



Full wwPDB EM Validation 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 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 : **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

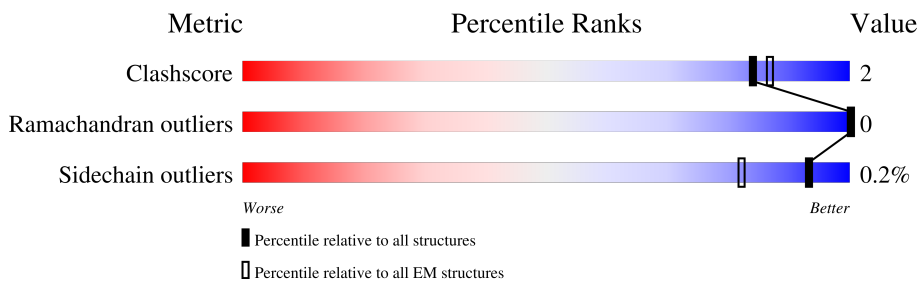
1 Overall quality at a glance i

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% .

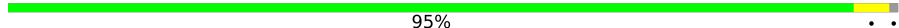
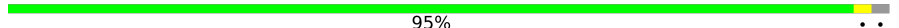
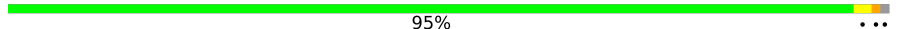
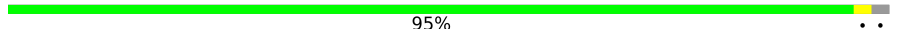




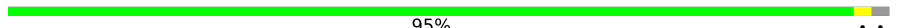
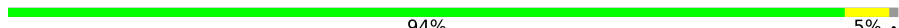

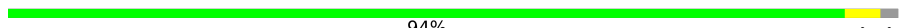
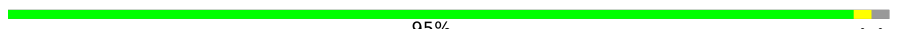
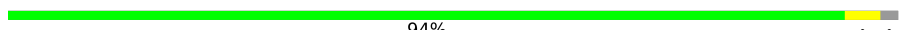

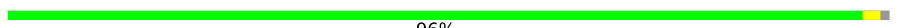
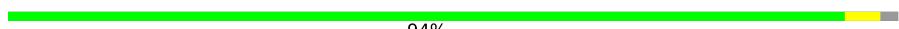


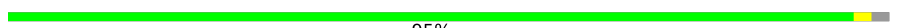





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Mol	Chain	Length	Quality of chain
3	1J	86	99%
4	1K	101	85% 11%
4	1L	101	88% 5% 7%
4	1M	101	85% 11%
4	1N	101	87% 12%
4	1O	101	82% 7% 11%
4	1P	101	86% 11%
5	1Z	141	100%
6	2A	80	76% 9% 15%
6	2B	80	74% 25%
6	2C	80	70% 26%
6	2D	80	98%
6	2E	80	84% 15%
6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

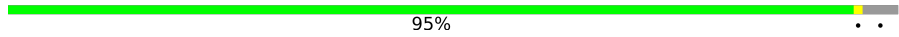
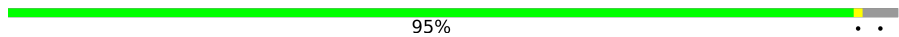








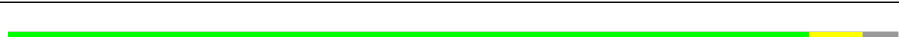


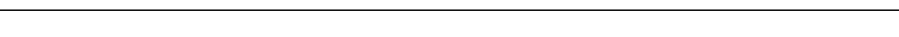
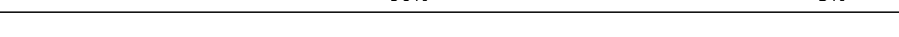
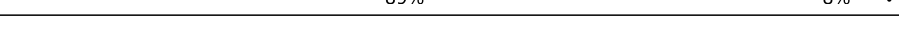

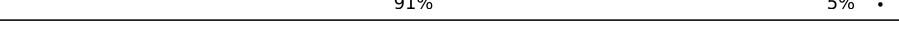

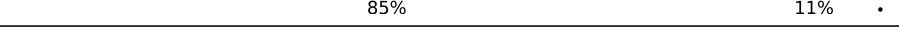




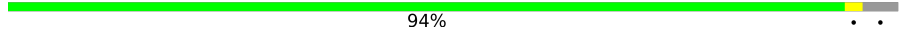
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Mol	Chain	Length	Quality of chain
6	2R	80	95% 
6	2S	80	95% 
6	2T	80	95% 
6	2U	80	95% 
6	2V	80	92% 
6	2W	80	94% 
6	2X	80	94% 
6	2Y	80	89% 
6	2Z	80	95% 
6	3A	80	94% 
6	3B	80	92% 
6	3C	80	94% 
6	3D	80	95% 
6	3E	80	94% 
6	3F	80	89% 
6	3G	80	96% 
6	3H	80	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% 









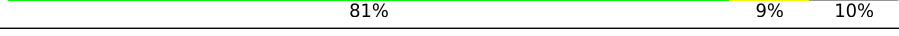

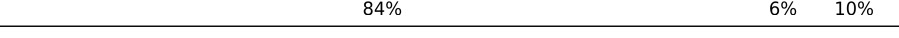
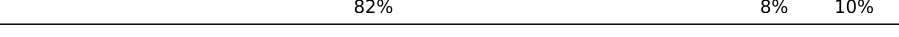

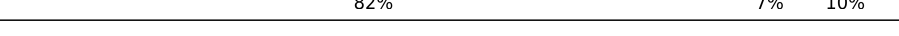


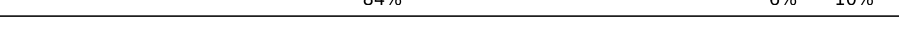

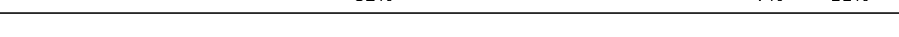






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Mol	Chain	Length	Quality of chain
6	3Q	80	 95% . .
6	3R	80	 95% . .
6	3S	80	 90% 6% .
6	3T	80	 84% 12% .
6	3U	80	 91% 5% .
6	3V	80	 89% 8% .
6	3W	80	 86% 10% .
6	3X	80	 84% 11% . .
6	3Y	80	 78% 19% .
6	3Z	80	 82% 14% .
6	4A	80	 90% 6% .
6	4B	80	 85% 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% .











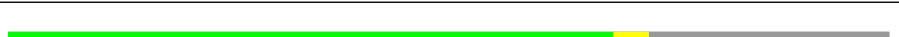


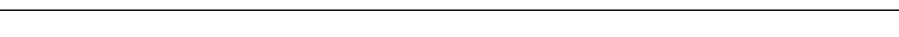
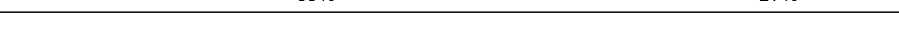
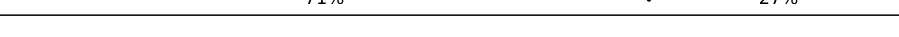



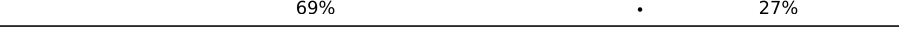





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Mol	Chain	Length	Quality of chain
6	4P	80	 82% 14%
6	4Q	80	 82% 14%
6	4R	80	 85% 11%
6	4S	80	 88% 9%
6	4T	80	 82% 14%
7	5A	562	 24% 75%
7	5B	562	 80% 9% 11%
7	5C	562	 82% 7% 11%
7	5D	562	 81% 9% 10%
7	5E	562	 84% 5% 10%
7	5F	562	 84% 6% 10%
7	5G	562	 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% 1% 11%
8	6A	252	 70% 27%
8	6B	252	 71% 27%
8	6C	252	 70% 27%
8	6D	252	 70% 27%

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Mol	Chain	Length	Quality of chain
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	
9	7A	392	
9	7B	392	
9	7C	392	
9	7D	392	
9	7E	392	

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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	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
			Total	C	H	N	O	S		
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
			Total	C	H	N	O	S		
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	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			

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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
			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

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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
			Total	C	H	N	O	S		
7	5A	141	Total 2241	C 719	H 1119	N 191	O 206	S 6	0	0
7	5B	502	Total 7884	C 2474	H 3971	N 680	O 747	S 12	0	0
7	5C	501	Total 7862	C 2468	H 3959	N 678	O 745	S 12	0	0
7	5D	506	Total 7953	C 2496	H 4007	N 685	O 753	S 12	0	0
7	5E	503	Total 7898	C 2479	H 3978	N 681	O 748	S 12	0	0
7	5F	506	Total 7953	C 2496	H 4007	N 685	O 753	S 12	0	0
7	5G	504	Total 7909	C 2482	H 3983	N 682	O 750	S 12	0	0
7	5H	506	Total 7952	C 2496	H 4006	N 685	O 753	S 12	0	0
7	5I	503	Total 7898	C 2479	H 3978	N 681	O 748	S 12	0	0
7	5J	508	Total 7981	C 2504	H 4021	N 687	O 756	S 13	0	0
7	5K	502	Total 7879	C 2473	H 3967	N 680	O 747	S 12	0	0
7	5L	506	Total 7954	C 2496	H 4008	N 685	O 753	S 12	0	0
7	5M	500	Total 7847	C 2463	H 3951	N 677	O 744	S 12	0	0
7	5N	501	Total 7873	C 2471	H 3966	N 679	O 745	S 12	0	0
7	5O	498	Total 7817	C 2454	H 3936	N 675	O 740	S 12	0	0
7	5P	500	Total 7851	C 2465	H 3953	N 677	O 744	S 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	Total 2849	C 899	H 1421	N 248	O 278	S 3	0	0
8	6B	183	Total 2849	C 899	H 1421	N 248	O 278	S 3	0	0
8	6C	183	Total 2849	C 899	H 1421	N 248	O 278	S 3	0	0
8	6D	183	Total 2849	C 899	H 1421	N 248	O 278	S 3	0	0

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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.

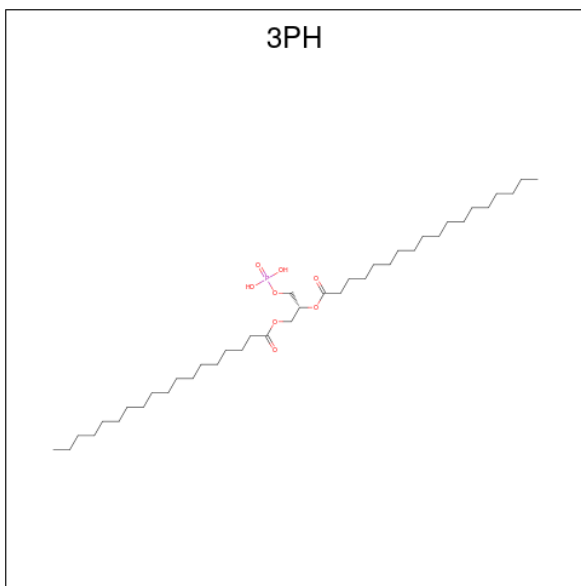
Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	7A	220	3602	1159	1782	324	332	5	0	0
9	7B	222	3636	1170	1800	326	335	5	0	0
9	7C	222	3636	1170	1800	326	335	5	0	0
9	7D	220	3602	1159	1782	324	332	5	0	0
9	7E	222	3636	1170	1800	326	335	5	0	0
9	7F	222	3636	1170	1800	326	335	5	0	0
9	7G	220	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

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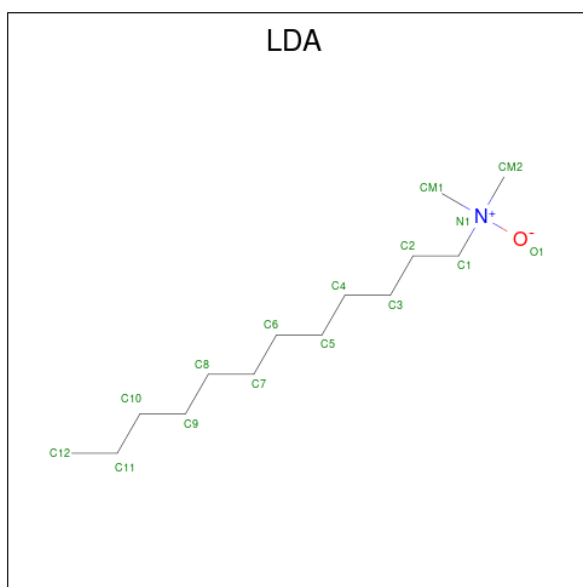
Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	7W	222	Total	C	H	N	O	S	0	0
			3636	1170	1800	326	335	5		
9	7X	222	Total	C	H	N	O	S	0	0
			3636	1170	1800	326	335	5		

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



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: $C_{14}H_{31}NO$).



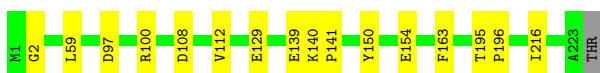
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
11	1A	1	Total	C	H	N	O	0
			47	14	31	1	1	
11	1D	1	Total	C	H	N	O	0
			47	14	31	1	1	
11	1G	1	Total	C	H	N	O	0
			47	14	31	1	1	
11	1H	1	Total	C	H	N	O	0
			47	14	31	1	1	
11	1I	1	Total	C	H	N	O	0
			47	14	31	1	1	
11	1I	1	Total	C	H	N	O	0
			47	14	31	1	1	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



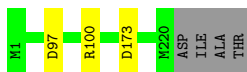
- Molecule 1: Surface presentation of antigens protein SpaP

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% ..

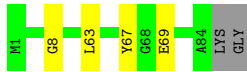


- Molecule 2: Surface presentation of antigens protein SpaR

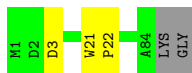
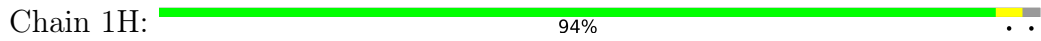
Chain 1F:  94% ..



- Molecule 3: Surface presentation of antigens protein SpaQ



- Molecule 3: Surface presentation of antigens protein SpaQ



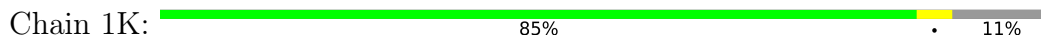
- Molecule 3: Surface presentation of antigens protein SpaQ



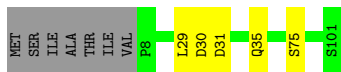
- Molecule 3: Surface presentation of antigens protein SpaQ



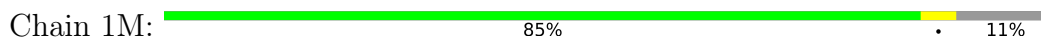
- Molecule 4: Protein PrgJ

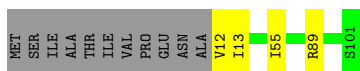


- Molecule 4: Protein PrgJ

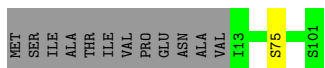


- Molecule 4: Protein PrgJ

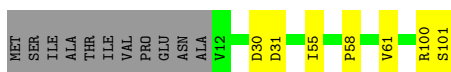
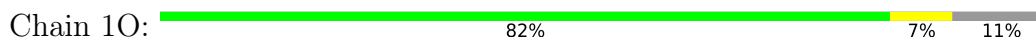




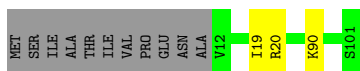
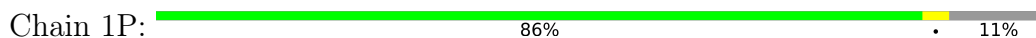
- Molecule 4: Protein PrgJ



- Molecule 4: Protein PrgJ



- Molecule 4: Protein PrgJ

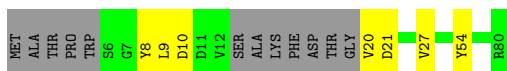
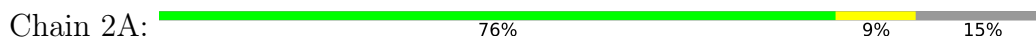


- Molecule 5: SptP3x-GFP-FLAG

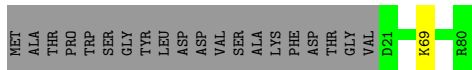
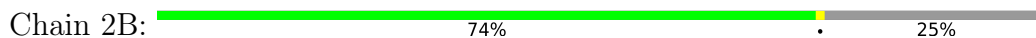


There are no outlier residues recorded for this chain.

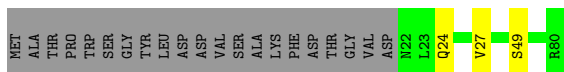
- Molecule 6: Protein PrgI



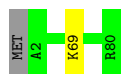
- Molecule 6: Protein PrgI



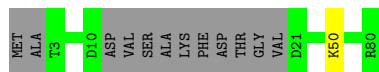
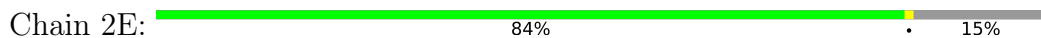
- Molecule 6: Protein PrgI



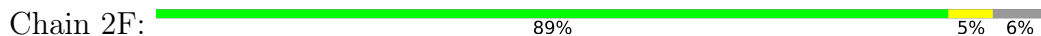
• Molecule 6: Protein PrgI



• Molecule 6: Protein PrgI



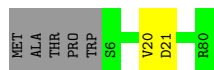
• Molecule 6: Protein PrgI



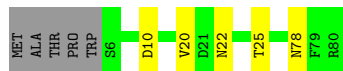
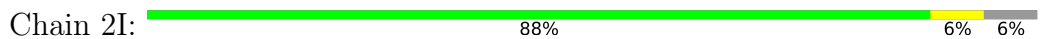
• Molecule 6: Protein PrgI



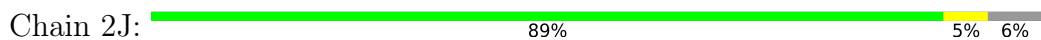
• Molecule 6: Protein PrgI



• Molecule 6: Protein PrgI

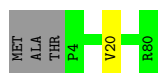


• Molecule 6: Protein PrgI



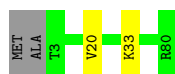
• Molecule 6: Protein PrgI

Chain 2K:  95% ..



● Molecule 6: Protein PrgI

Chain 2L:  95% ..



● Molecule 6: Protein PrgI

Chain 2M:  90% 8% .




● Molecule 6: Protein PrgI

Chain 2N:  92% 5% .



● Molecule 6: Protein PrgI

Chain 2O:  86% 11% .



● Molecule 6: Protein PrgI

Chain 2P:  92% ..



● Molecule 6: Protein PrgI

Chain 2Q:  92% 5% .



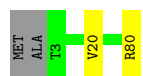
● Molecule 6: Protein PrgI

Chain 2R:  95% ..



● Molecule 6: Protein PrgI

Chain 2S:  95% ..



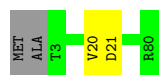
● Molecule 6: Protein PrgI

Chain 2T:  95% ...



● Molecule 6: Protein PrgI

Chain 2U:  95% ..



● Molecule 6: Protein PrgI

Chain 2V:  92% 6% .



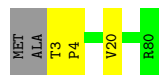
● Molecule 6: Protein PrgI

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%



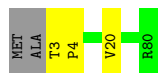
● Molecule 6: Protein PrgI

Chain 3D:  95%




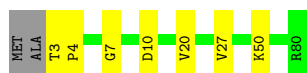
● Molecule 6: Protein PrgI

Chain 3E:  94%



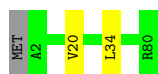
● Molecule 6: Protein PrgI

Chain 3F:  89% 9%



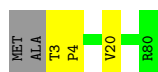
● Molecule 6: Protein PrgI

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%



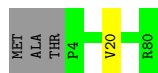
● Molecule 6: Protein PrgI

Chain 3O:  91% 5%



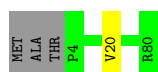
● Molecule 6: Protein PrgI

Chain 3P:  95%



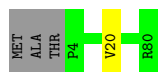
● Molecule 6: Protein PrgI

Chain 3Q:  95%




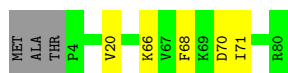
● Molecule 6: Protein PrgI

Chain 3R:  95%

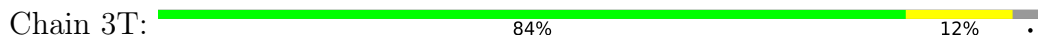


● Molecule 6: Protein PrgI

Chain 3S:  90% 6%



● Molecule 6: Protein PrgI



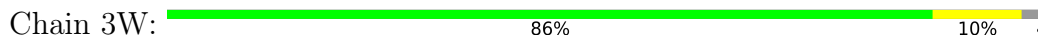
● Molecule 6: Protein PrgI



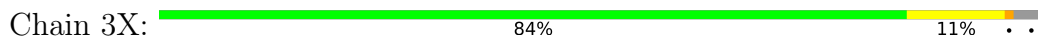
● Molecule 6: Protein PrgI



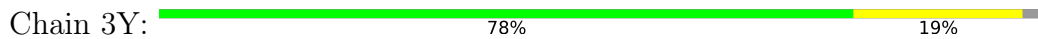
● Molecule 6: Protein PrgI



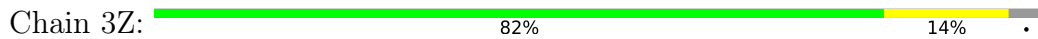
● Molecule 6: Protein PrgI




● Molecule 6: Protein PrgI

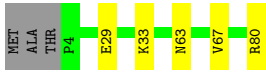


● Molecule 6: Protein PrgI




● Molecule 6: Protein PrgI

Chain 4A:  90% 6%




● Molecule 6: Protein PrgI

Chain 4B:  85% 11%



● Molecule 6: Protein PrgI

Chain 4C:  85% 11%




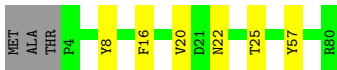
● Molecule 6: Protein PrgI

Chain 4D:  90% 5%




● Molecule 6: Protein PrgI

Chain 4E:  89% 8%



● Molecule 6: Protein PrgI

Chain 4F:  88% 9%

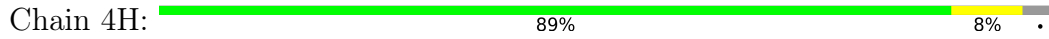


● Molecule 6: Protein PrgI

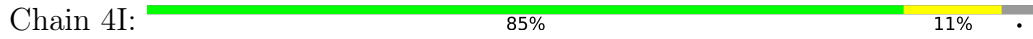
Chain 4G:  91% 5%



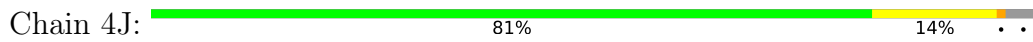
● Molecule 6: Protein PrgI



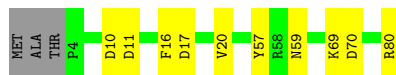
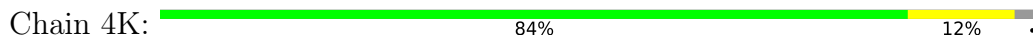
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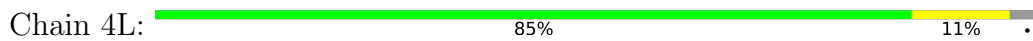
● Molecule 6: Protein PrgI



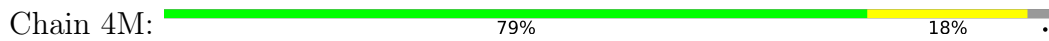
● Molecule 6: Protein PrgI



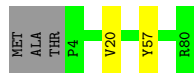
● Molecule 6: Protein PrgI



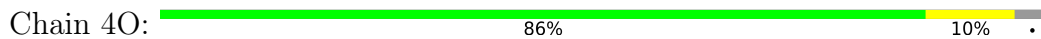
● Molecule 6: Protein PrgI



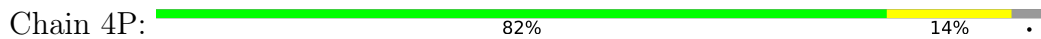
● Molecule 6: Protein PrgI



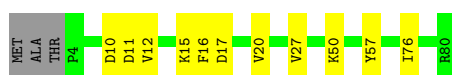
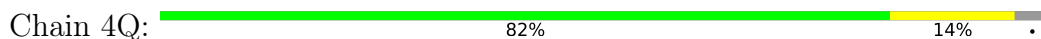
● Molecule 6: Protein PrgI



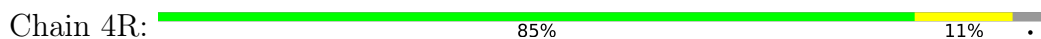
• Molecule 6: Protein PrgI



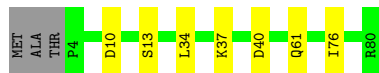
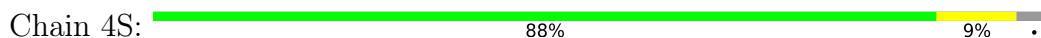
• Molecule 6: Protein PrgI



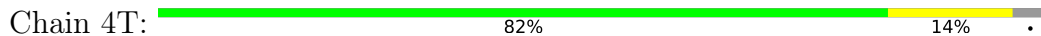
• Molecule 6: Protein PrgI



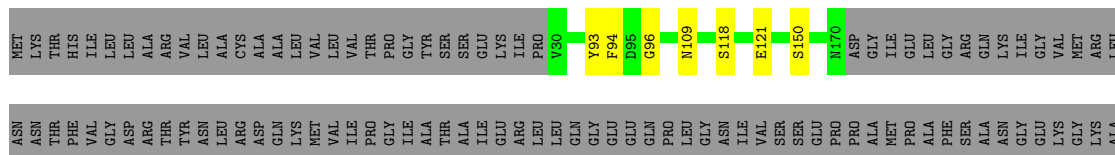
• Molecule 6: Protein PrgI

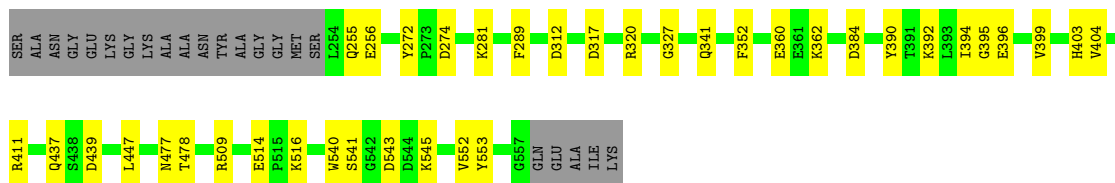


• Molecule 6: Protein PrgI

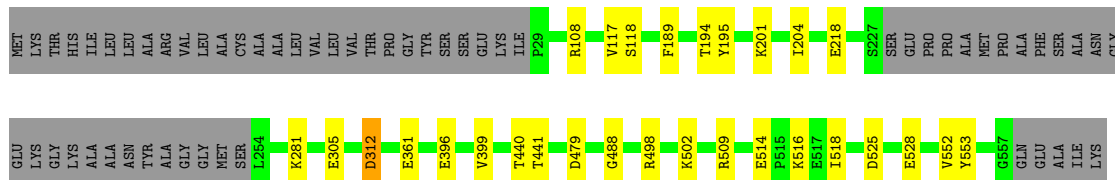
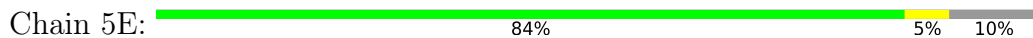


• Molecule 7: Type 3 secretion system secretin

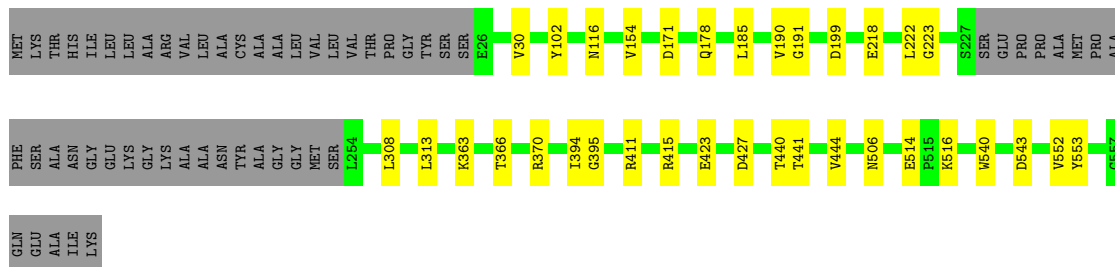
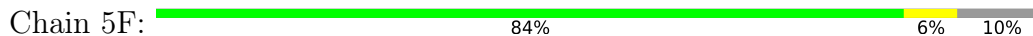




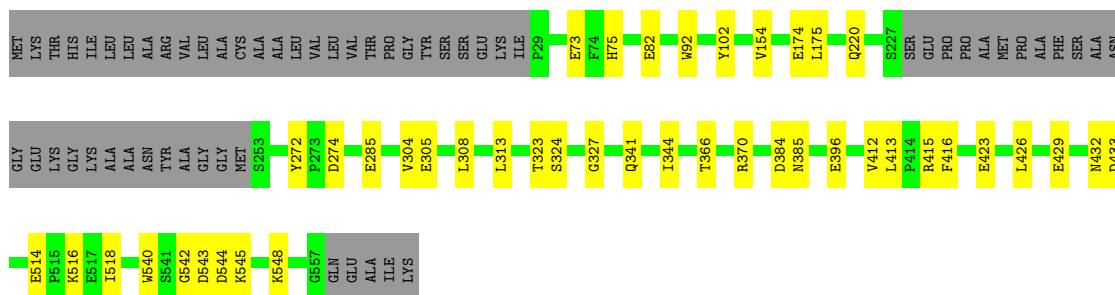
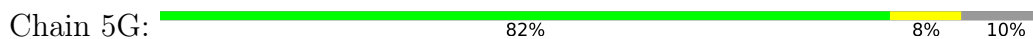
• Molecule 7: Type 3 secretion system secretin



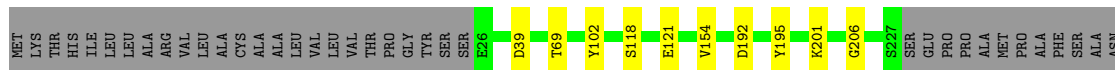
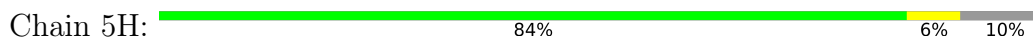
• Molecule 7: Type 3 secretion system secretin

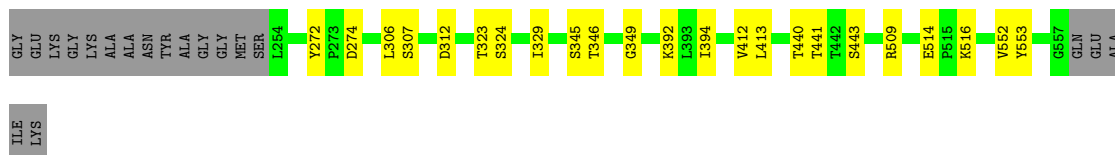


• Molecule 7: Type 3 secretion system secretin

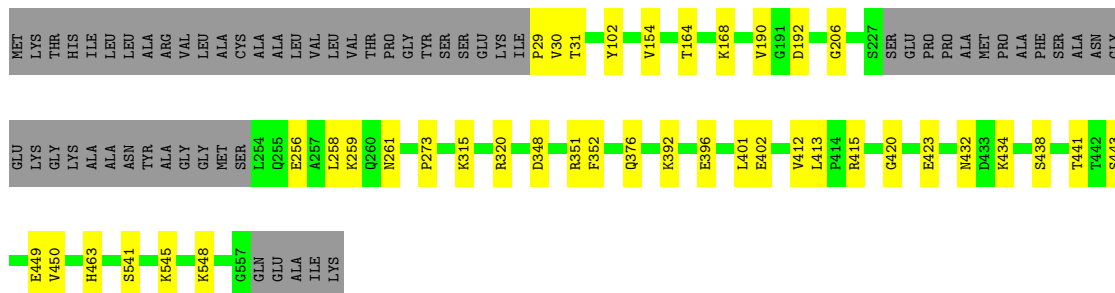
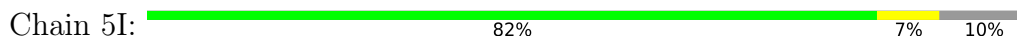


• Molecule 7: Type 3 secretion system secretin

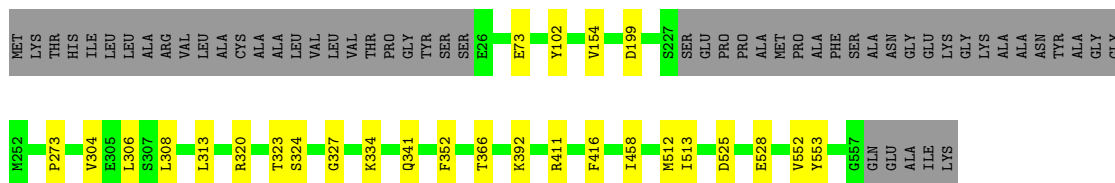
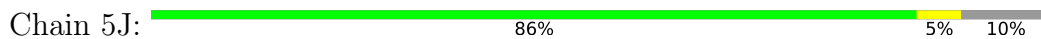




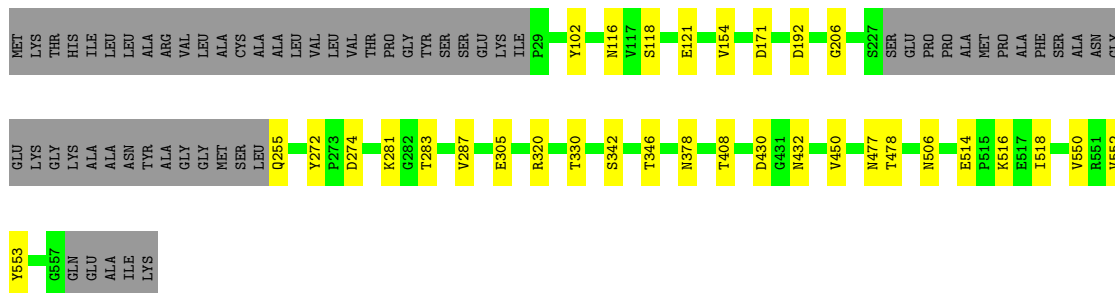
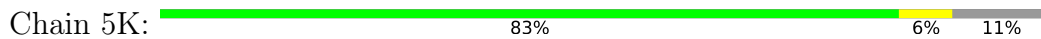
• Molecule 7: Type 3 secretion system secretin



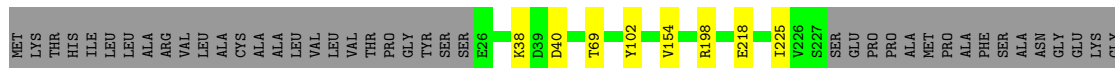
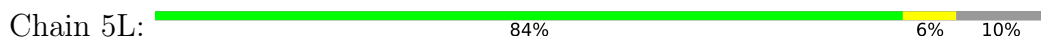
• Molecule 7: Type 3 secretion system secretin

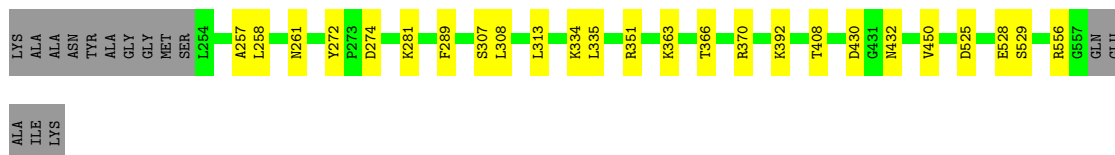


• Molecule 7: Type 3 secretion system secretin

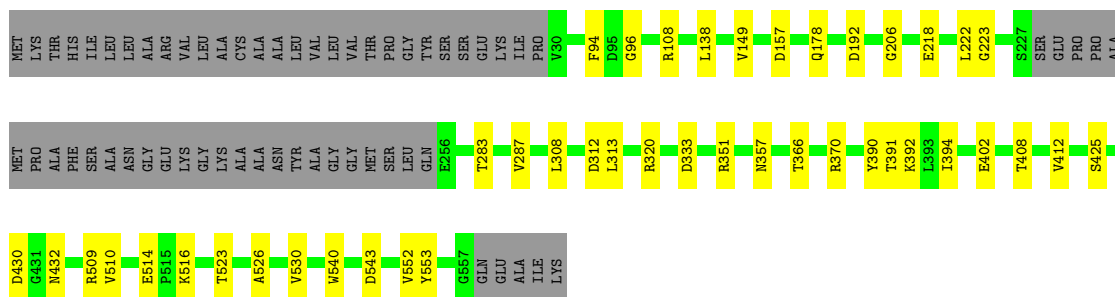
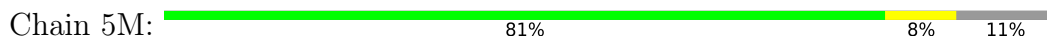


• Molecule 7: Type 3 secretion system secretin

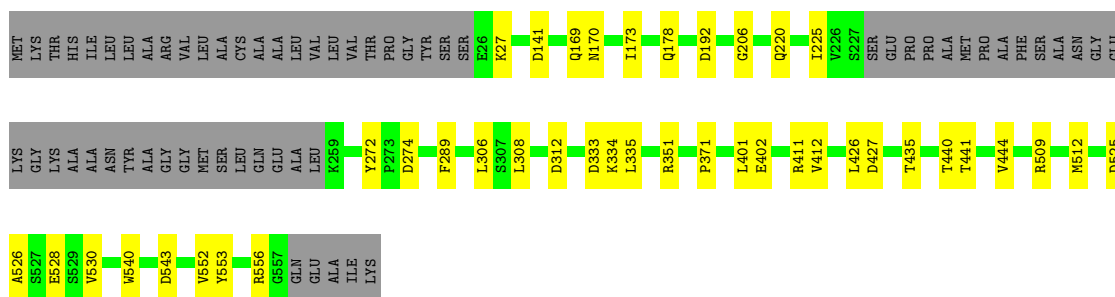
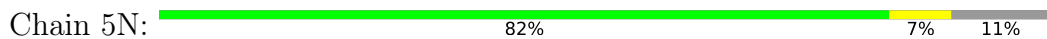




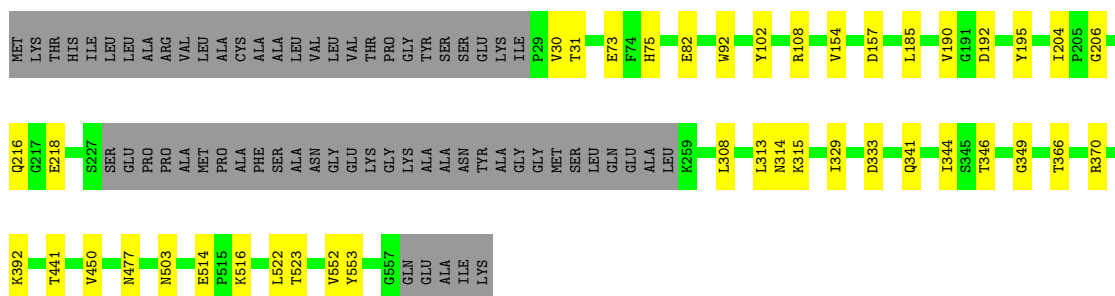
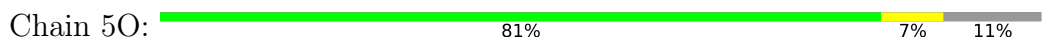
• Molecule 7: Type 3 secretion system secretin



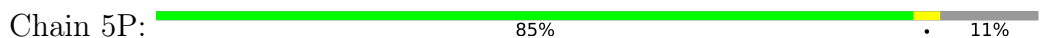
• Molecule 7: Type 3 secretion system secretin

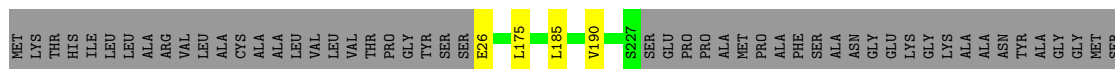


• Molecule 7: Type 3 secretion system secretin

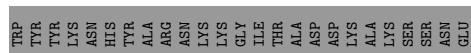


• Molecule 7: Type 3 secretion system secretin

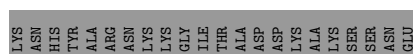
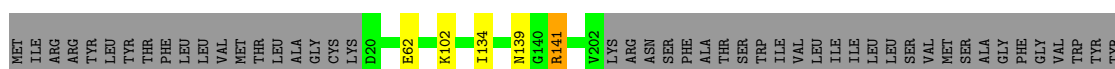




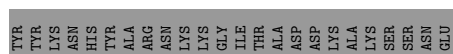
• Molecule 8: Lipoprotein PrgK



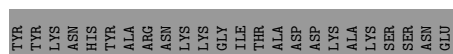
• Molecule 8: Lipoprotein PrgK



• Molecule 8: Lipoprotein PrgK

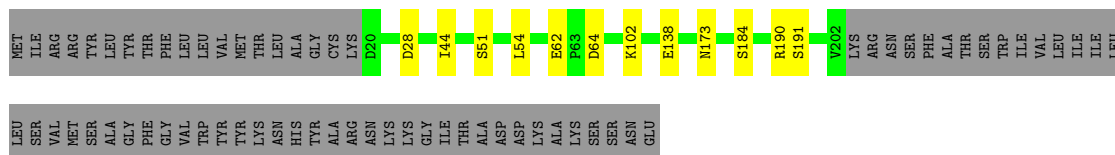


• Molecule 8: Lipoprotein PrgK

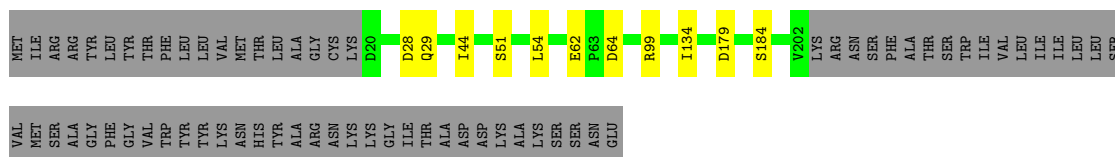


• Molecule 8: Lipoprotein PrgK

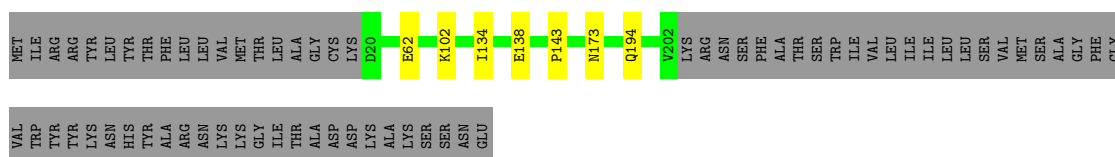




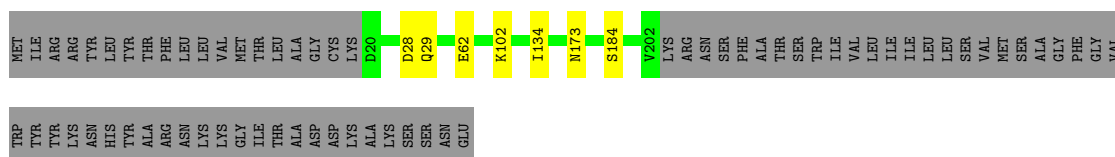
• Molecule 8: Lipoprotein PrgK



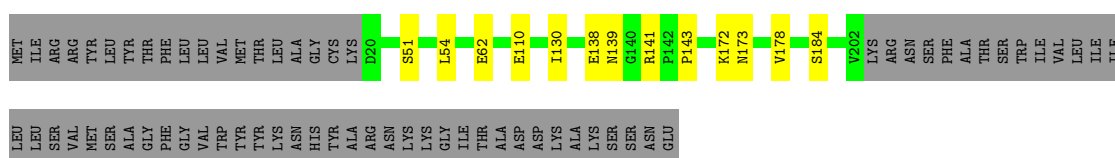
• Molecule 8: Lipoprotein PrgK



• Molecule 8: Lipoprotein PrgK



• Molecule 8: Lipoprotein PrgK



• Molecule 8: Lipoprotein PrgK



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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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• Molecule 8: Lipoprotein PrgK



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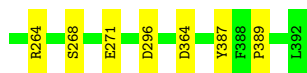
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• Molecule 8: Lipoprotein PrgK



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Molecule 9: Protein PrgH



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Molecule 9: Protein PrgH



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Molecule 9: Protein PrgH



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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

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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 (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

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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

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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

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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

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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.

All (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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
9:7L:246:TYR:OH	9:7L:296:ASP:OD1	2.08	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
6:4B:20:VAL:HG23	6:4B:20:VAL:O	1.94	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
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
6:2R:20:VAL:HG23	6:2R:20:VAL:O	1.96	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
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
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
9:7R:246:TYR:OH	9:7R:296:ASP:OD1	2.14	0.65
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
6:3B:20:VAL:HG23	6:3B:20:VAL:O	1.97	0.64
9:7P:264:ARG:NH1	9:7P:296:ASP:OD2	2.30	0.64
7:5J:102:TYR:OH	7:5J:154:VAL:HG23	1.98	0.64
6:4D:22:ASN:CG	6:4D:25:THR:HG1	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
6:4N:20:VAL:HG23	6:4N:20:VAL:O	1.98	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
6:4E:22:ASN:CG	6:4E:25:THR:HG1	2.02	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
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
7:5D:171:ASP:OD1	7:5D:172:GLY:N	2.32	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:514:GLU:OE2	7:5F:516:LYS:NZ	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
6:2X:20:VAL:O	6:2X:20:VAL:HG23	2.00	0.61
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
7:5H:69:THR:HG1	9:7F:387:TYR:HD1	1.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:5C:281:LYS:NZ	7:5D:218:GLU:OE1	2.30	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
7:5O: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
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
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
6:4J:20:VAL:HG23	6:4J:20:VAL:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
6:2A:8:TYR:C	6:2A:9:LEU:HD22	2.26	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
7:5B: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
9:7I:387:TYR:CE2	9:7I:389:PRO:HB3	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
6:3X:34:LEU:HD11	6:3X:44:LEU:HD23	1.90	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
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
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
8:6F:28:ASP:OD2	8:6F:29:GLN:N	2.42	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
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
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
6:4R:22:ASN:CG	6:4R:25:THR:HG1	2.12	0.52
7:5F:540:TRP:NE1	7:5F:543:ASP:OD1	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:4P:8:TYR:O	6:4P:12:VAL:HG23	2.10	0.52
7:5B:69:THR:HG1	9:7O:387:TYR:HD1	1.56	0.52
9:7D:365:TRP:O	9:7D:369:ARG:NH1	2.43	0.52
3:1G:69:GLU:CD	3:1G:69:GLU:H	2.13	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
8:6P:141:ARG:H	8:6P:141:ARG:HD2	1.75	0.52
6:3N:22:ASN:CG	6:3N:25:THR:HG1	2.13	0.52
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
6:2O:20:VAL:HG23	6:2O:20:VAL:O	2.11	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
4:1O:30:ASP:OD2	4:1O:31:ASP:N	2.43	0.51
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
7:5E:514:GLU:OE2	7:5E:516:LYS:NZ	2.42	0.51
6:4F:17:ASP:OD2	6:4F:57:TYR:OH	2.25	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
7:5D:392:LYS:NZ	7:5E:361:GLU:OE2	2.36	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
8:6S: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1H:3:ASP:OD1	3:1H:3:ASP:N	2.44	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
6:4S:10:ASP:N	6:4S:10:ASP:OD1	2.43	0.50
6:4B:34:LEU:C	6:4B:34:LEU:HD13	2.32	0.50
7:5B:552:VAL:HG13	7:5B:553:TYR:N	2.27	0.50
8:6W:190:ARG:NH1	8:6W:191:SER:O	2.45	0.50
6:3N:34:LEU:HD13	6:3N:34:LEU:C	2.32	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
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
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
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
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
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
7:5I: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
4:1K:45:ALA:HB1	4:1K:73:MET:CE	2.42	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
6:3Y:25:THR:O	6:3Y:28:THR:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:4L:34:LEU:HD13	6:4L:34:LEU:C	2.33	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
8:6V:62:GLU:H	8:6V:62:GLU:CD	2.16	0.49
4:1P:19:ILE:HG22	4:1P:20:ARG:N	2.28	0.48
7:5D:281:LYS:NZ	7:5E:218:GLU:OE1	2.29	0.48
7:5D:404:VAL:HG22	7:5D:447:LEU:HD13	1.95	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
7:5H:514:GLU:OE2	7:5H:516:LYS:NZ	2.34	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
8:6X: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
6:3X:80:ARG:HG2	6:3X:80:ARG:OXT	2.12	0.48
1:1C:137:GLU:O	1:1C:141:PRO:HD3	2.13	0.48
6:3A:34:LEU:HD13	6:3A:34:LEU:C	2.33	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
8:6E:62:GLU:H	8:6E:62:GLU:CD	2.17	0.48
8:6G:62:GLU:CD	8:6G:62:GLU:H	2.16	0.48
6:3F:7:GLY:O	6:3F:10:ASP:OD1	2.31	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
6:2Q:31:LEU:C	6:2Q:31:LEU:HD23	2.34	0.48
8:6P:62:GLU:H	8:6P:62:GLU:CD	2.16	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
6:3Z:34:LEU:HD13	6:3Z:34:LEU:C	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:6N:102:LYS:HD2	8:6N:134:ILE:HG12	1.96	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
7:5L:408:THR:OG1	7:5L:430:ASP:OD2	2.25	0.48
8:6X:62:GLU:H	8:6X:62:GLU:CD	2.18	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
6:4R:55:ASN:O	6:4R:59:ASN:ND2	2.37	0.47
7:5A:118:SER:HB2	7:5A:121:GLU:HG2	1.96	0.47
7:5H:552:VAL:HG13	7:5H:553:TYR:N	2.29	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
7:5O:30:VAL:HG23	7:5O:31:THR:HG23	1.97	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
6:2P:20:VAL:HG23	6:2P:20:VAL:O	2.14	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
6:4E: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
9:7B:264:ARG:NH1	9:7B:296:ASP:OD2	2.47	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
9:7B:332:ASP:OD2	9:7B:333:ASP:N	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:5N:552:VAL:HG13	7:5N:553:TYR:N	2.30	0.47
8:6A:62:GLU:H	8:6A:62:GLU:CD	2.19	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
7:5K:116:ASN:ND2	7:5K:171:ASP:OD2	2.47	0.46
8:6A:190:ARG:NH1	8:6A:191:SER:O	2.47	0.46
6:4C:34:LEU:HD13	6:4C:34:LEU:C	2.35	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
8:6M:62:GLU:H	8:6M:62:GLU:CD	2.19	0.46
4:1M:12:VAL:HG13	4:1M:13:ILE:N	2.28	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
7:5I:30:VAL:HG23	7:5I:31:THR:HG23	1.97	0.46
8:6N:62:GLU:H	8:6N:62:GLU:CD	2.17	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
6:3X:20:VAL:HG23	6:3X:20:VAL:O	2.15	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:6I:62:GLU:H	8:6I:62:GLU:CD	2.19	0.46
6:2Y:34:LEU:HD11	6:2Y:44:LEU:HD23	1.98	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
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
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
7:5H:118:SER:HB2	7:5H:121:GLU:HG2	1.97	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
2:1F:65:PHE:HB3	2:1F:160:MET:HE1	1.99	0.45
4:1O:30:ASP:OD2	4:1O:30:ASP:C	2.55	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
8:6X: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:401:LEU:HD21	7:5O:441:THR:HG22	1.98	0.45
8:6H:62:GLU:CD	8:6H:62:GLU:H	2.19	0.45
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
8:6F:62:GLU:H	8:6F:62:GLU:CD	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1D:173:ASP:C	1:1D:173:ASP:OD1	2.54	0.45
6:2U:20:VAL:HG23	6:2U:20:VAL:O	2.17	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
6:4T: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
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
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
8:6B:102:LYS:HB3	8:6B:134:ILE:HG12	1.99	0.45
8:6U:62:GLU:H	8:6U:62:GLU:CD	2.21	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
8:6T:62:GLU:H	8:6T:62:GLU:CD	2.20	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
7:5N: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
6:3N:22:ASN:OD1	6:3N:25:THR:OG1	2.32	0.44
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
8:6L:62:GLU:H	8:6L:62:GLU:CD	2.19	0.44
8:6S:62:GLU:H	8:6S:62:GLU:CD	2.21	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
3:1J:3:ASP:OD1	3:1J:3:ASP:N	2.50	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
7:5K:408:THR:OG1	7:5K:430:ASP:OD2	2.28	0.44
7:5L:351:ARG:NH1	7:5M:333:ASP:OD2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:6E:28:ASP:C	8:6E:28:ASP:OD1	2.56	0.44
9:7L:387:TYR:O	9:7L:387:TYR:CD1	2.70	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
6:2Z:34:LEU:C	6:2Z:34:LEU:HD23	2.38	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
6:4S:34:LEU:HD13	6:4S:34:LEU:C	2.38	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: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
6:4P:37:LYS:HE3	6:4P:40:ASP:HB2	1.99	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
7:5G: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
6:3H:3:THR:CB	6:3H:4:PRO:HD2	2.47	0.44
7:5B:26:GLU:OE2	9:7M:362:LYS:NZ	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5G:545:LYS:H	7:5G:545:LYS:HD2	1.83	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
7:5D:396:GLU:OE1	7:5E:441:THR:OG1	2.29	0.44
7:5K:281:LYS:NZ	7:5L:218:GLU:OE1	2.41	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
7:5H:394:ILE:HD11	7:5I:320:ARG:HD2	2.00	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
6:4G: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
8:6M:102:LYS:C	8:6M:134:ILE:HD13	2.38	0.43
6:3W:34:LEU:C	6:3W:34:LEU:HD13	2.39	0.43
7:5B:327:GLY:C	7:5B:341:GLN:HE21	2.21	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:441:THR:HG22	7:5I:443:SER:H	1.83	0.43
7:5M:222:LEU:HG	7:5M:223:GLY:H	1.83	0.43
1:1A:163:PHE:CE1	1:1B:200:VAL:CG2	3.01	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
6:3V: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
4:1P: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
8:6C:102:LYS:HD2	8:6C:134:ILE:HG12	1.99	0.43
8:6R:62:GLU:H	8:6R:62:GLU:CD	2.21	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
7:5E:479:ASP:OD2	7:5E:502:LYS:NZ	2.47	0.43
7:5H:272:TYR:CE2	7:5H:274:ASP:HB3	2.53	0.43
7:5L:556:ARG:NH2	7:5M:523:THR:O	2.50	0.43
8:6I:172:LYS:NZ	8:6I:178:VAL:O	2.46	0.43
8:6O:62:GLU:H	8:6O:62:GLU:CD	2.22	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:10:ASP:OD1	6:4C:10:ASP:N	2.52	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
7:5M:432:ASN:OD1	7:5M:432:ASN:C	2.57	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
6:3K:34:LEU:HD23	6:3K:34:LEU:C	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:5K: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
8:6J:62:GLU:H	8:6J:62:GLU:CD	2.20	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
6:3T:34:LEU:HD13	6:3T:34:LEU:C	2.40	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
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:327:GLY:C	7:5G:341:GLN:HE21	2.22	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:396:GLU:OE1	7:5F:441:THR:OG1	2.21	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
8:6Q: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
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
9:7U:201:GLU:CD	9:7U:201:GLU:H	2.21	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
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
8:6W:62:GLU:CD	8:6W:62:GLU:H	2.21	0.42
6:4J:20:VAL:HG21	6:4J:57:TYR:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:5C: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
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
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
8:6R:172:LYS:NZ	8:6R:178:VAL:O	2.49	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
6:4I:34:LEU:C	6:4I:34:LEU:HD13	2.40	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
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
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
9:7R: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
7:5G:384:ASP:OD1	7:5G:384:ASP:C	2.57	0.42
8:6I:110:GLU:HG3	8:6I:130:ILE:HD12	2.02	0.42
9:7F:264:ARG:NH1	9:7F:296:ASP:OD2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
8:6C:62:GLU:H	8:6C:62:GLU:CD	2.23	0.42
8:6K:62:GLU:H	8:6K:62:GLU:CD	2.21	0.42
1:1E:116:GLU:HA	1:1E:116:GLU:OE1	2.19	0.41
6:3J:59:ASN:O	6:3J:63:ASN:ND2	2.42	0.41
6:4A:29:GLU:CD	6:4A:33:LYS:HZ2	2.24	0.41
7:5D:118:SER:O	7:5D:121:GLU:N	2.52	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
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
9:7X:258:PHE:CE2	9:7X:260:LEU:HD21	2.55	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
9:7S:387:TYR:C	9:7S:387:TYR:CD2	2.93	0.41
4:1K:61:VAL:O	4:1K:61:VAL:HG12	2.20	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
7:5E: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
7:5H:306:LEU:HD23	7:5H:306:LEU:C	2.40	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
7:5H: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:5P:175:LEU:HD13	7:5P:262:ALA:HB2	2.03	0.41
8:6Q:62:GLU:H	8:6Q:62:GLU:CD	2.24	0.41
1:1A:129:GLU:OE2	1:1A:129:GLU:N	2.46	0.41
6:2M:34:LEU:HD13	6:2M:34:LEU:C	2.41	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
7:5C: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
6:3X:34:LEU:HD23	6:3X:34:LEU:C	2.41	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
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
6:2C:49:SER:OG	6:2I:10:ASP:OD1	2.36	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
7:5N:27:LYS:HG2	9:7S:365:TRP:CE3	2.55	0.41
7:5N:141:ASP:C	7:5N:141:ASP:OD1	2.59	0.41
7:5N:334:LYS:HG3	7:5N:335:LEU:H	1.86	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
6:3G:34:LEU:HD23	6:3G:34:LEU:C	2.41	0.41
6:3I:38:PRO:O	6:3I:39:SER:OG	2.32	0.41
6:3L:34:LEU:HD11	6:3L:44:LEU:HD23	2.03	0.41
6:3V:34:LEU:HD13	6:3V:34:LEU:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3Y:20:VAL:O	6:3Y:20:VAL:CG2	2.68	0.41
6:3Z:22:ASN:OD1	6:3Z:25:THR:OG1	2.39	0.41
6:3Z:55:ASN:O	6:3Z:59:ASN:ND2	2.51	0.41
6:4M:69:LYS:NZ	6:4M:70:ASP:OD1	2.42	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:285:GLU:CD	7:5G:285:GLU:H	2.24	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
7:5N:306:LEU:C	7:5N:306:LEU:HD23	2.41	0.41
8:6B:62:GLU:H	8:6B:62:GLU:CD	2.21	0.41
8:6F:99:ARG:HG3	8:6F:134:ILE:CG2	2.51	0.41
8:6Q:102:LYS:C	8:6Q:134:ILE:HD13	2.41	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
9:7D:172:GLU:HB2	9:7D:174:ASP:OD1	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
6:3B:34:LEU:HD11	6:3B:44:LEU:HD23	2.02	0.41
6:3P:20:VAL:HG23	6:3P:20:VAL:O	2.21	0.41
6:4D:20:VAL:O	6:4D:20:VAL:CG2	2.68	0.41
6:4J:22:ASN:CG	6:4J:25:THR:HG1	2.23	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
7:5J:304:VAL:HG22	7:5J:416:PHE:CZ	2.56	0.41
8:6F:51:SER:HB2	8:6F:54:LEU:HB2	2.03	0.41
6:3I:34:LEU:C	6:3I:34:LEU:HD23	2.42	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
7:5M:178:GLN:CG	7:5N:220:GLN:HB2	2.51	0.40
7:5O:73:GLU:OE1	7:5O:75:HIS:NE2	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:1C:101:ASP:O	1:1C:104:ILE:HG22	2.21	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
7:5J: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
9:7V: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
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
6:3H:3:THR:HB	6:3H:4:PRO:CD	2.52	0.40
6:4M:34:LEU:C	6:4M:34:LEU:HD13	2.42	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
6:3N:10:ASP:N	6:3N:10:ASP:OD1	2.53	0.40
6:3W:16:PHE:O	6:3W:20:VAL:HG22	2.22	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
8:6U:134:ILE:O	8:6U:134:ILE:HG22	2.21	0.40
8:6X:137:GLY:O	8:6X:138:GLU:HB2	2.22	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
9:7U:182:GLU:H	9:7U:182:GLU:CD	2.25	0.40
6:2J:37:LYS:O	6:2J:39:SER:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:5G: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
7:5M: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
8:6D:62:GLU:H	8:6D:62:GLU:CD	2.22	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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1B	109	ARG
1	1C	109	ARG
2	1F	238	ASN

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Mol	Chain	Res	Type
4	1M	89	ARG
6	2F	57	TYR
6	2L	33	LYS
6	2T	57	TYR
6	2U	21	ASP
6	2V	57	TYR
6	3D	57	TYR
6	3T	57	TYR
6	3X	48	GLN
6	3X	57	TYR
6	4B	57	TYR
6	4D	48	GLN
6	4H	57	TYR
6	4J	57	TYR
6	4N	57	TYR
6	4R	8	TYR
7	5D	26	GLU
7	5D	317	ASP
7	5D	352	PHE
7	5E	312	ASP
7	5F	427	ASP
7	5L	198	ARG
7	5L	363	LYS
7	5M	357	ASN
7	5M	392	LYS
7	5P	351	ARG
8	6B	141	ARG
8	6U	80	ARG
9	7B	388	PHE
9	7H	388	PHE
9	7J	332	ASP
9	7K	388	PHE
9	7N	388	PHE
9	7Q	388	PHE
9	7S	385	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
6	3I	78	ASN
6	3T	59	ASN
6	3W	61	GLN

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-

All (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
11	1I	503	LDA	O1-N1	-7.32	1.25	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1I	502	LDA	O1-N1	-7.30	1.25	1.42
11	1D	301	LDA	O1-N1	-7.22	1.25	1.42
11	1A	402	LDA	O1-N1	-7.21	1.25	1.42
10	1P	201	3PH	O21-C2	-2.85	1.39	1.46
10	1N	601	3PH	O21-C2	-2.80	1.39	1.46
10	1L	201	3PH	O21-C2	-2.68	1.39	1.46
10	1A	401	3PH	O31-C3	-2.61	1.39	1.45
10	1M	201	3PH	O21-C2	-2.51	1.40	1.46
10	1P	201	3PH	O31-C3	-2.46	1.39	1.45
10	1L	201	3PH	O31-C3	-2.34	1.39	1.45
10	1N	601	3PH	O31-C3	-2.33	1.39	1.45
10	1A	401	3PH	O21-C21	2.32	1.40	1.34
10	1M	201	3PH	O31-C3	-2.31	1.39	1.45
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	2.19	1.39	1.33
10	1L	201	3PH	O21-C21	2.16	1.40	1.34
10	1A	401	3PH	O31-C31	2.13	1.39	1.33
10	1P	201	3PH	O21-C21	2.04	1.40	1.34
10	1P	201	3PH	O31-C31	2.03	1.39	1.33

All (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
11	1J	401	LDA	CM1-N1-C1	2.81	116.14	110.23
10	1N	601	3PH	O31-C31-C32	2.42	119.50	111.91
10	1A	401	3PH	O31-C31-C32	2.39	119.42	111.91
10	1P	201	3PH	O31-C31-C32	2.19	118.79	111.91
10	1L	201	3PH	O31-C31-C32	2.16	118.69	111.91
10	1M	201	3PH	O21-C21-O22	-2.12	118.58	123.70

There are no chirality outliers.

All (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

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Mol	Chain	Res	Type	Atoms
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
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	1N	601	3PH	C26-C27-C28-C29
10	1A	401	3PH	C23-C24-C25-C26
10	1L	201	3PH	C25-C26-C27-C28
11	1A	402	LDA	C7-C8-C9-C10
10	1N	601	3PH	C32-C33-C34-C35
10	1P	201	3PH	C2A-C2B-C2C-C2D
10	1L	201	3PH	C28-C29-C2A-C2B
10	1M	201	3PH	C24-C25-C26-C27
10	1P	201	3PH	C2C-C2D-C2E-C2F
10	1M	201	3PH	C35-C36-C37-C38
10	1A	401	3PH	C32-C33-C34-C35
10	1P	201	3PH	C35-C36-C37-C38
10	1P	201	3PH	C2D-C2E-C2F-C2G
10	1P	201	3PH	O32-C31-O31-C3

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

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Mol	Chain	Res	Type	Atoms
11	1J	402	LDA	C2-C3-C4-C5
10	1P	201	3PH	C24-C25-C26-C27
10	1N	601	3PH	C23-C24-C25-C26
10	1M	201	3PH	C1-C2-O21-C21
10	1N	601	3PH	C34-C35-C36-C37
11	1I	502	LDA	C3-C4-C5-C6
10	1P	201	3PH	C27-C28-C29-C2A
11	1A	402	LDA	C4-C5-C6-C7
11	1J	402	LDA	C5-C6-C7-C8
11	1H	101	LDA	C6-C7-C8-C9
10	1N	601	3PH	O11-C1-C2-O21
10	1M	201	3PH	C28-C29-C2A-C2B
11	1D	301	LDA	C6-C7-C8-C9
10	1M	201	3PH	C1-C2-C3-O31
11	1G	201	LDA	C5-C6-C7-C8
10	1N	601	3PH	C33-C34-C35-C36
10	1N	601	3PH	C1-O11-P-O12
11	1I	502	LDA	C4-C5-C6-C7
10	1N	601	3PH	O31-C31-C32-C33
11	1G	201	LDA	N1-C1-C2-C3
10	1N	601	3PH	C27-C28-C29-C2A
10	1N	601	3PH	O32-C31-C32-C33
11	1D	301	LDA	C2-C3-C4-C5
10	1A	401	3PH	O21-C21-C22-C23
10	1M	201	3PH	O31-C31-C32-C33
10	1P	201	3PH	O31-C31-C32-C33

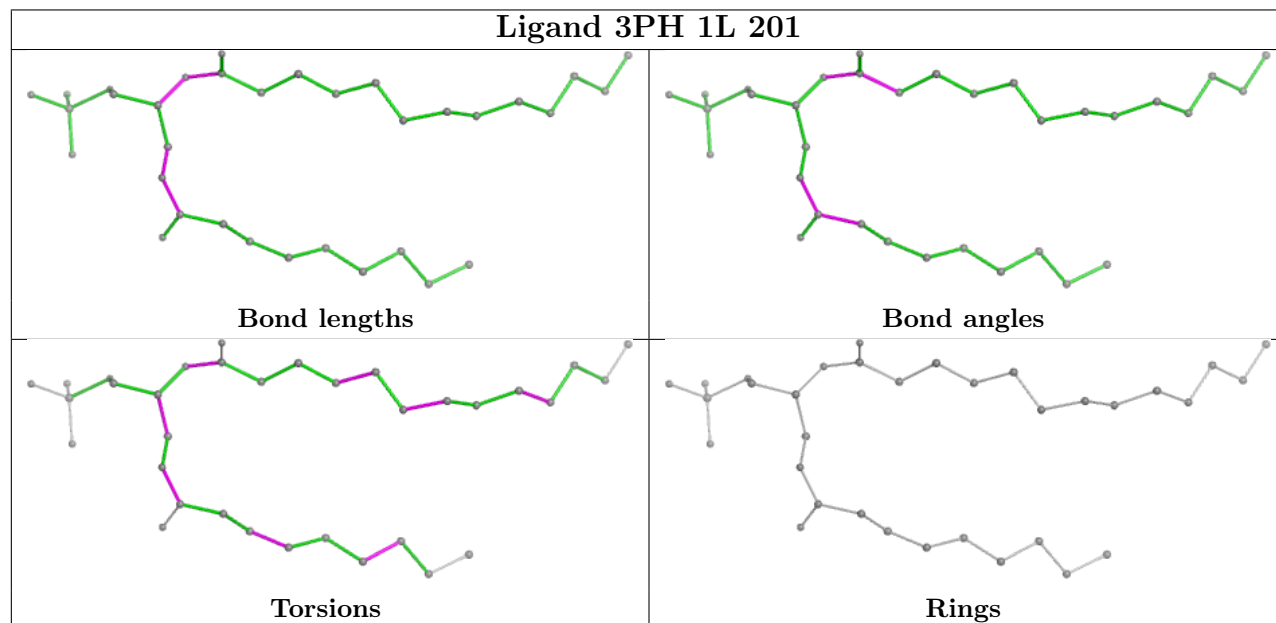
There are no ring outliers.

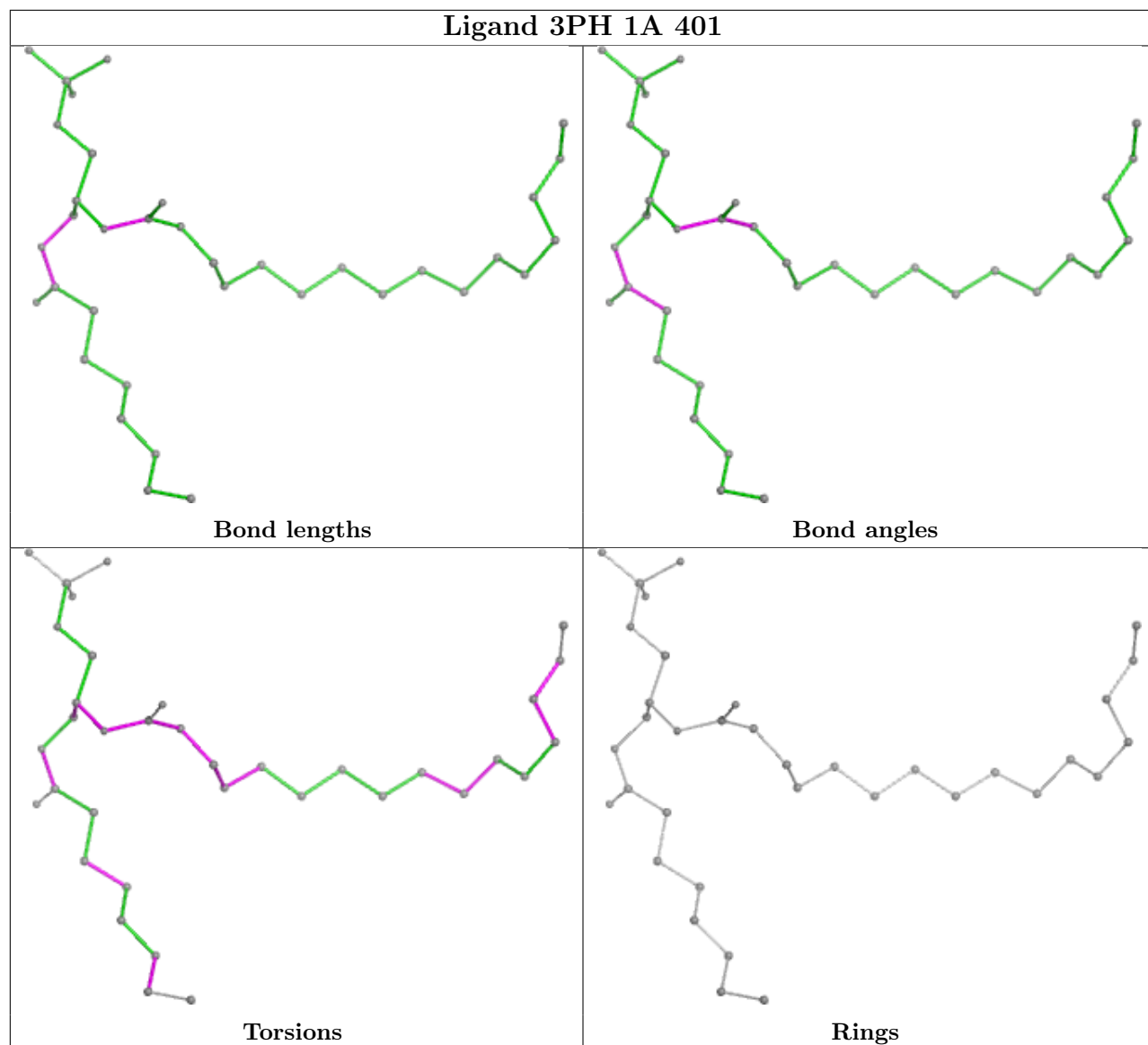
4 monomers are involved in 4 short contacts:

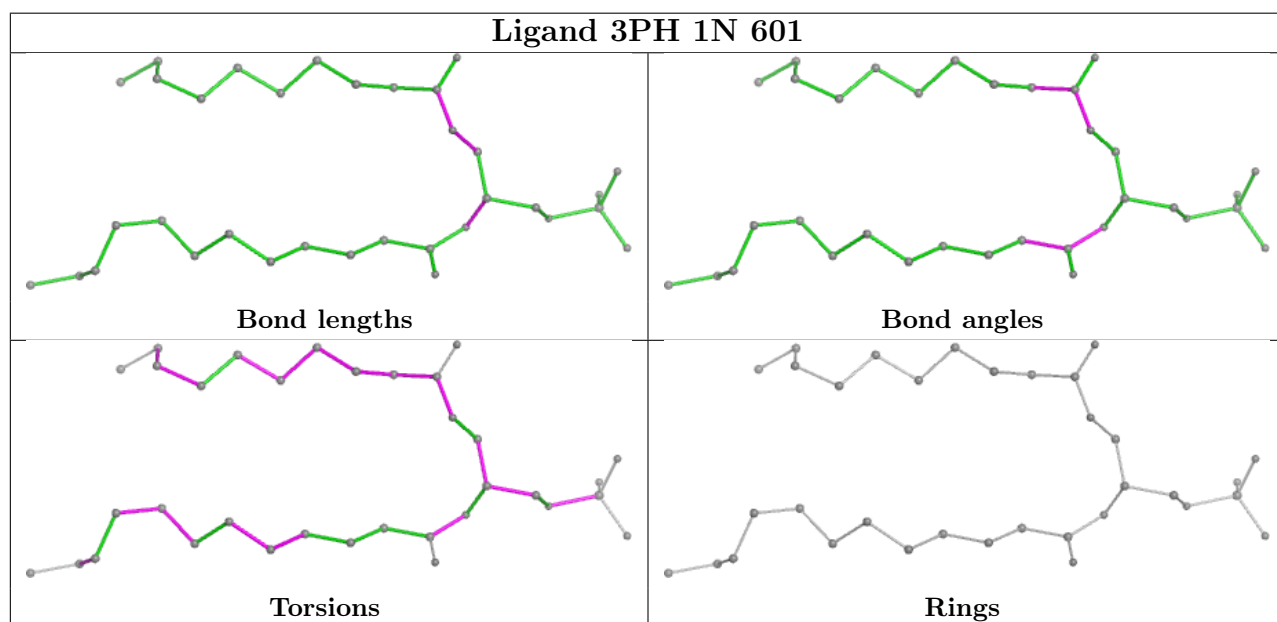
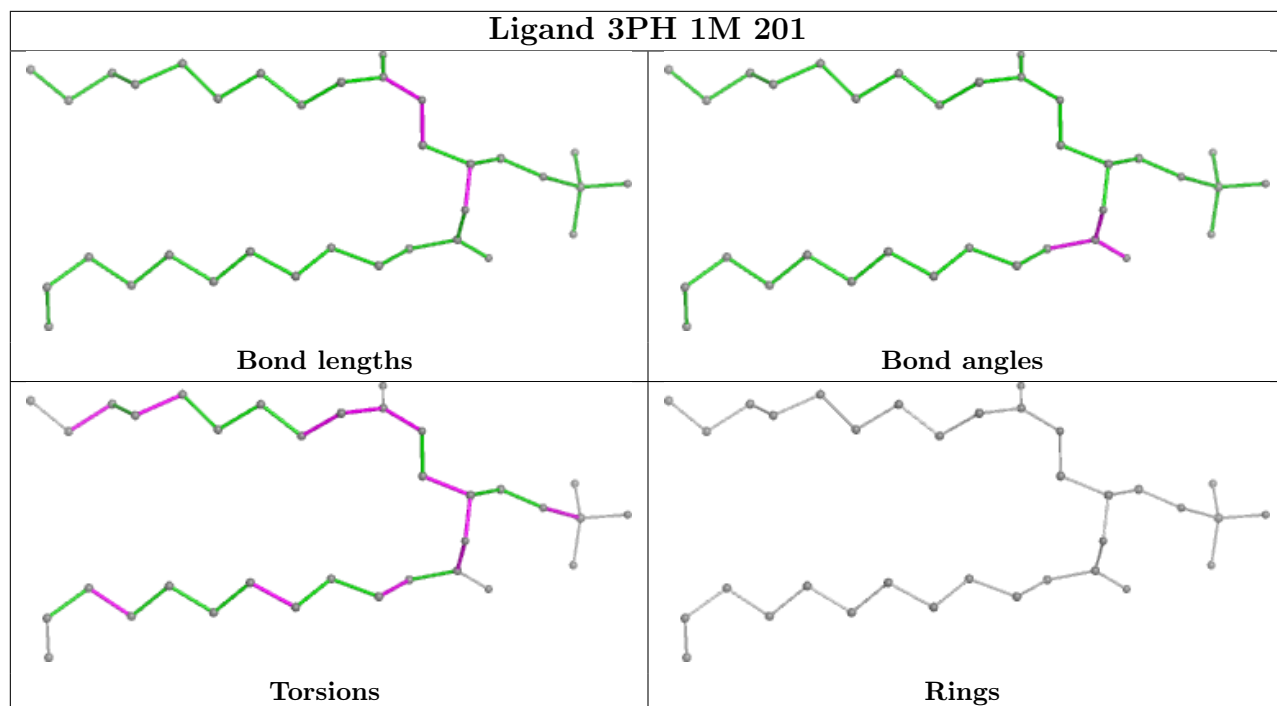
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	1I	501	LDA	1	0
11	1G	201	LDA	1	0
10	1A	401	3PH	1	0
10	1N	601	3PH	1	0

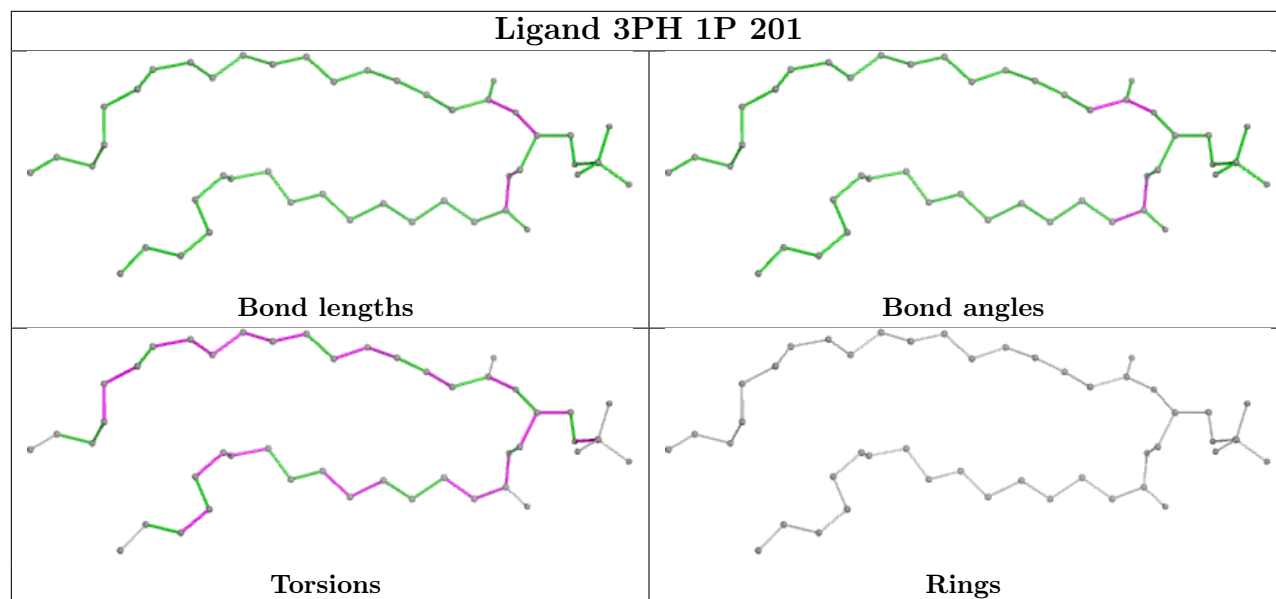
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.