



wwPDB EM Validation Summary Report ⓘ

Apr 22, 2024 – 04:13 pm BST

PDB ID : 7AH9
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 wwPDB EM Validation Summary 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 : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

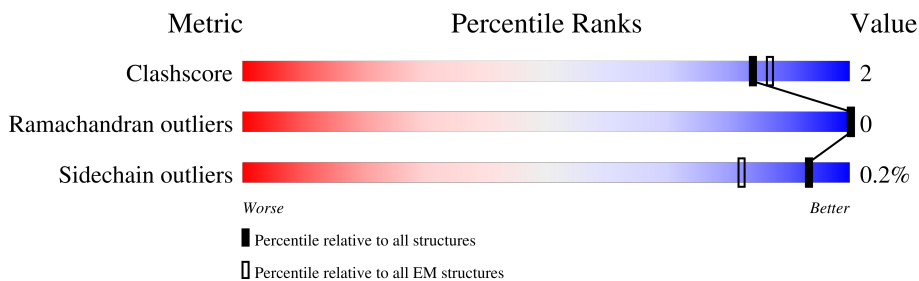
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1A	224	92% 7%
1	1B	224	94% 5%
1	1C	224	96% .
1	1D	224	97% ..
1	1E	224	98% ..
2	1F	263	94% . .
3	1G	86	93% 5% .
3	1H	86	94% . .
3	1I	86	99% .

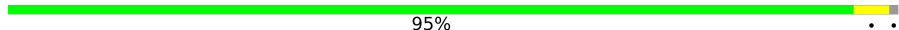

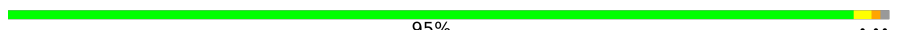
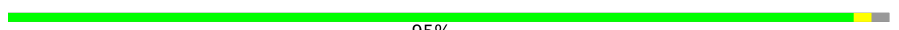






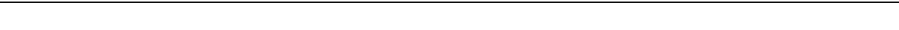

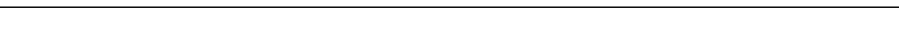
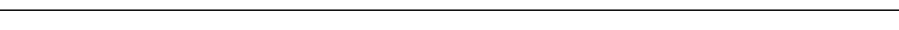
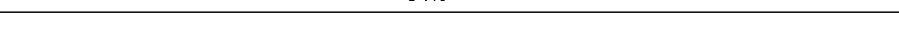

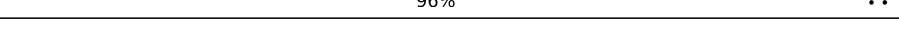
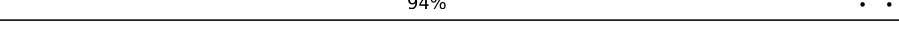


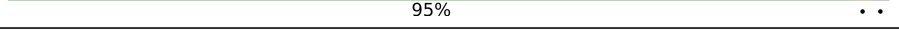
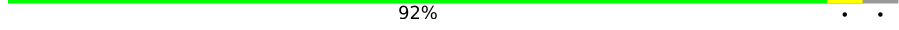



Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	1J	86	99%
4	1K	101	85% 11%
4	1L	101	88% 5% 7%
4	1M	101	85% 11%
4	1N	101	87% 12%
4	1O	101	82% 7% 11%
4	1P	101	86% 11%
5	1Z	141	100%
6	2A	80	76% 9% 15%
6	2B	80	74% 25%
6	2C	80	70% 26%
6	2D	80	98%
6	2E	80	84% 15%
6	2F	80	89% 5% 6%
6	2G	80	91% 5%
6	2H	80	91% 6%
6	2I	80	88% 6% 6%
6	2J	80	89% 5% 6%
6	2K	80	95%
6	2L	80	95%
6	2M	80	90% 8%
6	2N	80	92% 5%
6	2O	80	86% 11%
6	2P	80	92%
6	2Q	80	92% 5%

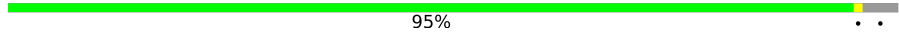
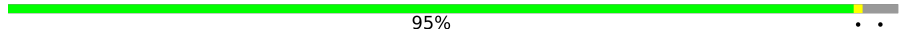





















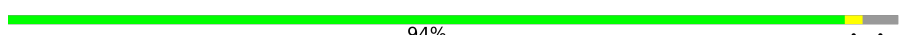

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	3Q	80	 95% . .
6	3R	80	 95% . .
6	3S	80	 90% 6% .
6	3T	80	 84% 12% .
6	3U	80	 91% 5% .
6	3V	80	 89% 8% .
6	3W	80	 86% 10% .
6	3X	80	 84% 11% . .
6	3Y	80	 78% 19% .
6	3Z	80	 82% 14% .
6	4A	80	 90% 6% .
6	4B	80	 85% 11% .
6	4C	80	 85% 11% .
6	4D	80	 90% 5% . .
6	4E	80	 89% 8% .
6	4F	80	 88% 9% .
6	4G	80	 91% 5% .
6	4H	80	 89% 8% .
6	4I	80	 85% 11% .
6	4J	80	 81% 14% . .
6	4K	80	 84% 12% .
6	4L	80	 85% 11% .
6	4M	80	 79% 18% .
6	4N	80	 94% . .
6	4O	80	 86% 10% .











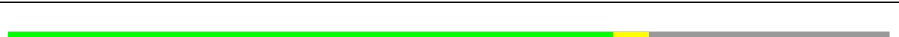


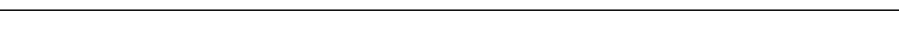
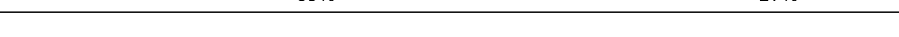
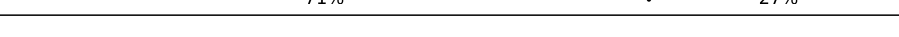



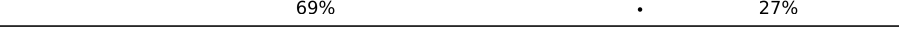





Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	4P	80	82% 14%
6	4Q	80	82% 14%
6	4R	80	85% 11%
6	4S	80	88% 9%
6	4T	80	82% 14%
7	5A	562	24% 75%
7	5B	562	80% 9% 11%
7	5C	562	82% 7% 11%
7	5D	562	81% 9% 10%
7	5E	562	84% 5% 10%
7	5F	562	84% 6% 10%
7	5G	562	82% 8% 10%
7	5H	562	84% 6% 10%
7	5I	562	82% 7% 10%
7	5J	562	86% 5% 10%
7	5K	562	83% 6% 11%
7	5L	562	84% 6% 10%
7	5M	562	81% 8% 11%
7	5N	562	82% 7% 11%
7	5O	562	81% 7% 11%
7	5P	562	85% 11%
8	6A	252	70% 27%
8	6B	252	71% 27%
8	6C	252	70% 27%
8	6D	252	70% 27%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	6E	252	 68% 5% 27%
8	6F	252	 68% . 27%
8	6G	252	 70% . 27%
8	6H	252	 70% . 27%
8	6I	252	 67% 5% 27%
8	6J	252	 70% . 27%
8	6K	252	 69% . 27%
8	6L	252	 69% . 27%
8	6M	252	 70% . 27%
8	6N	252	 69% . 27%
8	6O	252	 68% . 27%
8	6P	252	 71% . 27%
8	6Q	252	 69% . 27%
8	6R	252	 69% . 27%
8	6S	252	 71% . 27%
8	6T	252	 69% . 27%
8	6U	252	 69% . 27%
8	6V	252	 69% . 27%
8	6W	252	 69% . 27%
8	6X	252	 67% 5% 27%
9	7A	392	 53% . 44%
9	7B	392	 54% . 43%
9	7C	392	 55% . 43%
9	7D	392	 54% . 44%
9	7E	392	 55% . 43%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
9	7F	392	53%	43%
9	7G	392	52%	44%
9	7H	392	54%	43%
9	7I	392	52%	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	53%	43%
9	7P	392	54%	44%
9	7Q	392	52%	43%
9	7R	392	54%	43%
9	7S	392	53%	44%
9	7T	392	55%	43%
9	7U	392	54%	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
			Total	C	H	N	O	S		
1	1A	223	Total 3573	C 1166	H 1806	N 267	O 322	S 12	0	0
1	1B	223	Total 3551	C 1166	H 1784	N 267	O 322	S 12	0	0
1	1C	223	Total 3577	C 1166	H 1810	N 267	O 322	S 12	0	0
1	1D	220	Total 3536	C 1153	H 1790	N 264	O 317	S 12	0	0
1	1E	221	Total 3545	C 1157	H 1791	N 265	O 320	S 12	0	0

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

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

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

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

- Molecule 4 is a protein called Protein PrgJ.

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

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

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

- Molecule 6 is a protein called Protein PrgI.

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

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

- Molecule 8 is a protein called Lipoprotein PrgK.

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

Continued on next page...

Continued from previous page...

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

- Molecule 9 is a protein called Protein PrgH.

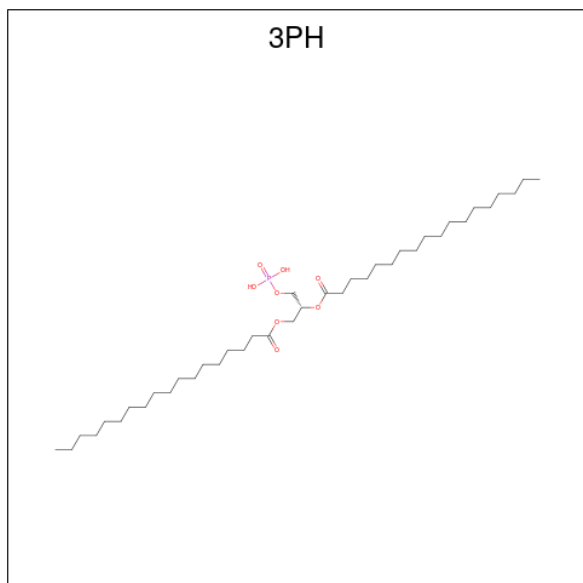
Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	7A	220	3602	1159	1782	324	332	5	0	0
9	7B	222	3636	1170	1800	326	335	5	0	0
9	7C	222	3636	1170	1800	326	335	5	0	0
9	7D	220	3602	1159	1782	324	332	5	0	0
9	7E	222	3636	1170	1800	326	335	5	0	0
9	7F	222	3636	1170	1800	326	335	5	0	0
9	7G	220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

Continued on next page...

Continued from previous page...

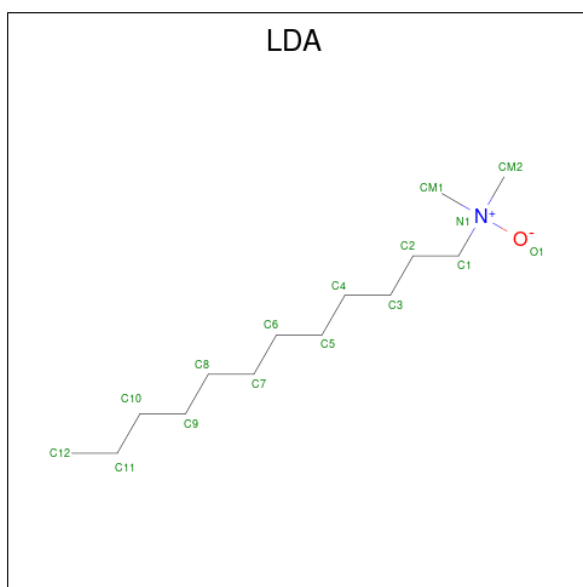
Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	7W	222	Total	C	H	N	O	S	0	0
			3636	1170	1800	326	335	5		
9	7X	222	Total	C	H	N	O	S	0	0
			3636	1170	1800	326	335	5		

- Molecule 10 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: C₃₉H₇₇O₈P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
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 (three-letter code: LDA) (formula: C₁₄H₃₁NO).



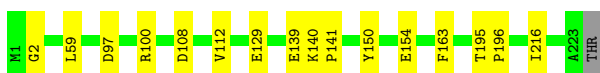
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
11	1A	1	Total 47	C 14	H 31	N 1	O 1	0
11	1D	1	Total 47	C 14	H 31	N 1	O 1	0
11	1G	1	Total 47	C 14	H 31	N 1	O 1	0
11	1H	1	Total 47	C 14	H 31	N 1	O 1	0
11	1I	1	Total 47	C 14	H 31	N 1	O 1	0
11	1I	1	Total 47	C 14	H 31	N 1	O 1	0
11	1I	1	Total 47	C 14	H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

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. 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. 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

Chain 1A:  92% 7%



- Molecule 1: Surface presentation of antigens protein SpaP

Chain 1B:  94% 5%



- Molecule 1: Surface presentation of antigens protein SpaP

Chain 1C:  96%



- Molecule 1: Surface presentation of antigens protein SpaP

Chain 1D:  97%



- Molecule 1: Surface presentation of antigens protein SpaP

Chain 1E:  98%

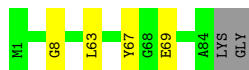


- Molecule 2: Surface presentation of antigens protein SpaR

Chain 1F:  94%



• Molecule 3: Surface presentation of antigens protein SpaQ



• Molecule 3: Surface presentation of antigens protein SpaQ



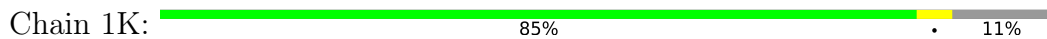
• Molecule 3: Surface presentation of antigens protein SpaQ



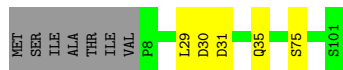
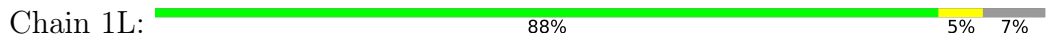
• Molecule 3: Surface presentation of antigens protein SpaQ



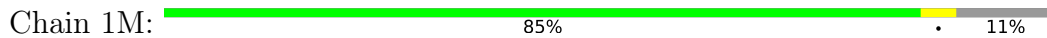
• Molecule 4: Protein PrgJ

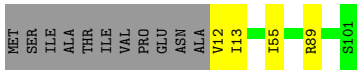


• Molecule 4: Protein PrgJ

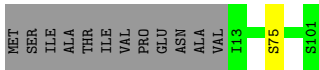
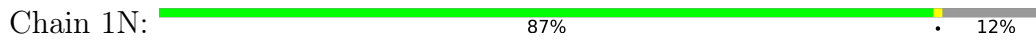


• Molecule 4: Protein PrgJ

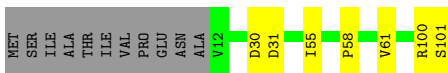
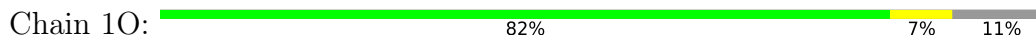




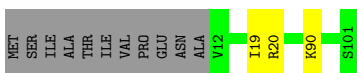
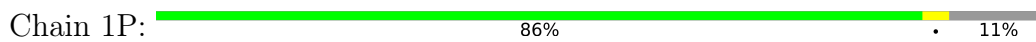
- Molecule 4: Protein PrgJ



- Molecule 4: Protein PrgJ



- Molecule 4: Protein PrgJ

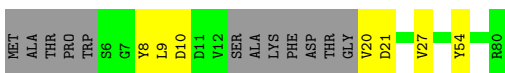
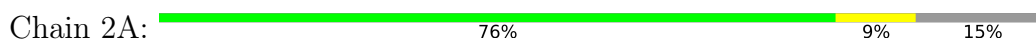


- Molecule 5: SptP3x-GFP-FLAG

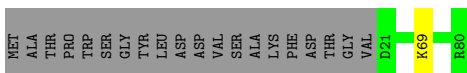
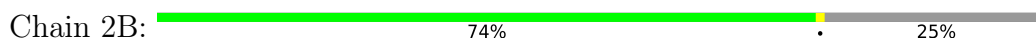


There are no outlier residues recorded for this chain.

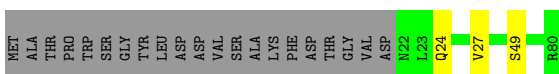
- Molecule 6: Protein PrgI



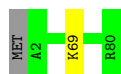
- Molecule 6: Protein PrgI



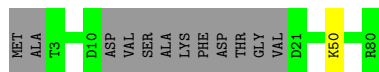
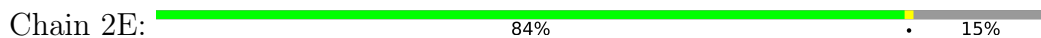
- Molecule 6: Protein PrgI



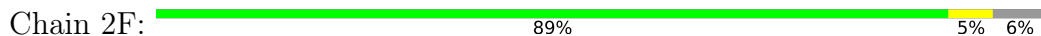
• Molecule 6: Protein PrgI



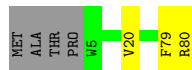
• Molecule 6: Protein PrgI



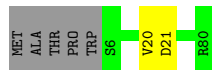
• Molecule 6: Protein PrgI



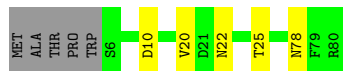
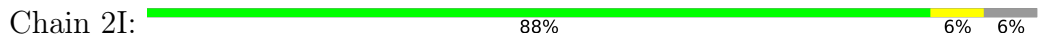
• Molecule 6: Protein PrgI



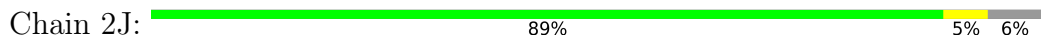
• Molecule 6: Protein PrgI



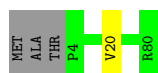
• Molecule 6: Protein PrgI



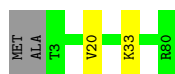
• Molecule 6: Protein PrgI



• Molecule 6: Protein PrgI



● Molecule 6: Protein PrgI



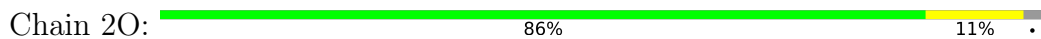
● Molecule 6: Protein PrgI



● Molecule 6: Protein PrgI



● Molecule 6: Protein PrgI



● Molecule 6: Protein PrgI



● Molecule 6: Protein PrgI



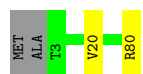
● Molecule 6: Protein PrgI

Chain 2R:  95% ..



● Molecule 6: Protein PrgI

Chain 2S:  95% ..



● Molecule 6: Protein PrgI

Chain 2T:  95% ...



● Molecule 6: Protein PrgI

Chain 2U:  95% ..



● Molecule 6: Protein PrgI

Chain 2V:  92% 6% .



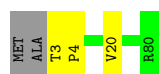
● Molecule 6: Protein PrgI

Chain 2W:  94% 5% .




● Molecule 6: Protein PrgI

Chain 2X:  94% ..



● Molecule 6: Protein PrgI

Chain 2Y:  89% 9%



● Molecule 6: Protein PrgI

Chain 2Z:  95%



● Molecule 6: Protein PrgI

Chain 3A:  94% 5%



● Molecule 6: Protein PrgI

Chain 3B:  92% 6%



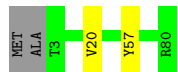
● Molecule 6: Protein PrgI

Chain 3C:  94%



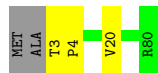
● Molecule 6: Protein PrgI

Chain 3D:  95%




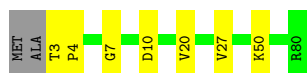
● Molecule 6: Protein PrgI

Chain 3E:  94%



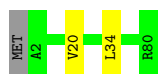
● Molecule 6: Protein PrgI

Chain 3F:  89% 9%



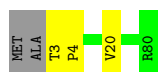
● Molecule 6: Protein PrgI

Chain 3G:  96%




● Molecule 6: Protein PrgI

Chain 3H:  94%



● Molecule 6: Protein PrgI

Chain 3I:  86% 11%



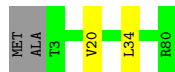
● Molecule 6: Protein PrgI

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:  90% 8%



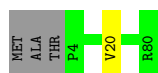
● Molecule 6: Protein PrgI

Chain 3O:  91% 5%



● Molecule 6: Protein PrgI

Chain 3P:  95% 2%



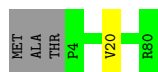
● Molecule 6: Protein PrgI

Chain 3Q:  95% 2%



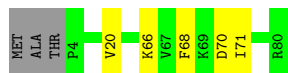
● Molecule 6: Protein PrgI

Chain 3R:  95% 2%

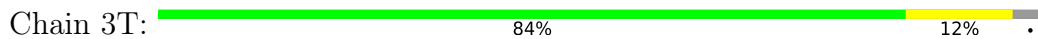


● Molecule 6: Protein PrgI

Chain 3S:  90% 6%



● Molecule 6: Protein PrgI



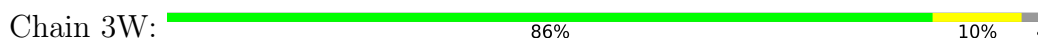
● Molecule 6: Protein PrgI



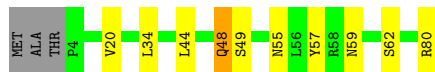
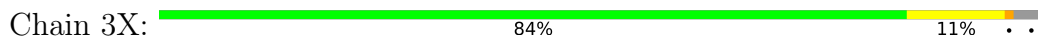
● Molecule 6: Protein PrgI



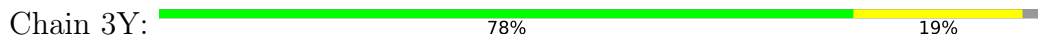
● Molecule 6: Protein PrgI



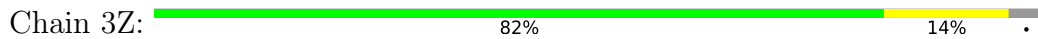
● Molecule 6: Protein PrgI



● Molecule 6: Protein PrgI

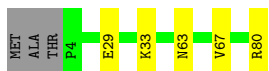


● Molecule 6: Protein PrgI




● Molecule 6: Protein PrgI

Chain 4A:  90% 6%




● Molecule 6: Protein PrgI

Chain 4B:  85% 11%



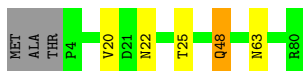
● Molecule 6: Protein PrgI

Chain 4C:  85% 11%



● Molecule 6: Protein PrgI

Chain 4D:  90% 5%




● Molecule 6: Protein PrgI

Chain 4E:  89% 8%



● Molecule 6: Protein PrgI

Chain 4F:  88% 9%

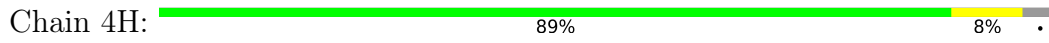


● Molecule 6: Protein PrgI

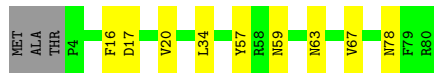
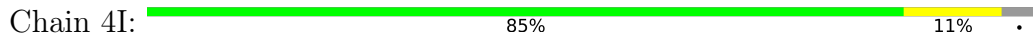
Chain 4G:  91% 5%



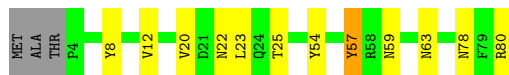
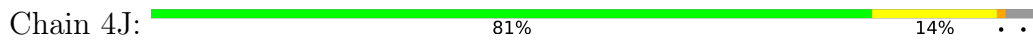
● Molecule 6: Protein PrgI



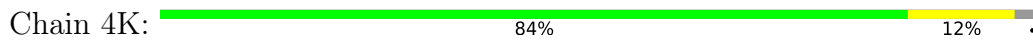
• Molecule 6: Protein PrgI



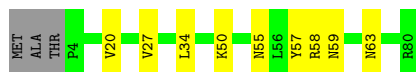
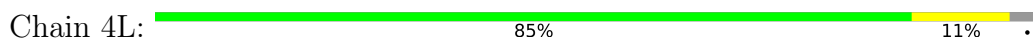
• Molecule 6: Protein PrgI



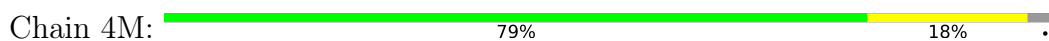
• Molecule 6: Protein PrgI



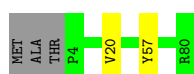
• Molecule 6: Protein PrgI



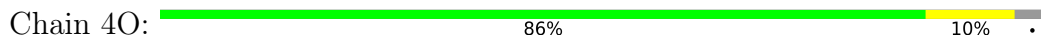
• Molecule 6: Protein PrgI



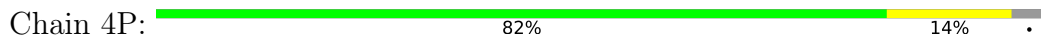
• Molecule 6: Protein PrgI



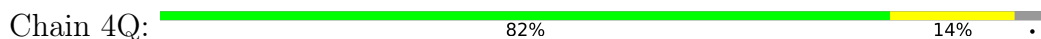
• Molecule 6: Protein PrgI



• Molecule 6: Protein PrgI



• Molecule 6: Protein PrgI



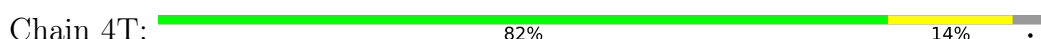
• Molecule 6: Protein PrgI



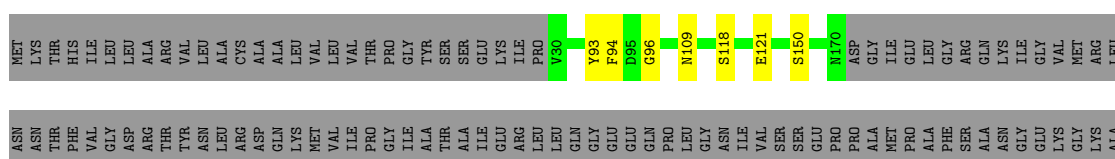
• Molecule 6: Protein PrgI

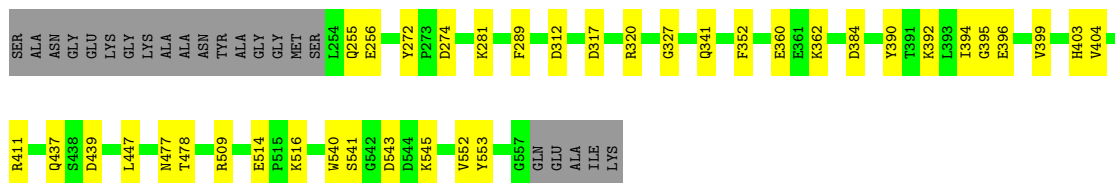


• Molecule 6: Protein PrgI

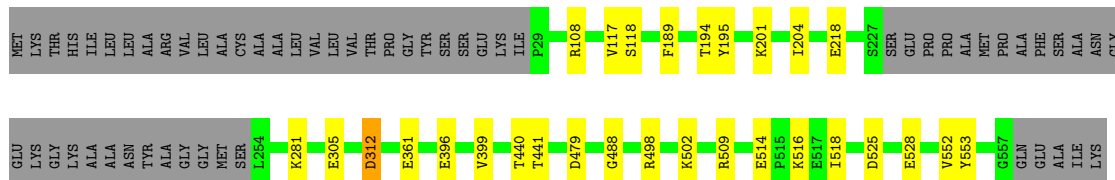
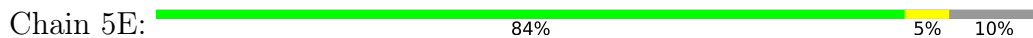


• Molecule 7: Type 3 secretion system secretin

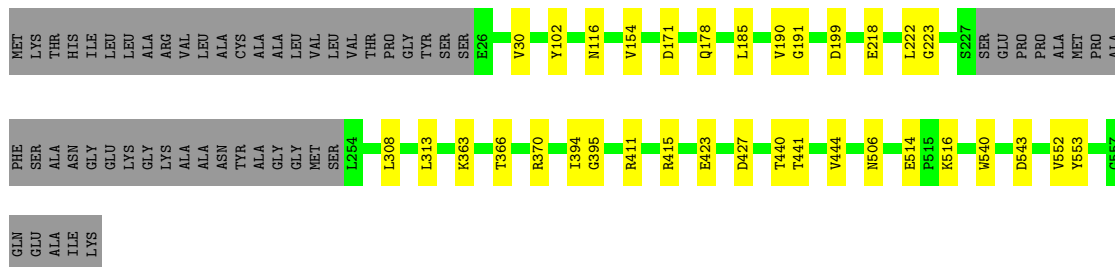
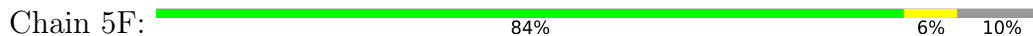




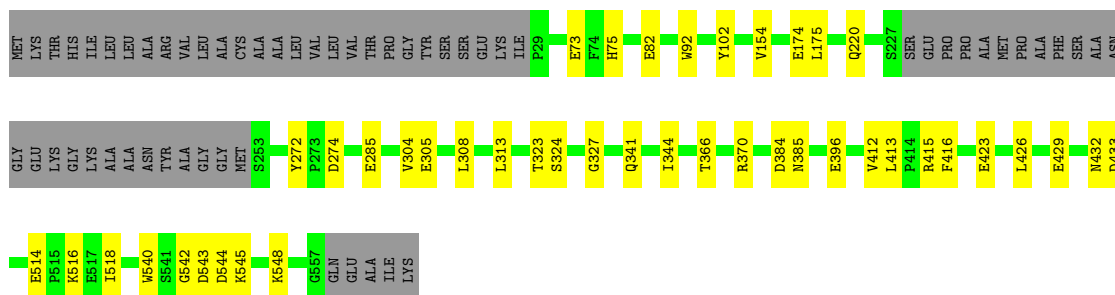
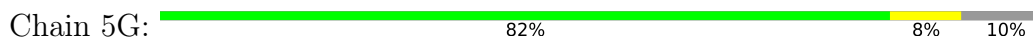
• Molecule 7: Type 3 secretion system secretin



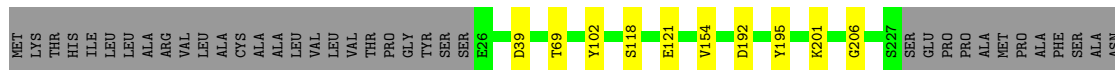
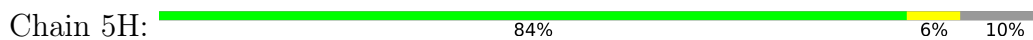
• Molecule 7: Type 3 secretion system secretin

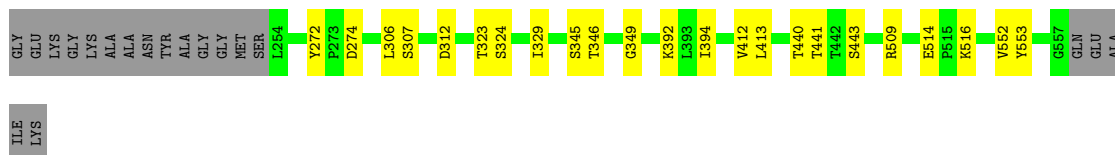


• Molecule 7: Type 3 secretion system secretin



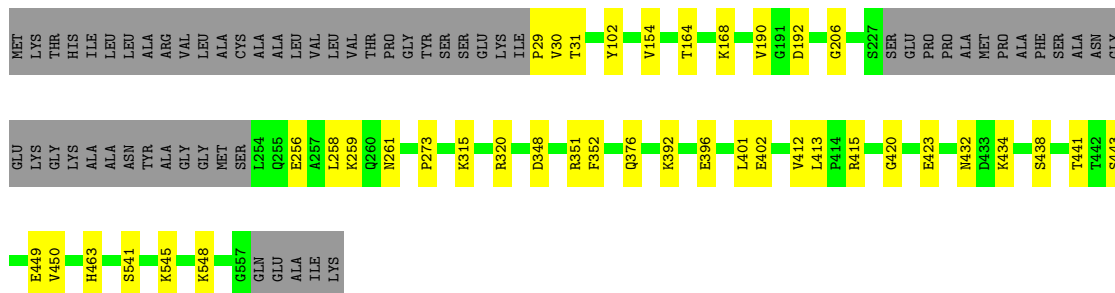
• Molecule 7: Type 3 secretion system secretin





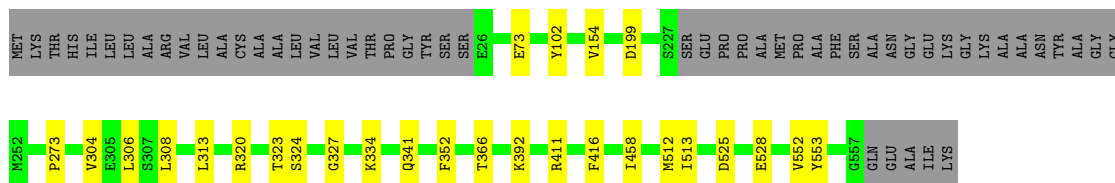
• Molecule 7: Type 3 secretion system secretin

Chain 5I: 82% 7% 10%



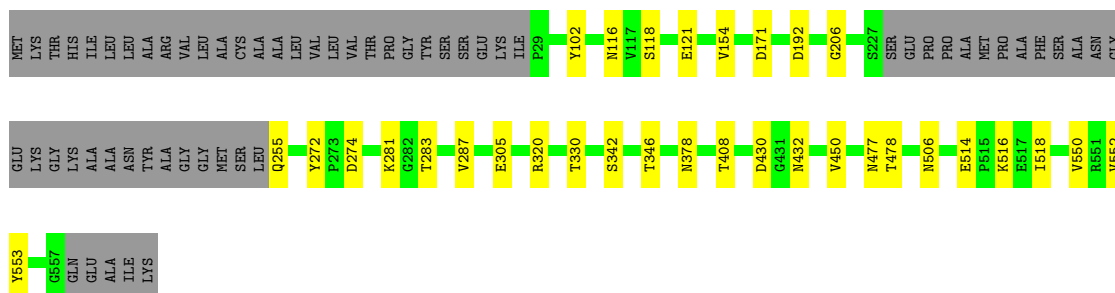
• Molecule 7: Type 3 secretion system secretin

Chain 5J: 86% 5% 10%



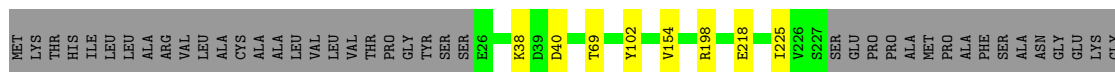
• Molecule 7: Type 3 secretion system secretin

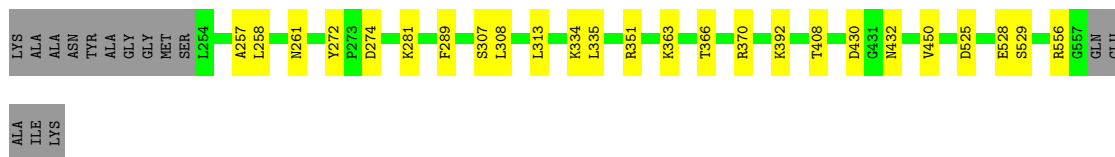
Chain 5K: 83% 6% 11%



• Molecule 7: Type 3 secretion system secretin

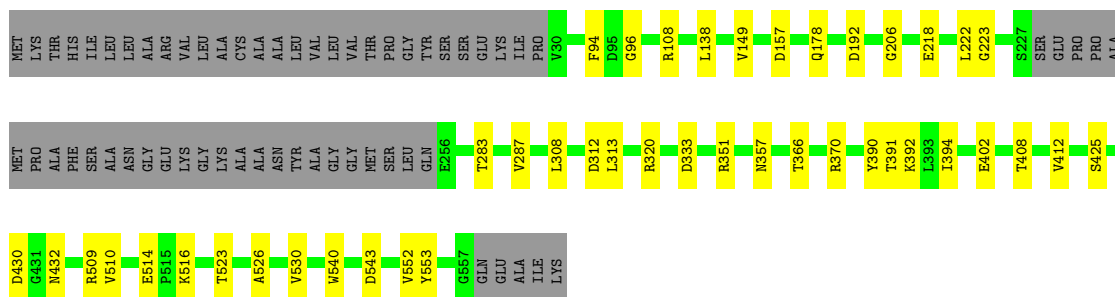
Chain 5L: 84% 6% 10%





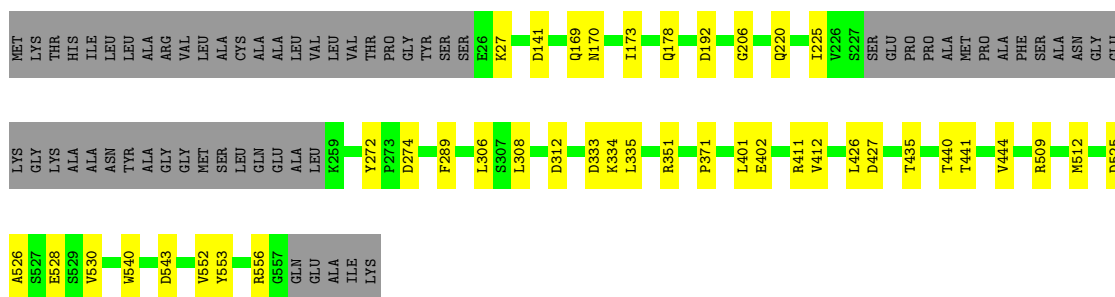
• Molecule 7: Type 3 secretion system secretin

Chain 5M: 81% 8% 11%



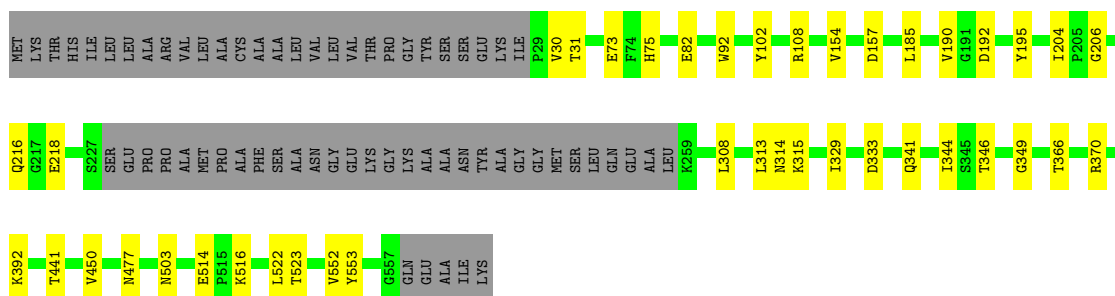
• Molecule 7: Type 3 secretion system secretin

Chain 5N: 82% 7% 11%



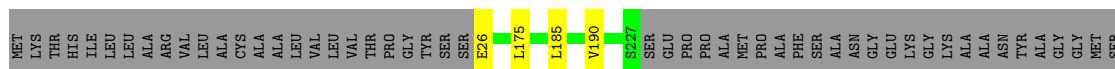
• Molecule 7: Type 3 secretion system secretin

Chain 5O: 81% 7% 11%

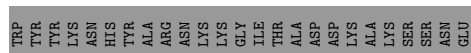


• Molecule 7: Type 3 secretion system secretin

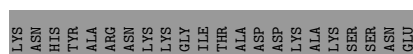
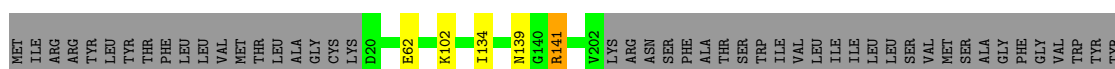
Chain 5P: 85% 11%



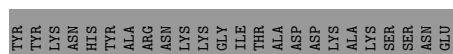
• Molecule 8: Lipoprotein PrgK



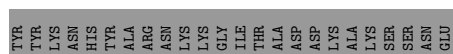
• Molecule 8: Lipoprotein PrgK



• Molecule 8: Lipoprotein PrgK

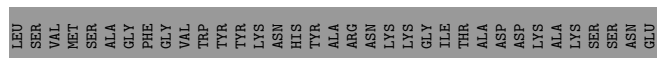


• Molecule 8: Lipoprotein PrgK



• Molecule 8: Lipoprotein PrgK

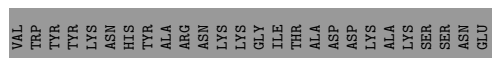




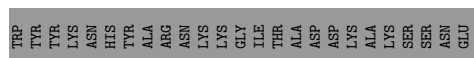
• Molecule 8: Lipoprotein PrgK



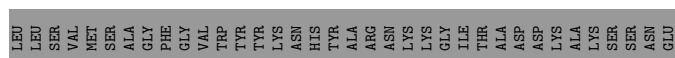
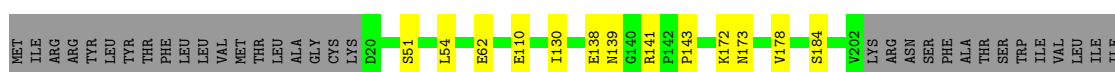
• Molecule 8: Lipoprotein PrgK



• Molecule 8: Lipoprotein PrgK



• Molecule 8: Lipoprotein PrgK



• Molecule 8: Lipoprotein PrgK



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

• Molecule 8: Lipoprotein PrgK



MET
ILE
ARG
TYR
LEU
THR
PHE
LEU
LEU
VAL
MET
THR
LEU
ALA
GLY
CYS
LYS
D20
E62
K102
I134
D166
N173
S184
R190
S191
V202
LYS
ARG
ASN
PHE
SER
PHE
ALA
THR
SER
TRP
ILE
VAL
LEU
ILE
LEU
SER
VAL
MET
SER
ALA
GLY
PHE

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

• Molecule 8: Lipoprotein PrgK



MET
ILE
ARG
TYR
LEU
THR
PHE
LEU
LEU
VAL
MET
THR
LEU
ALA
GLY
CYS
LYS
D20
E62
K102
I134
N139
G140
R141
N173
S184
Q194
V202
LYS
ARG
ASN
SER
PHE
PHE
ALA
THR
SER
TRP
ILE
VAL
LEU
ILE
LEU
SER
VAL
MET
SER
ALA
GLY
PHE

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

• Molecule 8: Lipoprotein PrgK



MET
ILE
ARG
TYR
LEU
THR
PHE
LEU
LEU
VAL
MET
THR
LEU
ALA
GLY
CYS
LYS
D20
E62
R80
K102
I134
N173
S184
V202
LYS
ARG
ASN
SER
PHE
PHE
ALA
THR
SER
TRP
ILE
VAL
LEU
ILE
LEU
SER
VAL
MET
SER
ALA
GLY
PHE
GLY
VAL
TRP

TYR
TYR
LYS
ASN
HIS
TYR
ALA
ARG
ASN
LYS
LYS
GLY
ILE
THR
ALA
ASP
ASP
LYS
LYS
ALA
SER
SER
ASN
GLU

• Molecule 8: Lipoprotein PrgK



MET
ILE
ARG
TYR
LEU
THR
PHE
LEU
LEU
VAL
MET
THR
LEU
ALA
GLY
CYS
LYS
D20
E62
R99
K102
E110
I130
I134
E138
N173
S184
Q194
V202
LYS
ARG
ASN
PHE
SER
PHE
ALA
THR
SER
TRP
ILE
VAL
LEU
ILE
LEU
SER
VAL
MET
SER
ALA
GLY
PHE
LEU
LEU
VAL

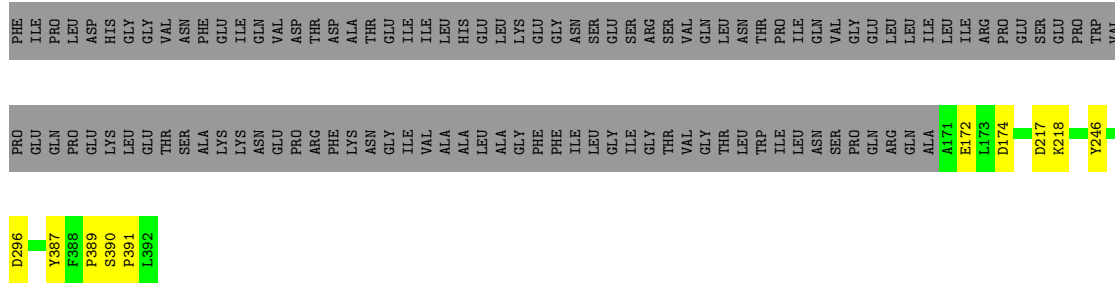
MET
SER
ALA
GLY
PHE
GLY
VAL
TRP
TYR
TYR
LYS
ASN
HIS
TYR
ALA
ARG
ASN
LYS
LYS
GLY
ILE
THR
ALA
ASP
ASP
LYS
LYS
ALA
SER
SER
ASN
GLU

• Molecule 8: Lipoprotein PrgK

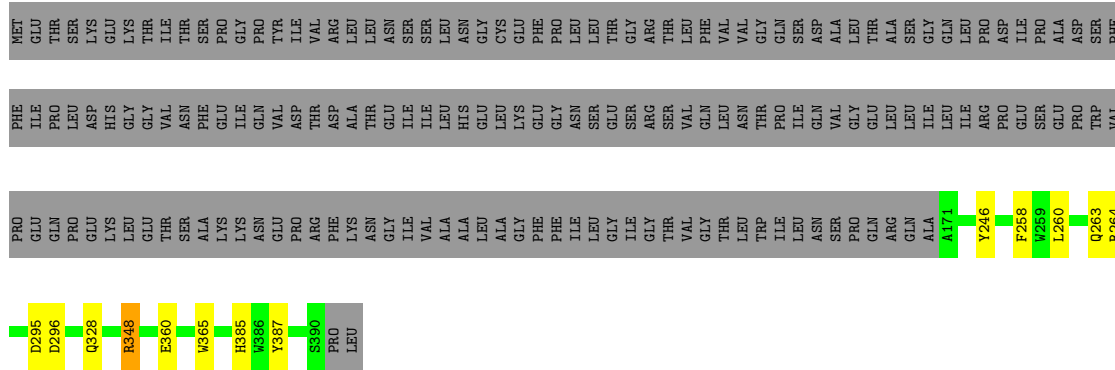


MET
ILE
ARG
TYR
LEU
THR
PHE
LEU
LEU
VAL
MET
THR
LEU
ALA
GLY
CYS
LYS
D20
I44
E62
P63
D64
E110
I130
S131
H147
N173
S184
R190
S191
V202
LYS
ARG
ASN
PHE
SER
PHE
ALA
THR
SER
TRP
ILE
VAL
LEU
ILE
LEU
SER
VAL
MET
SER
ALA
GLY
PHE
LEU
LEU
VAL

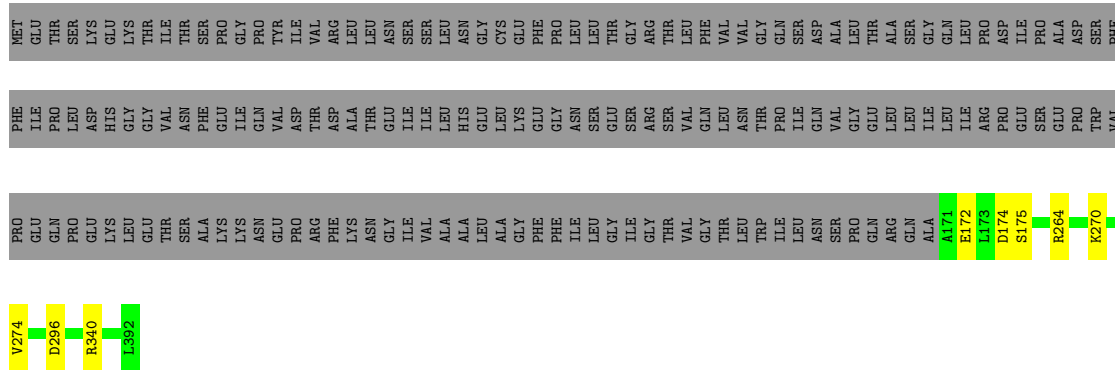
MET
SER
ALA
GLY
PHE
GLY
VAL
TRP
TYR
TYR
LYS
ASN
HIS
TYR
ALA
ARG
ASN
LYS
LYS
GLY
ILE
THR
ALA
ASP
ASP
LYS
LYS
ALA
SER
SER
ASN
GLU



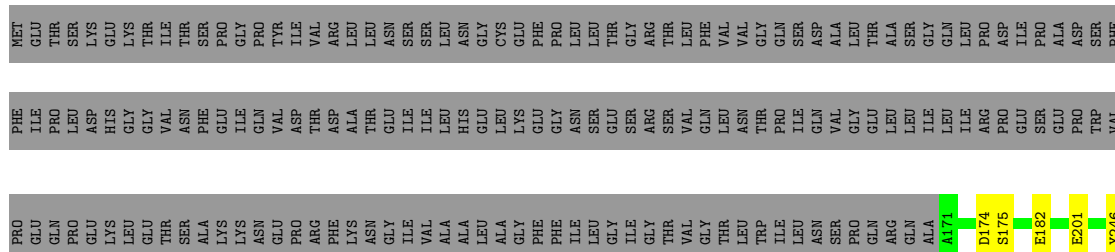
• Molecule 9: Protein PrgH



• Molecule 9: Protein PrgH



• Molecule 9: Protein PrgH





• Molecule 9: Protein PrgH



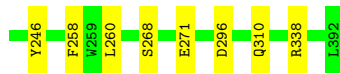
MET	GLU	THR	THR	LEU	ASP	GLY	LYS	THR	ILE	THR	THR	PRO	PRO	TYR	ILE	VAL	ARG	LEU	LEU	ASN	GLY	CYS	GLU	PHE	PRO	LEU	THR	ARG	THR	PHE	VAL	VAL	GLN	GLY	GLN	ASP	ALA	THR	LEU	GLN	PRO	ASP	ILE	PRO	ALA	ASP	TRP	ASP	PHE				
PHE	ILE	PRO	LEU	ASP	HIS	GLY	GLY	VAL	THR	ASN	PHE	GLU	LYS	ILE	GLN	VAL	THR	ASP	ALA	THR	LEU	HIS	GLU	LYS	PHE	GLY	ASN	LEU	THR	VAL	GLN	LEU	ASN	THR	TRP	THR	ILE	VAL	GLY	GLN	ARG	PRO	ASP	ILE	GLU	TRP	PRO	TRP	VAL				
PRO	GLU	GLN	PRO	GLY	LYS	LEU	GLY	THR	THR	ALA	ALA	LYS	ASN	GLU	PRO	ARG	PHE	LYS	ASN	GLY	ASN	ALA	ALA	PHE	PHE	ILE	LEU	THR	VAL	GLY	THR	VAL	THR	TRP	ILE	LEU	ASN	SER	ALA	PRO	GLY	GLN	ARG	LEU	GLN	ALA	A173	D174	S175	E182	N200	E201	R202



• Molecule 9: Protein PrgH



MET	GLU	THR	THR	LEU	ASP	GLY	LYS	THR	ILE	THR	THR	PRO	PRO	TYR	ILE	VAL	ARG	LEU	LEU	ASN	GLY	CYS	GLU	PHE	PRO	LEU	THR	ARG	THR	PHE	VAL	VAL	GLN	GLY	GLN	ASP	ALA	THR	LEU	GLN	PRO	ASP	ILE	PRO	ALA	ASP	TRP	ASP	PHE			
PHE	ILE	PRO	LEU	ASP	HIS	GLY	GLY	VAL	THR	ASN	PHE	GLU	LYS	ILE	GLN	VAL	THR	ALA	THR	LEU	HIS	GLU	LYS	PHE	GLY	ASN	LEU	THR	VAL	GLN	LEU	ASN	THR	TRP	THR	ILE	VAL	GLY	GLN	ARG	PRO	ASP	ILE	GLU	TRP	PRO	TRP	VAL				
PRO	GLU	GLN	PRO	GLY	LYS	LEU	GLY	THR	THR	ALA	ALA	LYS	ASN	GLU	PRO	ARG	PHE	LYS	ASN	GLY	ALA	ALA	PHE	PHE	ILE	LEU	THR	VAL	GLY	THR	VAL	THR	TRP	ILE	LEU	ASN	SER	ALA	PRO	GLY	GLN	ARG	LEU	GLN	ALA	A171	E172	L173	D174	N200	D203	I234



• Molecule 9: Protein PrgH



MET	GLU	THR	THR	LEU	ASP	GLY	LYS	THR	ILE	THR	THR	PRO	PRO	TYR	ILE	VAL	ARG	LEU	LEU	ASN	GLY	CYS	GLU	PHE	PRO	LEU	THR	ARG	THR	PHE	VAL	VAL	GLN	GLY	GLN	ASP	ALA	THR	LEU	GLN	PRO	ASP	ILE	PRO	ALA	ASP	TRP	ASP	PHE		
PHE	ILE	PRO	LEU	ASP	HIS	GLY	GLY	VAL	THR	ASN	PHE	GLU	LYS	ILE	GLN	VAL	THR	ALA	THR	LEU	HIS	GLU	LYS	PHE	GLY	ASN	LEU	THR	VAL	GLN	LEU	ASN	THR	TRP	THR	ILE	VAL	GLY	GLN	ARG	PRO	ASP	ILE	GLU	TRP	PRO	TRP	VAL			
PRO	GLU	GLN	PRO	GLY	LYS	LEU	GLY	THR	THR	ALA	ALA	LYS	ASN	GLU	PRO	ARG	PHE	LYS	ASN	GLY	ALA	ALA	PHE	PHE	ILE	LEU	THR	VAL	GLY	THR	VAL	THR	TRP	ILE	LEU	ASN	SER	ALA	PRO	GLY	GLN	ARG	LEU	GLN	ALA	A173	N200	D203	Y246	F258	W259



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

5 Model quality

5.1 Standard geometry

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

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	0.52	0/1805	0.56	0/2448
1	1B	0.52	0/1805	0.57	0/2448
1	1C	0.51	0/1805	0.58	0/2448
1	1D	0.55	0/1784	0.59	0/2419
1	1E	0.55	0/1792	0.59	0/2430
2	1F	0.54	0/2012	0.57	0/2754
3	1G	0.44	0/660	0.53	0/900
3	1H	0.48	0/660	0.56	0/900
3	1I	0.49	0/674	0.57	0/916
3	1J	0.50	0/674	0.59	0/916
4	1K	0.45	0/689	0.62	0/933
4	1L	0.51	0/719	0.58	0/974
4	1M	0.52	0/689	0.54	0/933
4	1N	0.51	0/682	0.59	0/923
4	1O	0.51	0/689	0.57	0/933
4	1P	0.52	0/689	0.56	0/933
6	2A	0.63	0/540	0.59	0/730
6	2B	0.64	0/480	0.56	0/649
6	2C	0.62	0/472	0.57	0/638
6	2D	0.58	0/628	0.57	0/853
6	2E	0.58	0/549	0.55	0/744
6	2F	0.63	0/592	0.57	0/801
6	2G	0.64	0/608	0.60	0/824
6	2H	0.63	0/592	0.57	0/801
6	2I	0.61	0/592	0.57	0/801
6	2J	0.64	0/592	0.58	0/801
6	2K	0.61	0/616	0.58	0/835
6	2L	0.62	0/623	0.58	0/846
6	2M	0.63	0/623	0.57	0/846
6	2N	0.61	0/623	0.56	0/846
6	2O	0.59	0/623	0.57	0/846
6	2P	0.60	0/616	0.61	0/835

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	2Q	0.59	0/623	0.59	0/846
6	2R	0.59	0/628	0.57	0/853
6	2S	0.58	0/623	0.58	0/846
6	2T	0.56	0/628	0.56	0/853
6	2U	0.55	0/623	0.53	0/846
6	2V	0.54	0/628	0.55	0/853
6	2W	0.55	0/628	0.56	0/853
6	2X	0.56	0/623	0.56	0/846
6	2Y	0.54	0/623	0.56	0/846
6	2Z	0.52	0/623	0.56	0/846
6	3A	0.49	0/628	0.55	0/853
6	3B	0.49	0/628	0.54	0/853
6	3C	0.48	0/623	0.55	0/846
6	3D	0.50	0/623	0.54	0/846
6	3E	0.49	0/623	0.53	0/846
6	3F	0.47	0/623	0.55	0/846
6	3G	0.46	0/628	0.52	0/853
6	3H	0.45	0/623	0.53	0/846
6	3I	0.45	0/623	0.53	0/846
6	3J	0.45	0/623	0.54	0/846
6	3K	0.43	0/623	0.52	0/846
6	3L	0.41	0/616	0.50	0/835
6	3M	0.39	0/623	0.50	0/846
6	3N	0.40	0/623	0.51	0/846
6	3O	0.39	0/616	0.51	0/835
6	3P	0.41	0/616	0.48	0/835
6	3Q	0.37	0/616	0.46	0/835
6	3R	0.38	0/616	0.51	0/835
6	3S	0.38	0/616	0.51	0/835
6	3T	0.36	0/616	0.48	0/835
6	3U	0.37	0/616	0.49	0/835
6	3V	0.37	0/616	0.49	0/835
6	3W	0.34	0/616	0.49	0/835
6	3X	0.34	0/616	0.51	0/835
6	3Y	0.35	0/616	0.49	0/835
6	3Z	0.34	0/616	0.50	0/835
6	4A	0.34	0/616	0.49	0/835
6	4B	0.32	0/616	0.48	0/835
6	4C	0.34	0/616	0.47	0/835
6	4D	0.33	0/616	0.48	0/835
6	4E	0.31	0/616	0.48	0/835
6	4F	0.34	0/616	0.51	0/835
6	4G	0.30	0/616	0.43	0/835

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	4H	0.31	0/616	0.46	0/835
6	4I	0.30	0/616	0.46	0/835
6	4J	0.31	0/616	0.49	0/835
6	4K	0.31	0/616	0.45	0/835
6	4L	0.31	0/616	0.44	0/835
6	4M	0.29	0/616	0.44	0/835
6	4N	0.29	0/616	0.44	0/835
6	4O	0.29	0/616	0.48	0/835
6	4P	0.29	0/616	0.48	0/835
6	4Q	0.29	0/616	0.47	0/835
6	4R	0.28	0/616	0.48	0/835
6	4S	0.27	0/616	0.45	0/835
6	4T	0.28	0/616	0.47	0/835
7	5A	0.55	0/1145	0.57	0/1545
7	5B	0.41	0/3978	0.57	0/5385
7	5C	0.40	0/3968	0.57	0/5372
7	5D	0.42	0/4011	0.56	0/5430
7	5E	0.43	0/3985	0.57	0/5395
7	5F	0.44	0/4011	0.58	0/5430
7	5G	0.44	0/3991	0.57	0/5403
7	5H	0.44	0/4011	0.60	0/5430
7	5I	0.44	0/3985	0.58	0/5395
7	5J	0.44	0/4025	0.58	0/5448
7	5K	0.42	0/3977	0.57	0/5384
7	5L	0.41	0/4011	0.57	0/5430
7	5M	0.41	0/3960	0.56	0/5361
7	5N	0.40	0/3972	0.56	0/5377
7	5O	0.40	0/3946	0.56	0/5342
7	5P	0.40	0/3963	0.54	0/5366
8	6A	0.52	0/1456	0.56	0/1978
8	6B	0.52	0/1456	0.55	0/1978
8	6C	0.53	0/1456	0.55	0/1978
8	6D	0.53	0/1456	0.55	0/1978
8	6E	0.52	0/1456	0.55	0/1978
8	6F	0.52	0/1456	0.54	0/1978
8	6G	0.51	0/1456	0.55	0/1978
8	6H	0.52	0/1456	0.56	0/1978
8	6I	0.51	0/1456	0.55	0/1978
8	6J	0.51	0/1456	0.56	0/1978
8	6K	0.51	0/1456	0.56	0/1978
8	6L	0.52	0/1456	0.55	0/1978
8	6M	0.52	0/1456	0.56	0/1978
8	6N	0.52	0/1456	0.56	0/1978

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	6O	0.51	0/1456	0.55	0/1978
8	6P	0.50	0/1456	0.56	0/1978
8	6Q	0.52	0/1456	0.54	0/1978
8	6R	0.51	0/1456	0.57	0/1978
8	6S	0.52	0/1456	0.56	0/1978
8	6T	0.52	0/1456	0.55	0/1978
8	6U	0.51	0/1456	0.53	0/1978
8	6V	0.51	0/1456	0.53	0/1978
8	6W	0.53	0/1456	0.56	0/1978
8	6X	0.52	0/1456	0.55	0/1978
9	7A	0.53	0/1864	0.54	0/2518
9	7B	0.51	0/1881	0.55	0/2541
9	7C	0.53	0/1881	0.56	0/2541
9	7D	0.54	0/1864	0.57	0/2518
9	7E	0.52	0/1881	0.56	0/2541
9	7F	0.53	0/1881	0.56	0/2541
9	7G	0.52	0/1864	0.56	0/2518
9	7H	0.51	0/1881	0.55	0/2541
9	7I	0.52	0/1881	0.55	0/2541
9	7J	0.53	0/1864	0.56	0/2518
9	7K	0.50	0/1881	0.55	0/2541
9	7L	0.52	0/1881	0.56	0/2541
9	7M	0.52	0/1864	0.56	0/2518
9	7N	0.51	0/1881	0.56	0/2541
9	7O	0.51	0/1881	0.56	0/2541
9	7P	0.52	0/1864	0.55	0/2518
9	7Q	0.49	0/1881	0.57	0/2541
9	7R	0.51	0/1881	0.55	0/2541
9	7S	0.51	0/1864	0.58	1/2518 (0.0%)
9	7T	0.49	0/1881	0.52	0/2541
9	7U	0.51	0/1881	0.54	0/2541
9	7V	0.52	0/1864	0.55	0/2518
9	7W	0.52	0/1881	0.56	0/2541
9	7X	0.53	0/1881	0.57	0/2541
All	All	0.48	0/202780	0.55	1/274731 (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

Continued on next page...

Continued from previous page...

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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
9	7S	348	ARG	NE-CZ-NH2	-7.24	116.68	120.30

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	10	0
1	1B	1767	1784	1810	8	0
1	1C	1767	1810	1810	5	0
1	1D	1746	1790	1790	2	0
1	1E	1754	1791	1794	2	0
2	1F	1960	2007	2008	5	0
3	1G	647	692	692	3	0
3	1H	647	692	692	2	0
3	1I	661	708	708	1	0
3	1J	661	708	708	1	0
4	1K	685	701	701	3	0
4	1L	714	726	726	4	0
4	1M	685	701	701	5	0
4	1N	678	692	692	1	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	3N	612	598	598	6	0
6	3O	605	592	592	3	0
6	3P	605	592	592	1	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	5	0
6	4B	605	592	592	7	0
6	4C	605	592	592	7	0
6	4D	605	592	592	6	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	7	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	5	0
6	4S	605	592	592	5	0
6	4T	605	592	592	7	0
7	5A	1122	1119	1119	4	0
7	5B	3913	3971	3970	33	0
7	5C	3903	3959	3958	25	0
7	5D	3946	4007	4006	36	0
7	5E	3920	3978	3977	20	0
7	5F	3946	4007	4006	21	0
7	5G	3926	3983	3982	28	0
7	5H	3946	4006	4006	21	0
7	5I	3920	3978	3977	27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	5J	3960	4021	4020	17	0
7	5K	3912	3967	3966	23	0
7	5L	3946	4008	4006	21	0
7	5M	3896	3951	3950	26	0
7	5N	3907	3966	3965	30	0
7	5O	3881	3936	3936	26	0
7	5P	3898	3953	3952	13	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	5	0
8	6E	1428	1421	1421	8	0
8	6F	1428	1421	1421	7	0
8	6G	1428	1421	1421	5	0
8	6H	1428	1421	1421	5	0
8	6I	1428	1421	1421	8	0
8	6J	1428	1421	1421	6	0
8	6K	1428	1421	1421	6	0
8	6L	1428	1421	1421	8	0
8	6M	1428	1421	1421	5	0
8	6N	1428	1421	1421	8	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	7	0
8	6S	1428	1420	1421	4	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	11	0
9	7A	1820	1782	1782	8	0
9	7B	1836	1800	1800	7	0
9	7C	1836	1800	1800	5	0
9	7D	1820	1782	1782	4	0
9	7E	1836	1800	1800	5	0
9	7F	1836	1800	1800	12	0
9	7G	1820	1782	1782	8	0
9	7H	1836	1800	1800	6	0
9	7I	1836	1800	1800	10	0
9	7J	1820	1782	1782	7	0
9	7K	1836	1800	1800	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	7L	1836	1800	1800	8	0
9	7M	1820	1782	1782	7	0
9	7N	1836	1800	1800	4	0
9	7O	1836	1800	1800	12	0
9	7P	1820	1782	1782	6	0
9	7Q	1836	1800	1800	10	0
9	7R	1836	1800	1800	6	0
9	7S	1820	1782	1782	7	0
9	7T	1836	1800	1800	5	0
9	7U	1836	1800	1800	9	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	924	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 2.

The worst 5 of 924 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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 [i](#)

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%)	197 (100%)	1 (0%)	88	93
1	1C	198/199 (100%)	197 (100%)	1 (0%)	88	93
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%)	88	93
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%)	78 (99%)	1 (1%)	69	82
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

Continued on next page...

Continued from previous page...

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%)	62 (98%)	1 (2%)	62	79
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%)	65 (98%)	1 (2%)	65	81
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%)	65 (98%)	1 (2%)	65	81
6	2U	66/67 (98%)	65 (98%)	1 (2%)	65	81
6	2V	66/67 (98%)	65 (98%)	1 (2%)	65	81
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%)	65 (98%)	1 (2%)	65	81
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

Continued on next page...

Continued from previous page...

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%)	64 (98%)	1 (2%)	65	81
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%)	63 (97%)	2 (3%)	40	67
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%)	64 (98%)	1 (2%)	65	81
6	4C	65/67 (97%)	65 (100%)	0	100	100
6	4D	65/67 (97%)	64 (98%)	1 (2%)	65	81
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%)	64 (98%)	1 (2%)	65	81
6	4I	65/67 (97%)	65 (100%)	0	100	100
6	4J	65/67 (97%)	64 (98%)	1 (2%)	65	81
6	4K	65/67 (97%)	65 (100%)	0	100	100
6	4L	65/67 (97%)	65 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	4M	65/67 (97%)	65 (100%)	0	100	100
6	4N	65/67 (97%)	64 (98%)	1 (2%)	65	81
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%)	64 (98%)	1 (2%)	65	81
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%)	434 (99%)	3 (1%)	84	90
7	5E	434/477 (91%)	433 (100%)	1 (0%)	93	97
7	5F	437/477 (92%)	436 (100%)	1 (0%)	93	97
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%)	435 (100%)	2 (0%)	88	93
7	5M	431/477 (90%)	429 (100%)	2 (0%)	88	93
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%)	431 (100%)	1 (0%)	93	97
8	6A	156/215 (73%)	156 (100%)	0	100	100
8	6B	156/215 (73%)	155 (99%)	1 (1%)	86	91
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

Continued on next page...

Continued from previous page...

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%)	155 (99%)	1 (1%)	86	91
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%)	189 (100%)	1 (0%)	88	93
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%)	189 (100%)	1 (0%)	88	93
9	7I	190/337 (56%)	190 (100%)	0	100	100
9	7J	188/337 (56%)	187 (100%)	1 (0%)	88	93
9	7K	190/337 (56%)	189 (100%)	1 (0%)	88	93
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%)	189 (100%)	1 (0%)	88	93

Continued on next page...

Continued from previous page...

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%)	189 (100%)	1 (0%)	88	93
9	7R	190/337 (56%)	190 (100%)	0	100	100
9	7S	188/337 (56%)	187 (100%)	1 (0%)	88	93
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%)	21501 (100%)	38 (0%)	93	97

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	5P	351	ARG
9	7N	388	PHE
8	6B	141	ARG
9	7H	388	PHE
9	7S	385	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
7	5J	341	GLN
7	5E	288	HIS
6	4B	61	GLN
6	4A	59	ASN
6	4L	59	ASN

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 monosaccharides 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	1L	201	-	33,33,47	1.03	4 (12%)	37,38,52	1.22	2 (5%)
11	LDA	1I	502	-	12,15,15	2.12	1 (8%)	14,17,17	0.67	0
11	LDA	1I	501	-	12,15,15	2.15	1 (8%)	14,17,17	0.66	0
11	LDA	1G	201	-	12,15,15	2.13	1 (8%)	14,17,17	0.82	0
10	3PH	1A	401	-	35,35,47	0.98	3 (8%)	39,40,52	1.24	2 (5%)
11	LDA	1H	101	-	12,15,15	2.14	1 (8%)	14,17,17	0.65	0
11	LDA	1D	301	-	12,15,15	2.10	1 (8%)	14,17,17	0.53	0
11	LDA	1J	402	-	12,15,15	2.15	1 (8%)	14,17,17	0.67	0
11	LDA	1A	402	-	12,15,15	2.09	1 (8%)	14,17,17	0.83	0
11	LDA	1I	503	-	12,15,15	2.12	1 (8%)	14,17,17	0.69	0
11	LDA	1J	401	-	12,15,15	2.17	1 (8%)	14,17,17	1.04	1 (7%)
10	3PH	1M	201	-	33,33,47	0.99	3 (9%)	37,38,52	1.16	2 (5%)
10	3PH	1N	601	-	33,33,47	1.02	3 (9%)	37,38,52	1.22	2 (5%)
10	3PH	1P	201	-	45,45,47	0.91	4 (8%)	49,50,52	1.05	2 (4%)

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	1L	201	-	-	11/35/35/49	-
11	LDA	1I	502	-	-	2/13/13/13	-
11	LDA	1I	501	-	-	0/13/13/13	-
11	LDA	1G	201	-	-	3/13/13/13	-
10	3PH	1A	401	-	-	16/37/37/49	-
11	LDA	1H	101	-	-	1/13/13/13	-
11	LDA	1D	301	-	-	5/13/13/13	-
11	LDA	1J	402	-	-	4/13/13/13	-
11	LDA	1A	402	-	-	2/13/13/13	-
11	LDA	1I	503	-	-	0/13/13/13	-
11	LDA	1J	401	-	-	0/13/13/13	-
10	3PH	1M	201	-	-	16/35/35/49	-
10	3PH	1N	601	-	-	23/35/35/49	-
10	3PH	1P	201	-	-	29/47/47/49	-

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1J	401	LDA	O1-N1	-7.46	1.24	1.42
11	1J	402	LDA	O1-N1	-7.43	1.24	1.42
11	1I	501	LDA	O1-N1	-7.39	1.24	1.42
11	1H	101	LDA	O1-N1	-7.38	1.24	1.42
11	1G	201	LDA	O1-N1	-7.34	1.25	1.42

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	1A	401	3PH	O21-C21-C22	5.11	122.52	111.50
10	1N	601	3PH	O21-C21-C22	4.51	121.22	111.50
10	1P	201	3PH	O21-C21-C22	4.37	120.91	111.50
10	1M	201	3PH	O21-C21-C22	4.33	120.84	111.50
10	1L	201	3PH	O21-C21-C22	4.29	120.74	111.50

There are no chirality outliers.

5 of 112 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

Continued on next page...

Continued from previous page...

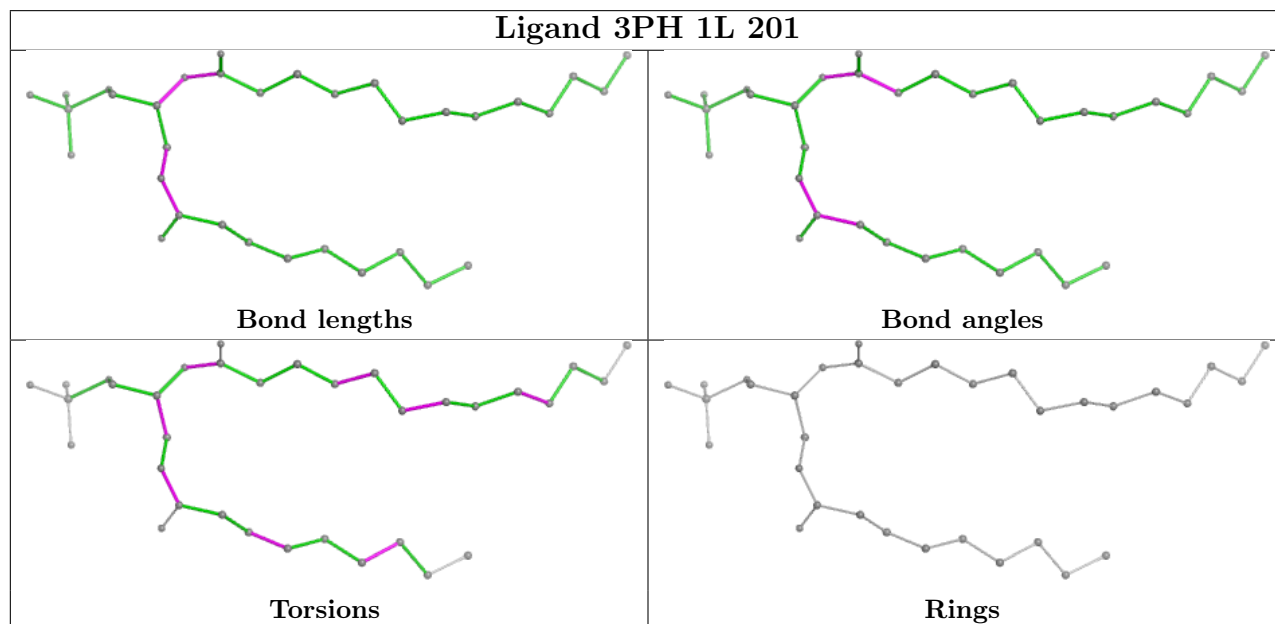
Mol	Chain	Res	Type	Atoms
10	1M	201	3PH	C1-O11-P-O13
10	1M	201	3PH	C1-O11-P-O14

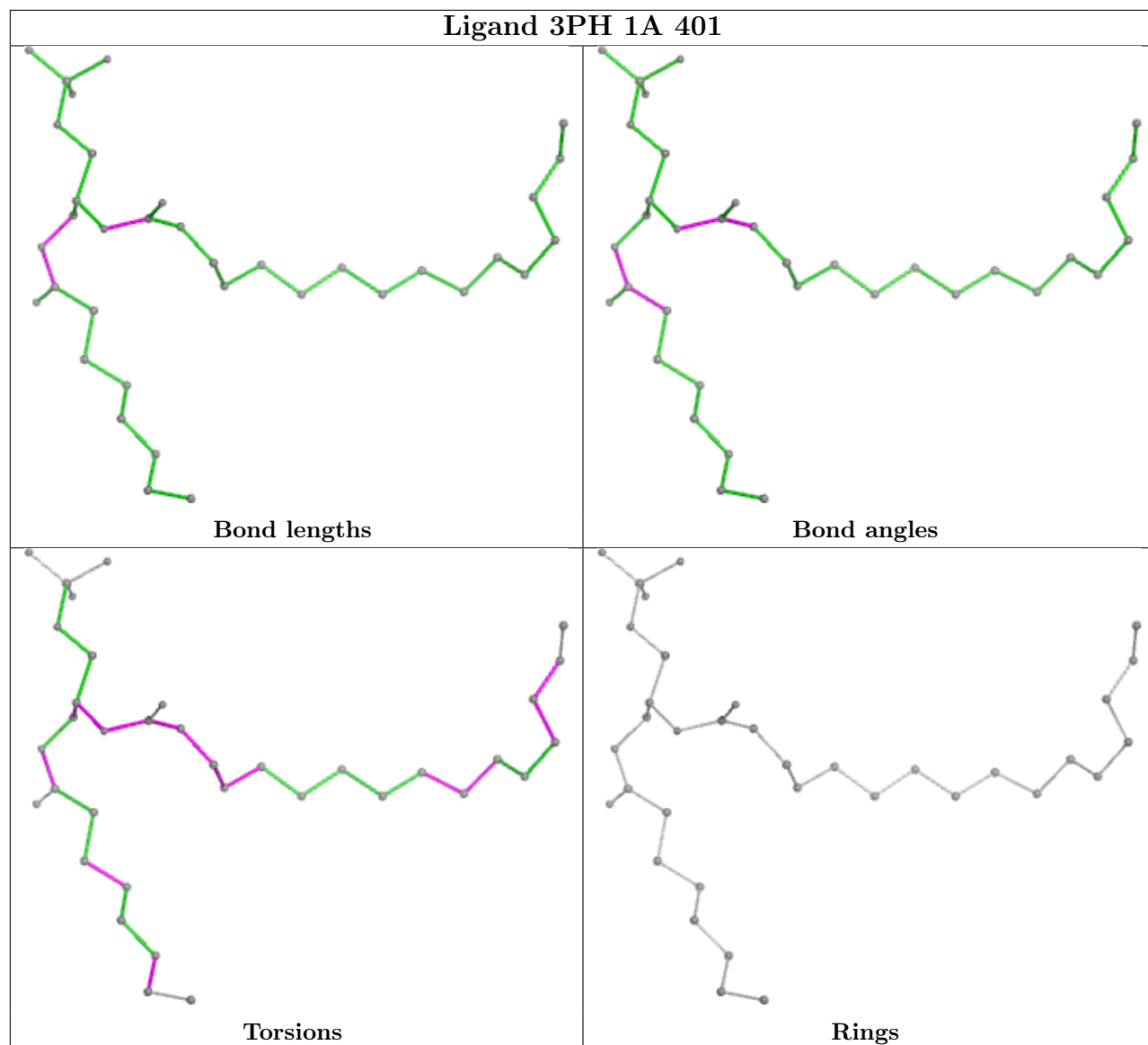
There are no ring outliers.

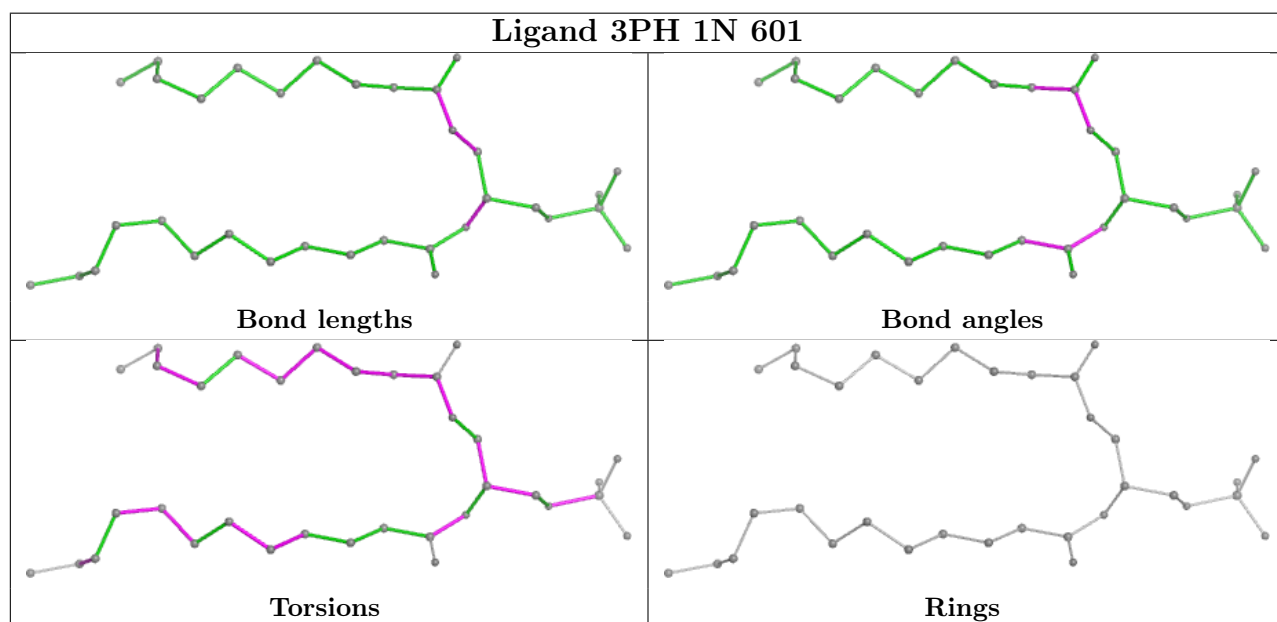
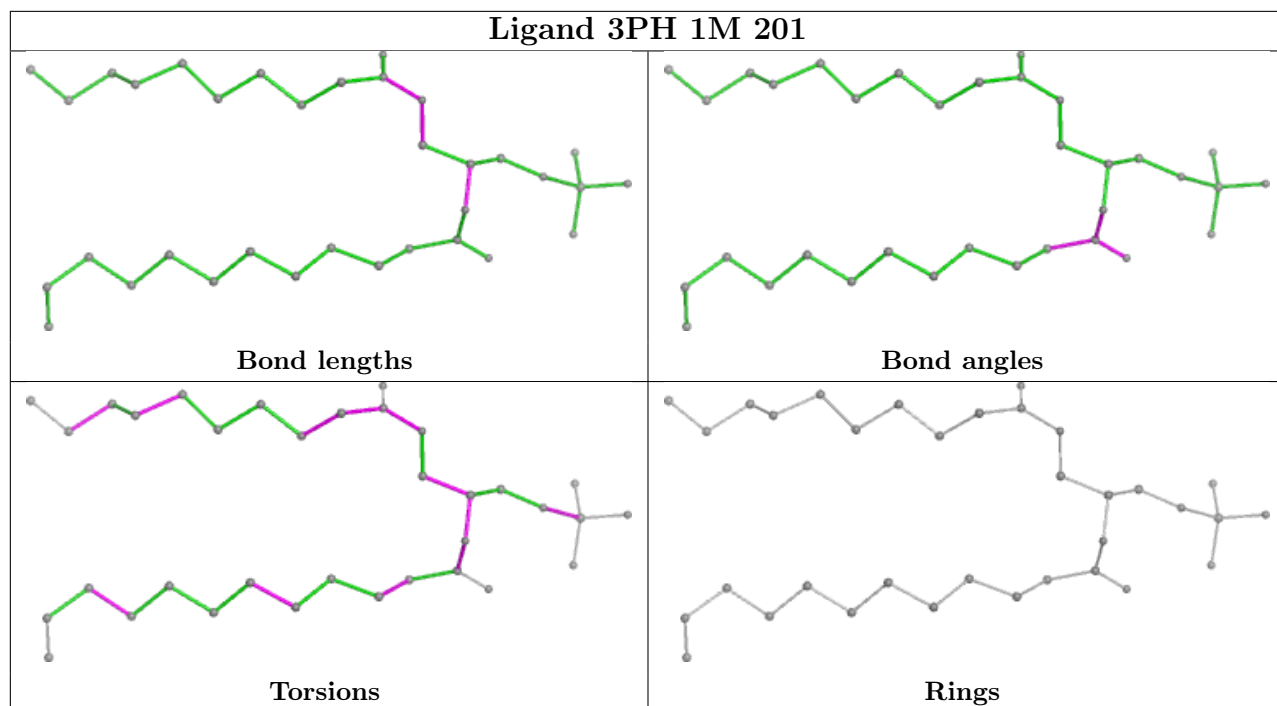
4 monomers are involved in 4 short contacts:

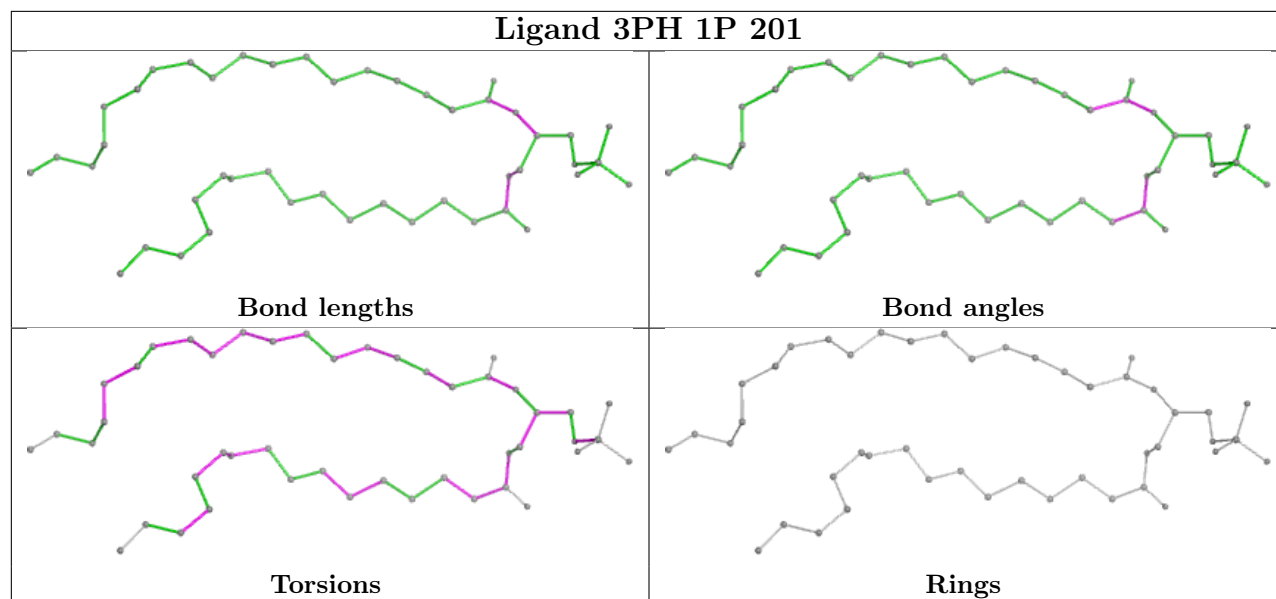
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	1I	501	LDA	1	0
11	1G	201	LDA	1	0
10	1A	401	3PH	1	0
10	1N	601	3PH	1	0

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.