-C21-O21-C2
10	1M	201	3PH	O22-C21-O21-C2
10	1N	601	3PH	O22-C21-O21-C2
10	1P	201	3PH	O22-C21-O21-C2
10	1A	401	3PH	C32-C31-O31-C3
10	1M	201	3PH	C32-C31-O31-C3
10	1N	601	3PH	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
10	1L	201	3PH	O32-C31-O31-C3
10	1L	201	3PH	C32-C31-O31-C3
10	1P	201	3PH	C3C-C3D-C3E-C3F
10	1M	201	3PH	C31-C32-C33-C34
10	1P	201	3PH	C21-C22-C23-C24
10	1P	201	3PH	C32-C31-O31-C3
10	1A	401	3PH	C23-C24-C25-C26
10	1N	601	3PH	C26-C27-C28-C29
10	1L	201	3PH	C25-C26-C27-C28
10	1N	601	3PH	C32-C33-C34-C35
10	1P	201	3PH	O32-C31-O31-C3
11	1A	402	LDA	C7-C8-C9-C10
10	1P	201	3PH	C2A-C2B-C2C-C2D
10	1M	201	3PH	C24-C25-C26-C27
10	1L	201	3PH	C28-C29-C2A-C2B
10	1M	201	3PH	C21-C22-C23-C24
10	1P	201	3PH	C2C-C2D-C2E-C2F
10	1P	201	3PH	C3A-C3B-C3C-C3D
10	1A	401	3PH	C21-C22-C23-C24
10	1N	601	3PH	C24-C25-C26-C27
10	1P	201	3PH	C31-C32-C33-C34
10	1M	201	3PH	C35-C36-C37-C38
10	1P	201	3PH	C2D-C2E-C2F-C2G
10	1A	401	3PH	C32-C33-C34-C35
10	1P	201	3PH	C35-C36-C37-C38
10	1L	201	3PH	C35-C36-C37-C38
10	1A	401	3PH	C2C-C2D-C2E-C2F
10	1P	201	3PH	C1-C2-C3-O31
10	1P	201	3PH	C34-C35-C36-C37
10	1A	401	3PH	C1-C2-O21-C21
10	1A	401	3PH	C28-C29-C2A-C2B
10	1P	201	3PH	C23-C24-C25-C26
10	1M	201	3PH	O21-C2-C3-O31
10	1N	601	3PH	C29-C2A-C2B-C2C
10	1N	601	3PH	C37-C38-C39-C3A
10	1L	201	3PH	C32-C33-C34-C35
11	1J	402	LDA	C11-C10-C9-C8
10	1A	401	3PH	C35-C36-C37-C38
10	1P	201	3PH	O11-C1-C2-O21
10	1N	601	3PH	C36-C37-C38-C39
10	1L	201	3PH	O21-C2-C3-O31
10	1P	201	3PH	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
10	1N	601	3PH	C31-C32-C33-C34
10	1P	201	3PH	O11-C1-C2-C3
10	1P	201	3PH	C29-C2A-C2B-C2C
10	1P	201	3PH	C28-C29-C2A-C2B
10	1P	201	3PH	C38-C39-C3A-C3B
10	1M	201	3PH	C37-C38-C39-C3A
11	1J	402	LDA	C7-C8-C9-C10
10	1A	401	3PH	C29-C2A-C2B-C2C
10	1A	401	3PH	C22-C23-C24-C25
11	1D	301	LDA	C4-C5-C6-C7
11	1G	201	LDA	C2-C1-N1-CM2
10	1A	401	3PH	C2D-C2E-C2F-C2G
10	1L	201	3PH	C23-C24-C25-C26
10	1P	201	3PH	C26-C27-C28-C29
11	1D	301	LDA	C3-C4-C5-C6
10	1P	201	3PH	C39-C3A-C3B-C3C
10	1N	601	3PH	O21-C2-C3-O31
10	1A	401	3PH	C1-C2-C3-O31
10	1L	201	3PH	C1-C2-C3-O31
10	1N	601	3PH	C1-C2-C3-O31
11	1J	402	LDA	C2-C3-C4-C5
10	1M	201	3PH	C1-C2-O21-C21
10	1P	201	3PH	C24-C25-C26-C27
10	1N	601	3PH	C23-C24-C25-C26
11	1I	502	LDA	C3-C4-C5-C6
10	1N	601	3PH	C34-C35-C36-C37
10	1N	601	3PH	O11-C1-C2-O21
11	1A	402	LDA	C4-C5-C6-C7
11	1J	402	LDA	C5-C6-C7-C8
10	1P	201	3PH	C27-C28-C29-C2A
11	1H	101	LDA	C6-C7-C8-C9
10	1M	201	3PH	C1-C2-C3-O31
11	1D	301	LDA	C6-C7-C8-C9
10	1M	201	3PH	C28-C29-C2A-C2B
10	1N	601	3PH	C1-O11-P-O12
11	1G	201	LDA	C5-C6-C7-C8
10	1N	601	3PH	C33-C34-C35-C36
11	1G	201	LDA	N1-C1-C2-C3
11	1I	502	LDA	C4-C5-C6-C7
10	1N	601	3PH	C27-C28-C29-C2A
10	1N	601	3PH	O31-C31-C32-C33
11	1D	301	LDA	C2-C3-C4-C5

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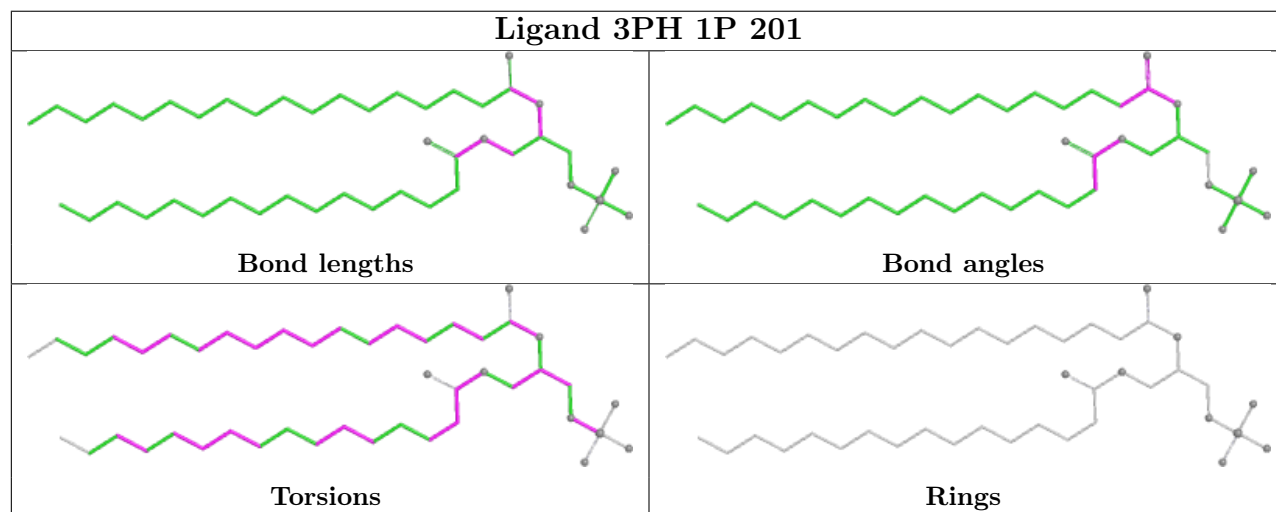
Mol	Chain	Res	Type	Atoms
10	1N	601	3PH	O32-C31-C32-C33
10	1A	401	3PH	C2B-C2C-C2D-C2E
10	1P	201	3PH	O31-C31-C32-C33

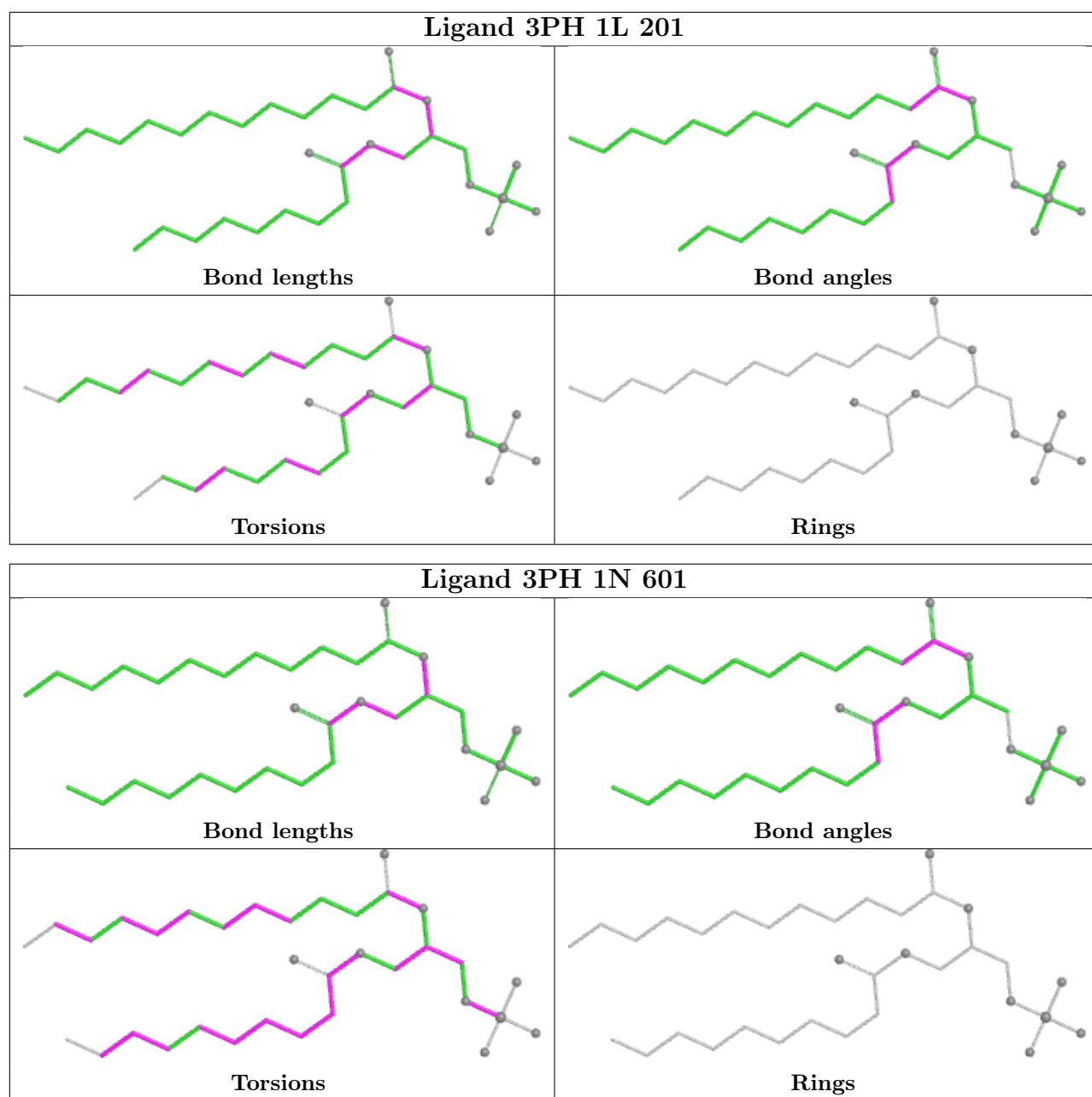
There are no ring outliers.

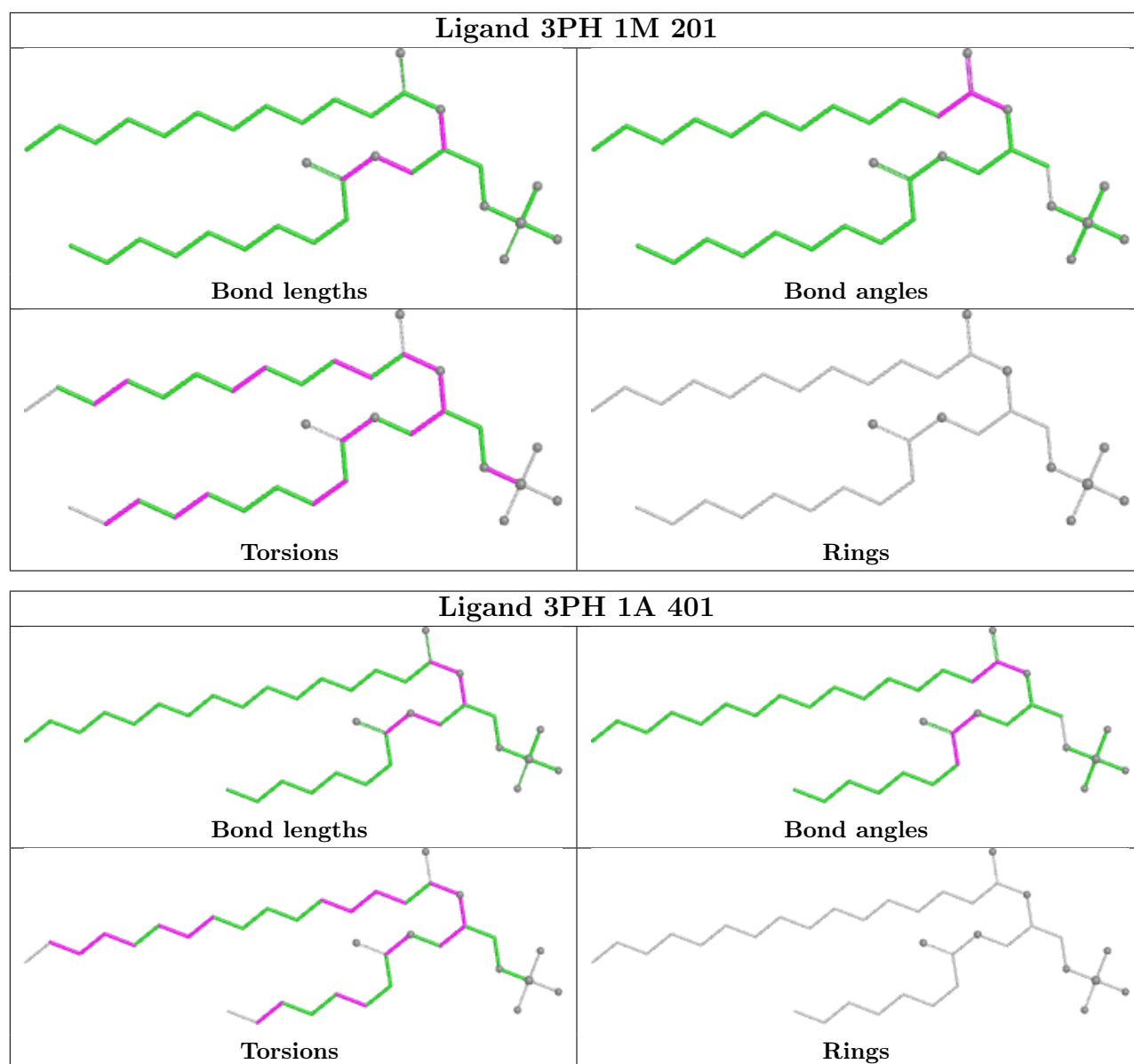
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	1N	601	3PH	1	0
11	1I	501	LDA	1	0
11	1G	201	LDA	1	0
10	1A	401	3PH	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

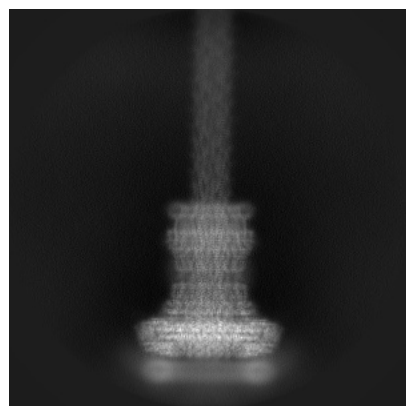
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11781. These allow visual inspection of the internal detail of the map and identification of artifacts.

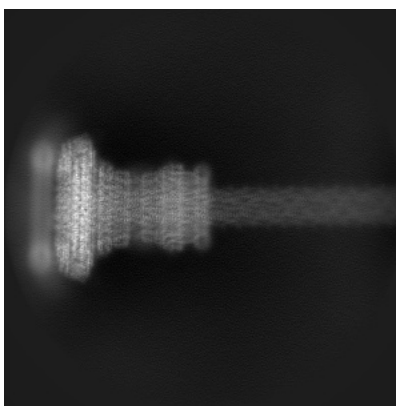
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

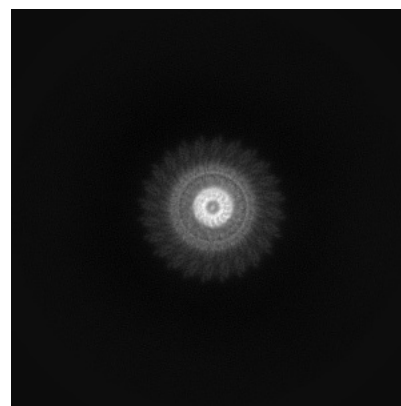
6.1.1 Primary map



X

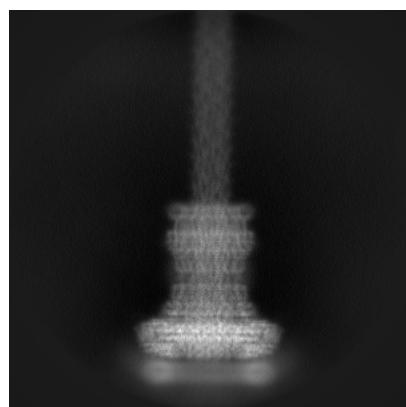


Y

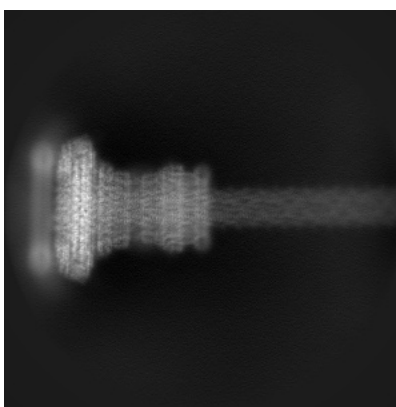


Z

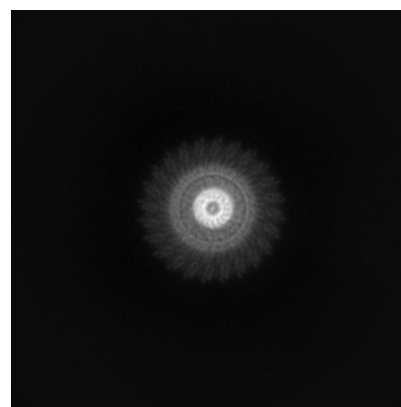
6.1.2 Raw map



X



Y

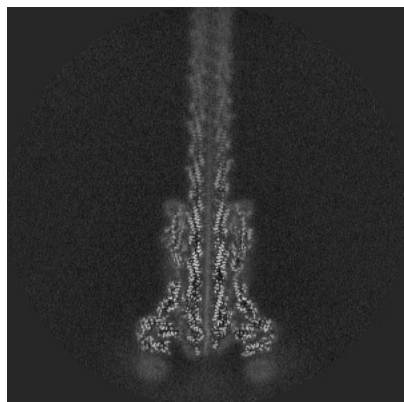


Z

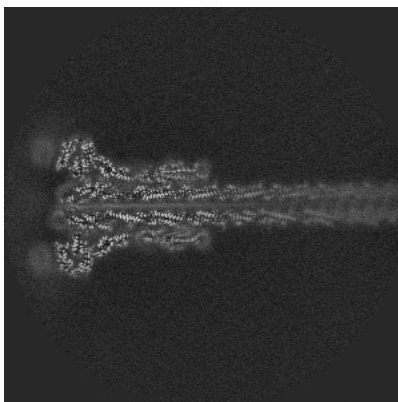
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

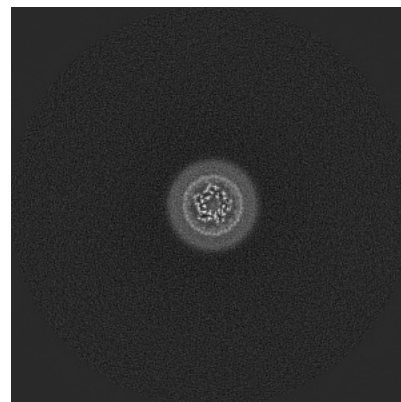
6.2.1 Primary map



X Index: 300

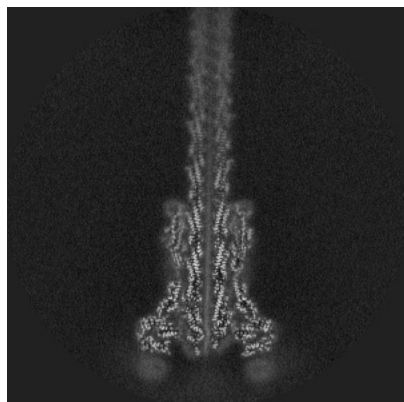


Y Index: 300

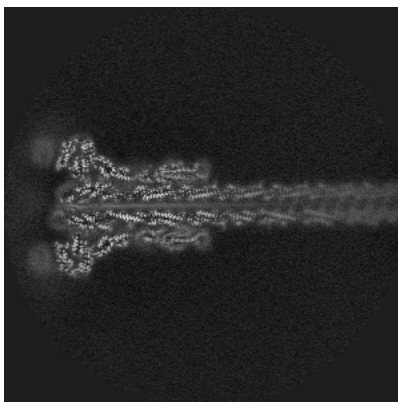


Z Index: 300

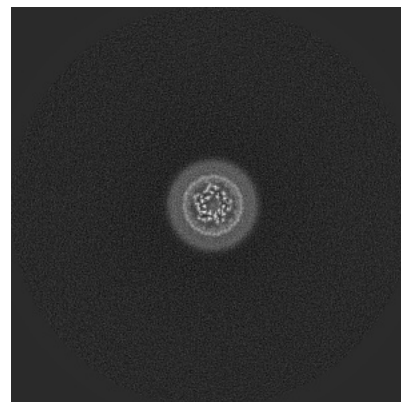
6.2.2 Raw map



X Index: 300



Y Index: 300

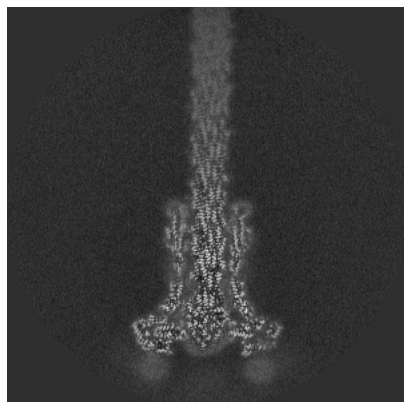


Z Index: 300

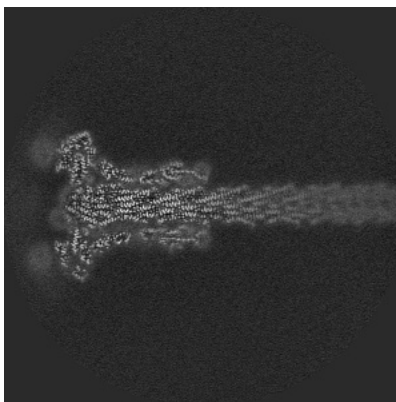
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

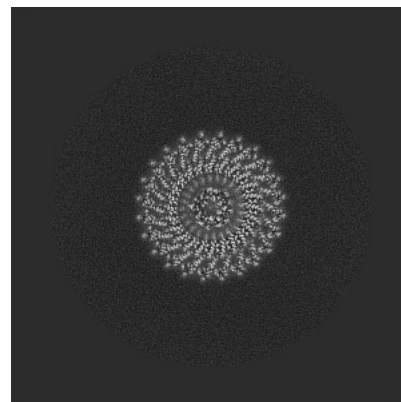
6.3.1 Primary map



X Index: 316

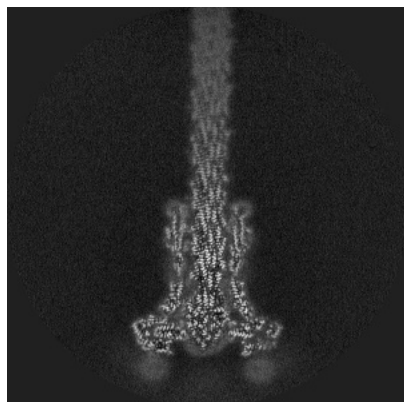


Y Index: 315

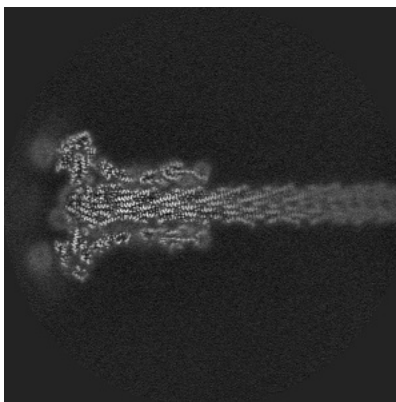


Z Index: 118

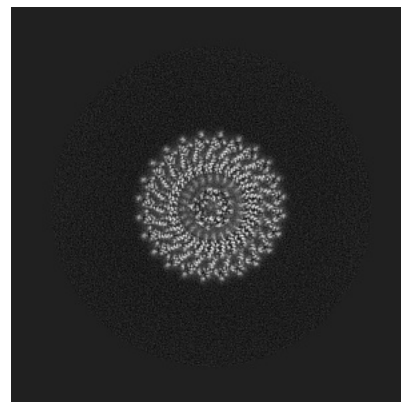
6.3.2 Raw map



X Index: 316



Y Index: 315

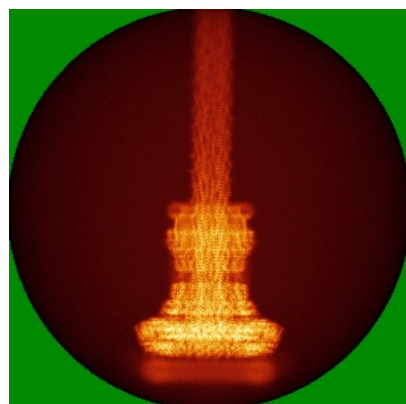


Z Index: 118

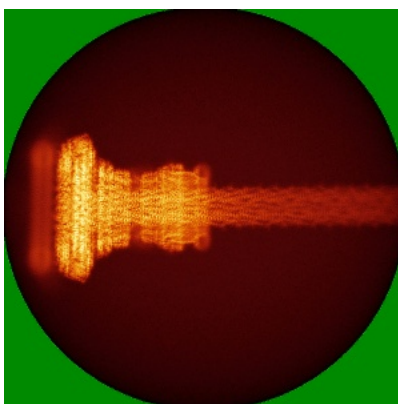
The images above show the largest variance slices of the map in three orthogonal directions.

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

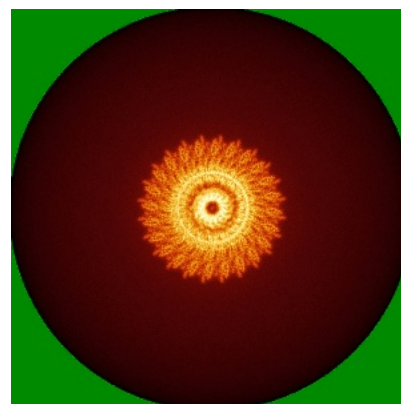
6.4.1 Primary map



X

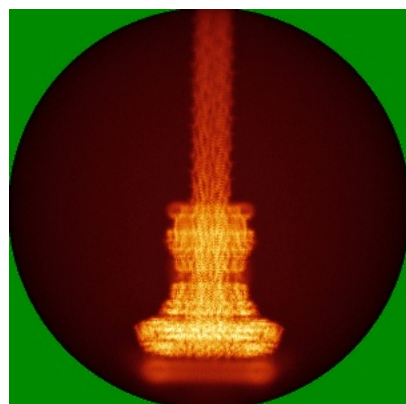


Y

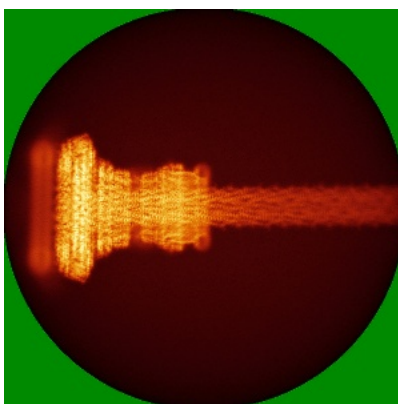


Z

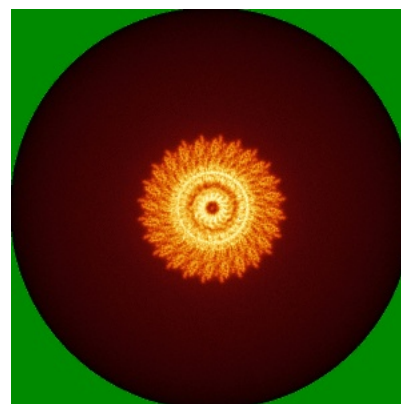
6.4.2 Raw map



X



Y

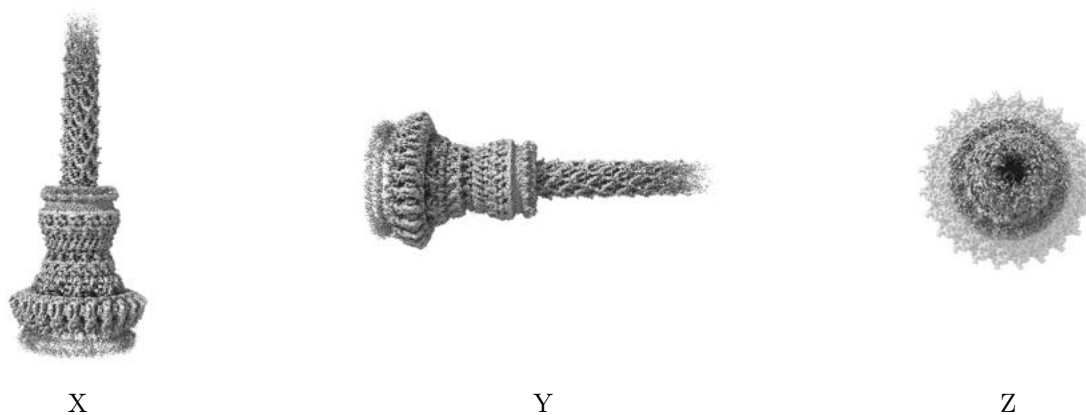


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.013. 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



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.

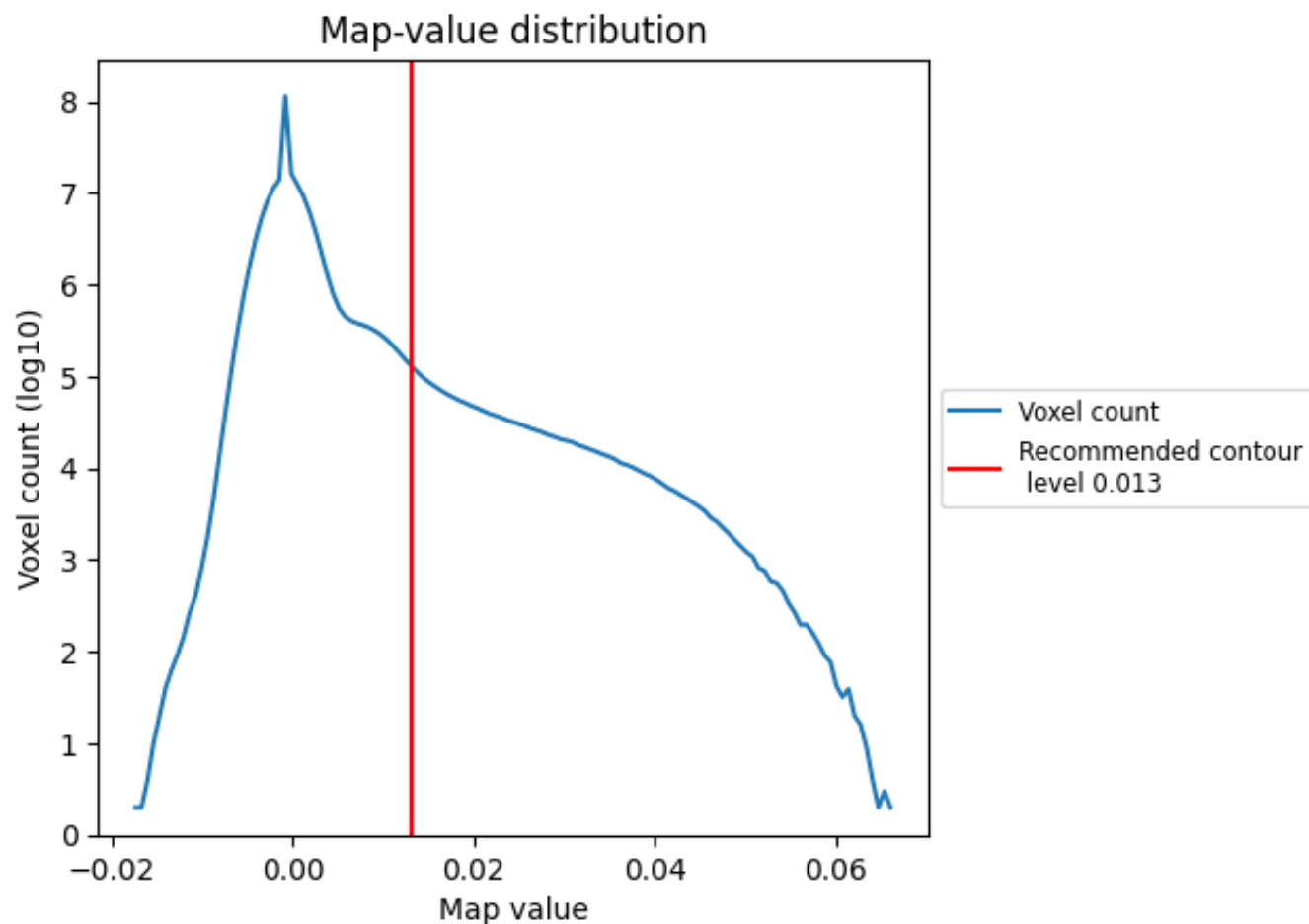
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

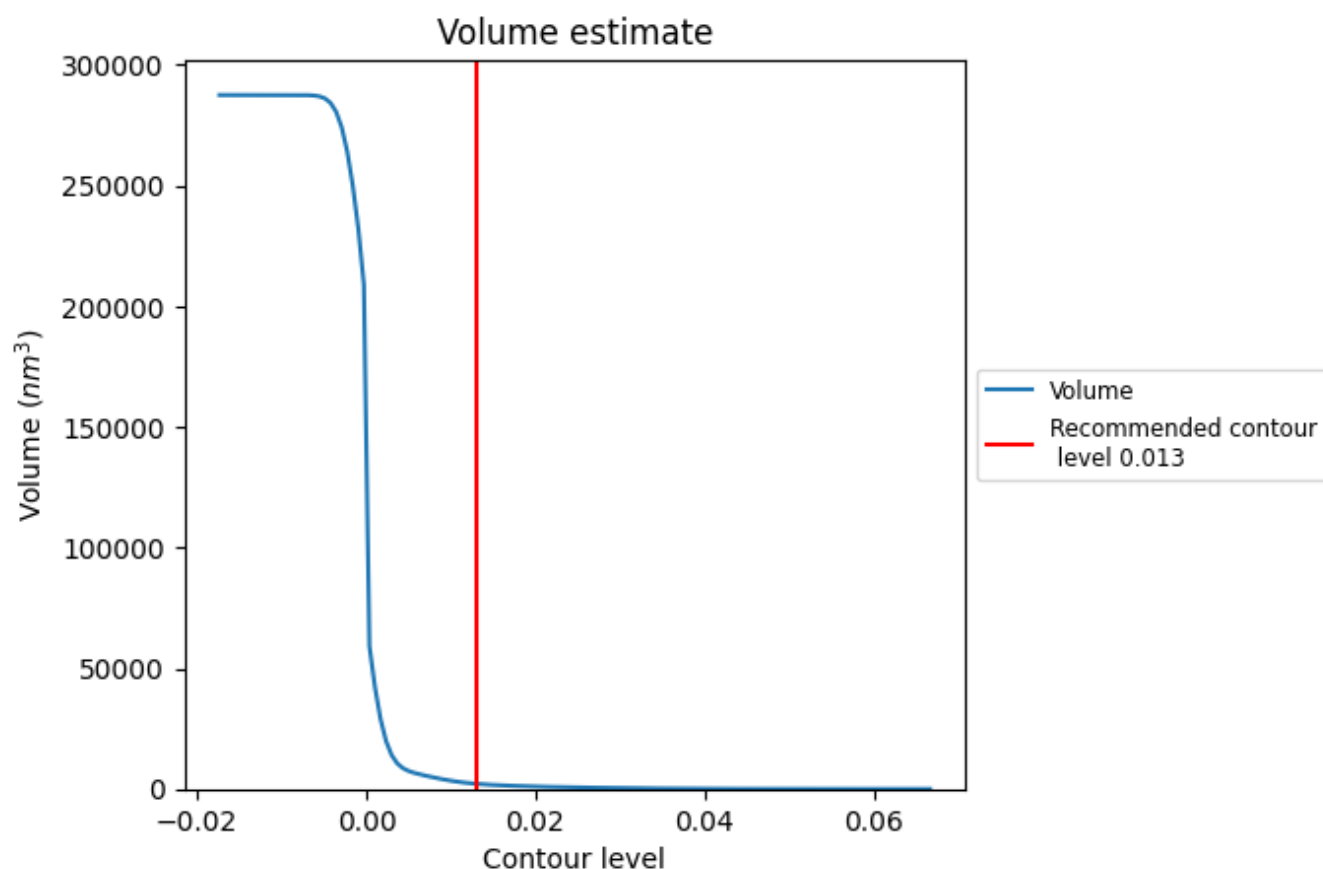
This section contains the results of statistical analysis of the map.

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.

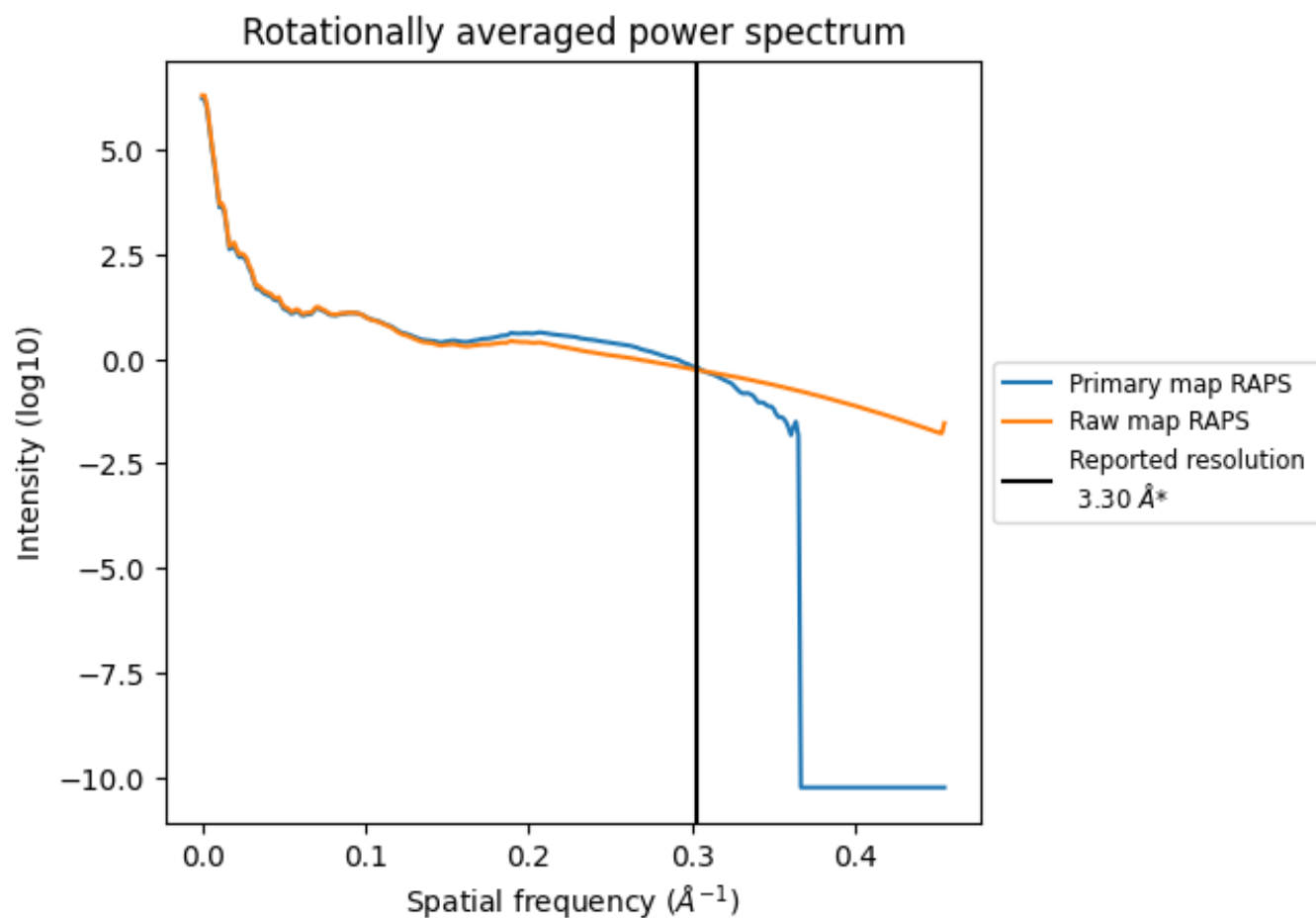
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2134 nm^3 ; this corresponds to an approximate mass of 1928 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

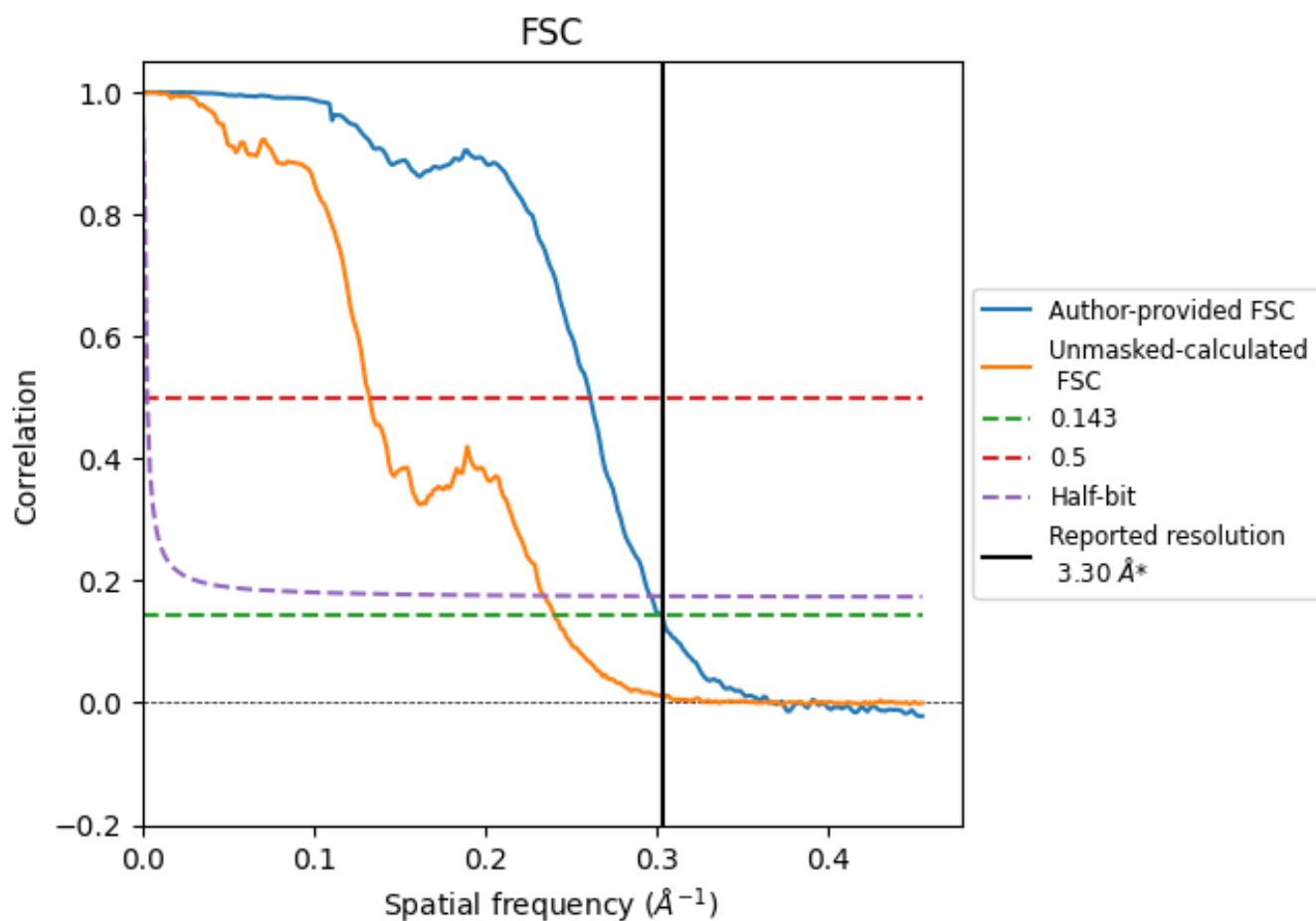


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

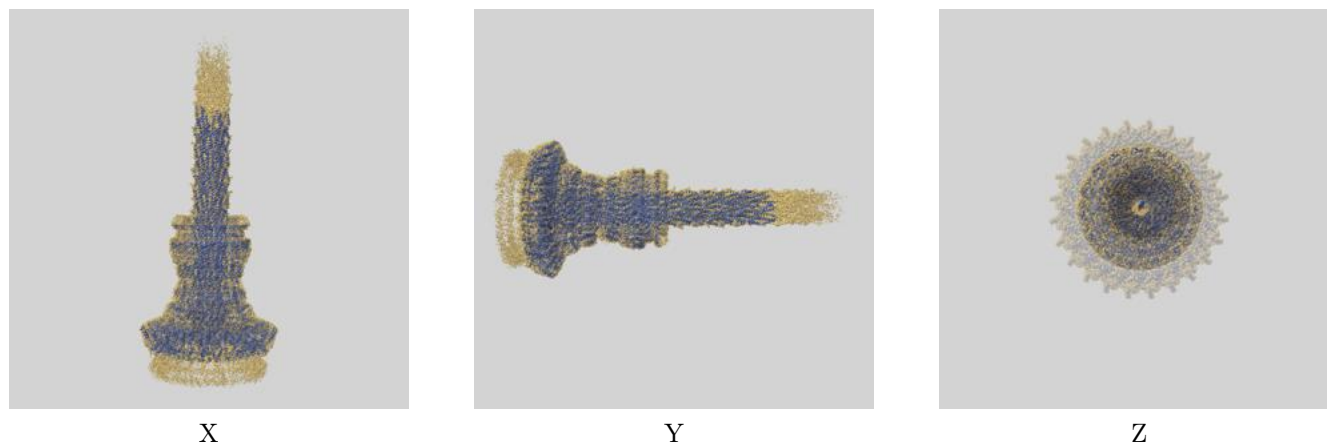
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	3.83	3.37
Unmasked-calculated*	4.16	7.55	4.27

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.16 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

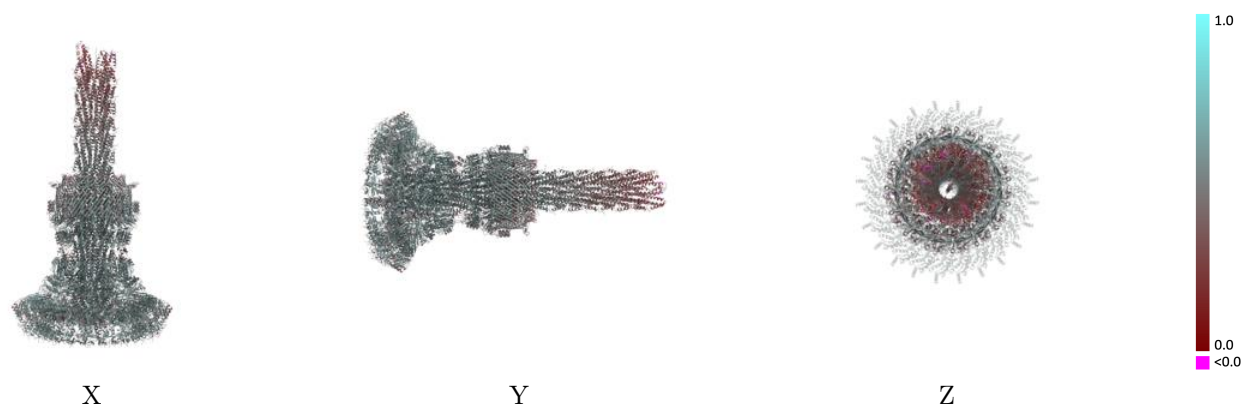
This section contains information regarding the fit between EMDB map EMD-11781 and PDB model 7AH9. Per-residue inclusion information can be found in section [3](#) on page [19](#).

9.1 Map-model overlay [i](#)



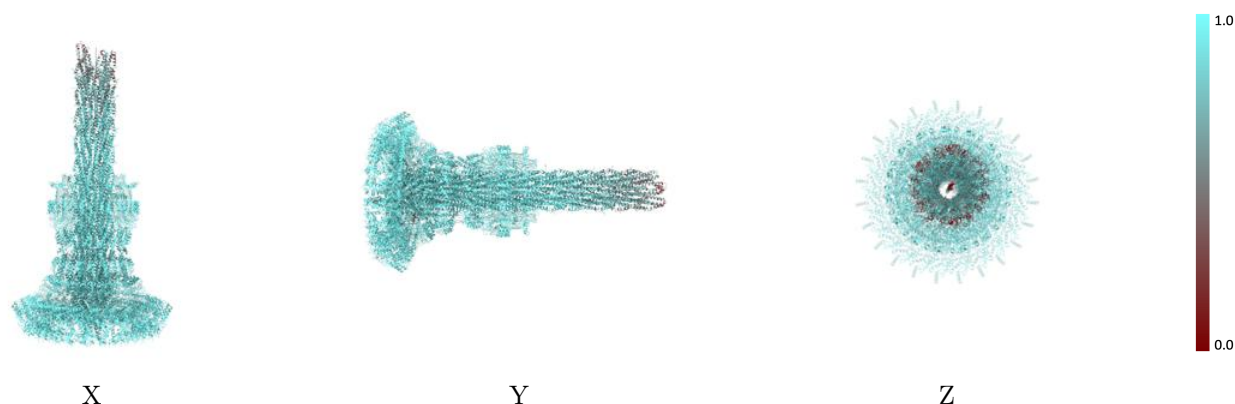
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



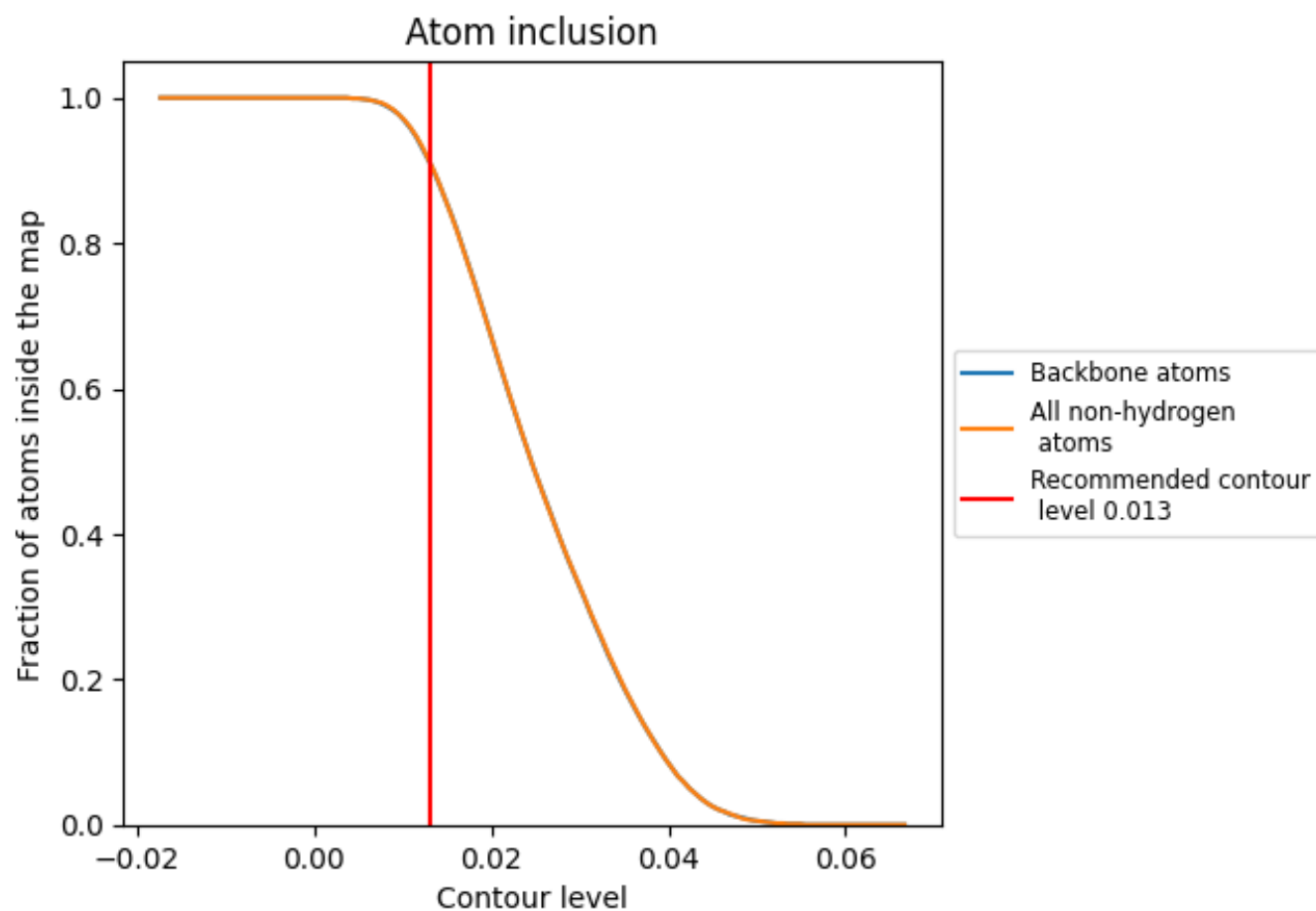
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 91% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9130	 0.5000
1A	 0.8990	 0.5140
1B	 0.9230	 0.5110
1C	 0.9380	 0.5100
1D	 0.9480	 0.5300
1E	 0.9580	 0.5380
1F	 0.9760	 0.5450
1G	 0.7710	 0.4560
1H	 0.9120	 0.4870
1I	 0.9060	 0.5120
1J	 0.9420	 0.5290
1K	 0.9060	 0.5070
1L	 0.9460	 0.5370
1M	 0.9600	 0.5310
1N	 0.9530	 0.5260
1O	 0.9600	 0.5390
1P	 0.9610	 0.5450
1Z	 0.5750	 0.3840
2A	 0.9600	 0.5530
2B	 0.9680	 0.5490
2C	 0.9780	 0.5440
2D	 0.9310	 0.5170
2E	 0.9680	 0.5420
2F	 0.9760	 0.5480
2G	 0.9730	 0.5650
2H	 0.9690	 0.5490
2I	 0.9790	 0.5520
2J	 0.9770	 0.5500
2K	 0.9660	 0.5440
2L	 0.9780	 0.5530
2M	 0.9820	 0.5510
2N	 0.9720	 0.5490
2O	 0.9770	 0.5350
2P	 0.9730	 0.5430
2Q	 0.9750	 0.5450



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Chain	Atom inclusion	Q-score
2R	 0.9770	 0.5440
2S	 0.9770	 0.5440
2T	 0.9790	 0.5450
2U	 0.9720	 0.5340
2V	 0.9660	 0.5300
2W	 0.9700	 0.5350
2X	 0.9720	 0.5410
2Y	 0.9740	 0.5410
2Z	 0.9640	 0.5270
3A	 0.9560	 0.5150
3B	 0.9570	 0.5150
3C	 0.9590	 0.5220
3D	 0.9500	 0.5200
3E	 0.9470	 0.5210
3F	 0.9450	 0.5040
3G	 0.9340	 0.4990
3H	 0.9190	 0.4920
3I	 0.9220	 0.4980
3J	 0.9250	 0.5070
3K	 0.9140	 0.4970
3L	 0.9140	 0.4900
3M	 0.8900	 0.4650
3N	 0.8940	 0.4760
3O	 0.8890	 0.4790
3P	 0.8890	 0.4910
3Q	 0.8730	 0.4710
3R	 0.8620	 0.4510
3S	 0.8260	 0.4320
3T	 0.8510	 0.4510
3U	 0.8340	 0.4490
3V	 0.8460	 0.4470
3W	 0.8140	 0.4280
3X	 0.7970	 0.4220
3Y	 0.7890	 0.4030
3Z	 0.7600	 0.3940
4A	 0.7750	 0.4160
4B	 0.7430	 0.3910
4C	 0.7650	 0.3890
4D	 0.7220	 0.3810
4E	 0.7300	 0.3920
4F	 0.7130	 0.3740
4G	 0.7230	 0.3740

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Chain	Atom inclusion	Q-score
4H	 0.7010	 0.3680
4I	 0.6810	 0.3460
4J	 0.6530	 0.3350
4K	 0.6120	 0.3300
4L	 0.6390	 0.3430
4M	 0.6170	 0.3300
4N	 0.6140	 0.3280
4O	 0.5650	 0.3090
4P	 0.5860	 0.3160
4Q	 0.5470	 0.3140
4R	 0.5490	 0.3160
4S	 0.4950	 0.2970
4T	 0.4880	 0.2730
5A	 0.9600	 0.5340
5B	 0.9210	 0.4790
5C	 0.9200	 0.4830
5D	 0.9270	 0.4880
5E	 0.9300	 0.5010
5F	 0.9370	 0.5030
5G	 0.9340	 0.5020
5H	 0.9390	 0.4980
5I	 0.9370	 0.5040
5J	 0.9300	 0.4970
5K	 0.9290	 0.4920
5L	 0.9280	 0.4870
5M	 0.9310	 0.4910
5N	 0.9210	 0.4760
5O	 0.9190	 0.4710
5P	 0.9190	 0.4730
6A	 0.9390	 0.5250
6B	 0.9430	 0.5300
6C	 0.9450	 0.5290
6D	 0.9410	 0.5240
6E	 0.9450	 0.5260
6F	 0.9410	 0.5240
6G	 0.9400	 0.5210
6H	 0.9450	 0.5210
6I	 0.9460	 0.5280
6J	 0.9440	 0.5280
6K	 0.9360	 0.5220
6L	 0.9430	 0.5300
6M	 0.9410	 0.5230

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Chain	Atom inclusion	Q-score
6N	 0.9410	 0.5280
6O	 0.9370	 0.5220
6P	 0.9390	 0.5180
6Q	 0.9390	 0.5250
6R	 0.9400	 0.5250
6S	 0.9370	 0.5190
6T	 0.9460	 0.5280
6U	 0.9410	 0.5290
6V	 0.9430	 0.5250
6W	 0.9390	 0.5270
6X	 0.9460	 0.5290
7A	 0.9440	 0.5260
7B	 0.9400	 0.5250
7C	 0.9430	 0.5240
7D	 0.9480	 0.5240
7E	 0.9470	 0.5260
7F	 0.9390	 0.5260
7G	 0.9500	 0.5290
7H	 0.9450	 0.5260
7I	 0.9400	 0.5210
7J	 0.9470	 0.5250
7K	 0.9440	 0.5250
7L	 0.9410	 0.5200
7M	 0.9470	 0.5220
7N	 0.9460	 0.5210
7O	 0.9440	 0.5180
7P	 0.9410	 0.5160
7Q	 0.9340	 0.5170
7R	 0.9380	 0.5150
7S	 0.9440	 0.5160
7T	 0.9310	 0.5170
7U	 0.9450	 0.5220
7V	 0.9460	 0.5180
7W	 0.9440	 0.5250
7X	 0.9420	 0.5220