Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 03:07 PM EST

PDB ID	:	7SGR
EMDB ID	:	EMD-25116
Title	:	Structure of hemolysin A secretion system HlyB/D complex
Authors	:	Zhao, H.; Chen, J.
Deposited on	:	2021-10-07
Resolution	:	2.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

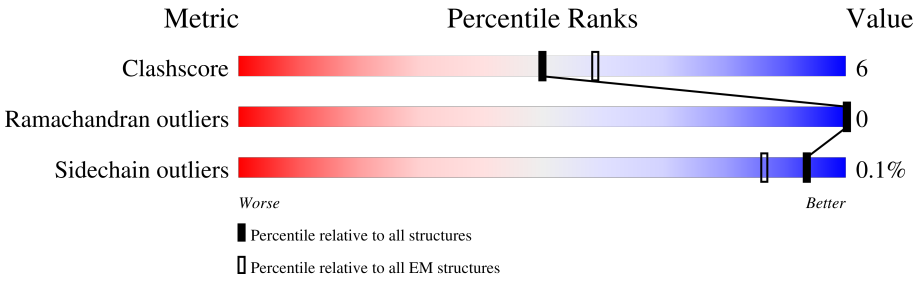
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	707	86% 13%
1	B	707	70% 11% 19%
1	E	707	83% 16%
1	F	707	65% 16% 19%
1	I	707	86% 13%
1	J	707	67% 14% 19%
2	C	356	14% 42% 53%
2	D	356	15% 81%

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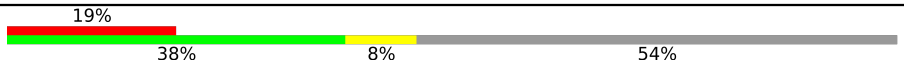
Mol	Chain	Length	Quality of chain
2	G	356	
2	H	356	
2	K	356	
2	L	356	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34989 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

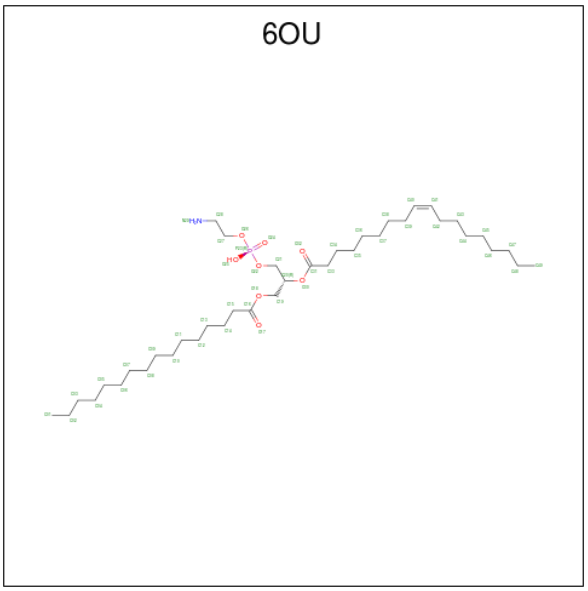
- Molecule 1 is a protein called Alpha-hemolysin translocation ATP-binding protein HlyB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	570	Total	C	N	O	S	0	0
			4505	2923	773	797	12		
1	I	700	Total	C	N	O	S	0	0
			5549	3595	953	989	12		
1	A	700	Total	C	N	O	S	0	0
			5543	3591	952	988	12		
1	B	570	Total	C	N	O	S	0	0
			4509	2926	774	797	12		
1	E	700	Total	C	N	O	S	0	0
			5535	3583	953	987	12		
1	F	570	Total	C	N	O	S	0	0
			4509	2926	774	797	12		

- Molecule 2 is a protein called Membrane fusion protein (MFP) family protein,Hemolysin secretion protein D, chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	69	Total	C	N	O	S	0	0
			581	385	97	98	1		
2	L	69	Total	C	N	O	S	0	0
			581	385	97	98	1		
2	D	69	Total	C	N	O	S	0	0
			581	385	97	98	1		
2	C	166	Total	C	N	O	S	0	0
			1035	648	186	199	2		
2	G	165	Total	C	N	O	S	0	0
			1026	640	185	199	2		
2	K	49	Total	C	N	O	S	0	0
			396	261	65	69	1		

- Molecule 3 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-propan-2-yl] ({Z})-octadec-9-enoate (three-letter code: 6OU) (formula: $C_{39}H_{76}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
3	J	1	Total C 82 82	0
3	J	1	Total C 82 82	0
3	J	1	Total C 82 82	0
3	J	1	Total C 82 82	0
3	J	1	Total C 82 82	0
3	J	1	Total C 82 82	0
3	I	1	Total C O P 131 122 8 1	0
3	I	1	Total C O P 131 122 8 1	0
3	I	1	Total C O P 131 122 8 1	0
3	I	1	Total C O P 131 122 8 1	0
3	I	1	Total C O P 131 122 8 1	0
3	I	1	Total C O P 131 122 8 1	0
3	I	1	Total C O P 131 122 8 1	0
3	I	1	Total C O P 131 122 8 1	0

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Mol	Chain	Residues	Atoms	AltConf
3	I	1	Total C O P 131 122 8 1	0
3	A	1	Total C N O P 147 114 1 29 3	0
3	A	1	Total C N O P 147 114 1 29 3	0
3	A	1	Total C N O P 147 114 1 29 3	0
3	A	1	Total C N O P 147 114 1 29 3	0
3	A	1	Total C N O P 147 114 1 29 3	0
3	A	1	Total C N O P 147 114 1 29 3	0
3	A	1	Total C N O P 147 114 1 29 3	0
3	B	1	Total C 26 26	0
3	B	1	Total C 26 26	0
3	E	1	Total C 38 38	0
3	E	1	Total C 38 38	0
3	E	1	Total C 38 38	0
3	E	1	Total C 38 38	0
3	F	1	Total C O 93 83 10	0
3	F	1	Total C O 93 83 10	0
3	F	1	Total C O 93 83 10	0
3	F	1	Total C O 93 83 10	0
3	H	1	Total C O P 53 44 8 1	0
3	H	1	Total C O P 53 44 8 1	0
3	L	1	Total C 29 29	0

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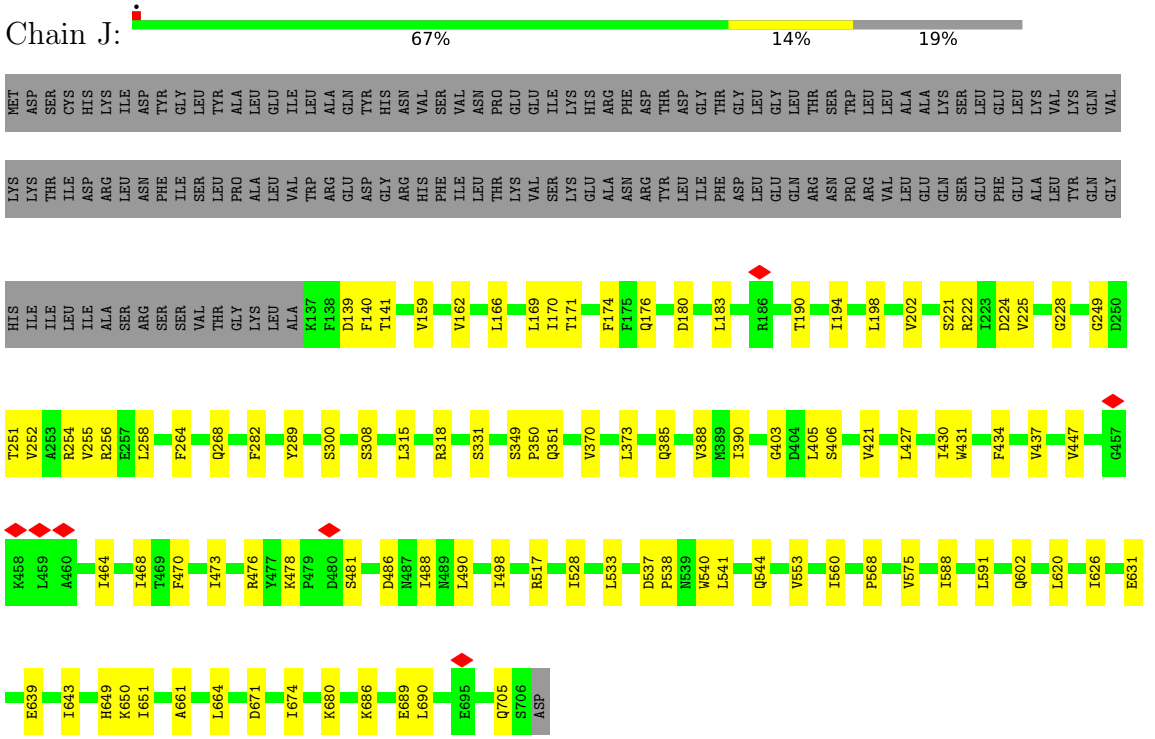
Mol	Chain	Residues	Atoms	AltConf
3	L	1	Total C 29 29	0
3	K	1	Total C O P 40 31 8 1	0

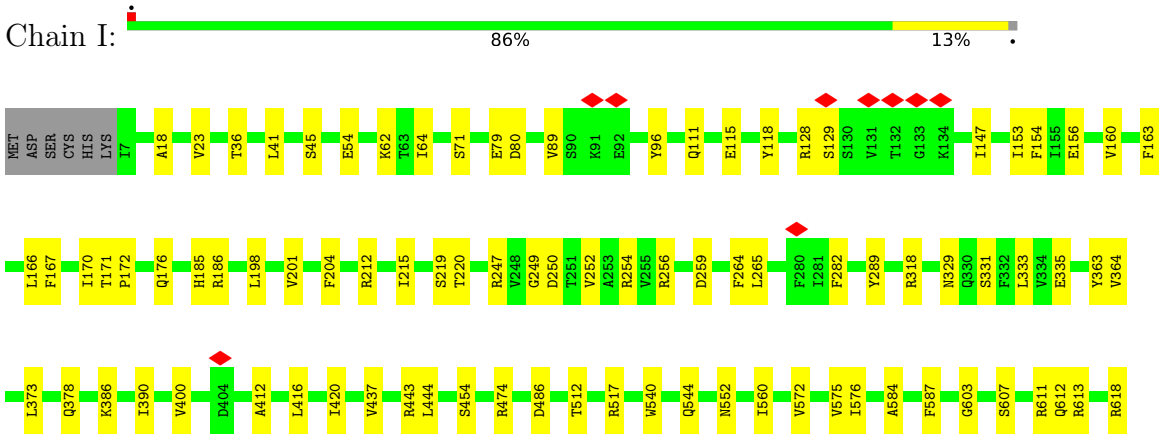
3 Residue-property plots (i)

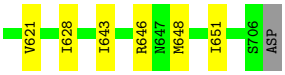
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Alpha-hemolysin translocation ATP-binding protein HlyB



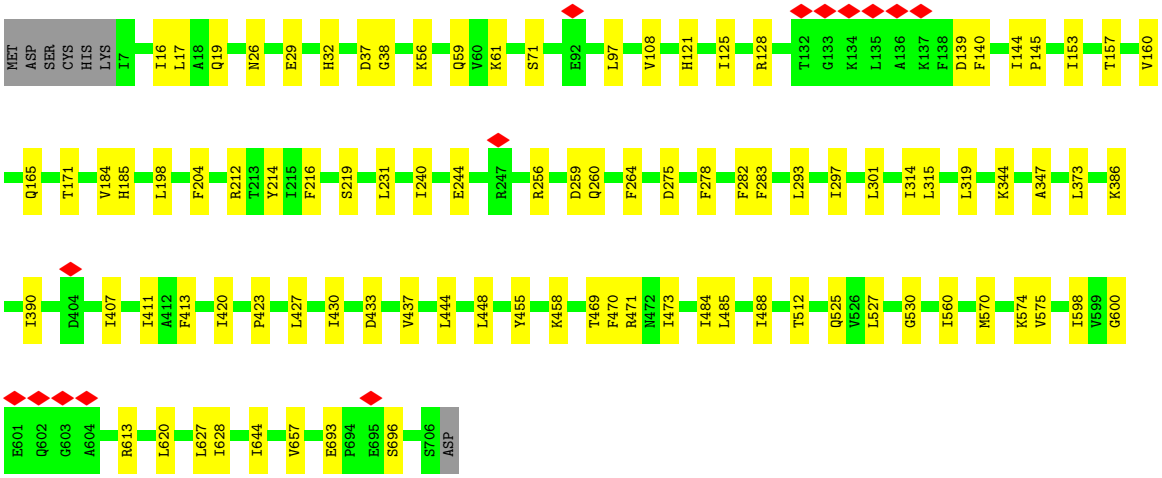
• Molecule 1: Alpha-hemolysin translocation ATP-binding protein HlyB





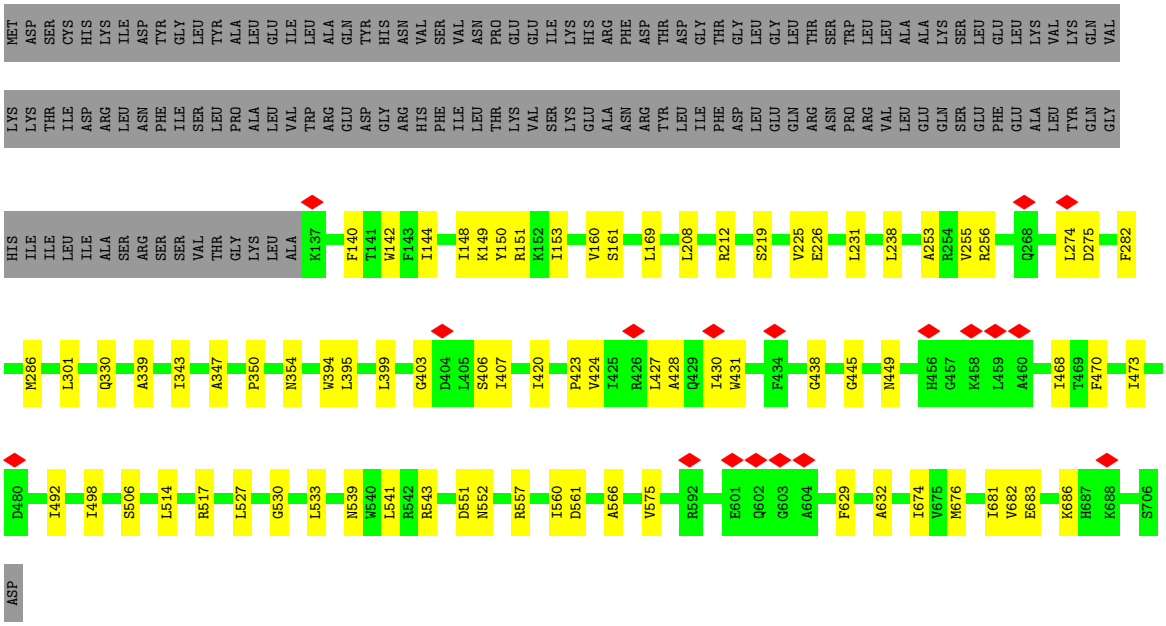
• Molecule 1: Alpha-hemolysin translocation ATP-binding protein HlyB

Chain A:



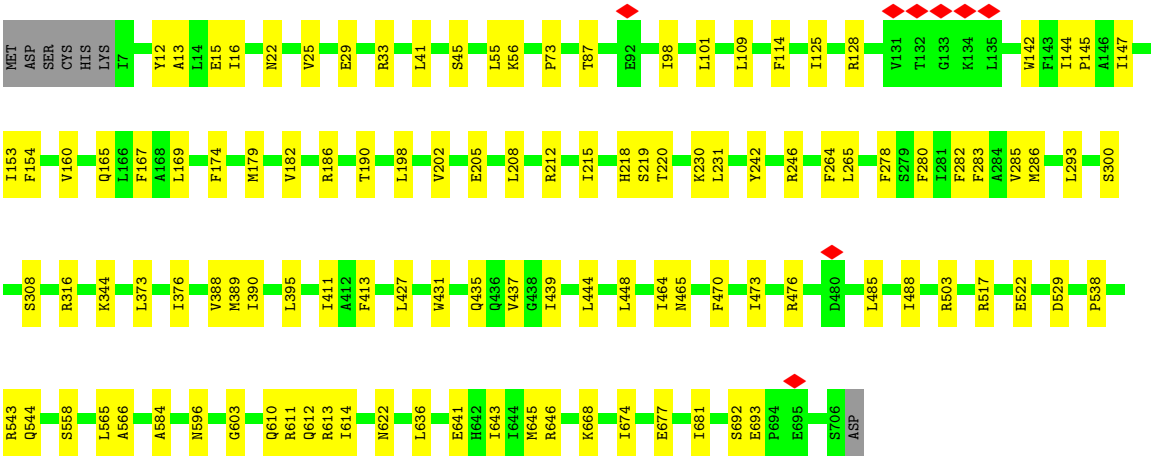
• Molecule 1: Alpha-hemolysin translocation ATP-binding protein HlyB

Chain B:



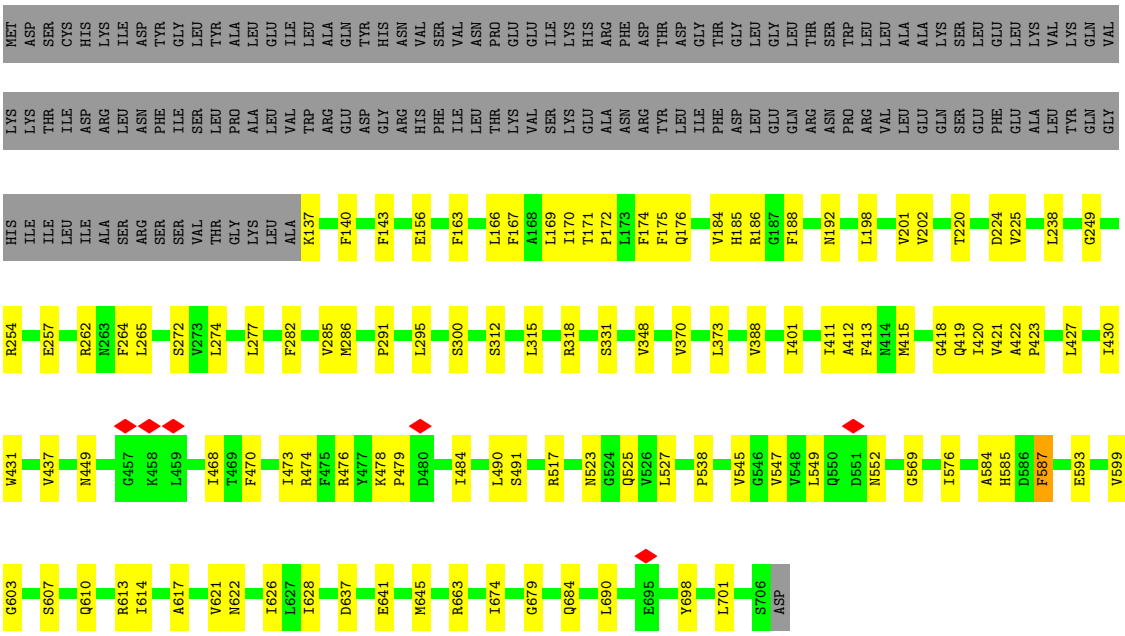
• Molecule 1: Alpha-hemolysin translocation ATP-binding protein HlyB

Chain E:



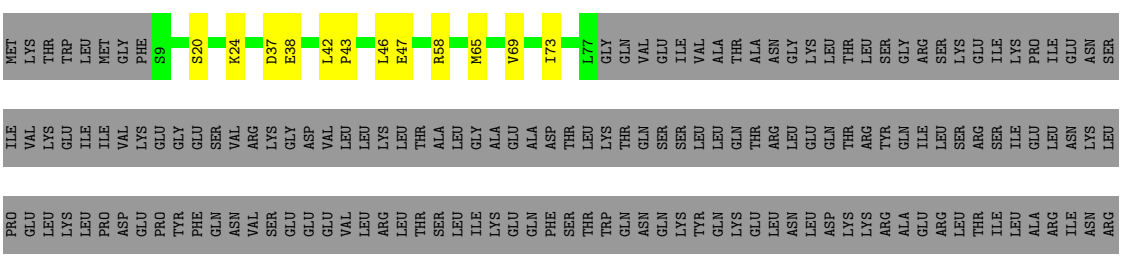
• Molecule 1: Alpha-hemolysin translocation ATP-binding protein HlyB

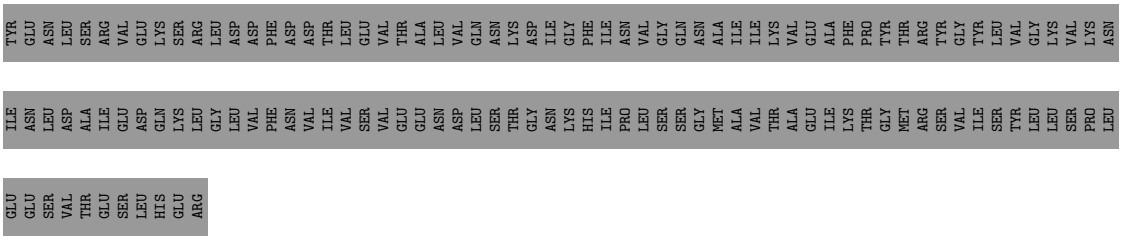
Chain F:



• Molecule 2: Membrane fusion protein (MFP) family protein,Hemolysin secretion protein D, chromosomal

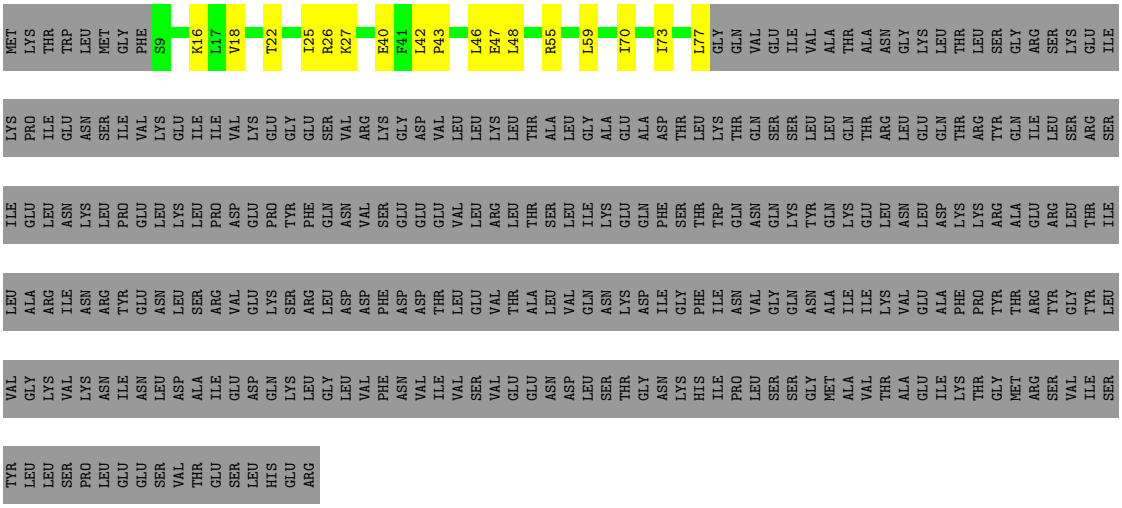
Chain H:





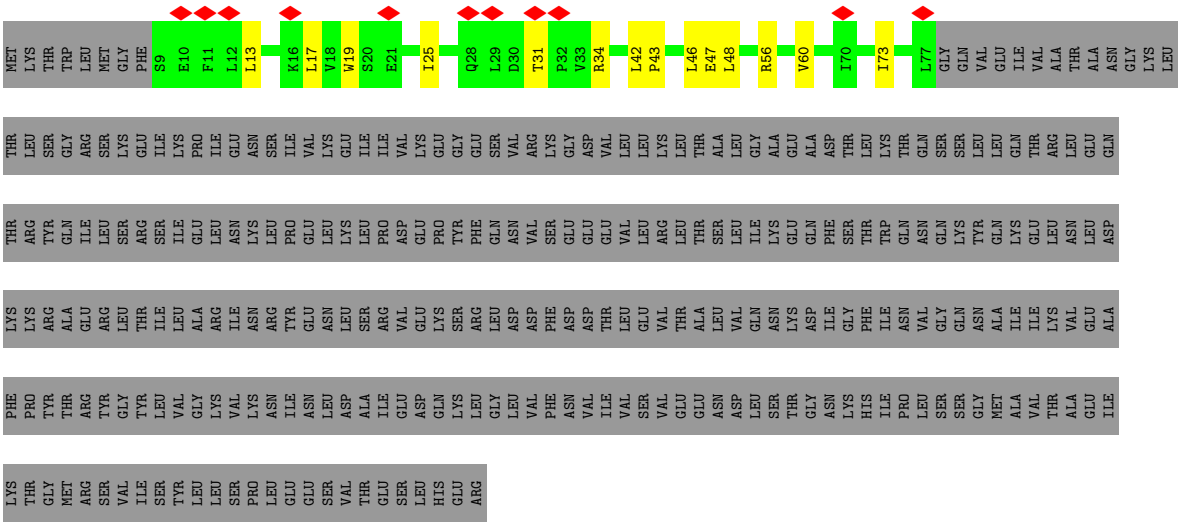
• Molecule 2: Membrane fusion protein (MFP) family protein,Hemolysin secretion protein D, chromosomal

Chain L:

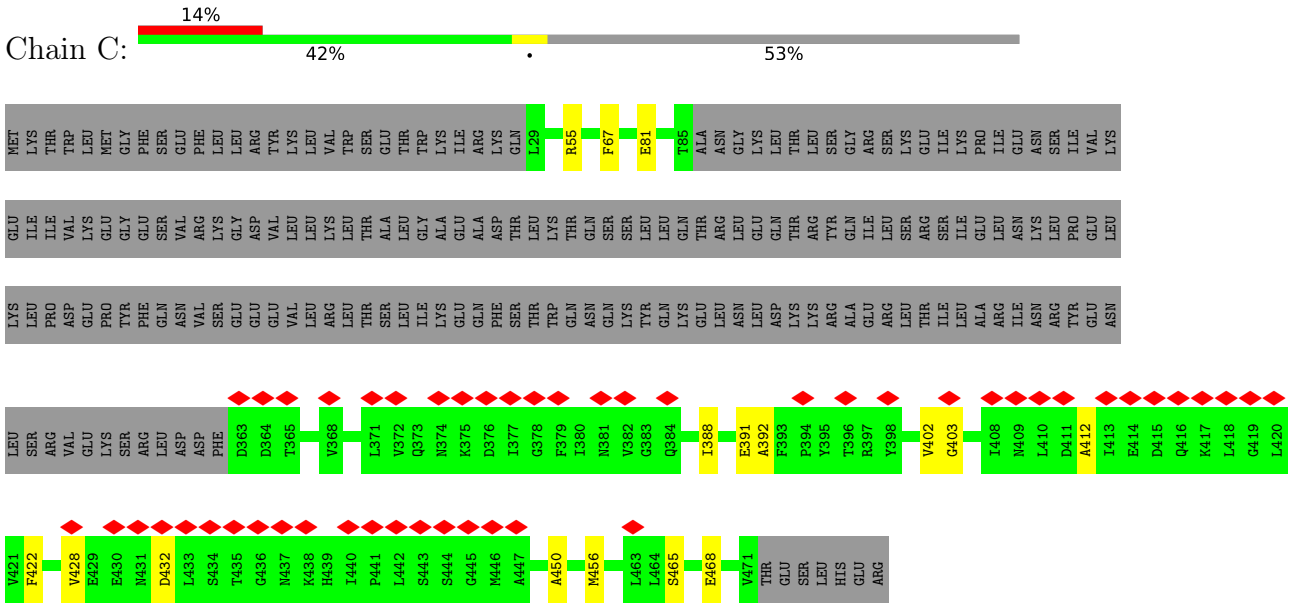


• Molecule 2: Membrane fusion protein (MFP) family protein,Hemolysin secretion protein D, chromosomal

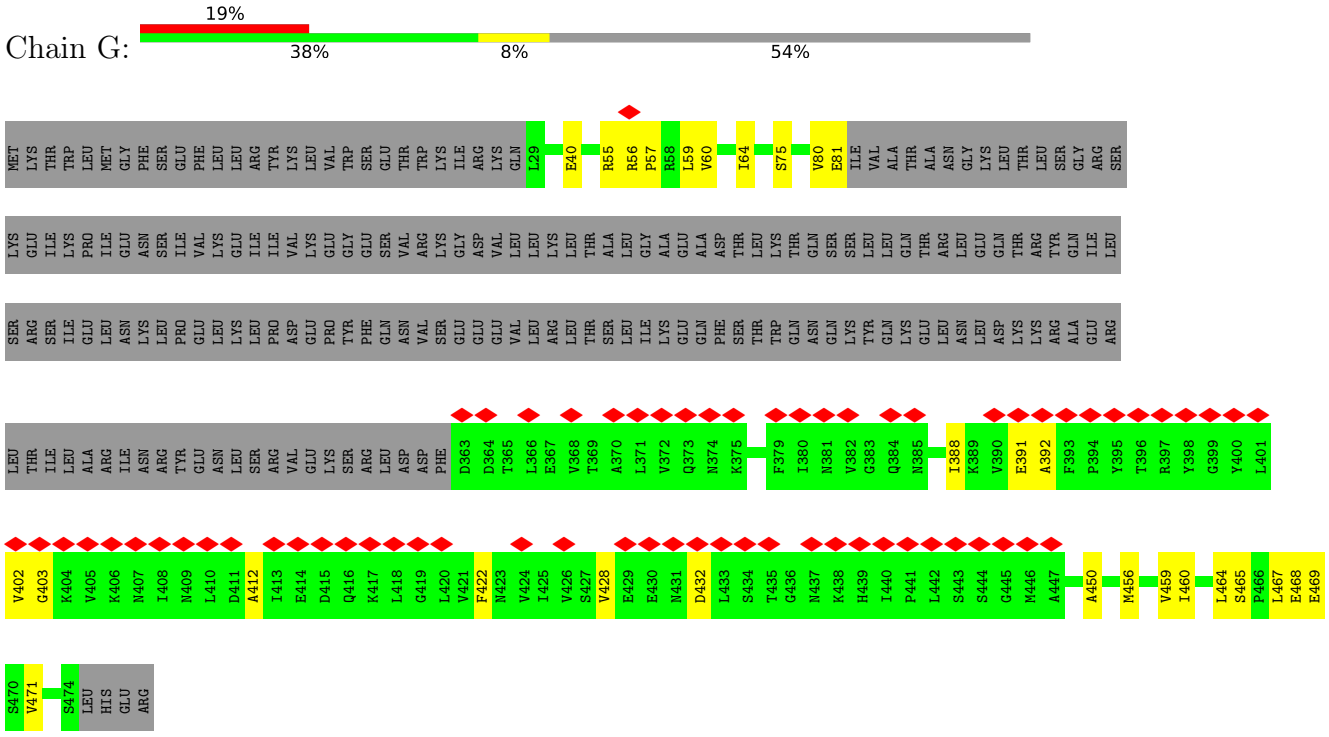
Chain D:



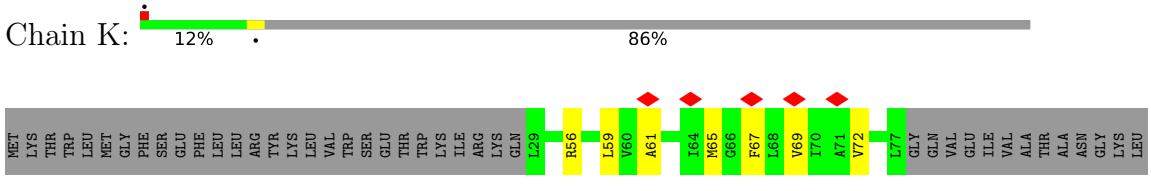
• Molecule 2: Membrane fusion protein (MFP) family protein,Hemolysin secretion protein D, chromosomal

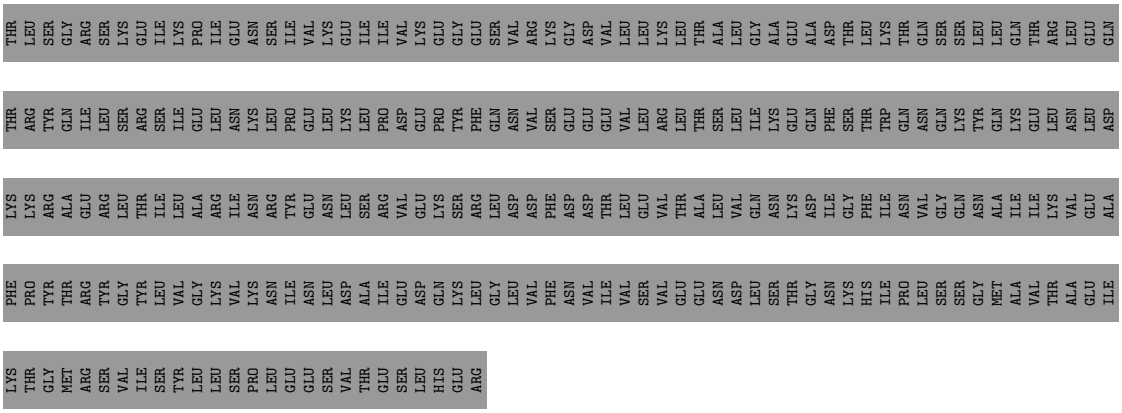


• Molecule 2: Membrane fusion protein (MFP) family protein,Hemolysin secretion protein D, chromosomal



• Molecule 2: Membrane fusion protein (MFP) family protein,Hemolysin secretion protein D, chromosomal




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

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136123	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	70	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.434	Depositor
Minimum map value	-2.384	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.104	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	410.88, 410.88, 410.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6OU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.30	0/5651	0.49	0/7663
1	B	0.25	0/4596	0.48	0/6232
1	E	0.26	0/5641	0.47	0/7648
1	F	0.27	0/4596	0.48	0/6232
1	I	0.25	0/5656	0.47	0/7669
1	J	0.25	0/4592	0.47	0/6228
2	C	0.25	0/1044	0.48	0/1433
2	D	0.24	0/595	0.53	0/807
2	G	0.24	0/1035	0.45	0/1420
2	H	0.24	0/595	0.51	0/807
2	K	0.23	0/404	0.47	0/550
2	L	0.25	0/595	0.53	0/807
All	All	0.26	0/35000	0.48	0/47496

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5543	0	5714	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4509	0	4683	52	0
1	E	5535	0	5706	76	0
1	F	4509	0	4683	80	0
1	I	5549	0	5734	62	0
1	J	4505	0	4672	60	0
2	C	1035	0	815	9	0
2	D	581	0	609	12	0
2	G	1026	0	797	23	0
2	H	581	0	609	8	0
2	K	396	0	416	5	0
2	L	581	0	609	16	0
3	A	147	0	0	0	0
3	B	26	0	0	0	0
3	E	38	0	0	0	0
3	F	93	0	0	0	0
3	H	53	0	0	0	0
3	I	131	0	0	0	0
3	J	82	0	0	0	0
3	K	40	0	0	0	0
3	L	29	0	0	0	0
All	All	34989	0	35047	421	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 6.

All (421) 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)
1:E:128:ARG:HH21	2:L:47:GLU:HG2	1.42	0.85
1:F:315:LEU:HD11	1:F:370:VAL:HG13	1.70	0.72
1:I:128:ARG:NH2	2:D:42:LEU:O	2.24	0.70
1:I:282:PHE:HB2	1:I:420:ILE:HD11	1.75	0.69
1:A:283:PHE:HZ	1:A:301:LEU:HD11	1.56	0.68
2:G:56:ARG:HG2	2:G:59:LEU:HD12	1.77	0.67
1:E:98:ILE:HD12	1:E:109:LEU:HD12	1.76	0.66
1:E:128:ARG:HH22	2:L:42:LEU:H	1.41	0.66
1:A:470:PHE:HD2	1:A:473:ILE:HG13	1.60	0.65
1:F:220:THR:HB	1:F:265:LEU:HB3	1.77	0.65
2:C:388:ILE:HA	2:C:450:ALA:HA	1.79	0.65
1:B:140:PHE:HZ	1:B:438:GLY:HA2	1.62	0.64
1:E:179:MET:HG3	1:E:411:ILE:HD11	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:648:MET:HA	1:I:651:ILE:HB	1.79	0.64
2:G:388:ILE:HA	2:G:450:ALA:HA	1.80	0.64
1:E:344:LYS:NZ	1:F:238:LEU:O	2.32	0.63
1:E:220:THR:HB	1:E:265:LEU:HB3	1.79	0.63
1:F:427:LEU:HD12	1:F:430:ILE:HD11	1.80	0.62
1:I:318:ARG:HG3	1:I:373:LEU:HD12	1.81	0.62
1:A:430:ILE:HA	1:A:433:ASP:HB2	1.81	0.62
1:E:283:PHE:HA	1:E:286:MET:HE2	1.81	0.62
1:E:128:ARG:NH2	2:L:42:LEU:O	2.33	0.61
1:I:247:ARG:NH2	1:I:335:GLU:OE1	2.33	0.61
1:E:503:ARG:NH1	1:E:677:GLU:OE2	2.34	0.61
1:B:150:TYR:HB3	1:B:153:ILE:HD11	1.81	0.61
1:E:286:MET:HB3	1:E:413:PHE:CE2	2.37	0.60
1:A:128:ARG:NH2	2:H:47:GLU:OE1	2.33	0.60
1:E:264:PHE:CG	1:E:437:VAL:HG21	2.36	0.60
1:J:252:VAL:O	1:J:256:ARG:HG2	2.02	0.60
1:B:253:ALA:HA	1:B:256:ARG:HG2	1.83	0.60
1:F:641:GLU:O	1:F:645:MET:HG2	2.01	0.60
1:F:576:ILE:HD12	1:F:585:HIS:CE1	2.36	0.60
2:G:80:VAL:CG2	2:G:459:VAL:HG22	2.32	0.59
1:A:283:PHE:CZ	1:A:301:LEU:HD11	2.37	0.59
1:E:603:GLY:HA3	1:E:611:ARG:HD3	1.84	0.59
1:E:641:GLU:O	1:E:645:MET:HG2	2.02	0.59
2:G:80:VAL:HG23	2:G:459:VAL:CG2	2.33	0.59
1:E:29:GLU:OE2	1:E:543:ARG:NH1	2.34	0.59
1:I:128:ARG:NH1	2:D:47:GLU:OE1	2.34	0.59
1:I:264:PHE:CG	1:I:437:VAL:HG21	2.38	0.59
1:A:620:LEU:HD21	1:A:627:LEU:HD11	1.84	0.59
1:B:428:ALA:HA	1:B:431:TRP:HE3	1.68	0.58
1:B:468:ILE:HB	1:B:492:ILE:HD12	1.84	0.58
1:J:468:ILE:HD11	1:J:626:ILE:HD13	1.85	0.58
1:J:620:LEU:HD21	1:J:651:ILE:HG23	1.86	0.58
1:A:427:LEU:HA	1:A:430:ILE:HG12	1.86	0.58
1:B:160:VAL:HG13	1:B:208:LEU:HG	1.84	0.58
1:A:171:THR:HG23	1:A:198:LEU:HD11	1.85	0.58
1:F:584:ALA:HB2	1:F:613:ARG:HB3	1.86	0.58
1:A:153:ILE:HG21	1:A:219:SER:HB3	1.84	0.58
1:E:56:LYS:HD3	1:E:128:ARG:HH11	1.68	0.58
1:I:167:PHE:HD2	1:I:201:VAL:HG13	1.69	0.58
1:E:282:PHE:O	1:E:286:MET:HG3	2.04	0.58
2:D:13:LEU:O	2:D:17:LEU:HG	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:185:HIS:O	1:I:186:ARG:HG3	2.03	0.57
1:F:474:ARG:HB3	1:F:523:ASN:HB3	1.86	0.57
1:E:153:ILE:HG21	1:E:219:SER:OG	2.04	0.57
1:A:444:LEU:HG	1:A:448:LEU:HD12	1.87	0.57
1:J:385:GLN:HG3	1:J:421:VAL:HG11	1.86	0.57
1:F:545:VAL:HG12	1:F:626:ILE:HB	1.86	0.57
1:I:153:ILE:HG21	1:I:219:SER:OG	2.03	0.57
1:F:476:ARG:HD2	1:F:479:PRO:HA	1.87	0.56
1:F:137:LYS:N	1:F:449:ASN:OD1	2.39	0.56
1:F:584:ALA:HB1	1:F:587:PHE:HE2	1.69	0.56
2:L:26:ARG:HD2	2:L:27:LYS:HG2	1.86	0.56
1:I:252:VAL:O	1:I:256:ARG:HG2	2.05	0.56
1:F:176:GLN:HB2	1:F:412:ALA:HB2	1.86	0.56
1:F:315:LEU:HD23	1:F:431:TRP:CD1	2.41	0.56
1:J:351:GLN:NE2	1:I:36:THR:O	2.39	0.56
1:F:610:GLN:O	1:F:614:ILE:HG12	2.06	0.56
1:E:41:LEU:O	1:E:45:SER:OG	2.22	0.55
1:J:560:ILE:HG13	1:J:575:VAL:HG11	1.88	0.55
1:I:256:ARG:NH2	1:I:259:ASP:OD2	2.40	0.55
1:A:165:GLN:HG3	1:A:278:PHE:CD2	2.42	0.55
1:F:517:ARG:HH11	1:F:538:PRO:HG3	1.72	0.55
1:I:643:ILE:HG13	1:I:646:ARG:HH21	1.71	0.55
1:J:300:SER:HB2	1:J:388:VAL:HG11	1.88	0.55
1:B:225:VAL:HG21	2:D:48:LEU:HD22	1.89	0.55
1:E:692:SER:OG	1:E:693:GLU:OE2	2.24	0.55
2:C:403:GLY:HA2	2:C:428:VAL:HA	1.89	0.55
1:I:163:PHE:O	1:I:167:PHE:HD1	1.90	0.55
1:B:470:PHE:HD2	1:B:473:ILE:HG13	1.72	0.55
1:F:584:ALA:HB1	1:F:587:PHE:CE2	2.42	0.55
1:B:423:PRO:O	1:B:427:LEU:HD23	2.07	0.54
1:F:224:ASP:OD1	1:F:225:VAL:N	2.40	0.54
1:J:176:GLN:OE1	1:J:289:TYR:OH	2.23	0.54
1:I:54:GLU:HB3	1:I:129:SER:HA	1.89	0.54
1:B:169:LEU:HB2	1:B:282:PHE:HE1	1.72	0.54
1:J:139:ASP:OD1	1:J:140:PHE:N	2.35	0.54
1:B:543:ARG:HH12	1:B:566:ALA:HB1	1.72	0.54
2:G:403:GLY:HA2	2:G:428:VAL:HA	1.89	0.54
1:B:560:ILE:HG13	1:B:575:VAL:HG11	1.89	0.54
1:F:171:THR:HG23	1:F:198:LEU:HD11	1.90	0.54
1:I:250:ASP:O	1:I:254:ARG:HG2	2.08	0.53
1:A:71:SER:HB2	2:H:42:LEU:HD23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:VAL:HG11	1:A:212:ARG:HB2	1.89	0.53
1:A:344:LYS:NZ	1:B:238:LEU:O	2.41	0.53
2:C:402:VAL:H	2:C:432:ASP:CB	2.22	0.53
1:J:476:ARG:NH2	1:J:481:SER:O	2.41	0.53
1:A:282:PHE:HB3	1:A:420:ILE:HD12	1.90	0.53
1:F:300:SER:HB2	1:F:388:VAL:HG21	1.89	0.53
1:F:470:PHE:HD2	1:F:473:ILE:HG13	1.73	0.53
2:K:56:ARG:HB3	2:K:59:LEU:HD13	1.90	0.53
1:F:576:ILE:HD12	1:F:585:HIS:HE1	1.74	0.53
1:B:142:TRP:HH2	1:B:226:GLU:HG2	1.73	0.53
1:E:182:VAL:HG12	1:F:401:ILE:HD11	1.90	0.53
1:F:264:PHE:CG	1:F:437:VAL:HG21	2.44	0.53
1:I:171:THR:HG23	1:I:172:PRO:HD3	1.91	0.53
1:F:254:ARG:HA	1:F:257:GLU:HG3	1.91	0.53
1:I:540:TRP:O	1:I:544:GLN:NE2	2.40	0.52
1:I:603:GLY:O	1:I:611:ARG:NH1	2.42	0.52
1:F:188:PHE:O	1:F:192:ASN:ND2	2.41	0.52
1:J:318:ARG:HG3	1:J:373:LEU:HD12	1.89	0.52
1:A:17:LEU:HD13	1:A:125:ILE:HD13	1.89	0.52
2:G:402:VAL:H	2:G:432:ASP:CB	2.22	0.52
1:F:411:ILE:O	1:F:415:MET:HG3	2.09	0.52
1:F:610:GLN:HG2	1:F:613:ARG:NH2	2.24	0.52
1:J:498:ILE:HD11	1:J:674:ILE:HD12	1.92	0.52
1:J:169:LEU:HB2	1:J:282:PHE:HE1	1.75	0.52
1:F:286:MET:HB3	1:F:413:PHE:CE2	2.45	0.52
1:J:202:VAL:HG11	1:I:386:LYS:HB3	1.92	0.51
1:I:584:ALA:HB2	1:I:613:ARG:HB3	1.92	0.51
1:E:565:LEU:HG	1:F:348:VAL:HG11	1.92	0.51
2:G:412:ALA:HA	2:G:422:PHE:HA	1.93	0.51
1:I:204:PHE:HD2	2:K:67:PHE:HB2	1.75	0.51
1:A:264:PHE:CG	1:A:437:VAL:HG21	2.45	0.51
1:E:390:ILE:HD11	1:F:202:VAL:HG21	1.91	0.51
2:C:412:ALA:HA	2:C:422:PHE:HA	1.92	0.51
1:F:140:PHE:HA	1:F:143:PHE:HD1	1.76	0.51
1:A:598:ILE:HG22	1:A:600:GLY:H	1.76	0.51
1:B:394:TRP:HE3	1:B:395:LEU:HD22	1.76	0.51
1:B:140:PHE:CZ	1:B:438:GLY:HA2	2.45	0.51
1:J:470:PHE:HD2	1:J:490:LEU:HB3	1.76	0.51
2:G:81:GLU:HA	2:G:456:MET:HG2	1.93	0.51
1:J:689:GLU:OE1	1:J:690:LEU:HG	2.11	0.50
1:A:627:LEU:HB2	1:A:657:VAL:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:156:GLU:OE2	2:H:58:ARG:NH1	2.45	0.50
1:J:166:LEU:O	1:J:170:ILE:HG12	2.11	0.50
1:J:171:THR:HG23	1:J:198:LEU:HD11	1.92	0.50
1:A:16:ILE:O	1:A:19:GLN:HB3	2.11	0.50
2:L:55:ARG:HG2	2:L:59:LEU:HD13	1.94	0.50
1:B:427:LEU:HA	1:B:430:ILE:HG12	1.92	0.50
1:I:71:SER:HB2	2:D:42:LEU:HD23	1.93	0.50
2:D:25:ILE:HG22	2:D:25:ILE:O	2.12	0.50
2:G:80:VAL:HG21	2:G:459:VAL:HG22	1.93	0.50
1:J:568:PRO:HG2	1:E:22:ASN:HB3	1.93	0.50
1:E:169:LEU:HD11	1:E:285:VAL:HG21	1.94	0.50
1:A:293:LEU:O	1:A:297:ILE:HG12	2.12	0.50
1:F:274:LEU:HD23	1:F:277:LEU:HD21	1.94	0.50
1:F:468:ILE:HD11	1:F:626:ILE:HD13	1.94	0.50
1:F:262:ARG:HG3	1:F:262:ARG:HH11	1.77	0.50
1:I:416:LEU:O	1:I:420:ILE:HG12	2.12	0.49
1:I:618:ARG:O	1:I:621:VAL:HG12	2.12	0.49
1:F:420:ILE:O	1:F:423:PRO:HD2	2.12	0.49
1:I:160:VAL:HG11	1:I:212:ARG:HB2	1.94	0.49
1:A:471:ARG:HH22	1:A:525:GLN:HE21	1.60	0.49
1:E:464:ILE:HD12	1:E:544:GLN:HB2	1.93	0.49
1:A:32:HIS:NE2	1:B:347:ALA:HB1	2.28	0.49
1:A:256:ARG:HD2	1:B:330:GLN:OE1	2.11	0.49
1:A:314:ILE:HG13	1:A:373:LEU:HD21	1.94	0.49
1:J:390:ILE:HG12	1:I:198:LEU:HD23	1.93	0.49
1:F:610:GLN:HG2	1:F:613:ARG:HH21	1.78	0.49
1:J:308:SER:HA	1:J:431:TRP:HH2	1.78	0.49
1:J:486:ASP:OD2	1:J:680:LYS:NZ	2.40	0.49
1:I:64:ILE:HD13	1:I:115:GLU:HG2	1.93	0.49
1:E:218:HIS:NE2	2:G:40:GLU:OE2	2.46	0.49
1:E:230:LYS:HE3	1:E:448:LEU:HD22	1.95	0.49
1:B:551:ASP:OD1	1:B:552:ASN:N	2.40	0.49
1:B:161:SER:HB3	1:B:274:LEU:HD13	1.93	0.48
1:F:312:SER:HA	1:F:431:TRP:HZ2	1.77	0.48
1:J:228:GLY:HA2	1:J:258:LEU:HD21	1.95	0.48
1:A:214:TYR:OH	2:C:55:ARG:NE	2.45	0.48
1:A:693:GLU:OE1	1:A:696:SER:N	2.46	0.48
1:B:144:ILE:HG23	2:D:19:TRP:CE3	2.48	0.48
1:E:186:ARG:HG2	1:F:401:ILE:HG23	1.95	0.48
1:F:617:ALA:O	1:F:621:VAL:HG13	2.12	0.48
2:C:81:GLU:HA	2:C:456:MET:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:60:VAL:O	2:G:64:ILE:HG12	2.13	0.48
1:B:682:VAL:HG23	1:B:683:GLU:HG2	1.95	0.48
2:L:18:VAL:O	2:L:22:THR:HG22	2.13	0.48
1:A:275:ASP:HB3	1:A:423:PRO:HB3	1.96	0.48
1:B:160:VAL:HG11	1:B:212:ARG:HB2	1.96	0.48
1:E:167:PHE:HE2	1:E:208:LEU:HD12	1.77	0.48
1:J:315:LEU:HD23	1:J:431:TRP:CD1	2.48	0.48
1:I:474:ARG:NH1	1:I:486:ASP:OD1	2.46	0.48
1:A:61:LYS:HD3	1:A:121:HIS:CE1	2.49	0.48
1:B:676:MET:HB3	1:B:681:ILE:HD13	1.96	0.48
1:F:163:PHE:CG	2:H:65:MET:HG2	2.49	0.48
1:F:637:ASP:OD1	1:F:637:ASP:N	2.46	0.48
1:E:73:PRO:HB3	1:E:87:THR:HG22	1.96	0.48
1:F:607:SER:HB2	1:F:610:GLN:HG3	1.96	0.48
1:J:180:ASP:OD1	1:J:406:SER:OG	2.31	0.48
1:A:37:ASP:OD1	1:A:38:GLY:N	2.41	0.48
1:F:166:LEU:O	1:F:170:ILE:HG12	2.14	0.48
1:F:517:ARG:NH1	1:F:538:PRO:HG3	2.29	0.48
1:I:79:GLU:N	1:I:79:GLU:OE1	2.47	0.48
1:E:147:ILE:HA	1:E:154:PHE:HE2	1.78	0.48
1:I:176:GLN:HB2	1:I:412:ALA:HB2	1.95	0.47
1:A:259:ASP:OD1	1:A:260:GLN:N	2.47	0.47
1:A:484:ILE:HG22	1:A:485:LEU:HD12	1.95	0.47
1:B:148:ILE:HA	1:B:151:ARG:HG3	1.95	0.47
1:J:517:ARG:NH2	1:J:538:PRO:HG3	2.29	0.47
1:B:445:GLY:O	1:B:449:ASN:N	2.47	0.47
2:G:80:VAL:CG2	2:G:459:VAL:CG2	2.90	0.47
1:J:190:THR:O	1:J:194:ILE:HG12	2.14	0.47
1:E:476:ARG:NH1	1:E:522:GLU:OE1	2.41	0.47
1:F:621:VAL:HG23	1:F:622:ASN:H	1.79	0.47
2:H:43:PRO:HG2	2:H:46:LEU:HD12	1.96	0.47
1:A:26:ASN:HB3	1:A:29:GLU:HB3	1.96	0.47
1:J:671:ASP:HA	1:J:686:LYS:NZ	2.30	0.47
1:A:613:ARG:HG2	1:A:644:ILE:HD11	1.96	0.47
1:B:557:ARG:NH2	1:B:561:ASP:OD2	2.48	0.47
1:E:128:ARG:NH2	2:L:47:GLU:HG2	2.20	0.47
1:E:202:VAL:HA	1:E:205:GLU:HG2	1.97	0.47
1:I:443:ARG:HA	1:I:443:ARG:HD3	1.73	0.47
1:E:316:ARG:HG3	1:E:439:ILE:HD11	1.96	0.47
1:F:291:PRO:O	1:F:295:LEU:HD13	2.14	0.47
1:A:97:LEU:HD13	1:A:108:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:584:ALA:HB2	1:E:613:ARG:HB3	1.96	0.47
1:F:593:GLU:N	1:F:593:GLU:OE1	2.48	0.47
1:J:639:GLU:O	1:J:643:ILE:HG12	2.15	0.47
1:A:570:MET:SD	1:A:574:LYS:HE3	2.55	0.47
1:F:547:VAL:HG22	1:F:628:ILE:HB	1.97	0.47
1:A:455:TYR:HB3	1:A:458:LYS:HE2	1.97	0.46
1:B:153:ILE:HD12	1:B:219:SER:OG	2.15	0.46
1:F:167:PHE:HD1	1:F:201:VAL:HG13	1.79	0.46
1:A:56:LYS:HB3	1:A:56:LYS:HE2	1.71	0.46
1:A:184:VAL:HG23	1:A:185:HIS:CD2	2.51	0.46
1:J:553:VAL:HG13	1:J:602:GLN:HB3	1.97	0.46
1:E:293:LEU:HB2	1:E:413:PHE:CZ	2.51	0.46
1:J:403:GLY:O	1:J:405:LEU:N	2.49	0.46
1:A:693:GLU:HB3	1:A:696:SER:HB3	1.96	0.46
1:E:300:SER:HB2	1:E:388:VAL:HG21	1.96	0.46
1:F:315:LEU:HD23	1:F:431:TRP:HD1	1.80	0.46
1:F:484:ILE:O	1:F:679:GLY:HA3	2.15	0.46
1:F:490:LEU:HD12	1:F:491:SER:H	1.80	0.46
1:A:471:ARG:HH21	1:A:527:LEU:HD23	1.81	0.46
1:B:301:LEU:HD22	1:B:424:VAL:HG11	1.97	0.46
1:B:527:LEU:HD12	1:B:530:GLY:HA2	1.97	0.46
2:G:55:ARG:O	2:G:57:PRO:HD3	2.15	0.46
1:J:249:GLY:HA3	1:J:331:SER:HA	1.98	0.46
1:F:318:ARG:HG3	1:F:373:LEU:HD12	1.98	0.46
1:I:18:ALA:HB1	1:I:23:VAL:HG23	1.98	0.45
1:I:220:THR:HB	1:I:265:LEU:HB3	1.97	0.45
2:H:20:SER:O	2:H:24:LYS:HG2	2.16	0.45
1:J:473:ILE:HB	1:J:488:ILE:HG23	1.97	0.45
1:I:552:ASN:ND2	1:I:612:GLN:OE1	2.49	0.45
1:J:221:SER:HA	1:J:224:ASP:OD2	2.17	0.45
1:E:558:SER:HB2	1:E:596:ASN:HA	1.99	0.45
1:J:256:ARG:HG3	1:J:256:ARG:HH11	1.81	0.45
1:E:160:VAL:HG11	1:E:212:ARG:HB2	1.98	0.45
1:I:560:ILE:HG13	1:I:575:VAL:HG11	1.98	0.45
1:E:389:MET:SD	1:F:175:PHE:HZ	2.40	0.45
1:J:141:THR:HB	2:L:18:VAL:HG11	1.99	0.45
1:A:59:GLN:HE21	1:A:121:HIS:HB3	1.81	0.45
1:B:539:ASN:O	1:B:543:ARG:HG2	2.16	0.45
1:E:373:LEU:HD12	1:E:376:ILE:HD11	1.99	0.45
1:A:347:ALA:HB3	1:B:543:ARG:CD	2.47	0.45
1:E:465:ASN:N	1:E:529:ASP:OD2	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:37:ASP:OD1	2:H:38:GLU:N	2.50	0.45
2:L:42:LEU:HB2	2:L:47:GLU:HB3	1.98	0.45
1:J:225:VAL:HG22	1:I:364:VAL:HG21	1.99	0.44
1:A:560:ILE:HD12	1:A:575:VAL:HG11	1.98	0.44
1:I:62:LYS:O	1:I:118:TYR:OH	2.28	0.44
1:A:347:ALA:HB3	1:B:543:ARG:HD3	1.99	0.44
1:A:407:ILE:O	1:A:411:ILE:HG12	2.17	0.44
1:E:144:ILE:HB	1:E:145:PRO:HD3	1.98	0.44
1:A:469:THR:HB	1:A:527:LEU:HD11	1.99	0.44
1:E:15:GLU:HA	1:E:25:VAL:HG11	1.98	0.44
1:E:231:LEU:HD22	1:E:444:LEU:HD11	1.99	0.44
2:L:16:LYS:HA	2:L:16:LYS:HD2	1.73	0.44
1:J:268:GLN:NE2	1:I:378:GLN:OE1	2.47	0.44
1:E:55:LEU:HD13	1:E:125:ILE:HG23	1.99	0.44
1:E:485:LEU:HD22	1:E:488:ILE:HG13	1.98	0.44
2:H:69:VAL:O	2:H:73:ILE:HG12	2.17	0.44
1:J:537:ASP:HB3	1:J:540:TRP:HB3	2.00	0.44
1:E:174:PHE:HD2	1:E:198:LEU:HD13	1.83	0.44
1:B:629:PHE:HD1	1:B:632:ALA:HB3	1.83	0.44
1:E:165:GLN:HG3	1:E:278:PHE:HB3	2.00	0.44
1:E:517:ARG:HH11	1:E:517:ARG:HG2	1.83	0.44
1:I:156:GLU:O	1:I:160:VAL:HG23	2.18	0.44
1:A:231:LEU:HD13	1:A:448:LEU:HD11	2.00	0.44
1:I:572:VAL:O	1:I:576:ILE:HG12	2.18	0.43
1:B:406:SER:OG	1:B:407:ILE:N	2.51	0.43
1:E:435:GLN:O	1:E:439:ILE:HG12	2.18	0.43
1:F:272:SER:HB2	1:F:427:LEU:HD13	1.99	0.43
1:J:174:PHE:HD2	1:J:198:LEU:HD13	1.82	0.43
1:B:517:ARG:HA	1:B:517:ARG:HD2	1.72	0.43
1:E:517:ARG:NH2	1:E:538:PRO:HG3	2.34	0.43
1:A:240:ILE:O	1:A:244:GLU:HG2	2.18	0.43
1:B:533:LEU:HD22	1:B:541:LEU:HD22	2.01	0.43
1:I:89:VAL:HG22	1:I:96:TYR:HD2	1.83	0.43
1:J:159:VAL:O	1:J:162:VAL:HG12	2.18	0.43
1:J:434:PHE:O	1:J:437:VAL:HG12	2.18	0.43
1:E:470:PHE:HD2	1:E:473:ILE:HG13	1.84	0.43
1:E:643:ILE:HG12	1:E:646:ARG:NH2	2.32	0.43
2:G:56:ARG:CG	2:G:59:LEU:HD12	2.46	0.43
1:J:255:VAL:HB	1:I:333:LEU:HD21	2.01	0.43
1:E:98:ILE:HD11	1:E:114:PHE:CE1	2.54	0.43
1:F:576:ILE:HG23	1:F:585:HIS:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:329:ASN:HD21	1:I:363:TYR:HB2	1.83	0.43
1:J:251:THR:O	1:J:255:VAL:HG23	2.19	0.43
1:A:485:LEU:HD23	1:A:488:ILE:HG13	2.00	0.43
2:K:69:VAL:HA	2:K:72:VAL:HG12	2.00	0.43
1:J:649:HIS:CE1	1:J:650:LYS:HG3	2.54	0.42
1:A:301:LEU:HD23	1:A:301:LEU:HA	1.74	0.42
1:B:286:MET:SD	1:B:420:ILE:HD12	2.59	0.42
2:L:22:THR:HA	2:L:25:ILE:HG22	2.00	0.42
2:L:43:PRO:HG2	2:L:46:LEU:HD12	2.01	0.42
1:J:533:LEU:HD22	1:J:541:LEU:HD22	1.99	0.42
1:J:588:ILE:HA	1:J:591:LEU:HD12	2.01	0.42
1:J:631:GLU:HG3	1:J:661:ALA:HA	2.00	0.42
1:I:96:TYR:HE1	1:I:111:GLN:HA	1.84	0.42
1:I:176:GLN:OE1	1:I:289:TYR:OH	2.37	0.42
1:A:204:PHE:CD2	2:C:67:PHE:HB2	2.55	0.42
1:F:174:PHE:HD2	1:F:198:LEU:HD13	1.84	0.42
1:F:525:GLN:HG3	1:F:527:LEU:HD11	2.00	0.42
1:F:641:GLU:OE1	1:F:663:ARG:NH2	2.52	0.42
1:B:506:SER:OG	1:B:676:MET:O	2.32	0.42
1:F:415:MET:O	1:F:419:GLN:HG3	2.19	0.42
1:J:202:VAL:HG21	1:I:390:ILE:HD11	2.02	0.42
1:I:41:LEU:O	1:I:45:SER:OG	2.32	0.42
1:F:185:HIS:O	1:F:186:ARG:HG2	2.18	0.42
2:K:61:ALA:O	2:K:65:MET:HG3	2.19	0.42
1:A:471:ARG:HE	1:A:527:LEU:HD21	1.84	0.42
1:A:512:THR:HG23	1:A:628:ILE:HG21	2.01	0.42
1:B:231:LEU:HD21	1:B:255:VAL:HG13	2.00	0.42
2:G:81:GLU:HA	2:G:456:MET:HA	2.00	0.42
1:A:139:ASP:CG	1:A:140:PHE:H	2.22	0.42
1:B:149:LYS:HE2	2:D:31:THR:HG23	2.01	0.42
1:J:427:LEU:HD12	1:J:430:ILE:HD11	2.01	0.42
1:E:308:SER:HA	1:E:431:TRP:CH2	2.55	0.42
1:F:169:LEU:HD11	1:F:285:VAL:HG21	2.02	0.42
1:A:527:LEU:HD13	1:A:530:GLY:HA2	2.02	0.42
1:E:427:LEU:HD23	1:E:427:LEU:HA	1.93	0.42
1:F:422:ALA:HB3	1:F:423:PRO:HD3	2.02	0.42
2:D:43:PRO:HG2	2:D:46:LEU:HD12	2.01	0.42
2:G:464:LEU:O	2:G:468:GLU:HB2	2.20	0.42
1:J:349:SER:HB2	1:J:350:PRO:HD3	2.01	0.42
1:J:664:LEU:HD23	1:J:705:GLN:HG3	2.01	0.42
1:I:153:ILE:HG23	1:I:215:ILE:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:ILE:HD11	1:B:674:ILE:HD12	2.01	0.42
1:F:418:GLY:HA2	1:F:421:VAL:HG22	2.02	0.42
2:G:56:ARG:HD2	2:G:56:ARG:N	2.34	0.42
1:J:528:ILE:HB	1:J:533:LEU:HD21	2.00	0.41
1:I:454:SER:O	1:I:517:ARG:NH2	2.53	0.41
1:B:274:LEU:HD12	1:B:275:ASP:N	2.35	0.41
1:B:350:PRO:O	1:B:354:ASN:ND2	2.51	0.41
1:B:514:LEU:HD23	1:B:514:LEU:HA	1.91	0.41
1:E:29:GLU:O	1:E:33:ARG:HG2	2.20	0.41
1:F:171:THR:HB	1:F:172:PRO:HD3	2.02	0.41
1:J:264:PHE:CD2	1:J:437:VAL:HG21	2.55	0.41
1:I:249:GLY:HA3	1:I:331:SER:HA	2.01	0.41
1:E:153:ILE:HG23	1:E:215:ILE:HG22	2.01	0.41
1:E:190:THR:OG1	2:G:80:VAL:HG13	2.19	0.41
1:E:674:ILE:HG23	1:E:681:ILE:HG23	2.02	0.41
1:F:169:LEU:HB2	1:F:282:PHE:HE1	1.86	0.41
1:F:249:GLY:HA3	1:F:331:SER:HA	2.02	0.41
1:J:183:LEU:HD13	1:I:400:VAL:HG11	2.03	0.41
1:J:315:LEU:HD11	1:J:370:VAL:HG13	2.00	0.41
1:A:19:GLN:NE2	1:F:569:GLY:O	2.51	0.41
1:A:315:LEU:O	1:A:319:LEU:HD23	2.19	0.41
1:E:128:ARG:NH2	2:L:40:GLU:O	2.54	0.41
1:E:610:GLN:O	1:E:614:ILE:HG12	2.20	0.41
1:A:386:LYS:O	1:A:390:ILE:HG12	2.21	0.41
1:B:399:LEU:O	1:B:403:GLY:N	2.47	0.41
1:F:549:LEU:O	1:F:552:ASN:ND2	2.54	0.41
1:F:674:ILE:HG12	1:F:684:GLN:HB3	2.03	0.41
2:G:467:LEU:O	2:G:471:VAL:HG23	2.20	0.41
1:I:444:LEU:HD23	1:I:444:LEU:HA	1.90	0.41
1:B:428:ALA:HA	1:B:431:TRP:CE3	2.52	0.41
1:E:142:TRP:O	1:E:145:PRO:HD2	2.21	0.41
1:E:208:LEU:HD23	1:E:208:LEU:HA	1.93	0.41
1:E:668:LYS:HE2	1:E:668:LYS:HB3	1.91	0.41
1:I:80:ASP:N	1:I:80:ASP:OD1	2.53	0.41
1:I:128:ARG:HD3	1:I:128:ARG:HA	1.80	0.41
1:E:612:GLN:HB3	1:E:636:LEU:HD21	2.01	0.41
1:F:599:VAL:HB	1:F:603:GLY:HA2	2.02	0.41
1:J:478:LYS:HB2	1:J:481:SER:OG	2.21	0.41
1:I:204:PHE:CD2	2:K:67:PHE:HB2	2.55	0.41
1:A:293:LEU:HB2	1:A:413:PHE:CZ	2.56	0.41
1:B:686:LYS:HE3	1:B:686:LYS:HB3	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:184:VAL:HG23	1:F:185:HIS:N	2.36	0.41
2:D:56:ARG:O	2:D:60:VAL:HG23	2.21	0.41
2:C:465:SER:HA	2:C:468:GLU:HG2	2.03	0.41
2:G:75:SER:HB3	2:G:460:ILE:HD13	2.03	0.41
1:E:242:TYR:O	1:E:246:ARG:HD3	2.20	0.41
1:E:395:LEU:HD23	1:E:395:LEU:HA	1.97	0.41
1:F:478:LYS:HD2	1:F:479:PRO:HD2	2.02	0.41
2:L:70:ILE:HA	2:L:73:ILE:HG22	2.03	0.41
2:C:391:GLU:O	2:C:392:ALA:C	2.59	0.41
2:G:80:VAL:HG23	2:G:459:VAL:HG23	2.02	0.41
1:I:147:ILE:HG23	1:I:154:PHE:CD2	2.56	0.40
1:I:254:ARG:HD2	1:I:443:ARG:HB3	2.01	0.40
1:I:512:THR:HG23	1:I:628:ILE:HG21	2.02	0.40
1:B:557:ARG:HE	1:B:561:ASP:HB3	1.85	0.40
1:E:12:TYR:CZ	1:E:16:ILE:HD11	2.55	0.40
1:E:566:ALA:HB3	1:E:622:ASN:OD1	2.21	0.40
1:J:222:ARG:HG2	2:L:48:LEU:O	2.21	0.40
1:A:144:ILE:N	1:A:145:PRO:HD2	2.36	0.40
1:B:339:ALA:O	1:B:343:ILE:HG12	2.20	0.40
1:B:420:ILE:O	1:B:423:PRO:HD2	2.21	0.40
1:E:13:ALA:HB2	1:E:101:LEU:HD11	2.04	0.40
1:F:169:LEU:HD21	1:F:285:VAL:HG21	2.03	0.40
1:J:254:ARG:HG2	1:J:447:VAL:HG23	2.04	0.40
1:E:280:PHE:HA	1:E:283:PHE:HB2	2.03	0.40
1:F:701:LEU:HD23	1:F:701:LEU:HA	1.96	0.40
2:L:77:LEU:HD23	2:L:77:LEU:HA	1.93	0.40
2:D:34:ARG:HH12	2:D:42:LEU:HD21	1.85	0.40
2:D:73:ILE:HD13	2:D:73:ILE:HA	1.90	0.40
1:J:464:ILE:HD12	1:J:544:GLN:HB2	2.03	0.40
1:I:166:LEU:O	1:I:170:ILE:HG13	2.21	0.40
1:F:171:THR:HG22	1:F:175:PHE:HE2	1.86	0.40
1:F:621:VAL:HG23	1:F:622:ASN:N	2.36	0.40
1:F:690:LEU:HB3	1:F:698:TYR:CD2	2.57	0.40
2:G:391:GLU:O	2:G:392:ALA:C	2.59	0.40
2:G:465:SER:O	2:G:469:GLU:HG2	2.22	0.40
1:I:607:SER:O	1:I:611:ARG:HG2	2.21	0.40
1:A:157:THR:HG21	1:A:216:PHE:HD1	1.85	0.40
1:E:169:LEU:HB2	1:E:282:PHE:HE1	1.87	0.40
1:E:677:GLU:OE1	1:E:677:GLU:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	698/707 (99%)	664 (95%)	34 (5%)	0	100	100
1	B	568/707 (80%)	543 (96%)	25 (4%)	0	100	100
1	E	698/707 (99%)	674 (97%)	24 (3%)	0	100	100
1	F	568/707 (80%)	547 (96%)	21 (4%)	0	100	100
1	I	698/707 (99%)	663 (95%)	35 (5%)	0	100	100
1	J	568/707 (80%)	545 (96%)	23 (4%)	0	100	100
2	C	162/356 (46%)	147 (91%)	15 (9%)	0	100	100
2	D	67/356 (19%)	65 (97%)	2 (3%)	0	100	100
2	G	161/356 (45%)	141 (88%)	20 (12%)	0	100	100
2	H	67/356 (19%)	66 (98%)	1 (2%)	0	100	100
2	K	47/356 (13%)	46 (98%)	1 (2%)	0	100	100
2	L	67/356 (19%)	64 (96%)	3 (4%)	0	100	100
All	All	4369/6378 (68%)	4165 (95%)	204 (5%)	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	A	603/615 (98%)	603 (100%)	0	100	100
1	B	494/615 (80%)	494 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	601/615 (98%)	601 (100%)	0	100 100
1	F	494/615 (80%)	493 (100%)	1 (0%)	93 98
1	I	605/615 (98%)	604 (100%)	1 (0%)	93 98
1	J	493/615 (80%)	493 (100%)	0	100 100
2	C	67/324 (21%)	67 (100%)	0	100 100
2	D	65/324 (20%)	65 (100%)	0	100 100
2	G	66/324 (20%)	66 (100%)	0	100 100
2	H	65/324 (20%)	65 (100%)	0	100 100
2	K	45/324 (14%)	45 (100%)	0	100 100
2	L	65/324 (20%)	65 (100%)	0	100 100
All	All	3663/5634 (65%)	3661 (100%)	2 (0%)	93 98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	587	PHE
1	F	587	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	HIS
1	E	539	ASN
1	F	585	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

37 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	$\#\|Z\| > 2$
3	6OU	A	803	-	32,32,48	1.45	6 (18%)	36,37,53	1.18	2 (5%)
3	6OU	F	803	-	31,31,48	1.32	3 (9%)	33,33,53	1.19	2 (6%)
3	6OU	F	804	-	11,11,48	0.70	0	10,10,53	0.81	0
3	6OU	I	802	-	9,9,48	0.74	0	8,8,53	0.79	0
3	6OU	J	803	-	11,11,48	0.68	0	10,10,53	0.82	0
3	6OU	B	801	-	13,13,48	0.80	0	12,12,53	0.74	0
3	6OU	F	801	-	31,31,48	1.34	4 (12%)	33,33,53	1.22	2 (6%)
3	6OU	E	803	-	7,7,48	0.72	0	6,6,53	0.72	0
3	6OU	H	402	-	11,11,48	0.70	0	10,10,53	0.81	0
3	6OU	I	806	-	10,10,48	0.67	0	9,9,53	0.81	0
3	6OU	J	801	-	16,16,48	1.43	2 (12%)	15,15,53	0.96	0
3	6OU	I	808	-	11,11,48	0.70	0	10,10,53	0.84	0
3	6OU	L	401	-	16,16,48	1.42	2 (12%)	15,15,53	1.03	1 (6%)
3	6OU	F	802	-	16,16,48	1.42	2 (12%)	15,15,53	0.96	1 (6%)
3	6OU	I	807	-	11,11,48	0.70	0	10,10,53	0.83	0
3	6OU	J	806	-	11,11,48	0.70	0	10,10,53	0.83	0
3	6OU	E	804	-	12,12,48	0.68	0	11,11,53	0.86	0
3	6OU	H	401	-	40,40,48	1.33	5 (12%)	44,45,53	1.13	2 (4%)
3	6OU	A	804	-	19,19,48	1.58	3 (15%)	21,21,53	1.37	2 (9%)
3	6OU	J	802	-	16,16,48	1.42	2 (12%)	15,15,53	0.98	1 (6%)
3	6OU	A	801	-	31,31,48	1.39	5 (16%)	34,36,53	1.15	2 (5%)
3	6OU	L	402	-	11,11,48	0.70	0	10,10,53	0.84	0
3	6OU	A	806	-	11,11,48	0.69	0	10,10,53	0.85	0
3	6OU	J	804	-	13,13,48	0.71	0	12,12,53	0.87	0
3	6OU	A	807	-	24,24,48	1.62	4 (16%)	28,29,53	1.26	2 (7%)
3	6OU	E	801	-	8,8,48	0.74	0	7,7,53	0.76	0
3	6OU	I	803	-	33,33,48	1.43	6 (18%)	37,38,53	1.17	2 (5%)
3	6OU	K	401	-	39,39,48	1.35	5 (12%)	43,44,53	1.09	2 (4%)
3	6OU	I	801	-	16,16,48	1.42	2 (12%)	15,15,53	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	6OU	I	804	-	10,10,48	0.67	0	9,9,53	0.84	0
3	6OU	A	805	-	7,7,48	0.64	0	6,6,53	0.73	0
3	6OU	I	809	-	12,12,48	0.70	0	11,11,53	0.83	0
3	6OU	B	802	-	11,11,48	0.69	0	10,10,53	0.83	0
3	6OU	J	805	-	9,9,48	0.74	0	8,8,53	0.80	0
3	6OU	I	805	-	10,10,48	0.67	0	9,9,53	0.81	0
3	6OU	E	802	-	7,7,48	0.71	0	6,6,53	0.74	0
3	6OU	A	802	-	16,16,48	1.43	2 (12%)	15,15,53	0.91	0

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
3	6OU	A	803	-	-	18/34/34/52	-
3	6OU	F	803	-	-	16/33/33/52	-
3	6OU	F	804	-	-	4/9/9/52	-
3	6OU	I	802	-	-	4/7/7/52	-
3	6OU	J	803	-	-	5/9/9/52	-
3	6OU	B	801	-	-	4/11/11/52	-
3	6OU	F	801	-	-	9/33/33/52	-
3	6OU	E	803	-	-	3/5/5/52	-
3	6OU	H	402	-	-	4/9/9/52	-
3	6OU	I	806	-	-	6/8/8/52	-
3	6OU	J	801	-	-	7/14/14/52	-
3	6OU	I	808	-	-	3/9/9/52	-
3	6OU	L	401	-	-	8/14/14/52	-
3	6OU	F	802	-	-	5/14/14/52	-
3	6OU	I	807	-	-	3/9/9/52	-
3	6OU	J	806	-	-	6/9/9/52	-
3	6OU	E	804	-	-	4/10/10/52	-
3	6OU	H	401	-	-	22/42/42/52	-
3	6OU	A	804	-	-	10/21/21/52	-
3	6OU	J	802	-	-	9/14/14/52	-
3	6OU	A	801	-	-	22/35/35/52	-
3	6OU	L	402	-	-	3/9/9/52	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6OU	A	806	-	-	5/9/9/52	-
3	6OU	J	804	-	-	5/11/11/52	-
3	6OU	A	807	-	-	10/26/26/52	-
3	6OU	E	801	-	-	2/6/6/52	-
3	6OU	I	803	-	-	16/35/35/52	-
3	6OU	K	401	-	-	13/41/41/52	-
3	6OU	I	801	-	-	10/14/14/52	-
3	6OU	I	804	-	-	3/8/8/52	-
3	6OU	A	805	-	-	2/5/5/52	-
3	6OU	I	809	-	-	5/10/10/52	-
3	6OU	B	802	-	-	6/9/9/52	-
3	6OU	J	805	-	-	4/7/7/52	-
3	6OU	I	805	-	-	3/8/8/52	-
3	6OU	E	802	-	-	3/5/5/52	-
3	6OU	A	802	-	-	7/14/14/52	-

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	802	6OU	C41-C40	4.24	1.56	1.31
3	L	401	6OU	C41-C40	4.23	1.56	1.31
3	I	801	6OU	C41-C40	4.23	1.56	1.31
3	J	801	6OU	C41-C40	4.23	1.56	1.31
3	A	802	6OU	C41-C40	4.22	1.56	1.31
3	F	802	6OU	C41-C40	4.21	1.56	1.31
3	F	801	6OU	O18-C16	3.82	1.44	1.33
3	I	803	6OU	O18-C16	3.78	1.44	1.33
3	F	803	6OU	O18-C16	3.78	1.44	1.33
3	A	807	6OU	O18-C16	3.78	1.44	1.33
3	H	401	6OU	O18-C16	3.77	1.44	1.33
3	K	401	6OU	O18-C16	3.77	1.44	1.33
3	A	801	6OU	O18-C16	3.77	1.44	1.33
3	A	804	6OU	O18-C16	3.76	1.44	1.33
3	A	803	6OU	O18-C16	3.75	1.44	1.33
3	K	401	6OU	O30-C31	3.29	1.43	1.34
3	A	803	6OU	O30-C31	3.29	1.43	1.34
3	A	807	6OU	O30-C31	3.28	1.43	1.34
3	F	803	6OU	O30-C31	3.28	1.43	1.34
3	I	803	6OU	O30-C31	3.26	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	804	6OU	O30-C31	3.26	1.43	1.34
3	A	801	6OU	O30-C31	3.22	1.43	1.34
3	F	801	6OU	O30-C31	3.21	1.43	1.34
3	H	401	6OU	O30-C31	3.20	1.43	1.34
3	A	807	6OU	P23-O26	2.88	1.65	1.54
3	A	803	6OU	P23-O26	2.87	1.65	1.54
3	I	803	6OU	P23-O26	2.86	1.65	1.54
3	K	401	6OU	P23-O26	2.86	1.65	1.54
3	H	401	6OU	P23-O26	2.86	1.65	1.54
3	F	802	6OU	C39-C40	-2.76	1.34	1.50
3	L	401	6OU	C39-C40	-2.74	1.34	1.50
3	J	801	6OU	C39-C40	-2.73	1.34	1.50
3	A	802	6OU	C39-C40	-2.73	1.34	1.50
3	J	802	6OU	C39-C40	-2.72	1.34	1.50
3	I	801	6OU	C39-C40	-2.72	1.34	1.50
3	I	803	6OU	P23-O22	2.23	1.67	1.60
3	H	401	6OU	P23-O22	2.23	1.67	1.60
3	K	401	6OU	P23-O22	2.22	1.67	1.60
3	A	807	6OU	P23-O22	2.22	1.67	1.60
3	A	803	6OU	P23-O22	2.20	1.67	1.60
3	F	801	6OU	O30-C20	-2.07	1.41	1.46
3	F	801	6OU	C33-C31	2.05	1.56	1.50
3	K	401	6OU	C33-C31	2.04	1.56	1.50
3	A	801	6OU	C33-C31	2.04	1.56	1.50
3	A	803	6OU	C33-C31	2.03	1.56	1.50
3	I	803	6OU	O30-C20	-2.02	1.41	1.46
3	A	801	6OU	O30-C20	-2.02	1.41	1.46
3	A	803	6OU	O30-C20	-2.02	1.41	1.46
3	H	401	6OU	O30-C20	-2.02	1.41	1.46
3	I	803	6OU	C33-C31	2.01	1.56	1.50
3	A	804	6OU	C33-C31	2.01	1.56	1.50
3	A	801	6OU	P23-O22	2.01	1.67	1.59
3	F	803	6OU	C33-C31	2.00	1.56	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	801	6OU	O30-C31-C33	4.05	120.23	111.50
3	A	807	6OU	O30-C31-C33	3.94	120.00	111.50
3	H	401	6OU	O30-C31-C33	3.94	119.98	111.50
3	A	801	6OU	O30-C31-C33	3.93	119.97	111.50
3	I	803	6OU	O30-C31-C33	3.91	119.94	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	804	6OU	O30-C31-C33	3.89	119.88	111.50
3	A	803	6OU	O30-C31-C33	3.89	119.88	111.50
3	F	803	6OU	O30-C31-C33	3.85	119.79	111.50
3	K	401	6OU	O30-C31-C33	3.60	119.26	111.50
3	F	803	6OU	O18-C16-C15	2.64	120.20	111.91
3	A	803	6OU	O18-C16-C15	2.61	120.10	111.91
3	H	401	6OU	O18-C16-C15	2.59	120.03	111.91
3	K	401	6OU	O18-C16-C15	2.58	120.01	111.91
3	I	803	6OU	O18-C16-C15	2.57	119.97	111.91
3	F	801	6OU	O18-C16-C15	2.56	119.94	111.91
3	A	801	6OU	O18-C16-C15	2.56	119.93	111.91
3	A	807	6OU	O18-C16-C15	2.54	119.89	111.91
3	A	804	6OU	O18-C16-C15	2.50	119.75	111.91
3	L	401	6OU	C42-C41-C40	-2.12	108.43	124.73
3	J	802	6OU	C42-C41-C40	-2.02	109.24	124.73
3	F	802	6OU	C42-C41-C40	-2.02	109.26	124.73

There are no chirality outliers.

All (269) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	803	6OU	O18-C19-C20-O30
3	A	801	6OU	C27-O26-P23-O22
3	A	801	6OU	C27-O26-P23-O24
3	A	801	6OU	C27-O26-P23-O25
3	A	801	6OU	O26-C27-C28-N29
3	F	801	6OU	O18-C19-C20-O30
3	H	401	6OU	C21-O22-P23-O25
3	H	401	6OU	C21-O22-P23-O26
3	A	804	6OU	C15-C16-O18-C19
3	K	401	6OU	C15-C16-O18-C19
3	J	801	6OU	C39-C40-C41-C42
3	A	802	6OU	C39-C40-C41-C42
3	F	802	6OU	C39-C40-C41-C42
3	L	401	6OU	C39-C40-C41-C42
3	A	807	6OU	C15-C16-O18-C19
3	K	401	6OU	O17-C16-O18-C19
3	A	804	6OU	O17-C16-O18-C19
3	A	802	6OU	C36-C37-C38-C39
3	A	802	6OU	C34-C35-C36-C37
3	A	807	6OU	O17-C16-O18-C19
3	A	801	6OU	C15-C16-O18-C19

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Mol	Chain	Res	Type	Atoms
3	F	803	6OU	C15-C16-O18-C19
3	A	803	6OU	O30-C20-C21-O22
3	A	804	6OU	C31-C33-C34-C35
3	F	803	6OU	C31-C33-C34-C35
3	F	803	6OU	O17-C16-O18-C19
3	A	801	6OU	O17-C16-O18-C19
3	A	803	6OU	C15-C16-O18-C19
3	I	803	6OU	C43-C44-C45-C46
3	F	801	6OU	C37-C38-C39-C40
3	J	805	6OU	C03-C04-C05-C06
3	I	803	6OU	C34-C35-C36-C37
3	F	803	6OU	C36-C37-C38-C39
3	J	802	6OU	C39-C40-C41-C42
3	I	806	6OU	C04-C05-C06-C07
3	I	806	6OU	C07-C08-C09-C10
3	J	803	6OU	C04-C05-C06-C07
3	J	806	6OU	C06-C07-C08-C09
3	I	805	6OU	C07-C08-C09-C10
3	A	803	6OU	C35-C36-C37-C38
3	A	804	6OU	O18-C19-C20-O30
3	A	801	6OU	C07-C08-C09-C10
3	L	401	6OU	C36-C37-C38-C39
3	J	801	6OU	C36-C37-C38-C39
3	A	805	6OU	C03-C04-C05-C06
3	E	804	6OU	C07-C08-C09-C10
3	H	401	6OU	C08-C09-C10-C11
3	H	402	6OU	C03-C04-C05-C06
3	A	803	6OU	O17-C16-O18-C19
3	J	801	6OU	C37-C38-C39-C40
3	I	804	6OU	C04-C05-C06-C07
3	A	806	6OU	C03-C04-C05-C06
3	E	803	6OU	C02-C03-C04-C05
3	F	804	6OU	C03-C04-C05-C06
3	H	401	6OU	C44-C45-C46-C47
3	A	806	6OU	C06-C07-C08-C09
3	I	805	6OU	C04-C05-C06-C07
3	J	803	6OU	C07-C08-C09-C10
3	E	802	6OU	C02-C03-C04-C05
3	F	803	6OU	C35-C36-C37-C38
3	L	402	6OU	C06-C07-C08-C09
3	I	801	6OU	C39-C40-C41-C42
3	J	806	6OU	C05-C06-C07-C08

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Mol	Chain	Res	Type	Atoms
3	K	401	6OU	C08-C09-C10-C11
3	A	801	6OU	C33-C31-O30-C20
3	I	805	6OU	C06-C07-C08-C09
3	I	808	6OU	C03-C04-C05-C06
3	J	802	6OU	C37-C38-C39-C40
3	I	801	6OU	C37-C38-C39-C40
3	A	802	6OU	C37-C38-C39-C40
3	F	802	6OU	C37-C38-C39-C40
3	F	803	6OU	C37-C38-C39-C40
3	L	401	6OU	C37-C38-C39-C40
3	H	401	6OU	C36-C37-C38-C39
3	I	801	6OU	C35-C36-C37-C38
3	A	806	6OU	C08-C09-C10-C11
3	A	801	6OU	O32-C31-O30-C20
3	J	802	6OU	C34-C35-C36-C37
3	I	808	6OU	C06-C07-C08-C09
3	B	802	6OU	C07-C08-C09-C10
3	A	801	6OU	C12-C13-C14-C15
3	F	801	6OU	C08-C09-C10-C11
3	H	401	6OU	C11-C12-C13-C14
3	J	804	6OU	C09-C10-C11-C12
3	E	801	6OU	C02-C03-C04-C05
3	H	401	6OU	C37-C38-C39-C40
3	A	801	6OU	C13-C14-C15-C16
3	I	809	6OU	C07-C08-C09-C10
3	I	802	6OU	C02-C03-C04-C05
3	A	803	6OU	C33-C31-O30-C20
3	A	807	6OU	C33-C31-O30-C20
3	H	401	6OU	C33-C31-O30-C20
3	A	807	6OU	O30-C20-C21-O22
3	J	804	6OU	C07-C08-C09-C10
3	A	803	6OU	C05-C06-C07-C08
3	F	803	6OU	O18-C19-C20-O30
3	A	807	6OU	C35-C36-C37-C38
3	J	803	6OU	C06-C07-C08-C09
3	F	804	6OU	C05-C06-C07-C08
3	I	807	6OU	C06-C07-C08-C09
3	A	801	6OU	C08-C09-C10-C11
3	H	402	6OU	C08-C09-C10-C11
3	I	806	6OU	C06-C07-C08-C09
3	H	401	6OU	C35-C36-C37-C38
3	A	803	6OU	O32-C31-O30-C20

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Mol	Chain	Res	Type	Atoms
3	A	807	6OU	O32-C31-O30-C20
3	H	401	6OU	O32-C31-O30-C20
3	J	806	6OU	C03-C04-C05-C06
3	I	803	6OU	C35-C36-C37-C38
3	H	401	6OU	C20-C21-O22-P23
3	A	803	6OU	C19-C20-C21-O22
3	A	801	6OU	C11-C12-C13-C14
3	L	402	6OU	C05-C06-C07-C08
3	A	803	6OU	O18-C19-C20-C21
3	A	804	6OU	O18-C19-C20-C21
3	A	807	6OU	O18-C19-C20-C21
3	H	401	6OU	O18-C19-C20-C21
3	I	804	6OU	C07-C08-C09-C10
3	H	401	6OU	C13-C14-C15-C16
3	I	802	6OU	C06-C07-C08-C09
3	B	802	6OU	C04-C05-C06-C07
3	J	805	6OU	C02-C03-C04-C05
3	I	801	6OU	C42-C43-C44-C45
3	I	801	6OU	C36-C37-C38-C39
3	A	801	6OU	C05-C06-C07-C08
3	A	803	6OU	C21-O22-P23-O24
3	H	401	6OU	C21-O22-P23-O24
3	K	401	6OU	C13-C14-C15-C16
3	H	402	6OU	C05-C06-C07-C08
3	A	803	6OU	O18-C19-C20-O30
3	A	807	6OU	O18-C19-C20-O30
3	I	803	6OU	C15-C16-O18-C19
3	I	803	6OU	C33-C31-O30-C20
3	B	801	6OU	C31-C33-C34-C35
3	K	401	6OU	C12-C13-C14-C15
3	E	801	6OU	C01-C02-C03-C04
3	A	801	6OU	C19-C20-C21-O22
3	A	807	6OU	C19-C20-C21-O22
3	H	401	6OU	C19-C20-C21-O22
3	F	801	6OU	O18-C19-C20-C21
3	F	803	6OU	O18-C19-C20-C21
3	J	804	6OU	C10-C11-C12-C13
3	L	401	6OU	C35-C36-C37-C38
3	B	801	6OU	C34-C35-C36-C37
3	A	801	6OU	O30-C20-C21-O22
3	H	401	6OU	O30-C20-C21-O22
3	I	803	6OU	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
3	A	803	6OU	C31-C33-C34-C35
3	F	802	6OU	C34-C35-C36-C37
3	I	803	6OU	O17-C16-O18-C19
3	A	803	6OU	C36-C37-C38-C39
3	J	801	6OU	C34-C35-C36-C37
3	I	806	6OU	C01-C02-C03-C04
3	A	803	6OU	C07-C08-C09-C10
3	A	804	6OU	C19-C20-C21-O22
3	F	803	6OU	C19-C20-C21-O22
3	I	801	6OU	C33-C34-C35-C36
3	L	401	6OU	C42-C43-C44-C45
3	E	803	6OU	C01-C02-C03-C04
3	I	803	6OU	C31-C33-C34-C35
3	I	803	6OU	O32-C31-O30-C20
3	K	401	6OU	C19-C20-C21-O22
3	A	806	6OU	C09-C10-C11-C12
3	F	801	6OU	C35-C36-C37-C38
3	I	804	6OU	C06-C07-C08-C09
3	I	803	6OU	O18-C19-C20-C21
3	K	401	6OU	O30-C20-C21-O22
3	F	803	6OU	C46-C47-C48-C49
3	I	809	6OU	C05-C06-C07-C08
3	H	401	6OU	O18-C19-C20-O30
3	J	803	6OU	C09-C10-C11-C12
3	L	401	6OU	C41-C42-C43-C44
3	A	801	6OU	C21-O22-P23-O26
3	A	801	6OU	C20-C21-O22-P23
3	I	802	6OU	C03-C04-C05-C06
3	A	806	6OU	C05-C06-C07-C08
3	A	807	6OU	C36-C37-C38-C39
3	B	802	6OU	C05-C06-C07-C08
3	B	802	6OU	C06-C07-C08-C09
3	J	804	6OU	C05-C06-C07-C08
3	J	801	6OU	C41-C42-C43-C44
3	B	801	6OU	C37-C38-C39-C40
3	K	401	6OU	C37-C38-C39-C40
3	I	803	6OU	O30-C20-C21-O22
3	A	804	6OU	C35-C36-C37-C38
3	A	805	6OU	C05-C06-C07-C08
3	J	806	6OU	C09-C10-C11-C12
3	A	803	6OU	C08-C09-C10-C11
3	I	802	6OU	C01-C02-C03-C04

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Mol	Chain	Res	Type	Atoms
3	F	804	6OU	C06-C07-C08-C09
3	A	801	6OU	C10-C11-C12-C13
3	E	804	6OU	C10-C11-C12-C13
3	K	401	6OU	C36-C37-C38-C39
3	F	803	6OU	C44-C45-C46-C47
3	J	801	6OU	C38-C39-C40-C41
3	I	801	6OU	C38-C39-C40-C41
3	A	802	6OU	C38-C39-C40-C41
3	L	401	6OU	C38-C39-C40-C41
3	I	803	6OU	C44-C45-C46-C47
3	J	805	6OU	C01-C02-C03-C04
3	J	803	6OU	C03-C04-C05-C06
3	I	801	6OU	C43-C44-C45-C46
3	J	806	6OU	C08-C09-C10-C11
3	J	806	6OU	C01-C02-C03-C04
3	E	802	6OU	C01-C02-C03-C04
3	F	804	6OU	C08-C09-C10-C11
3	F	803	6OU	C34-C35-C36-C37
3	A	803	6OU	C10-C11-C12-C13
3	E	804	6OU	C05-C06-C07-C08
3	B	801	6OU	C35-C36-C37-C38
3	I	809	6OU	C06-C07-C08-C09
3	I	809	6OU	C10-C11-C12-C13
3	B	802	6OU	C02-C03-C04-C05
3	F	801	6OU	C31-C33-C34-C35
3	I	803	6OU	C19-C20-C21-O22
3	I	809	6OU	C09-C10-C11-C12
3	A	803	6OU	C06-C07-C08-C09
3	B	802	6OU	C09-C10-C11-C12
3	I	801	6OU	C31-C33-C34-C35
3	J	801	6OU	C42-C43-C44-C45
3	I	807	6OU	C02-C03-C04-C05
3	J	802	6OU	C31-C33-C34-C35
3	H	401	6OU	C09-C10-C11-C12
3	F	801	6OU	C36-C37-C38-C39
3	I	806	6OU	C03-C04-C05-C06
3	I	808	6OU	C04-C05-C06-C07
3	H	402	6OU	C09-C10-C11-C12
3	E	802	6OU	C05-C06-C07-C08
3	L	402	6OU	C04-C05-C06-C07
3	J	805	6OU	C06-C07-C08-C09
3	J	802	6OU	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
3	A	804	6OU	O30-C20-C21-O22
3	F	803	6OU	O30-C20-C21-O22
3	I	803	6OU	C20-C21-O22-P23
3	I	806	6OU	C05-C06-C07-C08
3	A	803	6OU	C33-C34-C35-C36
3	K	401	6OU	C07-C08-C09-C10
3	A	804	6OU	O30-C31-C33-C34
3	J	802	6OU	C40-C41-C42-C43
3	I	801	6OU	C40-C41-C42-C43
3	F	801	6OU	C40-C41-C42-C43
3	F	802	6OU	C40-C41-C42-C43
3	H	401	6OU	C43-C44-C45-C46
3	E	803	6OU	C05-C06-C07-C08
3	F	803	6OU	C40-C41-C42-C43
3	I	807	6OU	C09-C10-C11-C12
3	K	401	6OU	O30-C31-C33-C34
3	F	801	6OU	C34-C35-C36-C37
3	H	401	6OU	C14-C15-C16-O18
3	J	802	6OU	C35-C36-C37-C38
3	A	802	6OU	C40-C41-C42-C43
3	A	802	6OU	C35-C36-C37-C38
3	I	803	6OU	C46-C47-C48-C49
3	J	802	6OU	C38-C39-C40-C41
3	F	802	6OU	C38-C39-C40-C41
3	K	401	6OU	O32-C31-C33-C34
3	A	801	6OU	C14-C15-C16-O18
3	A	801	6OU	C21-O22-P23-O24
3	K	401	6OU	C33-C34-C35-C36
3	A	804	6OU	O32-C31-C33-C34
3	J	802	6OU	C33-C34-C35-C36
3	E	804	6OU	C08-C09-C10-C11
3	J	804	6OU	C06-C07-C08-C09
3	H	401	6OU	C14-C15-C16-O17
3	L	401	6OU	C31-C33-C34-C35
3	H	401	6OU	C07-C08-C09-C10
3	F	803	6OU	O30-C31-C33-C34
3	F	803	6OU	O32-C31-C33-C34
3	A	801	6OU	C14-C15-C16-O17

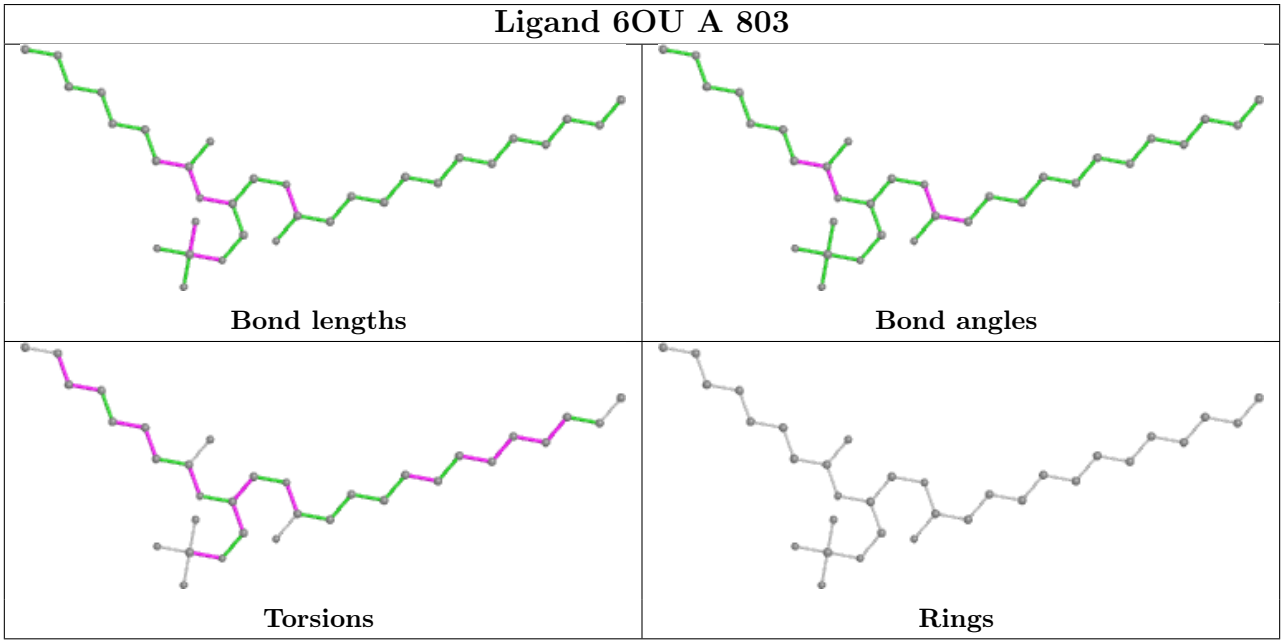
There are no ring outliers.

No monomer is involved in short contacts.

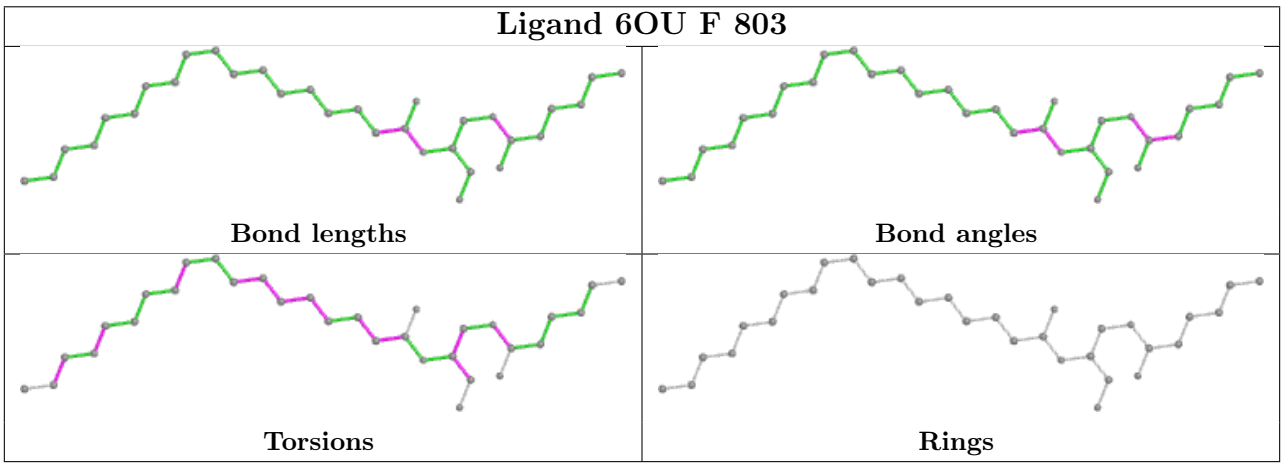
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 then 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.

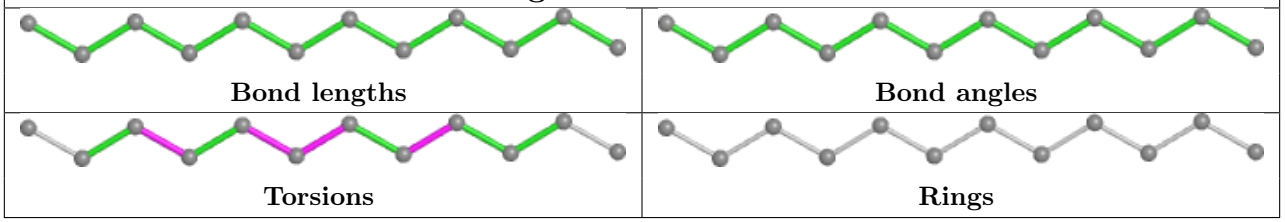
Ligand 6OU A 803



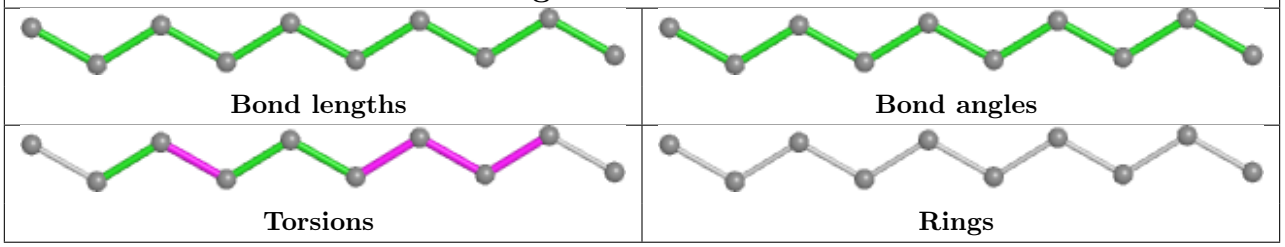
Ligand 6OU F 803



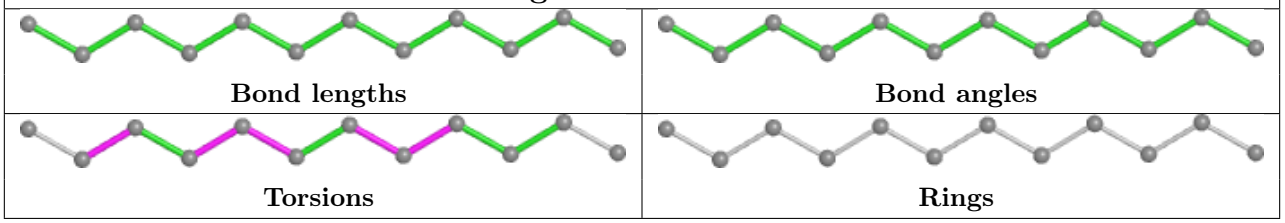
Ligand 6OU F 804



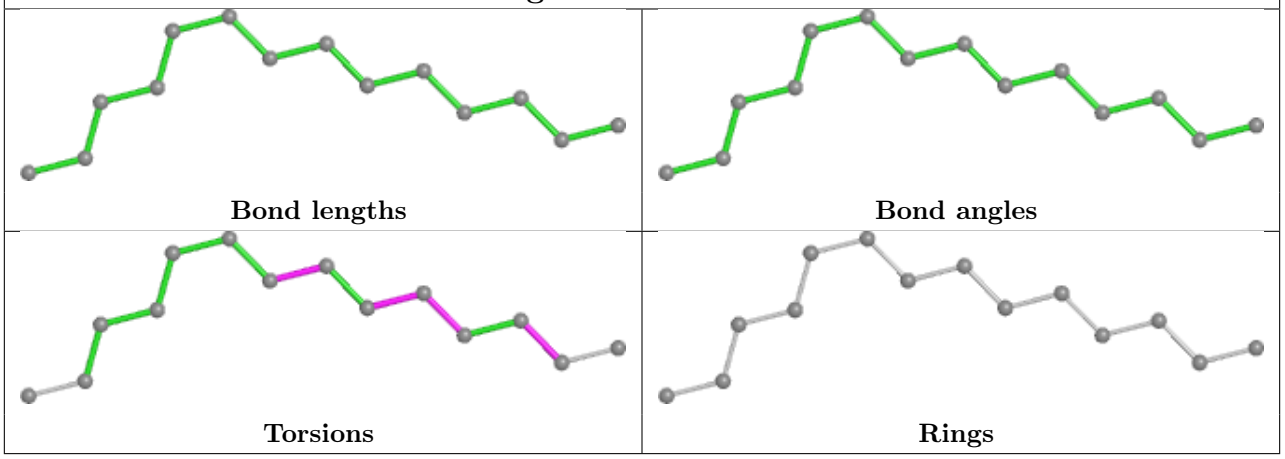
Ligand 6OU I 802



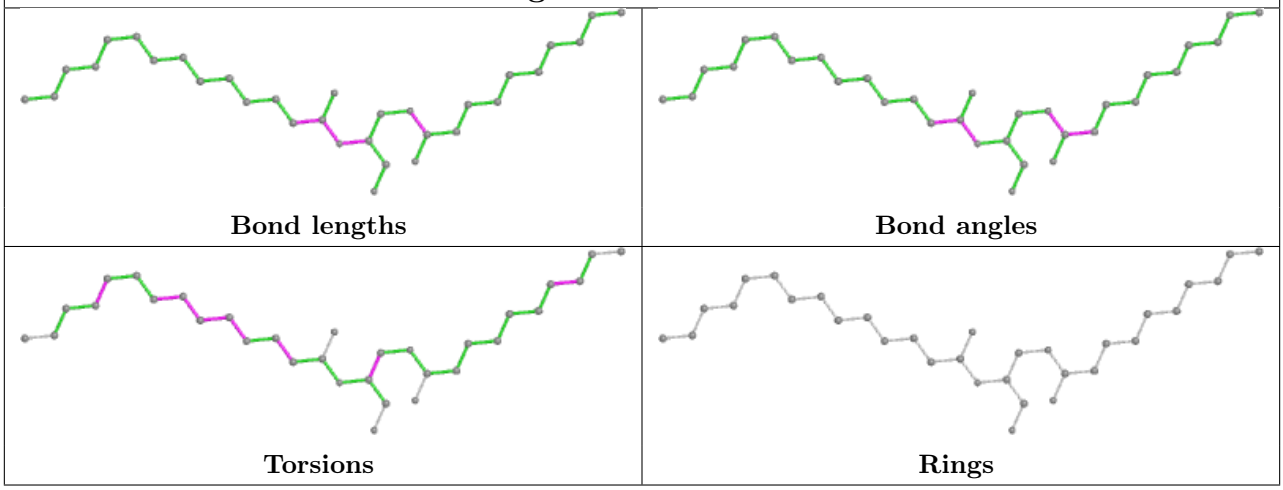
Ligand 6OU J 803



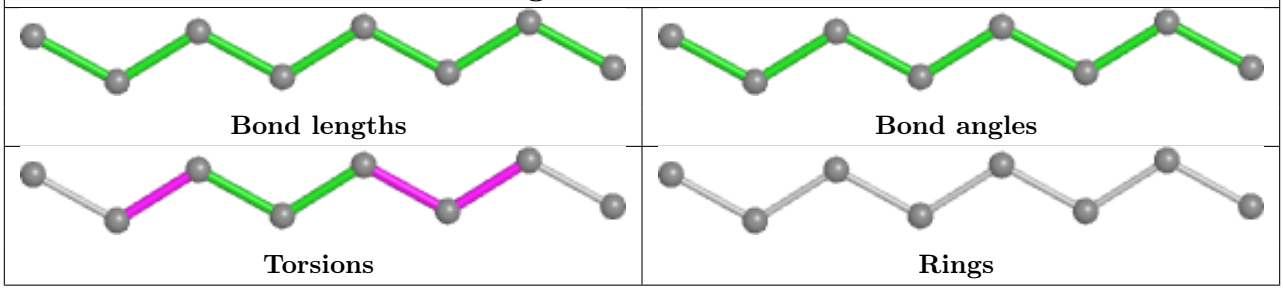
Ligand 6OU B 801



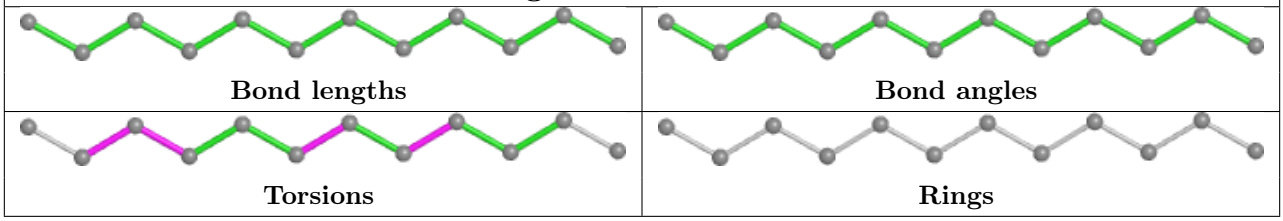
Ligand 6OU F 801



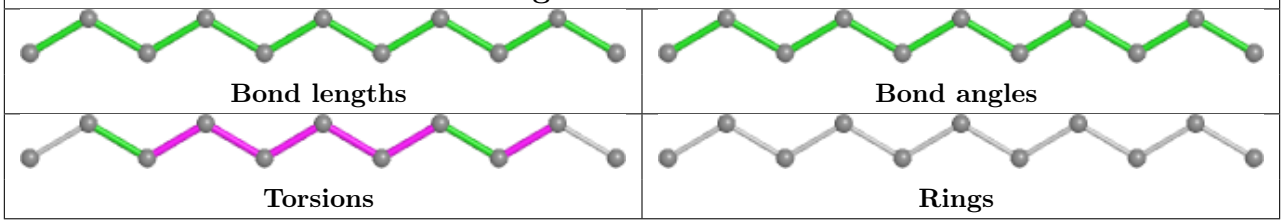
Ligand 6OU E 803



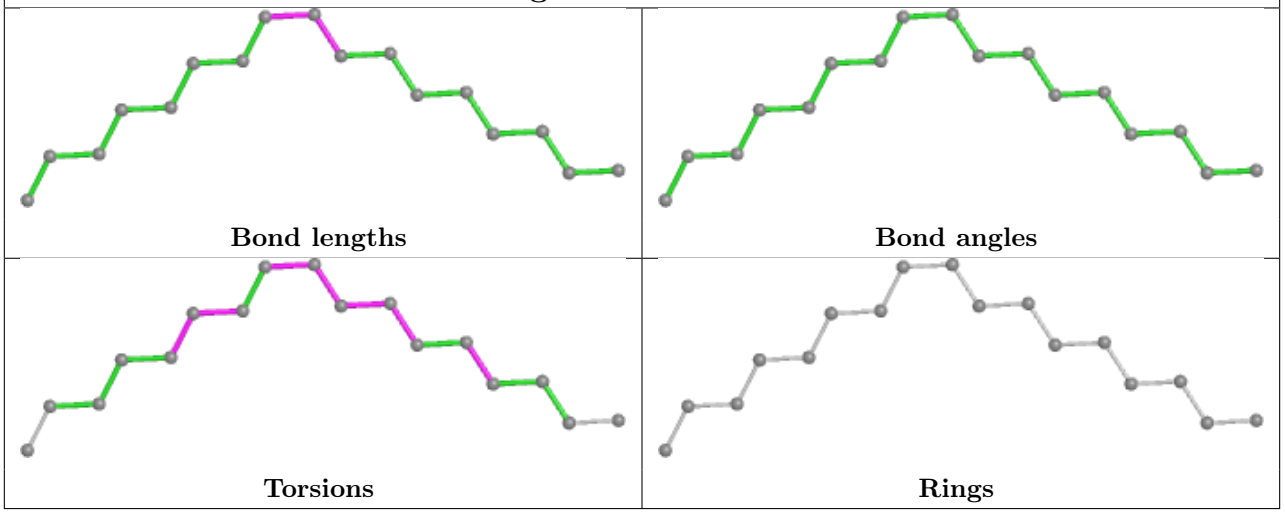
Ligand 6OU H 402



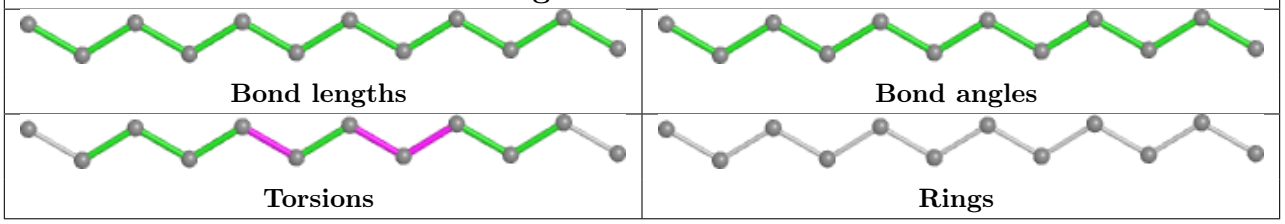
Ligand 6OU I 806



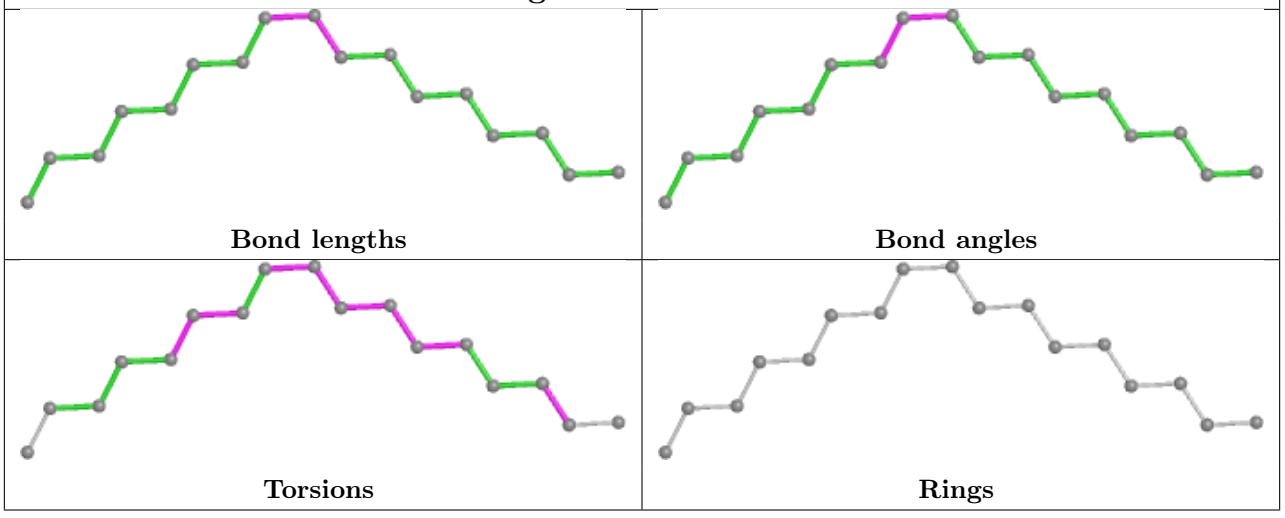
Ligand 6OU J 801



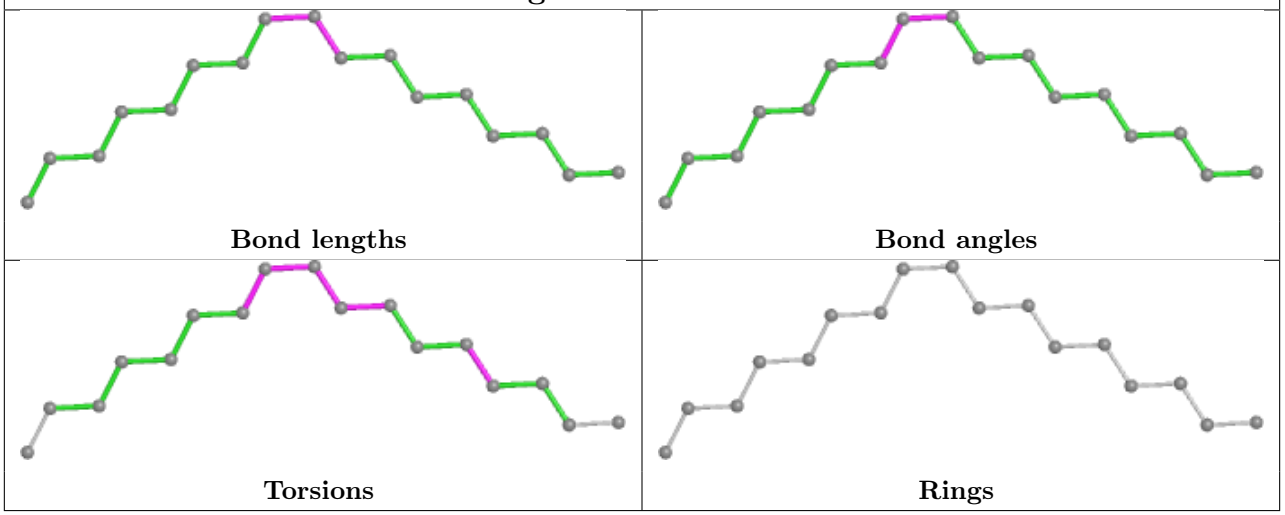
Ligand 6OU I 808



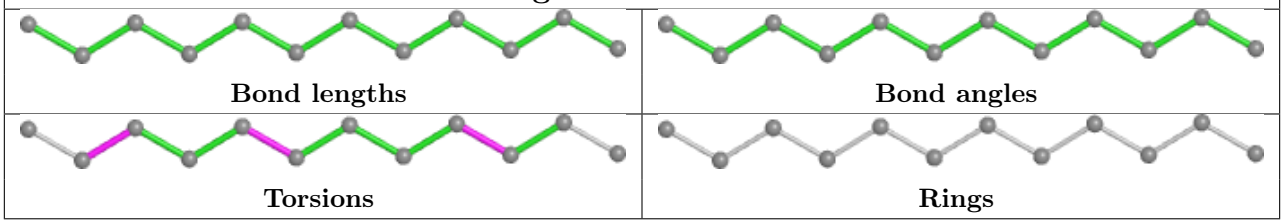
Ligand 6OU L 401



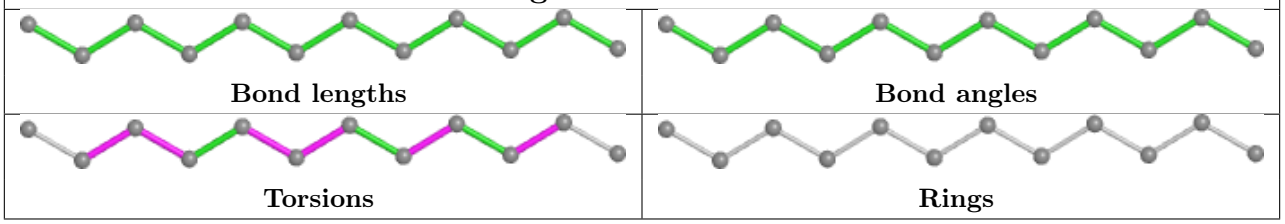
Ligand 6OU F 802



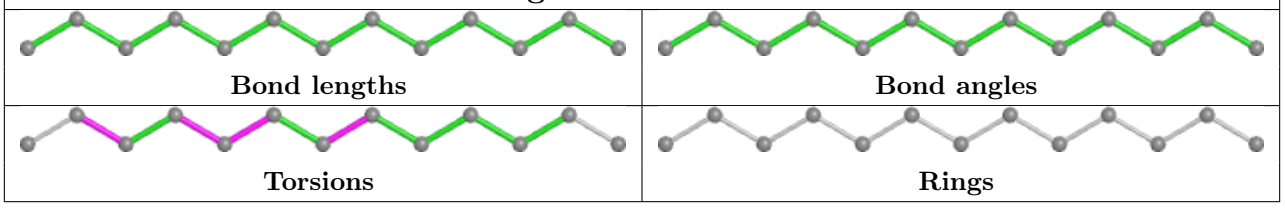
Ligand 6OU I 807



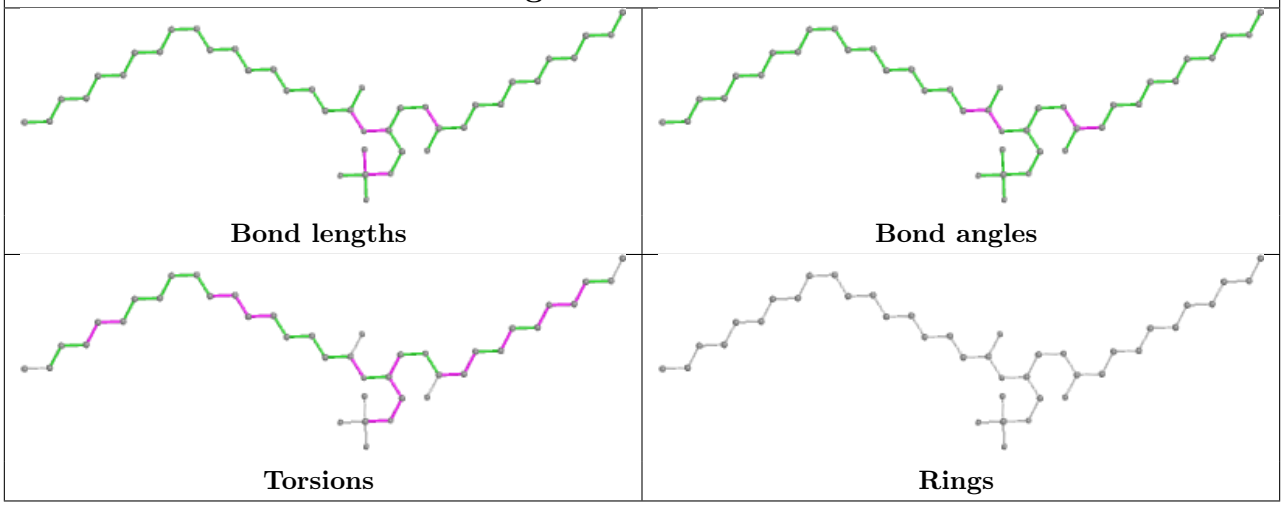
Ligand 6OU J 806



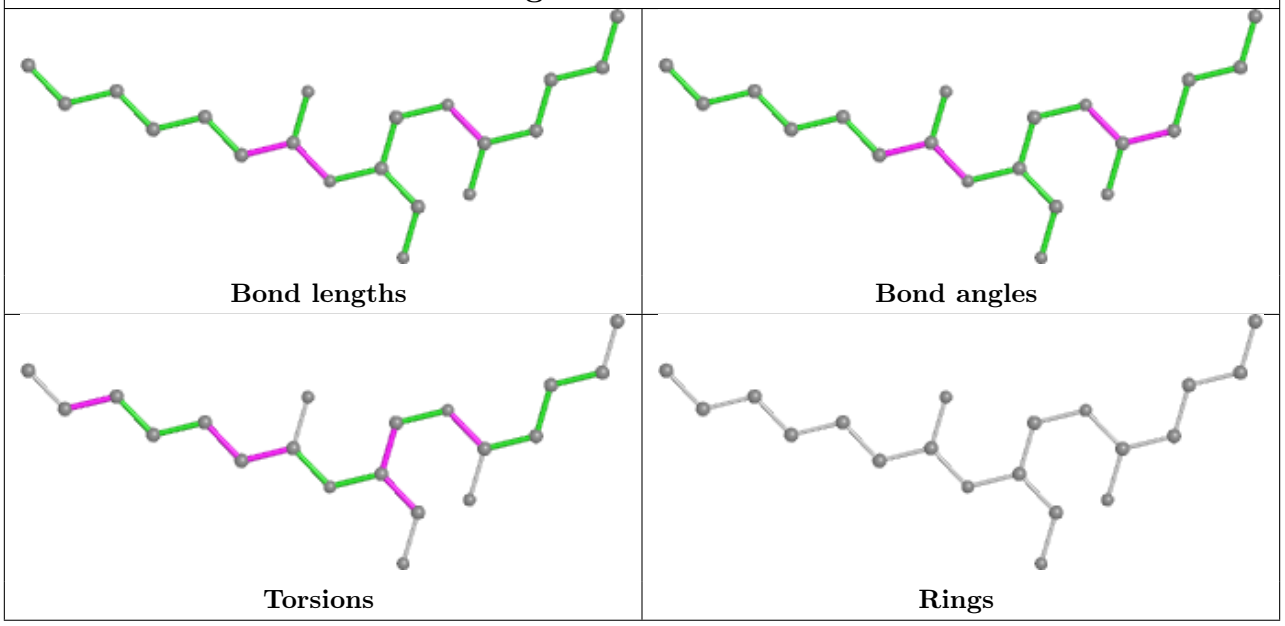
Ligand 6OU E 804



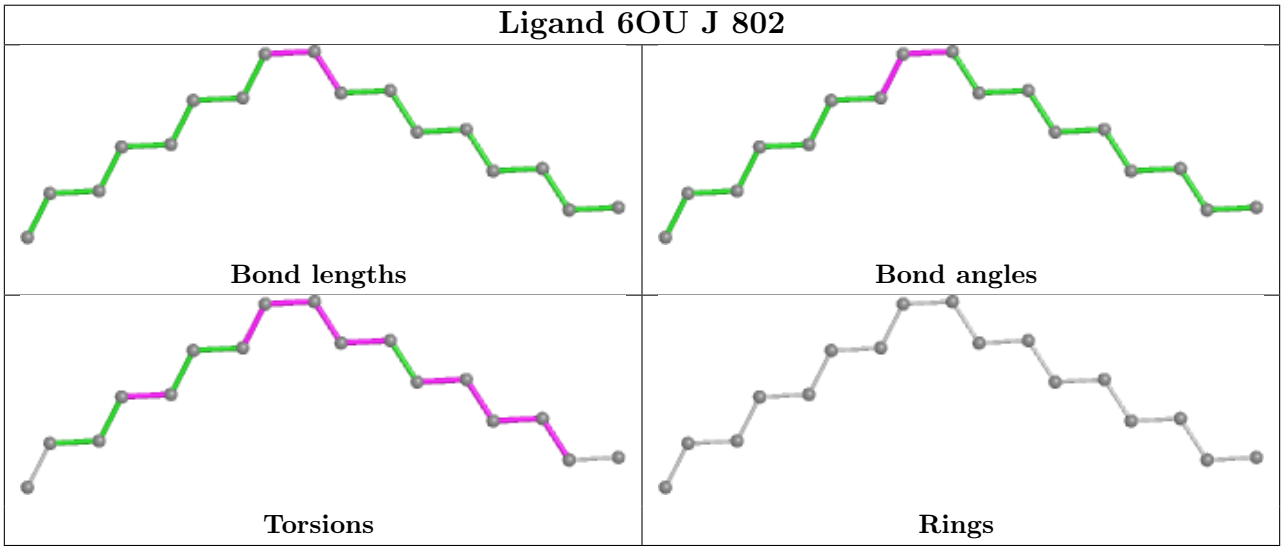
Ligand 6OU H 401



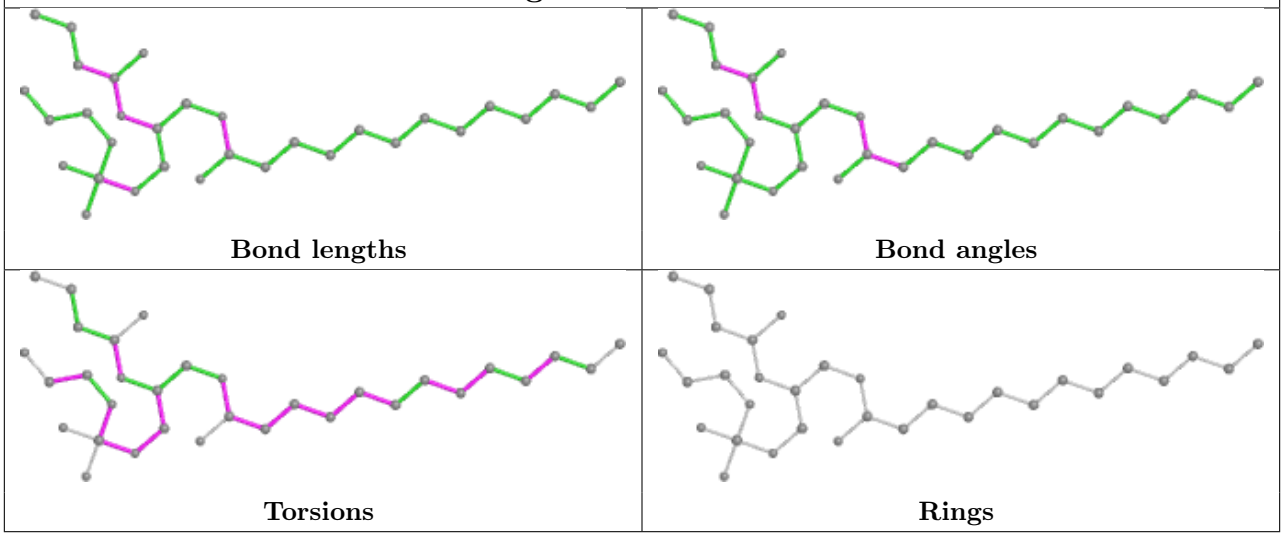
Ligand 6OU A 804



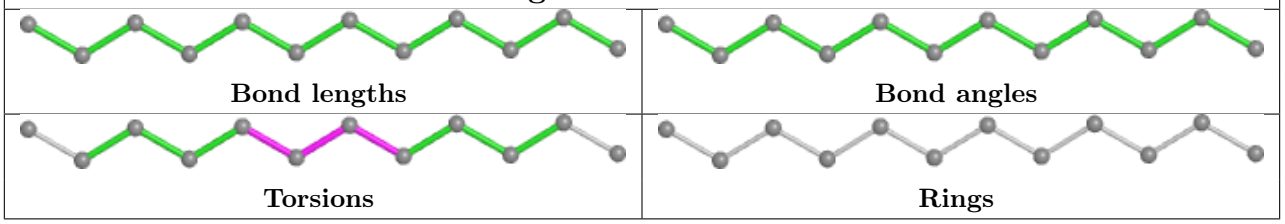
Ligand 6OU J 802



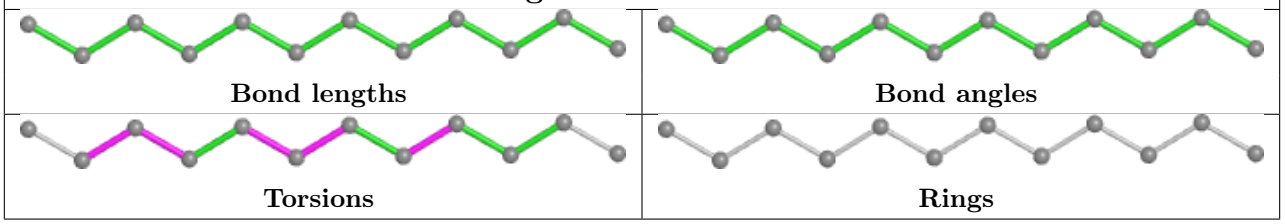
Ligand 6OU A 801



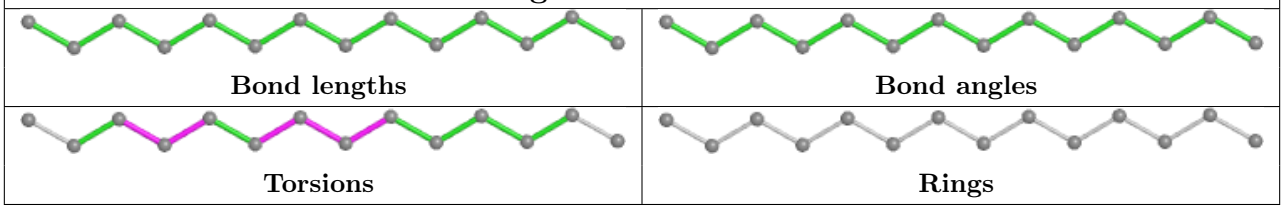
Ligand 6OU L 402



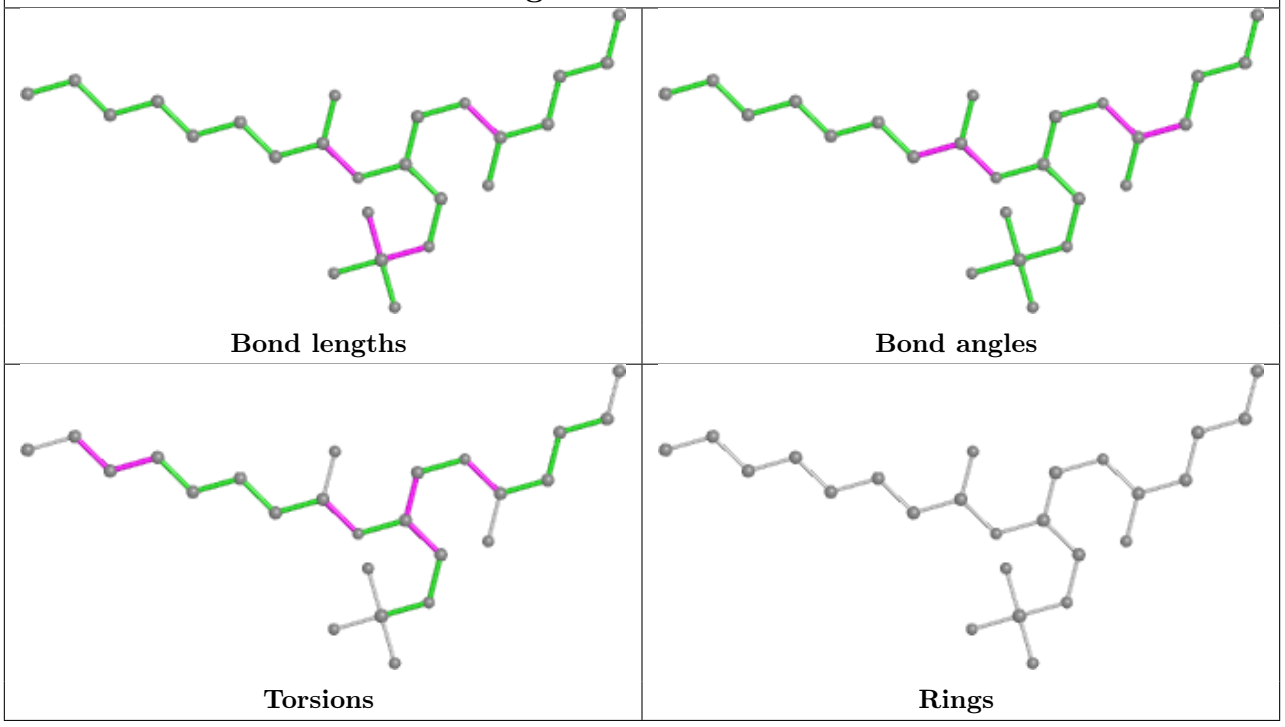
Ligand 6OU A 806



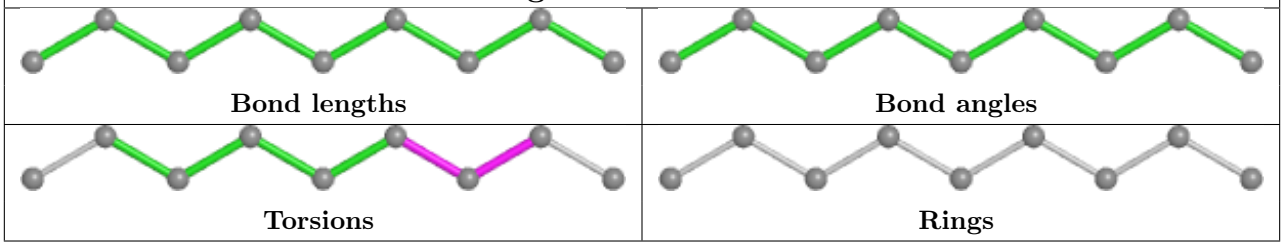
Ligand 6OU J 804



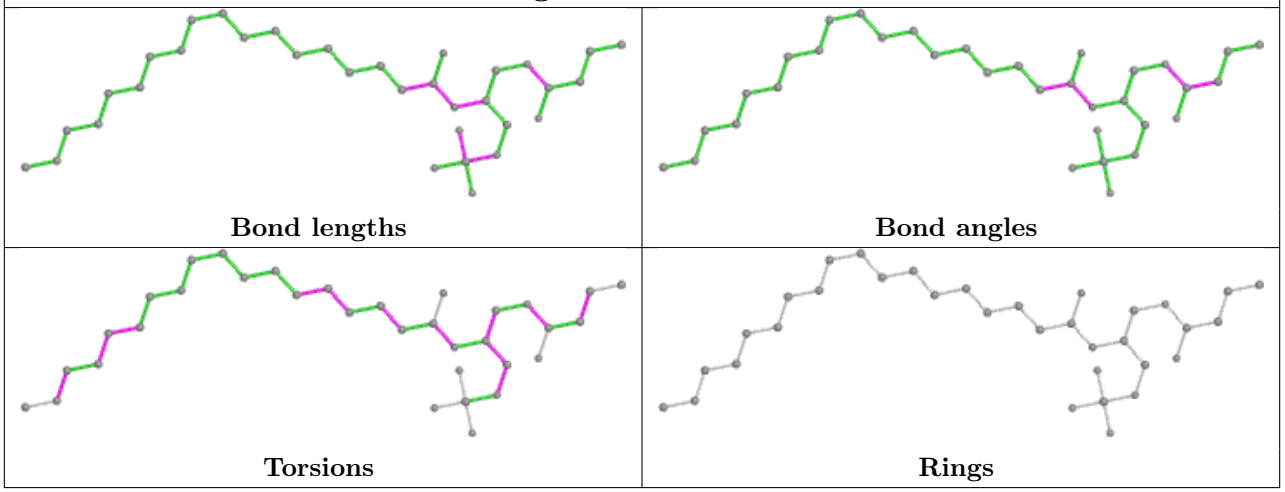
Ligand 6OU A 807



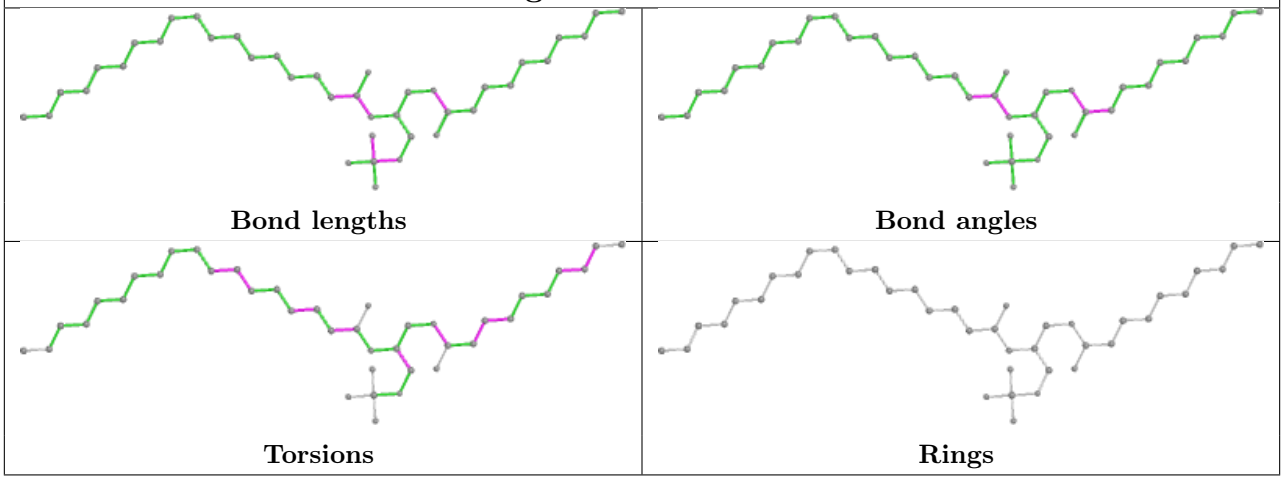
Ligand 6OU E 801



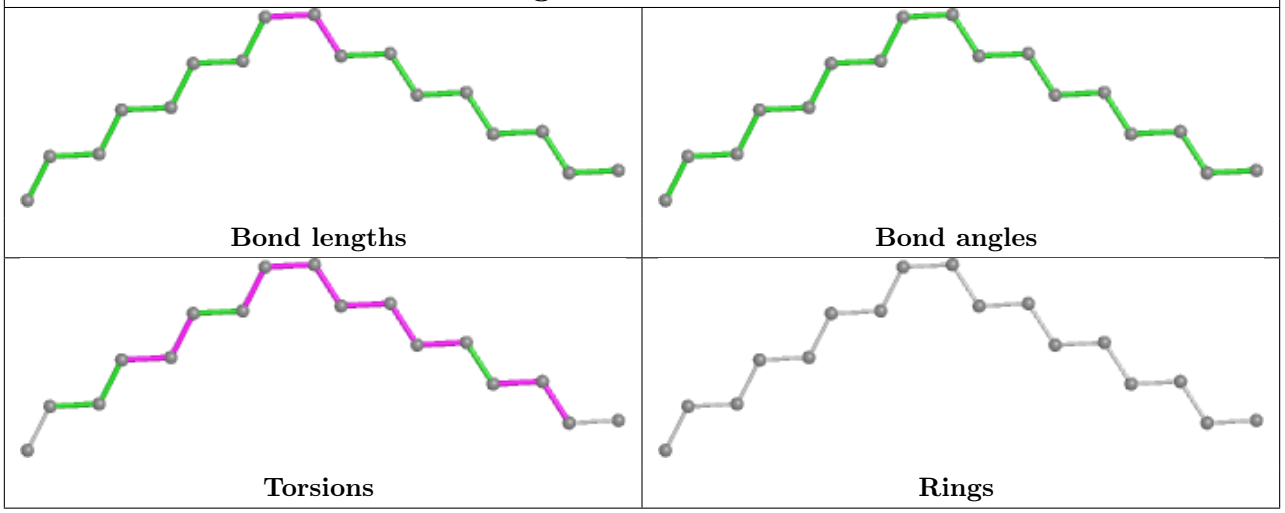
Ligand 6OU I 803



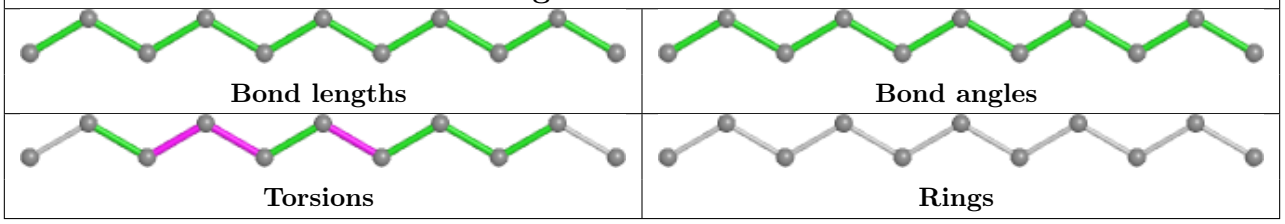
Ligand 6OU K 401



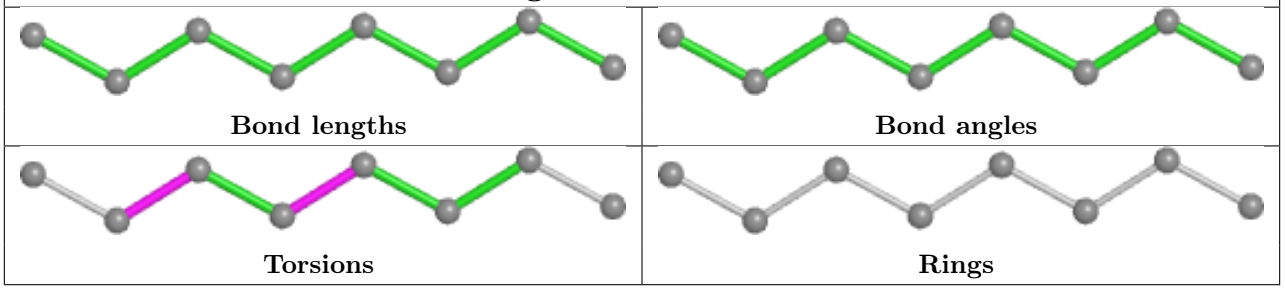
Ligand 6OU I 801



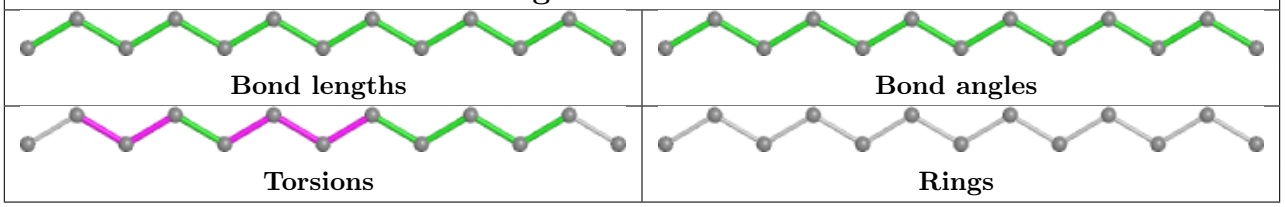
Ligand 6OU I 804



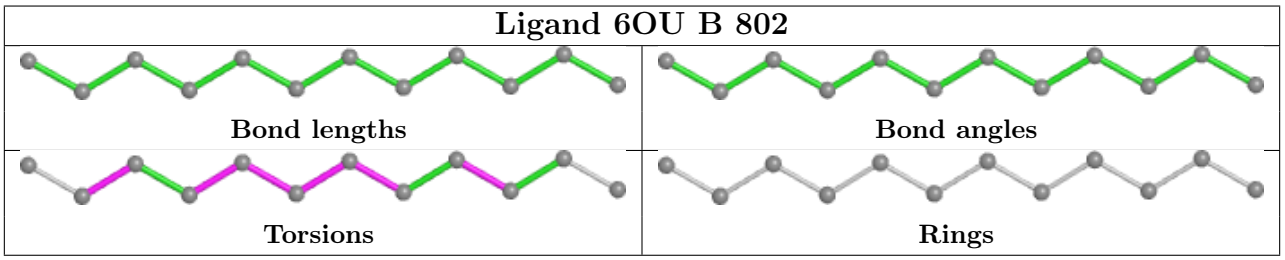
Ligand 6OU A 805



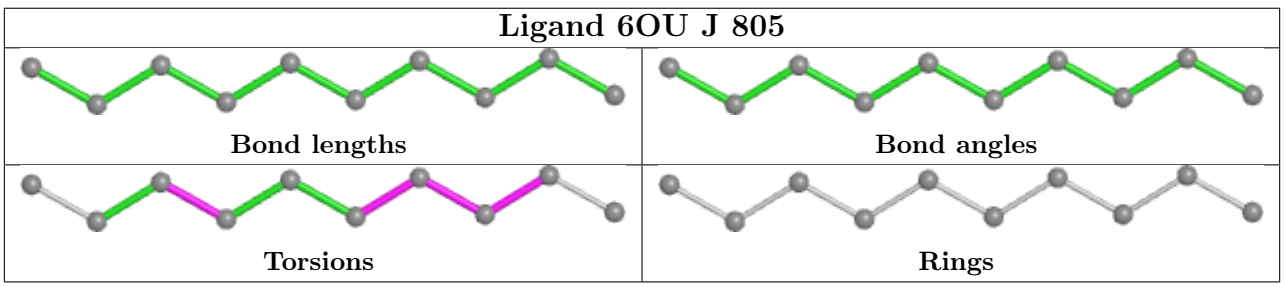
Ligand 6OU I 809



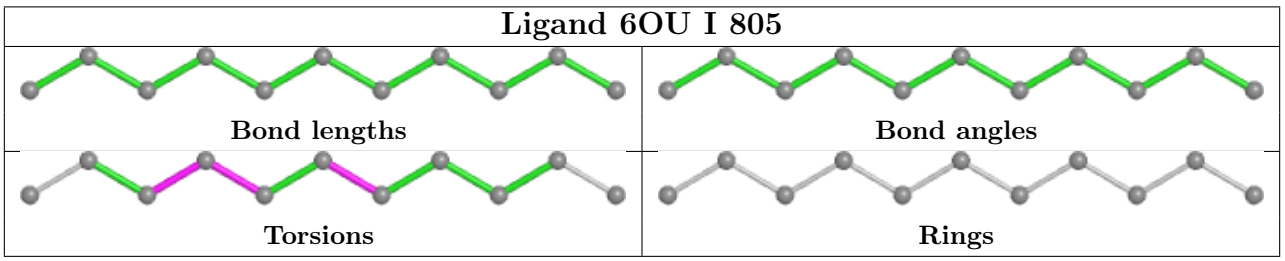
Ligand 6OU B 802



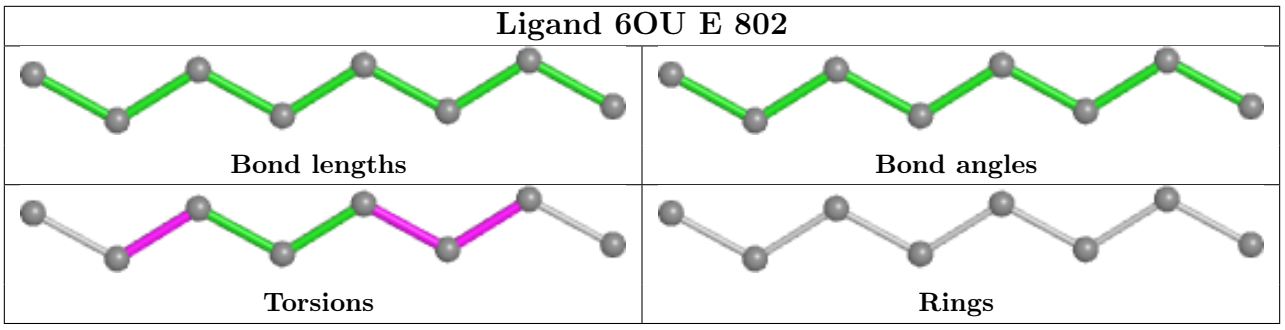
Ligand 6OU J 805

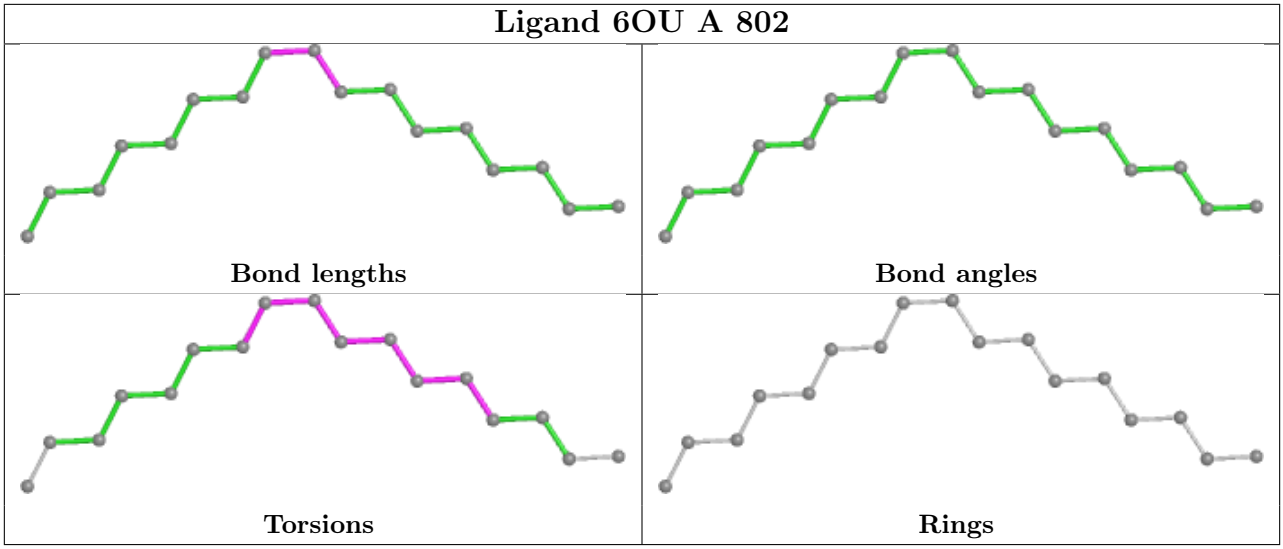


Ligand 6OU I 805



Ligand 6OU E 802





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

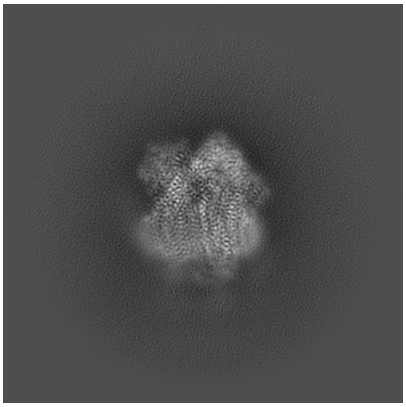
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25116. These allow visual inspection of the internal detail of the map and identification of artifacts.

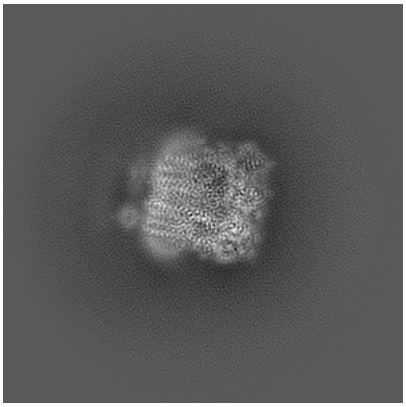
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

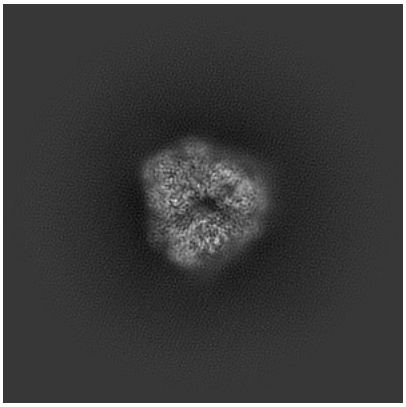
6.1.1 Primary map



X



Y

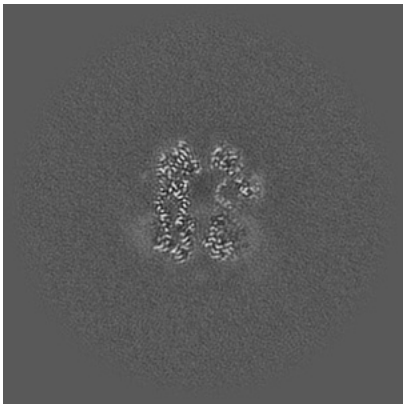


Z

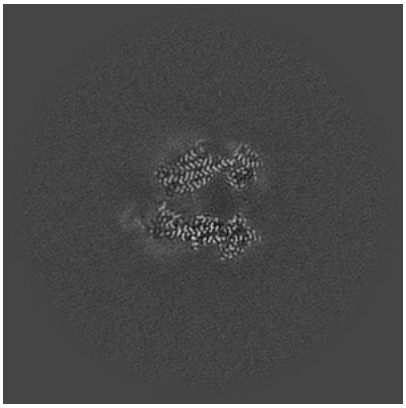
The images above show the map projected in three orthogonal directions.

6.2 Central slices

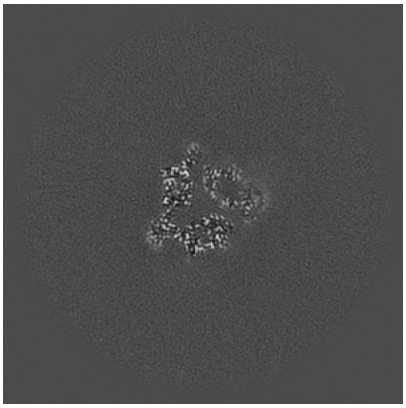
6.2.1 Primary map



X Index: 192



Y Index: 192

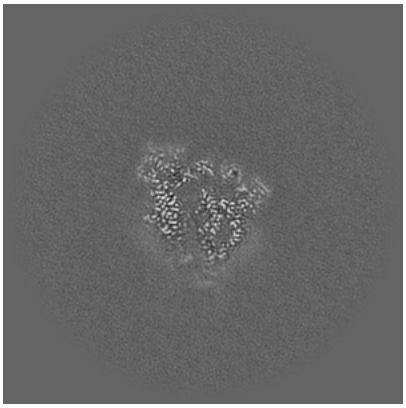


Z Index: 192

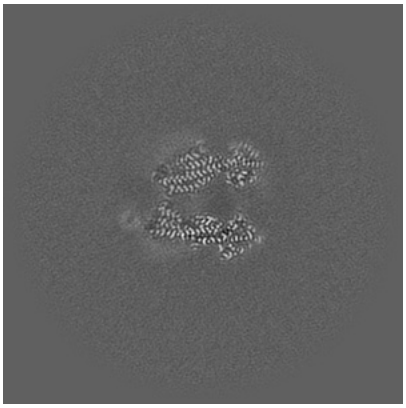
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

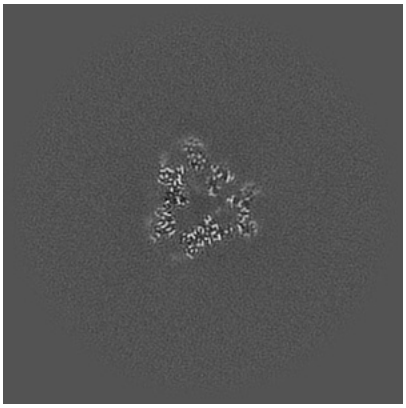
6.3.1 Primary map



X Index: 177



Y Index: 193

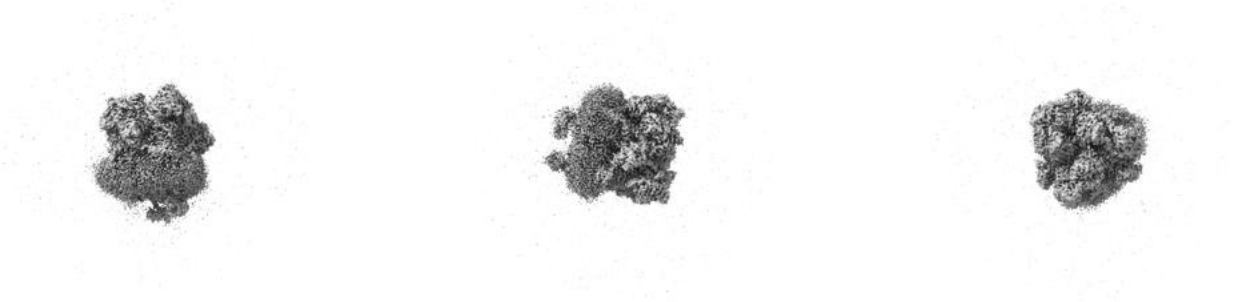


Z Index: 201

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

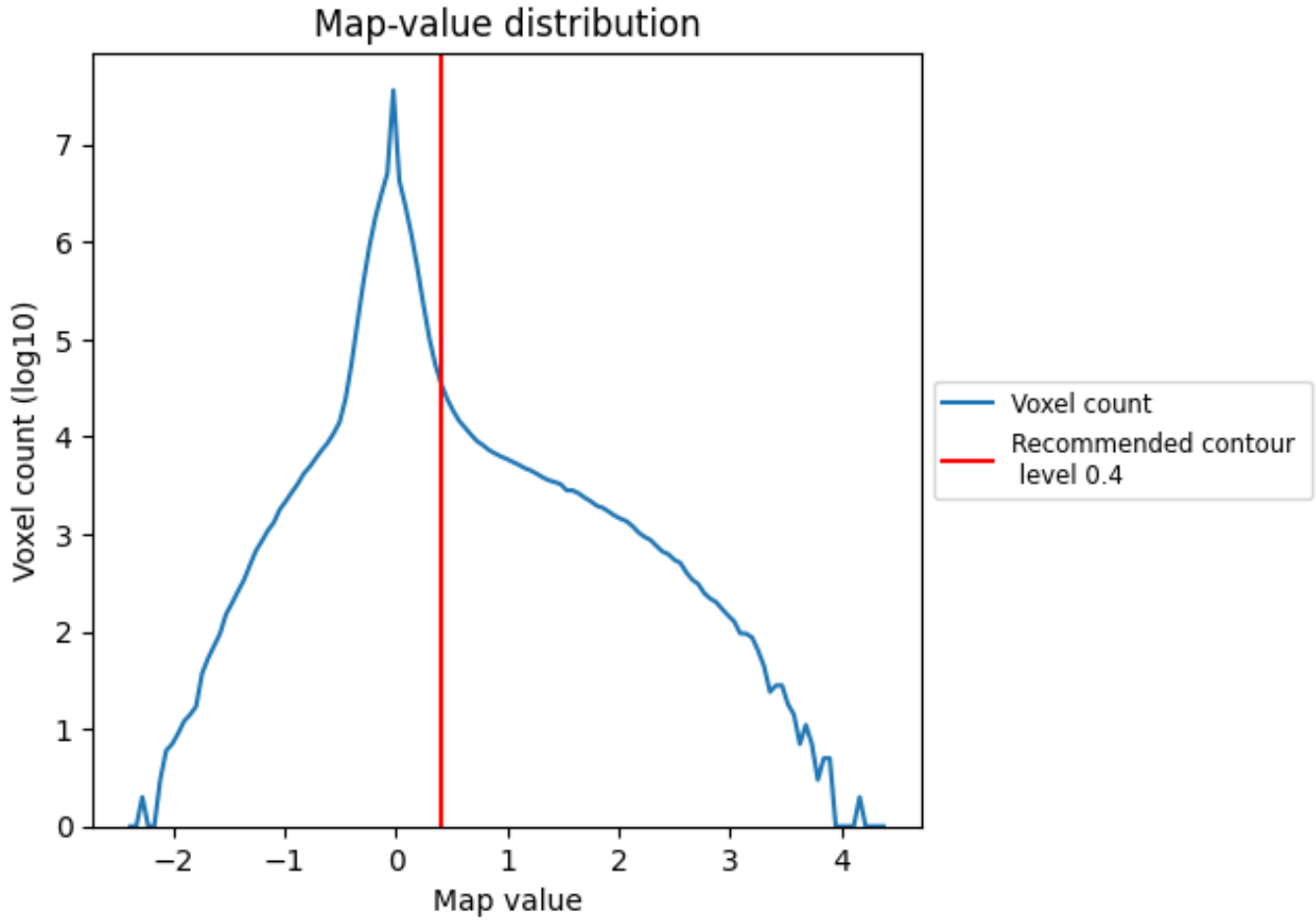
6.5 Mask visualisation (i)

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

7 Map analysis

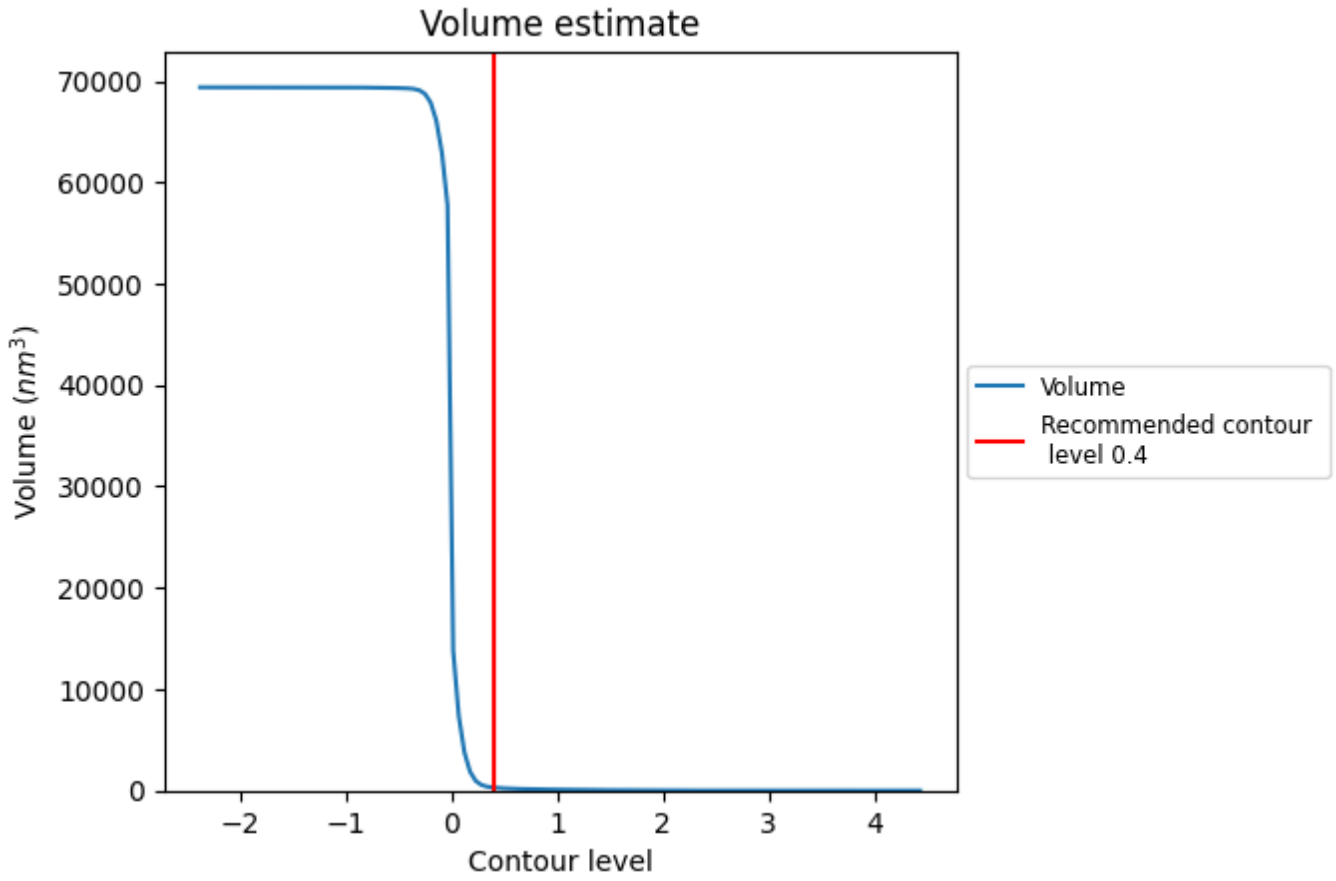
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

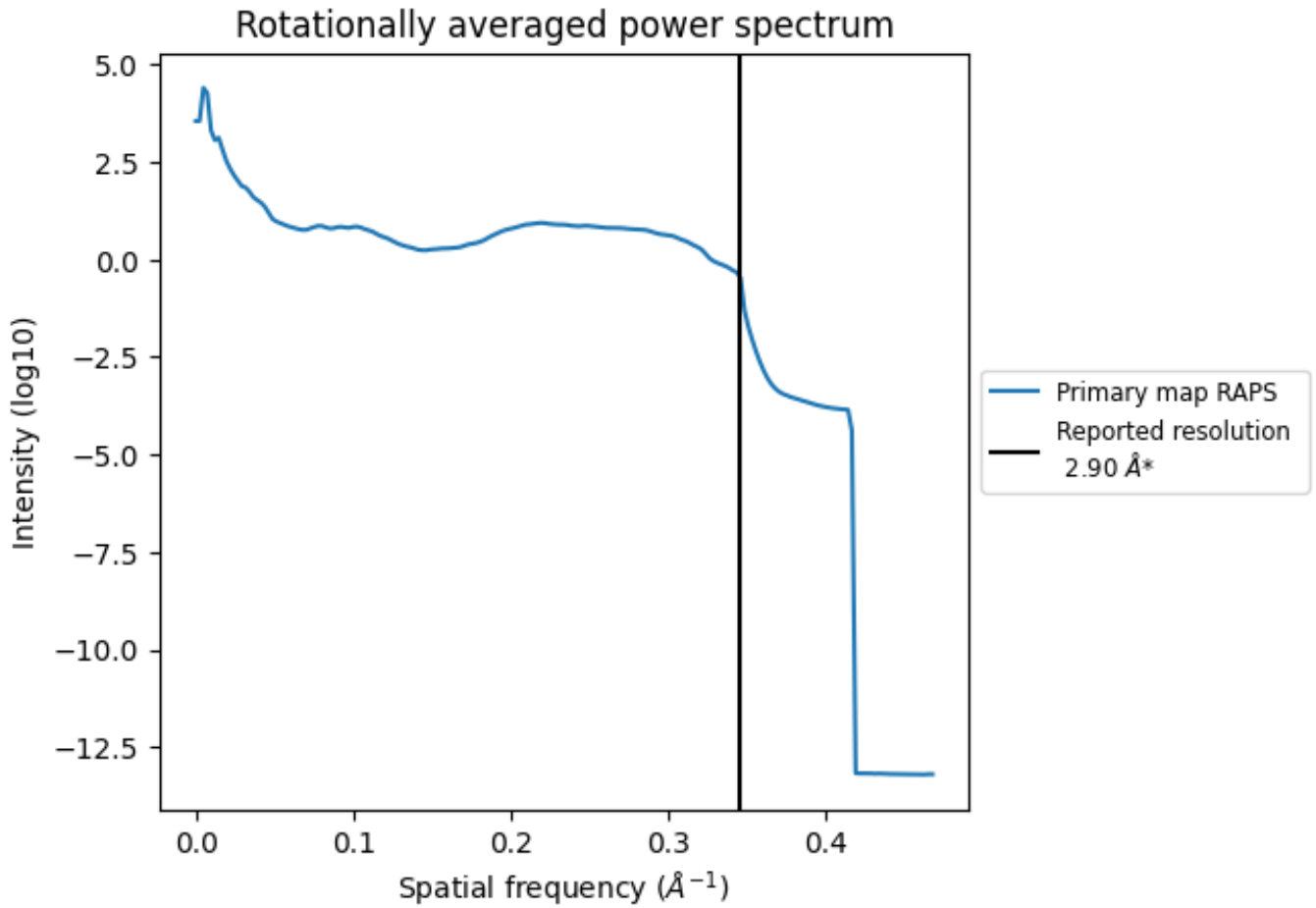
7.2 Volume estimate



The volume at the recommended contour level is 291 nm^3; this corresponds to an approximate mass of 262 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

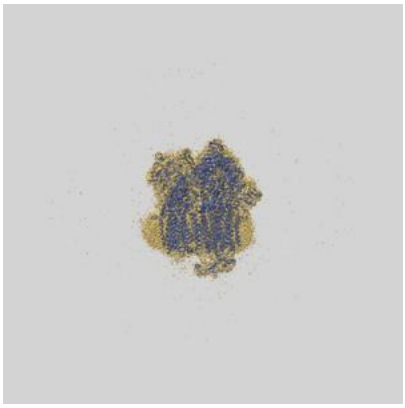
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

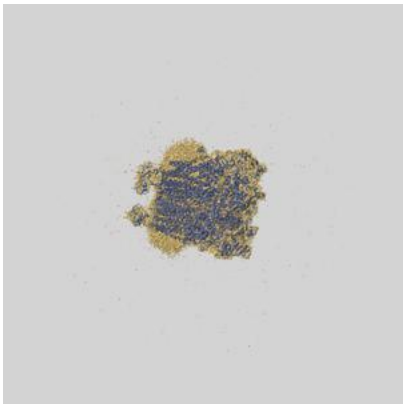
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-25116 and PDB model 7SGR. Per-residue inclusion information can be found in section 3 on page 8.

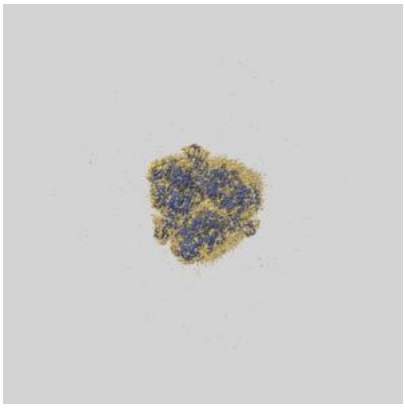
9.1 Map-model overlay



X



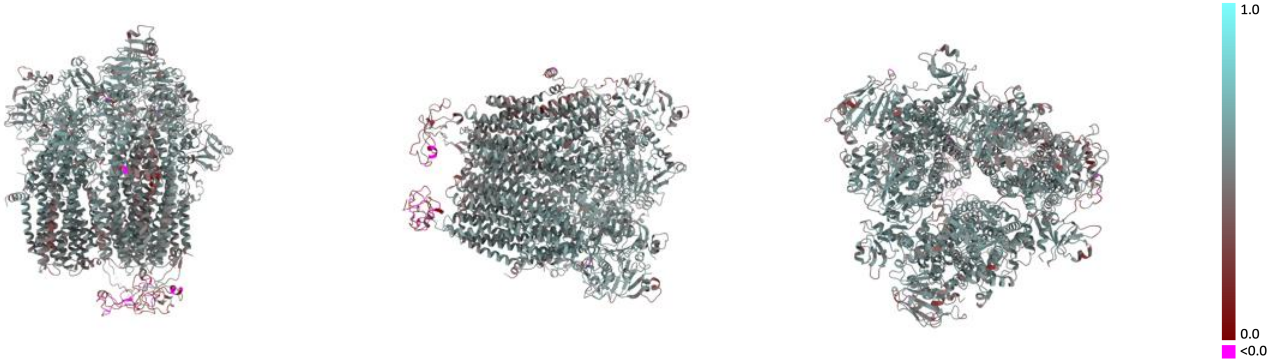
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

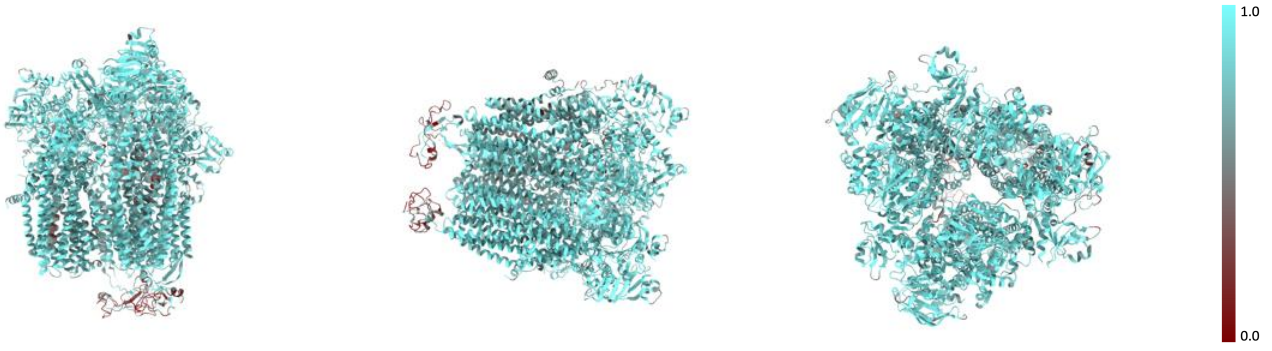
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

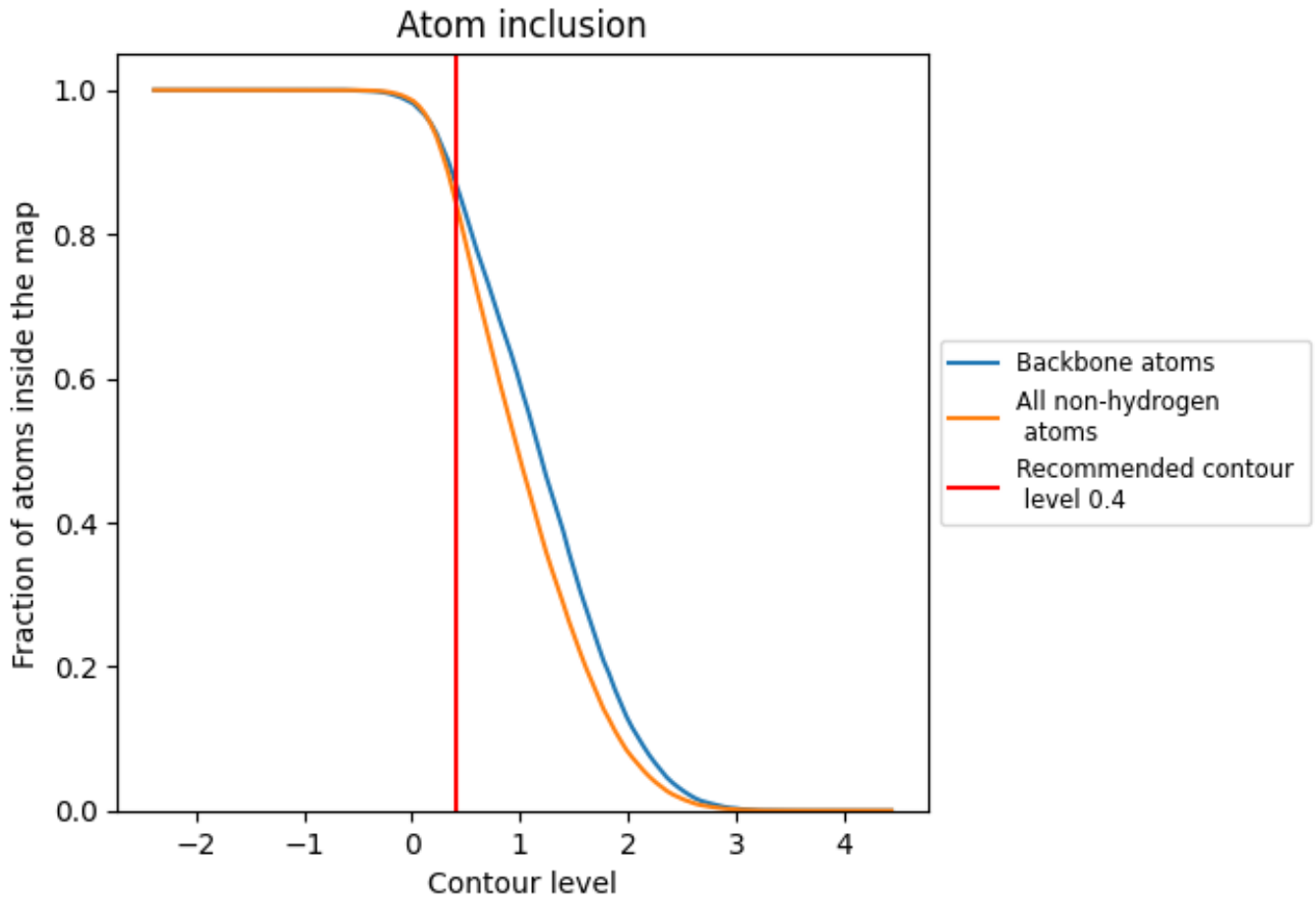
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8476	0.5180
A	0.8547	0.5260
B	0.8276	0.4990
C	0.6364	0.4040
D	0.6973	0.4320
E	0.8935	0.5530
F	0.8788	0.5330
G	0.5799	0.3200
H	0.8414	0.5200
I	0.8781	0.5420
J	0.8740	0.5280
K	0.7190	0.4620
L	0.8468	0.5010