



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:05 PM UTC

PDB ID : 7SGR / pdb_00007sgr
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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

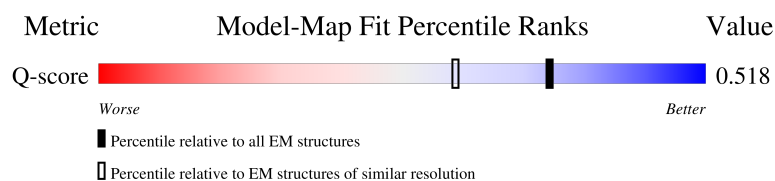
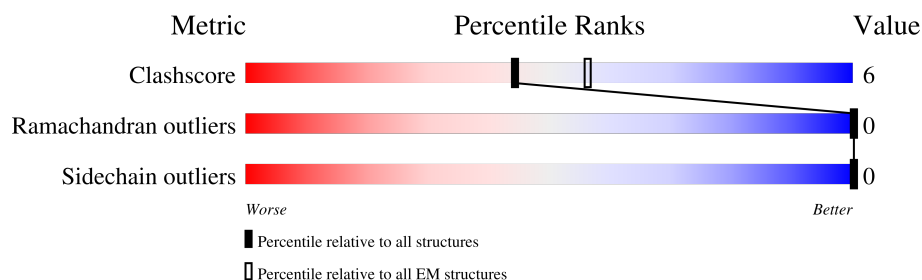
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	707	 85% 14% .
1	B	707	 69% 11% 19%
1	E	707	 82% 17% .
1	F	707	 64% 16% 19%

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Mol	Chain	Length	Quality of chain
1	I	707	85% 14%
1	J	707	66% 15% 19%
2	C	356	14% 42% 5% 53%
2	D	356	15% 81%
2	G	356	19% 37% 9% 54%
2	H	356	16% 81%
2	K	356	12% 86%
2	L	356	14% 5% 81%

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.

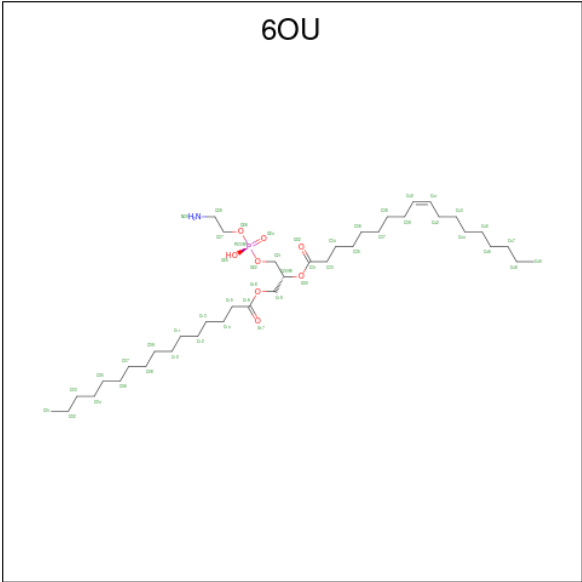
- Molecule 1 is a protein called Alpha-hemolysin translocation ATP-binding protein HlyB.

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-prop an-2-yl] ({Z})-octadec-9-enoate (CCD ID: 6OU) (formula: C₃₉H₇₆NO₈P).



Mol	Chain	Residues	Atoms				AltConf
3	J	1	Total	C			0
			17	17			
3	J	1	Total	C			0
			17	17			
3	J	1	Total	C			0
			12	12			
3	J	1	Total	C			0
			14	14			
3	J	1	Total	C			0
			10	10			
3	J	1	Total	C			0
			12	12			
3	I	1	Total	C			0
			17	17			
3	I	1	Total	C			0
			10	10			
3	I	1	Total	C	O	P	0
			34	25	8	1	
3	I	1	Total	C			0
			11	11			
3	I	1	Total	C			0
			11	11			
3	I	1	Total	C			0
			11	11			
3	I	1	Total	C			0
			12	12			
3	I	1	Total	C			0
			12	12			

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Mol	Chain	Residues	Atoms	AltConf
3	I	1	Total C 13 13	0
3	A	1	Total C N O P 32 22 1 8 1	0
3	A	1	Total C 17 17	0
3	A	1	Total C O P 33 24 8 1	0
3	A	1	Total C O 20 15 5	0
3	A	1	Total C 8 8	0
3	A	1	Total C 12 12	0
3	A	1	Total C O P 25 16 8 1	0
3	B	1	Total C 14 14	0
3	B	1	Total C 12 12	0
3	E	1	Total C 9 9	0
3	E	1	Total C 8 8	0
3	E	1	Total C 8 8	0
3	E	1	Total C 13 13	0
3	F	1	Total C O 32 27 5	0
3	F	1	Total C 17 17	0
3	F	1	Total C O 32 27 5	0
3	F	1	Total C 12 12	0
3	H	1	Total C O P 41 32 8 1	0
3	H	1	Total C 12 12	0
3	L	1	Total C 17 17	0

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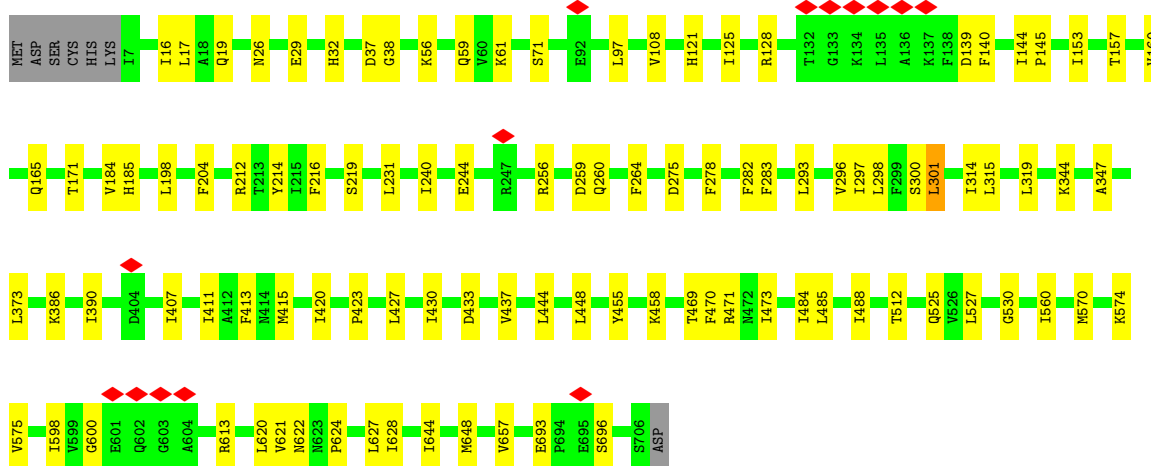
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Mol	Chain	Residues	Atoms				AltConf
3	L	1	Total	C			0
			12	12			
3	K	1	Total	C	O	P	0
			40	31	8	1	



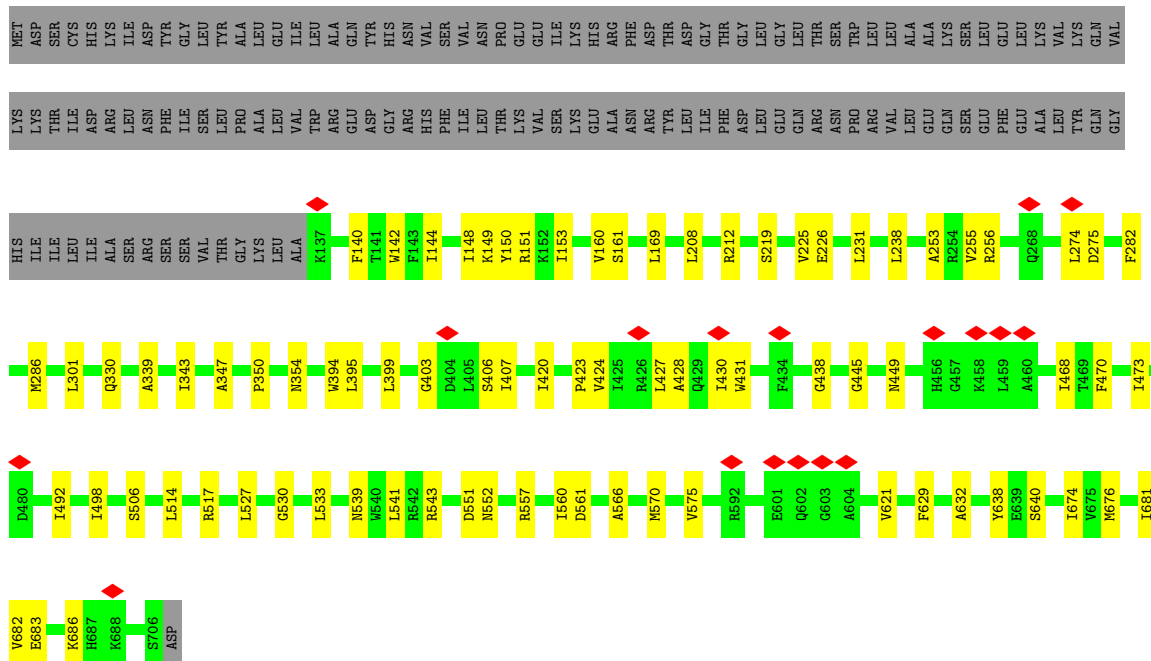
- Molecule 1: Alpha-hemolysin translocation ATP-binding protein HlyB

Chain A: 85% 14%



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

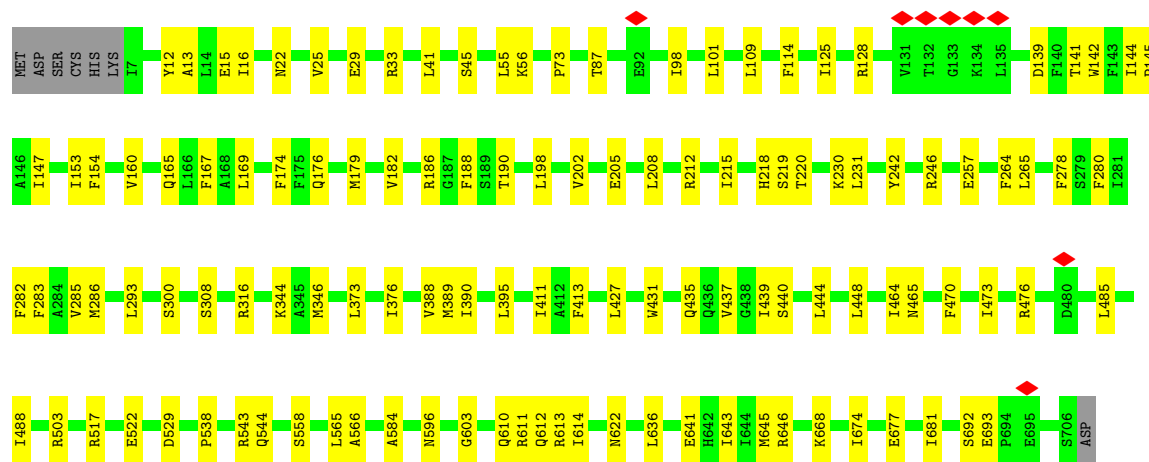
Chain B: 69% 11% 19%



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

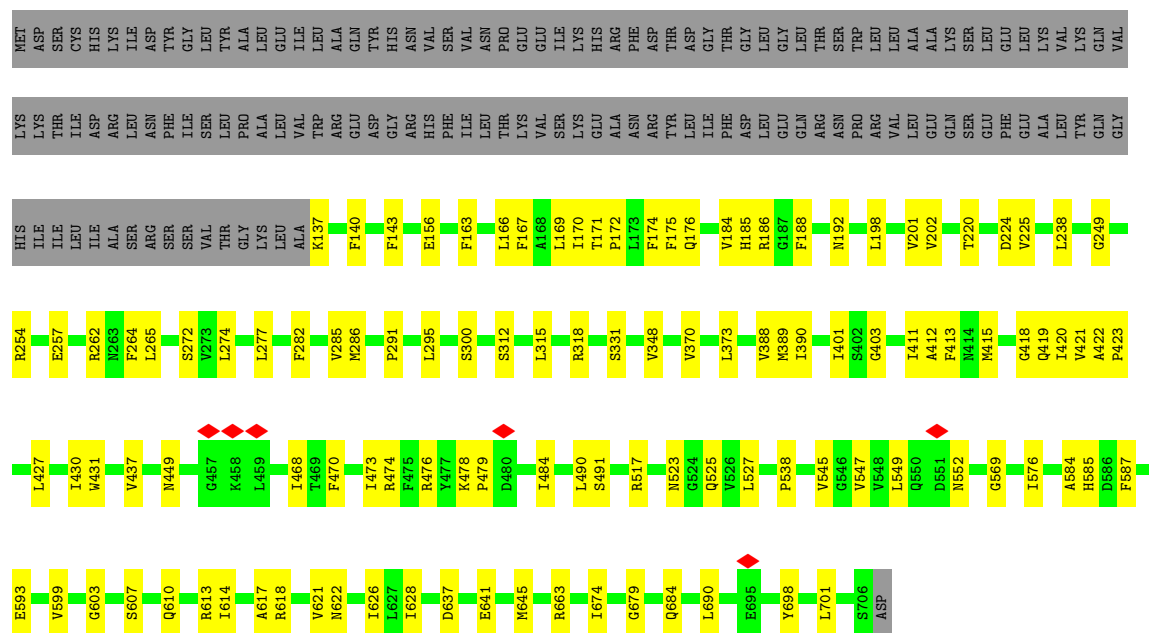
Chain E: 82% 17%





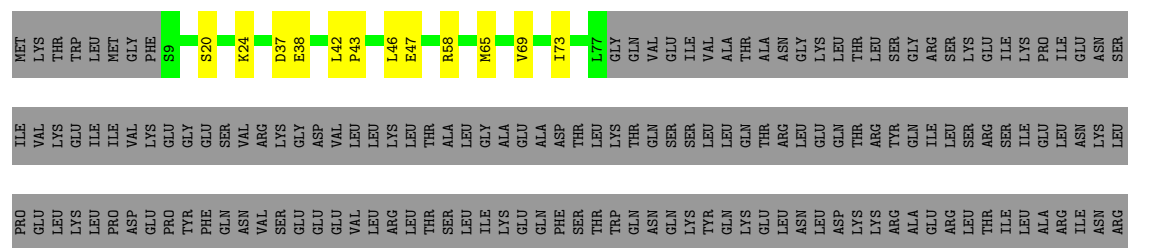
• Molecule 1: Alpha-hemolysin translocation ATP-binding protein HlyB

Chain F: 64% 16% 19%



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

Chain H: 16% 81%



[illegible]

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

Chain L: 14% 5% 81%

ILE	TYR	THR	ARG	GLU	MET
SER	LEU	ILE	ILE	ILE	LYS
TYR	VAL	LEU	ILE	LYS	THR
LEU	GLY	ALA	GLU	PRO	TRP
LEU	LYS	ARG	LEU	ILE	LEU
SER	VAL	ILE	ASN	GLU	MET
PRO	ASN	ASN	LYS	ASN	GLY
LEU	ASN	ARG	LEU	SER	PHE
GLU	ILE	TYR	PRO	ILE	SS
GLU	ASN	GLU	GLU	VAL	K16
SER	ASP	ASN	LEU	LYS	K17
VAL	ASP	LEU	LYS	GLU	V18
THR	ALA	SER	LEU	ILE	
GLU	ILE	ARG	PRO	ILE	T22
SER	GLU	VAL	ASP	VAL	
GLU	ASP	GLU	GLU	LYS	
HIS	GLN	LYS	PRO	GLU	I25
GLU	LEU	LYS	SER	GLY	R26
ARG	LEU	ARG	PHE	GLU	K27
	GLY	LEU	GLN	SER	
	LEU	ASP	ASN	VAL	E40
VAL	VAL	ASP	VAL	ARG	F41
PHE	PHE	PHE	SER	LYS	L42
ASN	ASN	ASP	GLU	GLY	P43
VAL	VAL	ASP	GLU	ASP	
ILE	ILE	THR	GLU	VAL	L46
VAL	VAL	LEU	VAL	LEU	E47
SER	SER	GLU	LEU	LEU	L48
VAL	VAL	VAL	ARG	LYS	
GLU	GLU	THR	LEU	LEU	T51
GLU	GLU	ALA	THR	THR	
ASN	ASN	LEU	SER	ALA	R55
ASP	ASP	GLN	LEU	LEU	
LEU	LEU	VAL	ILE	GLY	L59
SER	SER	ASN	LYS	ALA	
THR	THR	LYS	GLU	GLU	I70
GLY	GLY	ASP	GLN	ALA	
ASN	ASN	ILE	PHE	ASP	I73
LYS	LYS	GLY	SER	THR	
HIS	HIS	PHE	THR	LEU	L77
ILE	ILE	ILE	TPP	LYS	GLY
PRO	PRO	ASN	GLN	LYS	
LEU	LEU	VAL	GLN	THR	GLN
SER	SER	GLY	ASN	GLN	VAL
SER	SER	GLN	LYS	SER	GLU
GLY	GLY	ASN	TYR	ILE	VAL
MET	MET	ALA	GLN	LEU	VAL
ALA	ALA	ILE	LYS	LEU	ALA
VAL	VAL	ILE	GLU	GLN	THR
THR	THR	LYS	LEU	THR	ALA
ALA	ALA	VAL	ASN	ARG	GLY
GLU	GLU	VAL	LEU	GLY	GLY
ILE	ILE	ALA	ASP	GLN	LEU
LYS	LYS	PHE	LYS	THR	THR
THR	THR	PRO	LYS	ARG	THR
GLY	GLY	TYR	LYS	TYR	SER
MET	MET	THR	ALA	GLN	GLY
ARG	ARG	ARG	GLU	ILE	ARG
SER	SER	TYR	LEU	SER	LEU
VAL	VAL	GLY	THR	THR	LYS

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

Chain D: 15% . 81%

[illegible]

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

Lys	Thr	Phe	Lys	Lys	Thr	Thr
Thr	Arg	Pro	Lys	Arg	Arg	Arg
Gly	Tyr	Tyr	Arg	Ala	Tyr	Ser
Met	Thr	Thr	Ala	Glu	Gln	Gly
Arg	Arg	Arg	Glu	Leu	Ile	Arg
Ser	Tyr	Tyr	Arg	Leu	Ser	Ser
Val	Gly	Gly	Leu	Thr	Leu	Lys
Ile	Leu	Tyr	Thr	Leu	Arg	Arg
Ser	Leu	Leu	Ile	Ser	Leu	Ile
Tyr	Tyr	Val	Leu	Ala	Glu	Pro
Leu	Leu	Gly	Ala	Arg	Leu	Ile
Leu	Leu	Lys	Arg	Leu	Asn	Glu
Ser	Ser	Val	Ile	Ile	Asn	Glu
Pro	Leu	Lys	Asn	Asn	Lys	Asn
Glu	Leu	Asn	Arg	Leu	Leu	Thr
Glu	Glu	Ile	Tyr	Pro	Pro	Ile
Gly	Glu	Asn	Glu	Glu	Val	Lys
Ser	Ser	Leu	Asn	Leu	Leu	Glu
Val	Val	Asp	Leu	Leu	Lys	Gly
Thr	Thr	Ala	Ser	Ser	Leu	Ile
Glu	Glu	Ile	Arg	Pro	Pro	Ile
Ser	Ser	Glu	Val	Asp	Val	Val
His	His	Asp	Glu	Glu	Lys	Lys
Glu	Glu	Gln	Lys	Pro	Gly	Gly
Arg	Arg	Lys	Ser	Tyr	Ser	Ser
		Leu	Arg	Phe	Gln	Val
		Leu	Leu	Asn	Val	Arg
		Val	Asp	Ser	Val	Val
		Phe	Phe	Ser	Arg	Lys
		Asn	Asn	Glu	Val	Val
		Val	Asp	Glu	Leu	Leu
		Ile	Thr	Leu	Val	Leu
		Val	Leu	Val	Val	Leu
		Ser	Glu	Glu	Leu	Lys
		Val	Val	Arg	Leu	Lys
		Glu	Thr	Leu	Leu	Thr
		Glu	Ala	Thr	Ser	Ala
		Asn	Leu	Ser	Leu	Leu
		Asp	Val	Leu	Gly	Gly
		Thr	Val	Ile	Ala	Ala
		Ser	Asn	Lys	Ala	Glu
		Gly	Ile	Thr	Thr	Thr
		Pro	Thr	Trp	Lys	Lys
		Leu	Asn	Gln	Thr	Thr
		Leu	Val	Asn	Ser	Ser
		Ser	Gly	Gln	Leu	Leu
		Ser	Gln	Lys	Ser	Ser
		Gly	Asn	Tyr	Leu	Leu
		Met	Ala	Gln	Leu	Leu
		Ala	Ile	Lys	Gln	Gln
		Val	Ile	Lys	Leu	Thr
		Thr	Lys	Val	Arg	Arg
		Ala	Val	Asn	Leu	Leu
		Glu	Glu	Leu	Gln	Gln
		Thr	Ala	Arg	Leu	Thr

4 Experimental information

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 ($e^-/\text{\AA}^2$)	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	0.28	4/5651 (0.1%)	0.35	2/7663 (0.0%)
1	B	0.13	0/4596	0.33	0/6232
1	E	0.18	1/5641 (0.0%)	0.31	0/7648
1	F	0.20	0/4596	0.35	1/6232 (0.0%)
1	I	0.14	0/5656	0.31	0/7669
1	J	0.14	0/4592	0.33	0/6228
2	C	0.25	0/1044	0.59	0/1433
2	D	0.12	0/595	0.35	0/807
2	G	0.24	0/1035	0.63	0/1420
2	H	0.12	0/595	0.33	0/807
2	K	0.10	0/404	0.27	0/550
2	L	0.13	0/595	0.38	0/807
All	All	0.19	5/35000 (0.0%)	0.35	3/47496 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	301	LEU	C-O	-5.72	1.17	1.24
1	E	176	GLN	C-O	-5.69	1.17	1.24
1	A	296	VAL	C-O	-5.44	1.17	1.24
1	A	300	SER	C-O	-5.05	1.17	1.24
1	A	298	LEU	C-O	-5.00	1.17	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	403	GLY	N-CA-C	7.30	125.45	115.30
1	A	301	LEU	N-CA-C	5.70	122.41	109.81
1	A	296	VAL	CB-CA-C	-5.11	105.25	112.14

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	66	0
1	B	4509	0	4683	54	0
1	E	5535	0	5706	81	0
1	F	4509	0	4683	83	0
1	I	5549	0	5734	66	0
1	J	4505	0	4672	64	0
2	C	1035	0	815	10	0
2	D	581	0	609	13	0
2	G	1026	0	797	26	0
2	H	581	0	609	8	0
2	K	396	0	416	5	0
2	L	581	0	609	17	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	446	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 (446) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:128:ARG:NH2	2:D:42:LEU:O	2.24	0.70
1:A:411:ILE:HG22	1:A:415:MET:HE3	1.74	0.69
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
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:I:411:ILE:HG22	1:I:415:MET:HE2	1.82	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:E:283:PHE:HA	1:E:286:MET:HE2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:I:645:MET:HE1	1:I:666:THR:HG23	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:257:GLU:OE1	1:I:440:SER:OG	2.20	0.52
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:B:570:MET:HE1	1:B:621:VAL:HG22	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:346:MET:HE3	1:F:618:ARG:HE	1.76	0.51
1:B:140:PHE:CZ	1:B:438:GLY:HA2	2.45	0.51
2:L:47:GLU:O	2:L:51:THR:OG1	2.27	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:139:ASP:CG	1:A:140:PHE:H	2.22	0.47
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
2:D:47:GLU:O	2:D:51:THR:OG1	2.24	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
1:E:257:GLU:OE1	1:E:440:SER:OG	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:176:GLN:OE1	1:J:289:TYR:OH	2.23	0.45
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
2:C:391:GLU:O	2:C:392:ALA:C	2.59	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
2:G:391:GLU:O	2:G:392:ALA:C	2.59	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
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:A:622:ASN:C	1:A:624:PRO:HD3	2.42	0.45
1:J:175:PHE:CE2	1:J:415:MET:HE1	2.52	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:368:VAL:O	2:C:369:THR:C	2.60	0.44
1:I:156:GLU:O	1:I:160:VAL:HG23	2.18	0.44
1:I:175:PHE:HB2	1:I:415:MET:HE1	1.99	0.44
1:A:231:LEU:HD13	1:A:448:LEU:HD11	2.00	0.44
1:E:139:ASP:OD1	1:E:141:THR:OG1	2.32	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
2:G:368:VAL:O	2:G:369:THR:C	2.60	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
1:J:676:MET:HE2	1:J:676:MET:HB3	1.84	0.43
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
1:A:570:MET:HE1	1:A:621:VAL:HG21	2.01	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
1:E:346:MET:HE3	1:F:618:ARG:NE	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:533:LEU:HD22	1:J:541:LEU:HD22	1.99	0.42
1:E:188:PHE:C	1:E:190:THR:H	2.27	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:B:149:LYS:HE2	2:D:31:THR:HG23	2.01	0.42
2:G:458:SER:O	2:G:459:VAL:C	2.61	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
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:J:352:MET:HE1	1:I:557:ARG:NH2	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:389:MET:HE2	1:F:390:ILE:HG13	2.01	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:A:648:MET:HE2	1:A:648:MET:HB2	1.91	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: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
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:J:477:TYR:C	1:J:478:LYS:HD3	2.46	0.41
1:E:242:TYR:O	1:E:246:ARG:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:638:TYR:C	1:B:640:SER:H	2.29	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:457:ARG:O	2:G:458:SER:C	2.63	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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 ⓘ

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%)	494 (100%)	0	100	100
1	I	605/615 (98%)	605 (100%)	0	100	100
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%)	3663 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	165	GLN
1	J	326	ASN
1	J	398	HIS
1	J	523	ASN
1	J	531	HIS
1	J	556	ASN
1	J	610	GLN
1	J	622	ASN
1	I	326	ASN
1	I	419	GLN
1	I	467	ASN
1	I	525	GLN
1	I	610	GLN
1	A	59	GLN
1	A	121	HIS
1	A	185	HIS
1	A	192	ASN
1	A	326	ASN
1	A	330	GLN
1	A	531	HIS
1	B	185	HIS

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Mol	Chain	Res	Type
1	B	472	ASN
1	B	487	ASN
1	B	525	GLN
1	B	556	ASN
1	E	94	ASN
1	E	111	GLN
1	E	185	HIS
1	E	326	ASN
1	E	392	ASN
1	E	539	ASN
1	E	612	GLN
1	F	382	GLN
1	F	523	ASN
1	F	525	GLN
1	F	567	ASN
1	F	585	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	J	801	-	16,16,48	1.46	2 (12%)	15,15,53	0.96	0
3	6OU	I	809	-	12,12,48	0.75	0	11,11,53	0.84	0
3	6OU	J	805	-	9,9,48	0.80	0	8,8,53	0.81	0
3	6OU	J	803	-	11,11,48	0.74	0	10,10,53	0.82	0
3	6OU	I	807	-	11,11,48	0.75	0	10,10,53	0.84	0
3	6OU	L	401	-	16,16,48	1.46	2 (12%)	15,15,53	1.04	1 (6%)
3	6OU	K	401	-	39,39,48	1.37	6 (15%)	42,44,53	1.11	2 (4%)
3	6OU	A	806	-	11,11,48	0.75	0	10,10,53	0.85	0
3	6OU	L	402	-	11,11,48	0.76	0	10,10,53	0.84	0
3	6OU	A	807	-	24,24,48	1.64	6 (25%)	27,29,53	1.30	2 (7%)
3	6OU	B	802	-	11,11,48	0.74	0	10,10,53	0.83	0
3	6OU	I	805	-	10,10,48	0.73	0	9,9,53	0.82	0
3	6OU	E	802	-	7,7,48	0.78	0	6,6,53	0.76	0
3	6OU	I	803	-	33,33,48	1.45	6 (18%)	36,38,53	1.20	2 (5%)
3	6OU	A	805	-	7,7,48	0.70	0	6,6,53	0.75	0
3	6OU	E	804	-	12,12,48	0.74	0	11,11,53	0.87	0
3	6OU	F	801	-	31,31,48	1.37	4 (12%)	33,33,53	1.24	2 (6%)
3	6OU	J	806	-	11,11,48	0.76	0	10,10,53	0.83	0
3	6OU	I	802	-	9,9,48	0.81	0	8,8,53	0.81	0
3	6OU	E	801	-	8,8,48	0.81	0	7,7,53	0.77	0
3	6OU	A	804	-	19,19,48	1.60	4 (21%)	21,21,53	1.39	2 (9%)
3	6OU	I	808	-	11,11,48	0.75	0	10,10,53	0.84	0
3	6OU	I	806	-	10,10,48	0.72	0	9,9,53	0.82	0
3	6OU	F	803	-	31,31,48	1.34	4 (12%)	33,33,53	1.20	2 (6%)
3	6OU	J	804	-	13,13,48	0.76	0	12,12,53	0.87	0
3	6OU	A	802	-	16,16,48	1.47	2 (12%)	15,15,53	0.92	0
3	6OU	B	801	-	13,13,48	0.84	0	12,12,53	0.75	0
3	6OU	H	402	-	11,11,48	0.76	0	10,10,53	0.82	0
3	6OU	E	803	-	7,7,48	0.78	0	6,6,53	0.74	0
3	6OU	I	804	-	10,10,48	0.72	0	9,9,53	0.84	0
3	6OU	A	801	-	31,31,48	1.41	5 (16%)	34,36,53	1.16	2 (5%)
3	6OU	J	802	-	16,16,48	1.46	2 (12%)	15,15,53	0.98	1 (6%)
3	6OU	I	801	-	16,16,48	1.46	2 (12%)	15,15,53	0.97	0
3	6OU	F	802	-	16,16,48	1.46	2 (12%)	15,15,53	0.97	1 (6%)
3	6OU	F	804	-	11,11,48	0.76	0	10,10,53	0.82	0
3	6OU	H	401	-	40,40,48	1.36	6 (15%)	43,45,53	1.16	2 (4%)
3	6OU	A	803	-	32,32,48	1.48	6 (18%)	35,37,53	1.21	2 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6OU	J	801	-	-	7/14/14/52	-
3	6OU	I	809	-	-	5/10/10/52	-
3	6OU	J	805	-	-	4/7/7/52	-
3	6OU	J	803	-	-	5/9/9/52	-
3	6OU	I	807	-	-	3/9/9/52	-
3	6OU	L	401	-	-	8/14/14/52	-
3	6OU	K	401	-	-	13/41/41/52	-
3	6OU	A	806	-	-	5/9/9/52	-
3	6OU	L	402	-	-	3/9/9/52	-
3	6OU	A	807	-	-	10/26/26/52	-
3	6OU	B	802	-	-	6/9/9/52	-
3	6OU	I	805	-	-	3/8/8/52	-
3	6OU	E	802	-	-	3/5/5/52	-
3	6OU	I	803	-	-	16/35/35/52	-
3	6OU	A	805	-	-	2/5/5/52	-
3	6OU	E	804	-	-	4/10/10/52	-
3	6OU	F	801	-	-	9/33/33/52	-
3	6OU	J	806	-	-	6/9/9/52	-
3	6OU	I	802	-	-	4/7/7/52	-
3	6OU	E	801	-	-	2/6/6/52	-
3	6OU	A	804	-	-	10/21/21/52	-
3	6OU	I	808	-	-	3/9/9/52	-
3	6OU	I	806	-	-	6/8/8/52	-
3	6OU	F	803	-	-	15/33/33/52	-
3	6OU	J	804	-	-	5/11/11/52	-
3	6OU	A	802	-	-	7/14/14/52	-
3	6OU	B	801	-	-	4/11/11/52	-
3	6OU	H	402	-	-	4/9/9/52	-
3	6OU	E	803	-	-	3/5/5/52	-
3	6OU	I	804	-	-	3/8/8/52	-
3	6OU	A	801	-	-	20/35/35/52	-
3	6OU	J	802	-	-	9/14/14/52	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6OU	I	801	-	-	10/14/14/52	-
3	6OU	F	802	-	-	5/14/14/52	-
3	6OU	F	804	-	-	4/9/9/52	-
3	6OU	H	401	-	-	22/42/42/52	-
3	6OU	A	803	-	-	18/34/34/52	-

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	802	6OU	C41-C40	4.33	1.56	1.31
3	L	401	6OU	C41-C40	4.33	1.56	1.31
3	I	801	6OU	C41-C40	4.33	1.56	1.31
3	J	801	6OU	C41-C40	4.32	1.56	1.31
3	A	802	6OU	C41-C40	4.32	1.56	1.31
3	F	802	6OU	C41-C40	4.31	1.56	1.31
3	F	801	6OU	O18-C16	3.83	1.44	1.33
3	I	803	6OU	O18-C16	3.79	1.44	1.33
3	F	803	6OU	O18-C16	3.79	1.44	1.33
3	A	807	6OU	O18-C16	3.78	1.44	1.33
3	H	401	6OU	O18-C16	3.78	1.44	1.33
3	K	401	6OU	O18-C16	3.78	1.44	1.33
3	A	801	6OU	O18-C16	3.78	1.44	1.33
3	A	804	6OU	O18-C16	3.77	1.44	1.33
3	A	803	6OU	O18-C16	3.76	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	3.29	1.43	1.34
3	F	803	6OU	O30-C31	3.28	1.43	1.34
3	I	803	6OU	O30-C31	3.27	1.43	1.34
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	3.22	1.43	1.34
3	H	401	6OU	O30-C31	3.21	1.43	1.34
3	A	807	6OU	P23-O26	3.00	1.65	1.54
3	A	803	6OU	P23-O26	2.99	1.65	1.54
3	I	803	6OU	P23-O26	2.98	1.65	1.54
3	K	401	6OU	P23-O26	2.98	1.65	1.54
3	H	401	6OU	P23-O26	2.98	1.65	1.54
3	F	802	6OU	C39-C40	-2.82	1.34	1.50
3	L	401	6OU	C39-C40	-2.81	1.34	1.50
3	J	801	6OU	C39-C40	-2.80	1.34	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	6OU	C39-C40	-2.79	1.34	1.50
3	J	802	6OU	C39-C40	-2.79	1.34	1.50
3	I	801	6OU	C39-C40	-2.79	1.34	1.50
3	I	803	6OU	P23-O22	2.24	1.67	1.60
3	H	401	6OU	P23-O22	2.24	1.67	1.60
3	K	401	6OU	P23-O22	2.23	1.67	1.60
3	A	807	6OU	P23-O22	2.23	1.67	1.60
3	A	803	6OU	P23-O22	2.21	1.67	1.60
3	F	801	6OU	O30-C20	-2.20	1.41	1.46
3	I	803	6OU	O30-C20	-2.16	1.41	1.46
3	A	801	6OU	O30-C20	-2.15	1.41	1.46
3	A	803	6OU	O30-C20	-2.15	1.41	1.46
3	H	401	6OU	O30-C20	-2.15	1.41	1.46
3	A	804	6OU	O30-C20	-2.13	1.41	1.46
3	A	807	6OU	O30-C20	-2.13	1.41	1.46
3	F	803	6OU	O30-C20	-2.12	1.41	1.46
3	K	401	6OU	O30-C20	-2.12	1.41	1.46
3	F	801	6OU	C33-C31	2.07	1.56	1.50
3	K	401	6OU	C33-C31	2.05	1.56	1.50
3	A	801	6OU	C33-C31	2.05	1.56	1.50
3	A	801	6OU	P23-O22	2.05	1.67	1.59
3	A	803	6OU	C33-C31	2.05	1.56	1.50
3	I	803	6OU	C33-C31	2.03	1.56	1.50
3	A	804	6OU	C33-C31	2.02	1.56	1.50
3	F	803	6OU	C33-C31	2.02	1.56	1.50
3	H	401	6OU	C33-C31	2.01	1.56	1.50
3	A	807	6OU	C33-C31	2.01	1.56	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	801	6OU	O30-C31-C33	4.04	120.23	111.48
3	A	807	6OU	O30-C31-C33	3.94	120.00	111.48
3	H	401	6OU	O30-C31-C33	3.93	119.98	111.48
3	A	801	6OU	O30-C31-C33	3.93	119.97	111.48
3	I	803	6OU	O30-C31-C33	3.91	119.94	111.48
3	A	804	6OU	O30-C31-C33	3.88	119.88	111.48
3	A	803	6OU	O30-C31-C33	3.88	119.88	111.48
3	F	803	6OU	O30-C31-C33	3.84	119.79	111.48
3	K	401	6OU	O30-C31-C33	3.60	119.26	111.48
3	F	803	6OU	O18-C16-C15	2.74	120.20	111.83
3	A	803	6OU	O18-C16-C15	2.71	120.10	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	401	6OU	O18-C16-C15	2.69	120.03	111.83
3	K	401	6OU	O18-C16-C15	2.68	120.01	111.83
3	I	803	6OU	O18-C16-C15	2.67	119.97	111.83
3	F	801	6OU	O18-C16-C15	2.66	119.94	111.83
3	A	801	6OU	O18-C16-C15	2.66	119.93	111.83
3	A	807	6OU	O18-C16-C15	2.64	119.89	111.83
3	A	804	6OU	O18-C16-C15	2.60	119.75	111.83
3	L	401	6OU	C42-C41-C40	-2.19	108.43	124.83
3	J	802	6OU	C42-C41-C40	-2.08	109.24	124.83
3	F	802	6OU	C42-C41-C40	-2.08	109.26	124.83

There are no chirality outliers.

All (266) 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	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	J	801	6OU	C39-C40-C41-C42
3	A	802	6OU	C39-C40-C41-C42
3	F	802	6OU	C39-C40-C41-C42
3	A	807	6OU	O17-C16-O18-C19
3	A	801	6OU	C15-C16-O18-C19
3	F	803	6OU	C15-C16-O18-C19
3	A	802	6OU	C36-C37-C38-C39
3	A	802	6OU	C34-C35-C36-C37
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

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Mol	Chain	Res	Type	Atoms
3	A	803	6OU	C15-C16-O18-C19
3	J	802	6OU	C39-C40-C41-C42
3	F	801	6OU	C37-C38-C39-C40
3	A	803	6OU	O17-C16-O18-C19
3	I	803	6OU	C43-C44-C45-C46
3	A	804	6OU	O18-C19-C20-O30
3	I	801	6OU	C39-C40-C41-C42
3	J	805	6OU	C03-C04-C05-C06
3	I	803	6OU	C34-C35-C36-C37
3	A	801	6OU	C33-C31-O30-C20
3	J	806	6OU	C06-C07-C08-C09
3	I	806	6OU	C07-C08-C09-C10
3	E	804	6OU	C07-C08-C09-C10
3	F	803	6OU	C36-C37-C38-C39
3	I	805	6OU	C07-C08-C09-C10
3	I	806	6OU	C04-C05-C06-C07
3	A	803	6OU	C35-C36-C37-C38
3	H	401	6OU	C44-C45-C46-C47
3	J	803	6OU	C04-C05-C06-C07
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	J	801	6OU	C37-C38-C39-C40
3	J	803	6OU	C07-C08-C09-C10
3	H	401	6OU	C08-C09-C10-C11
3	H	402	6OU	C03-C04-C05-C06
3	A	801	6OU	O32-C31-O30-C20
3	A	805	6OU	C03-C04-C05-C06
3	K	401	6OU	C08-C09-C10-C11
3	F	804	6OU	C03-C04-C05-C06
3	H	401	6OU	C36-C37-C38-C39
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	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	806	6OU	C06-C07-C08-C09
3	J	802	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

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Mol	Chain	Res	Type	Atoms
3	I	805	6OU	C04-C05-C06-C07
3	I	808	6OU	C06-C07-C08-C09
3	B	802	6OU	C07-C08-C09-C10
3	F	801	6OU	C08-C09-C10-C11
3	A	807	6OU	O30-C20-C21-O22
3	E	802	6OU	C02-C03-C04-C05
3	L	402	6OU	C06-C07-C08-C09
3	A	801	6OU	C13-C14-C15-C16
3	F	803	6OU	C35-C36-C37-C38
3	I	801	6OU	C37-C38-C39-C40
3	F	803	6OU	O18-C19-C20-O30
3	H	401	6OU	C37-C38-C39-C40
3	L	401	6OU	C37-C38-C39-C40
3	J	806	6OU	C05-C06-C07-C08
3	I	801	6OU	C35-C36-C37-C38
3	I	805	6OU	C06-C07-C08-C09
3	I	808	6OU	C03-C04-C05-C06
3	H	401	6OU	C20-C21-O22-P23
3	A	806	6OU	C08-C09-C10-C11
3	J	804	6OU	C07-C08-C09-C10
3	I	807	6OU	C06-C07-C08-C09
3	J	802	6OU	C34-C35-C36-C37
3	J	804	6OU	C09-C10-C11-C12
3	A	803	6OU	C19-C20-C21-O22
3	A	803	6OU	O32-C31-O30-C20
3	H	401	6OU	O32-C31-O30-C20
3	A	801	6OU	C12-C13-C14-C15
3	E	801	6OU	C02-C03-C04-C05
3	H	401	6OU	C11-C12-C13-C14
3	I	803	6OU	C35-C36-C37-C38
3	A	807	6OU	O32-C31-O30-C20
3	I	809	6OU	C07-C08-C09-C10
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	H	402	6OU	C08-C09-C10-C11
3	I	802	6OU	C02-C03-C04-C05
3	A	803	6OU	C05-C06-C07-C08
3	I	804	6OU	C07-C08-C09-C10
3	J	803	6OU	C06-C07-C08-C09
3	A	807	6OU	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
3	A	803	6OU	C21-O22-P23-O24
3	H	401	6OU	C21-O22-P23-O24
3	F	804	6OU	C05-C06-C07-C08
3	A	801	6OU	C08-C09-C10-C11
3	I	803	6OU	C15-C16-O18-C19
3	H	401	6OU	C35-C36-C37-C38
3	J	806	6OU	C03-C04-C05-C06
3	I	806	6OU	C06-C07-C08-C09
3	H	401	6OU	C13-C14-C15-C16
3	L	402	6OU	C05-C06-C07-C08
3	A	801	6OU	C11-C12-C13-C14
3	A	803	6OU	O18-C19-C20-O30
3	A	807	6OU	O18-C19-C20-O30
3	B	802	6OU	C04-C05-C06-C07
3	I	802	6OU	C06-C07-C08-C09
3	I	803	6OU	C33-C31-O30-C20
3	I	801	6OU	C42-C43-C44-C45
3	J	805	6OU	C02-C03-C04-C05
3	I	801	6OU	C36-C37-C38-C39
3	A	801	6OU	C05-C06-C07-C08
3	H	402	6OU	C05-C06-C07-C08
3	K	401	6OU	C13-C14-C15-C16
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	B	801	6OU	C31-C33-C34-C35
3	I	803	6OU	C13-C14-C15-C16
3	I	803	6OU	O17-C16-O18-C19
3	K	401	6OU	C12-C13-C14-C15
3	E	801	6OU	C01-C02-C03-C04
3	F	801	6OU	O18-C19-C20-C21
3	F	803	6OU	O18-C19-C20-C21
3	A	804	6OU	C19-C20-C21-O22
3	F	803	6OU	C19-C20-C21-O22
3	A	801	6OU	O30-C20-C21-O22
3	H	401	6OU	O30-C20-C21-O22
3	J	804	6OU	C10-C11-C12-C13
3	B	801	6OU	C34-C35-C36-C37
3	L	401	6OU	C35-C36-C37-C38
3	I	806	6OU	C01-C02-C03-C04
3	F	802	6OU	C34-C35-C36-C37
3	J	801	6OU	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
3	A	803	6OU	C36-C37-C38-C39
3	A	803	6OU	C07-C08-C09-C10
3	I	801	6OU	C33-C34-C35-C36
3	K	401	6OU	C19-C20-C21-O22
3	L	401	6OU	C42-C43-C44-C45
3	A	803	6OU	C31-C33-C34-C35
3	E	803	6OU	C01-C02-C03-C04
3	L	401	6OU	C41-C42-C43-C44
3	I	803	6OU	O32-C31-O30-C20
3	K	401	6OU	O30-C20-C21-O22
3	I	804	6OU	C06-C07-C08-C09
3	F	801	6OU	C35-C36-C37-C38
3	I	803	6OU	O18-C19-C20-C21
3	I	803	6OU	C31-C33-C34-C35
3	A	806	6OU	C09-C10-C11-C12
3	H	401	6OU	O18-C19-C20-O30
3	J	803	6OU	C09-C10-C11-C12
3	I	809	6OU	C05-C06-C07-C08
3	K	401	6OU	C37-C38-C39-C40
3	F	803	6OU	C46-C47-C48-C49
3	J	801	6OU	C41-C42-C43-C44
3	B	801	6OU	C37-C38-C39-C40
3	I	802	6OU	C03-C04-C05-C06
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	A	806	6OU	C05-C06-C07-C08
3	I	803	6OU	O30-C20-C21-O22
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	A	807	6OU	C36-C37-C38-C39
3	A	803	6OU	C08-C09-C10-C11
3	A	801	6OU	C21-O22-P23-O24
3	A	801	6OU	C20-C21-O22-P23
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	801	6OU	C10-C11-C12-C13
3	F	804	6OU	C06-C07-C08-C09
3	I	802	6OU	C01-C02-C03-C04

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Mol	Chain	Res	Type	Atoms
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	I	803	6OU	C44-C45-C46-C47
3	J	805	6OU	C01-C02-C03-C04
3	J	803	6OU	C03-C04-C05-C06
3	J	806	6OU	C08-C09-C10-C11
3	J	806	6OU	C01-C02-C03-C04
3	I	801	6OU	C43-C44-C45-C46
3	F	804	6OU	C08-C09-C10-C11
3	E	802	6OU	C01-C02-C03-C04
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	803	6OU	C19-C20-C21-O22
3	I	809	6OU	C10-C11-C12-C13
3	I	809	6OU	C06-C07-C08-C09
3	B	802	6OU	C02-C03-C04-C05
3	A	804	6OU	O30-C20-C21-O22
3	F	803	6OU	O30-C20-C21-O22
3	I	807	6OU	C02-C03-C04-C05
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	F	801	6OU	C31-C33-C34-C35
3	I	801	6OU	C31-C33-C34-C35
3	I	808	6OU	C04-C05-C06-C07
3	J	802	6OU	C31-C33-C34-C35
3	J	801	6OU	C42-C43-C44-C45
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	J	802	6OU	C40-C41-C42-C43
3	I	801	6OU	C40-C41-C42-C43
3	H	402	6OU	C09-C10-C11-C12
3	J	802	6OU	C43-C44-C45-C46
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	F	802	6OU	C40-C41-C42-C43
3	I	806	6OU	C05-C06-C07-C08

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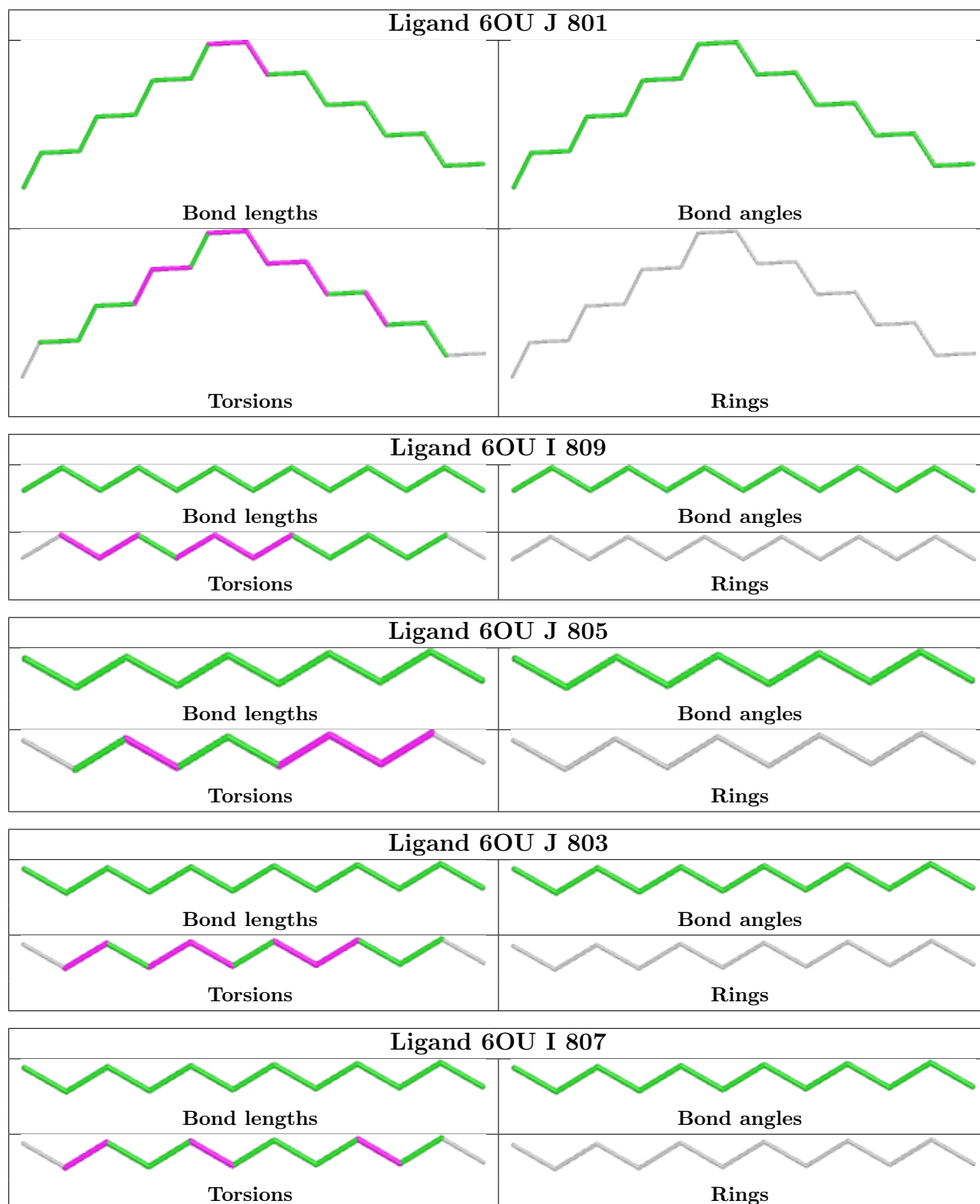
Mol	Chain	Res	Type	Atoms
3	I	803	6OU	C20-C21-O22-P23
3	F	801	6OU	C40-C41-C42-C43
3	A	803	6OU	C33-C34-C35-C36
3	K	401	6OU	C07-C08-C09-C10
3	A	802	6OU	C40-C41-C42-C43
3	F	803	6OU	C40-C41-C42-C43
3	H	401	6OU	C43-C44-C45-C46
3	E	803	6OU	C05-C06-C07-C08
3	I	807	6OU	C09-C10-C11-C12
3	F	801	6OU	C34-C35-C36-C37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

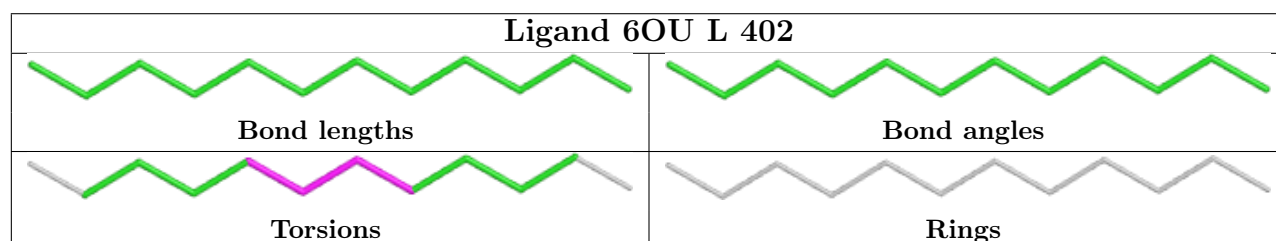
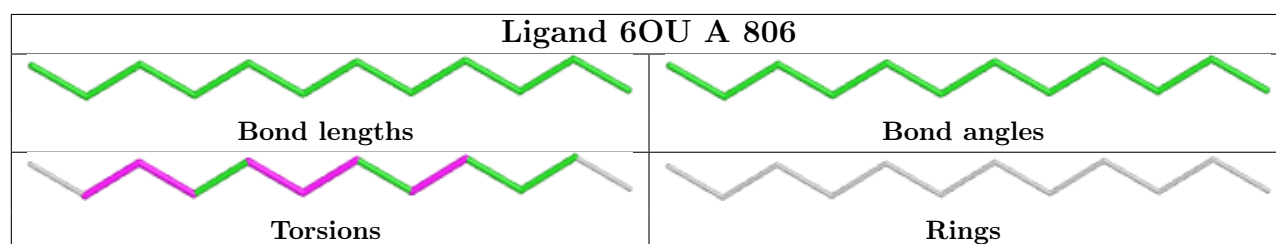
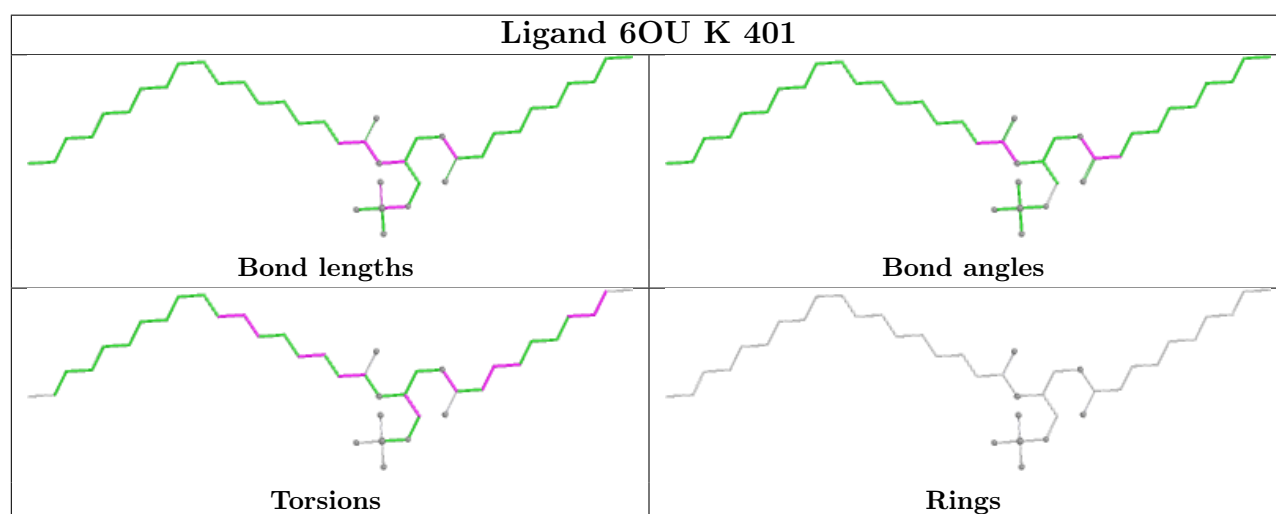
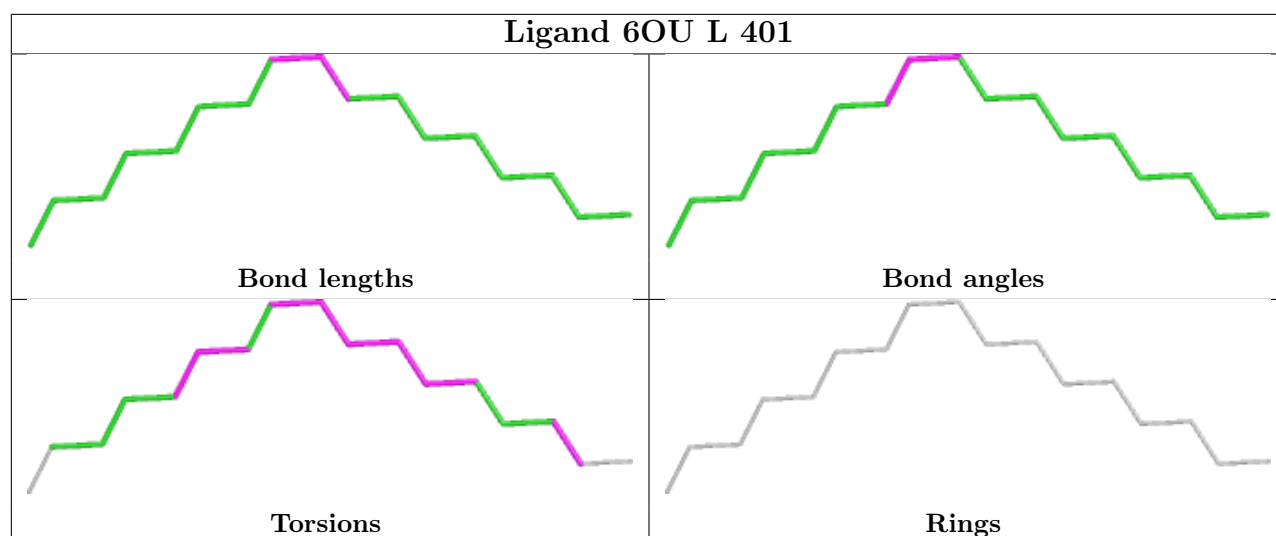
There are no ring outliers.

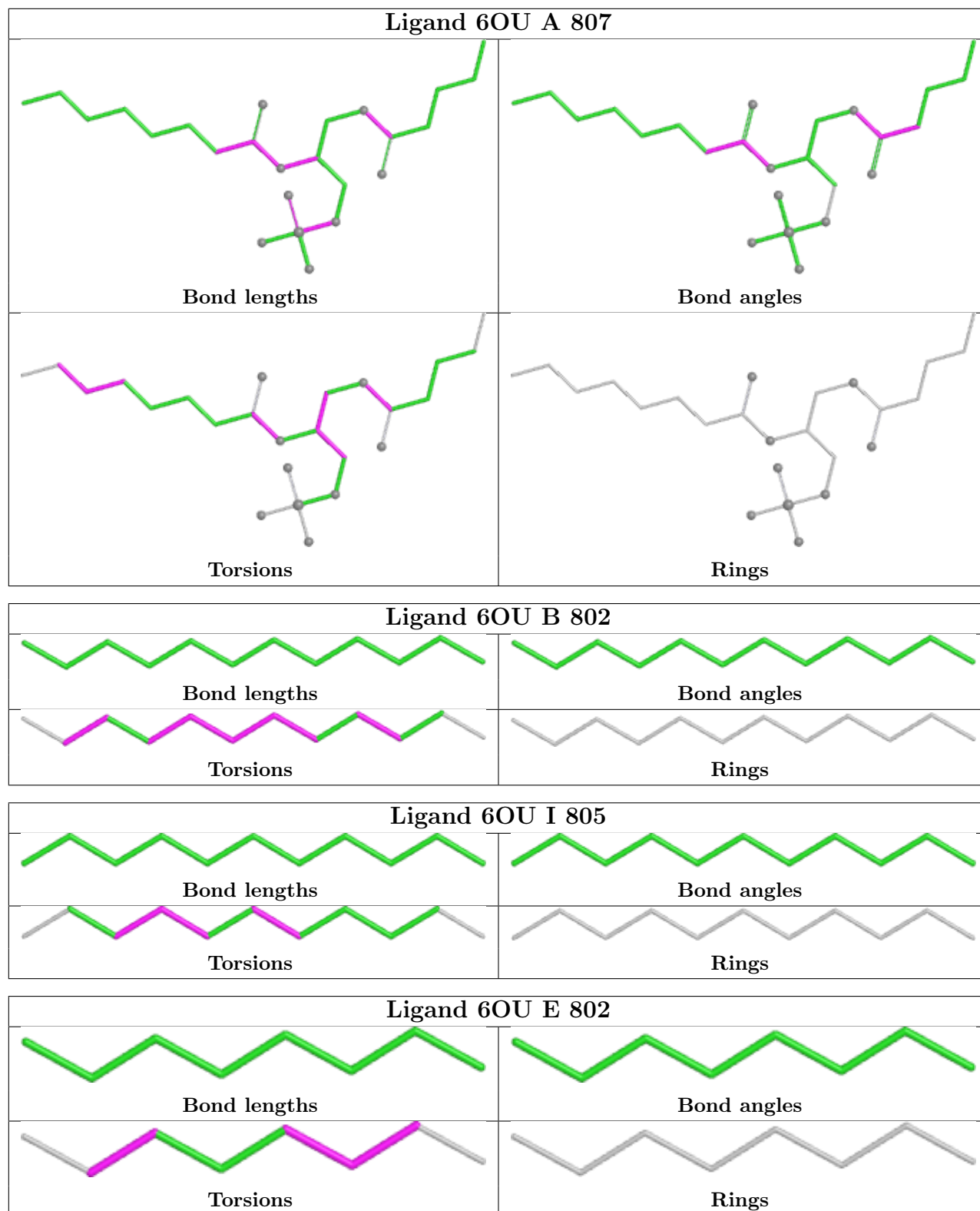
No monomer is involved in short contacts.

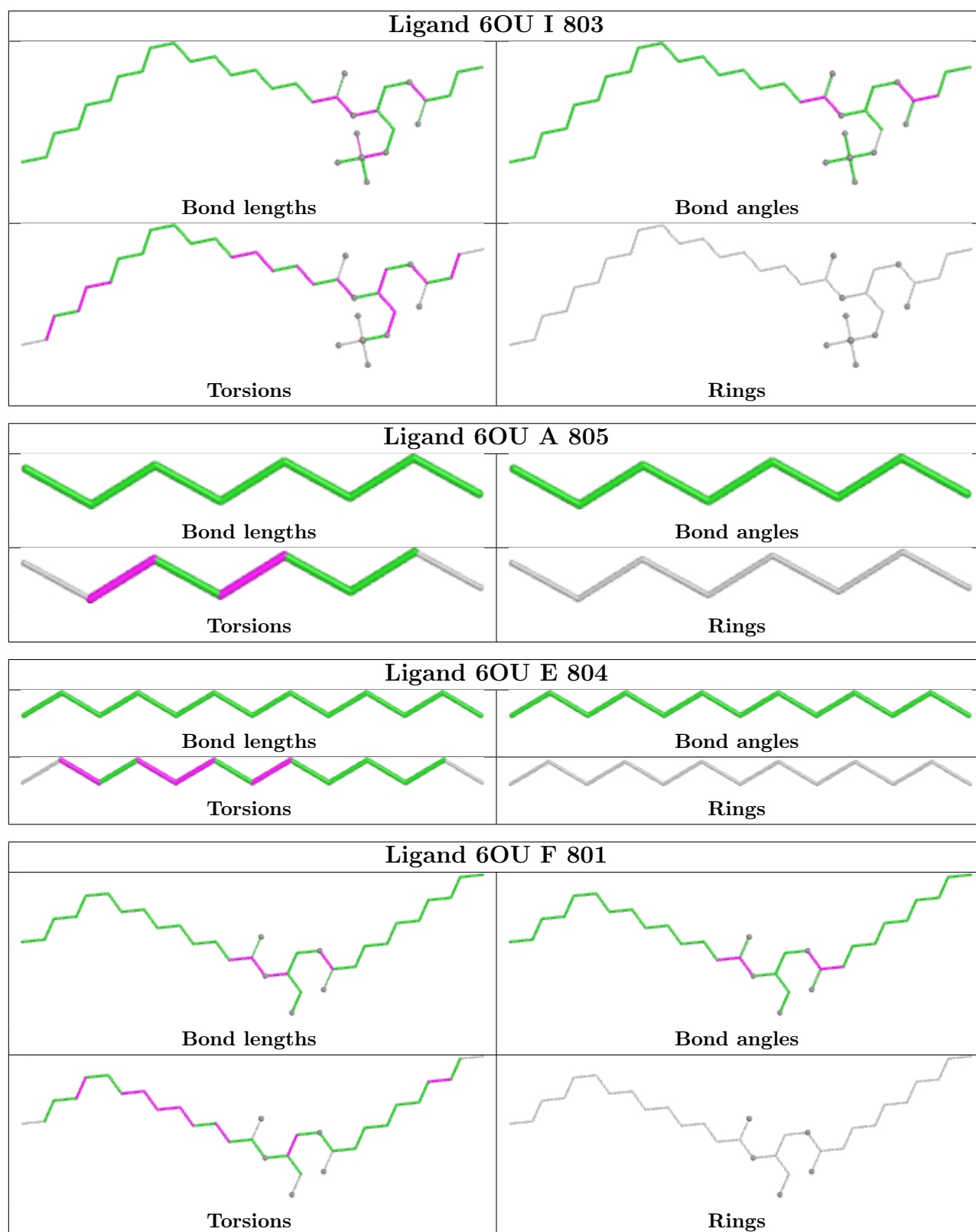
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

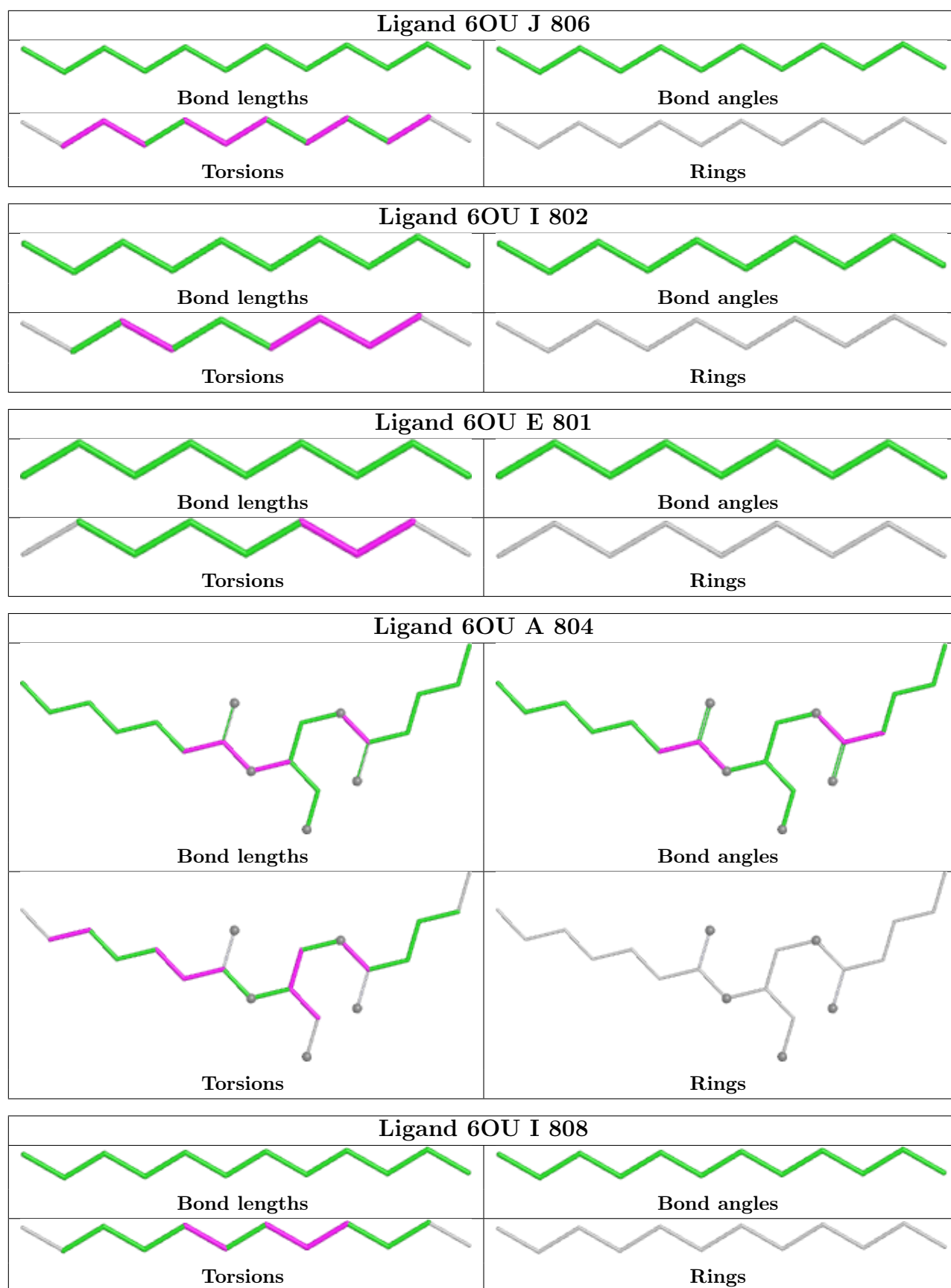
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

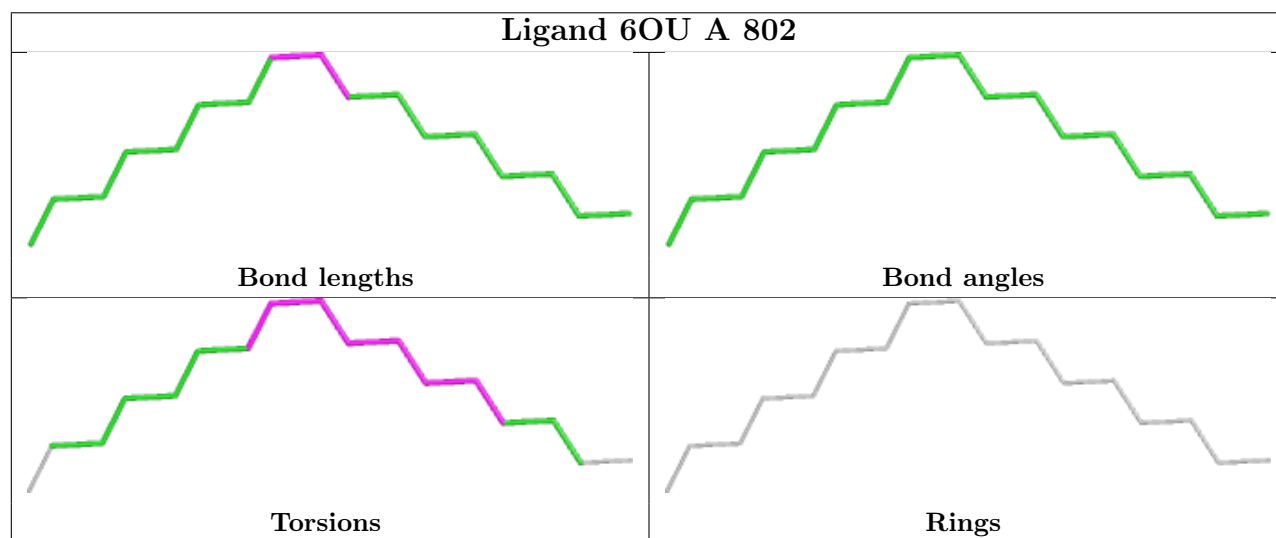
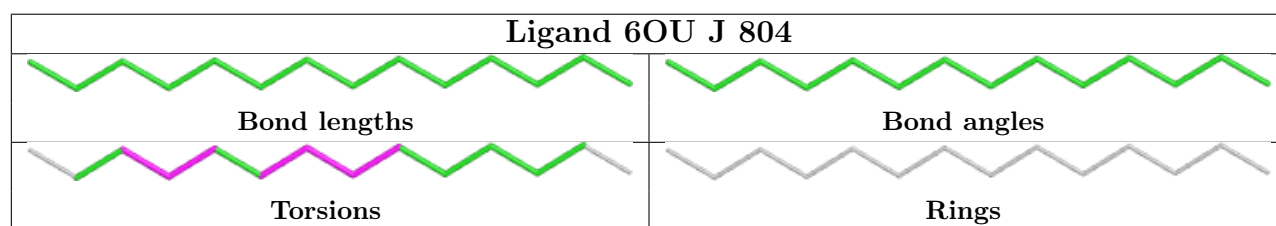
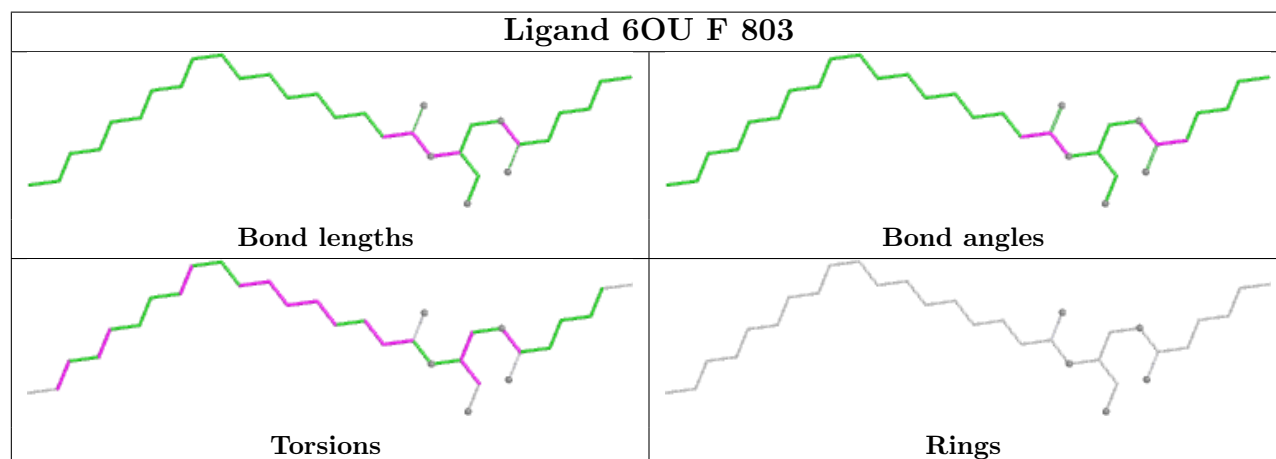
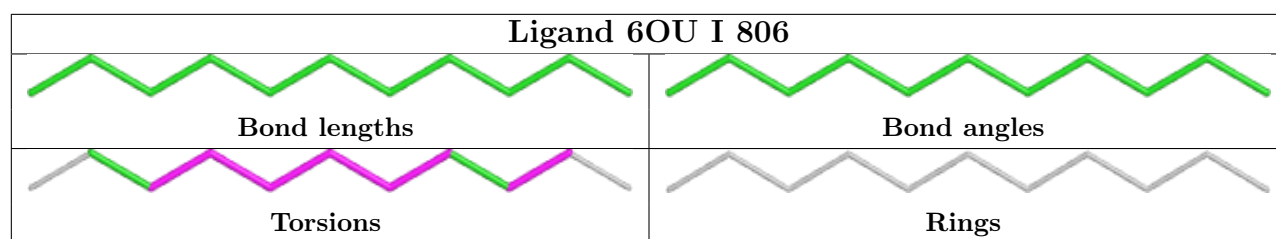


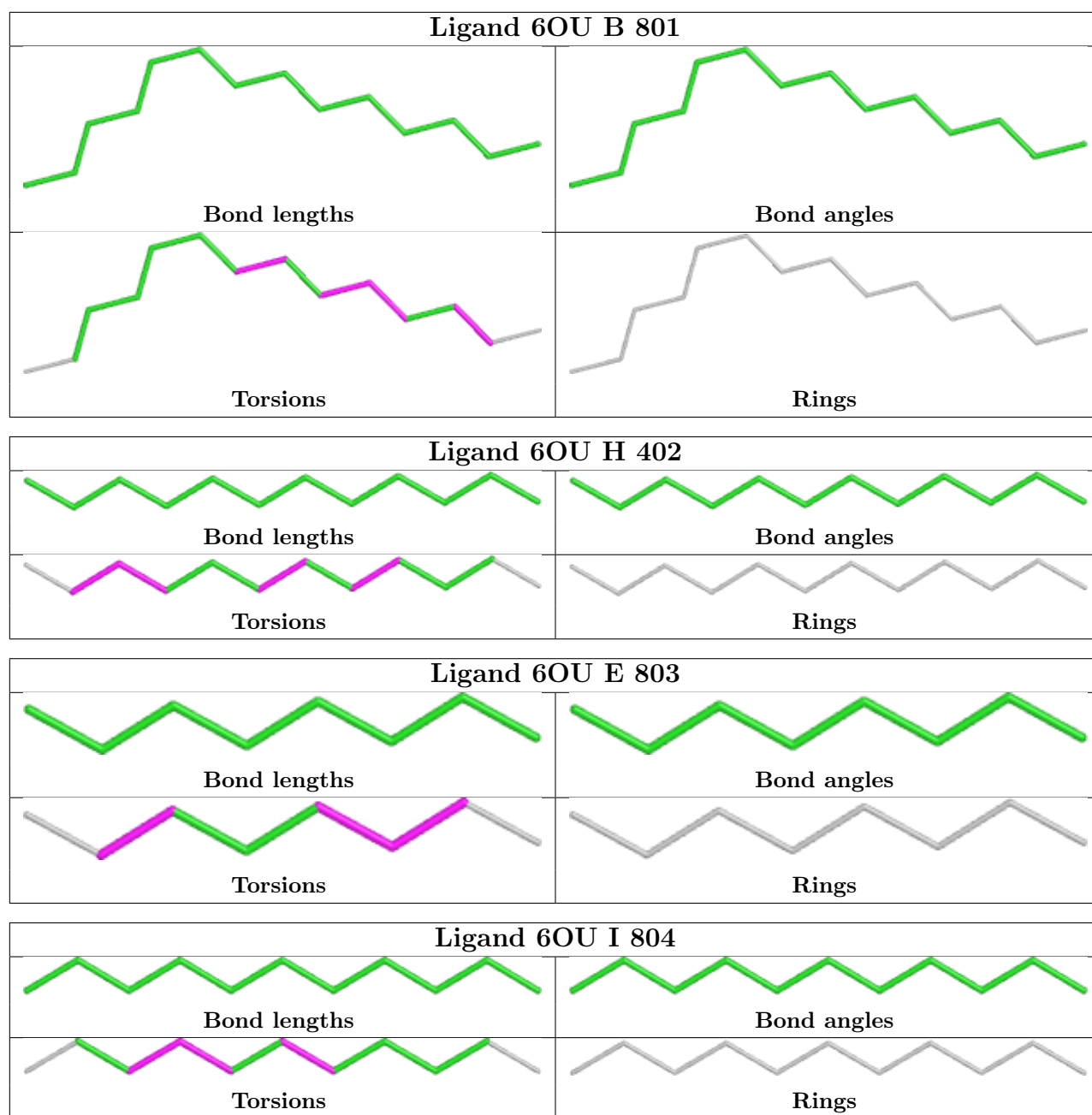


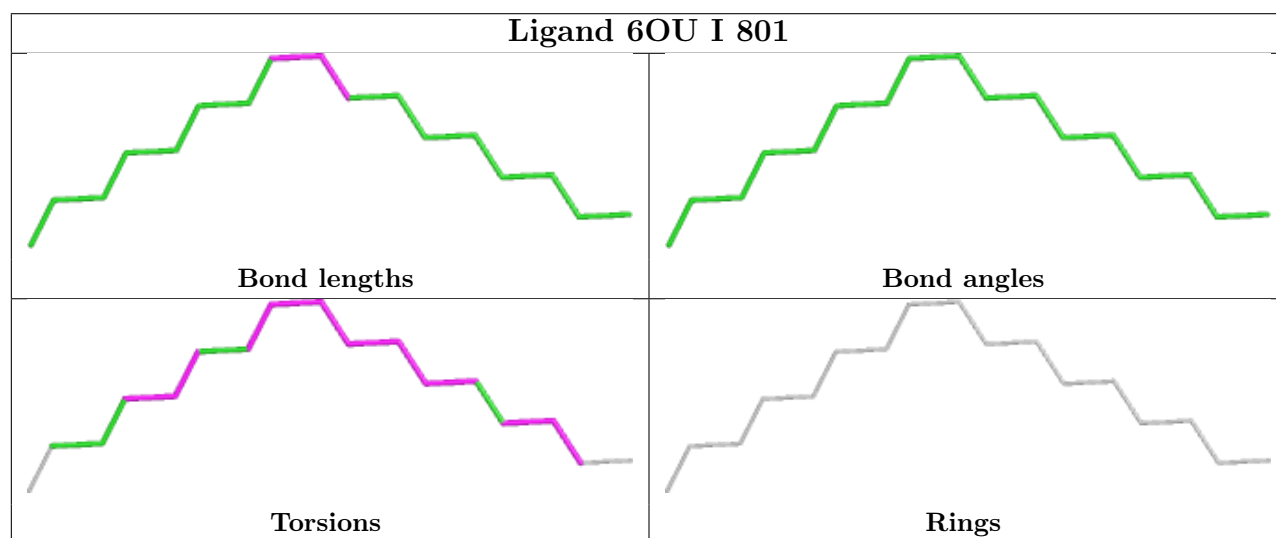
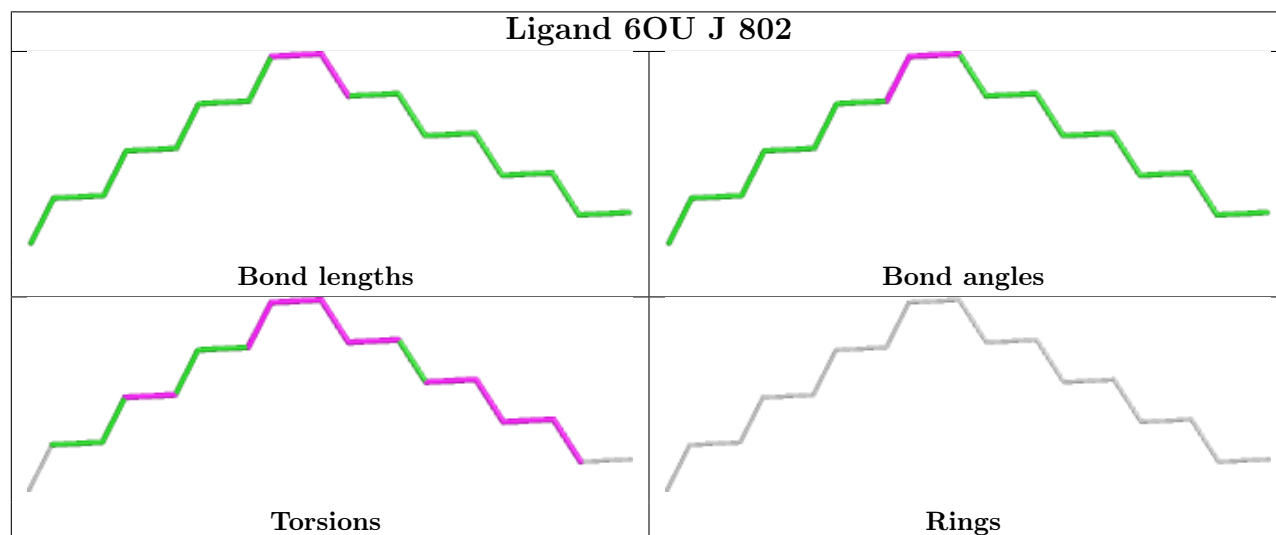
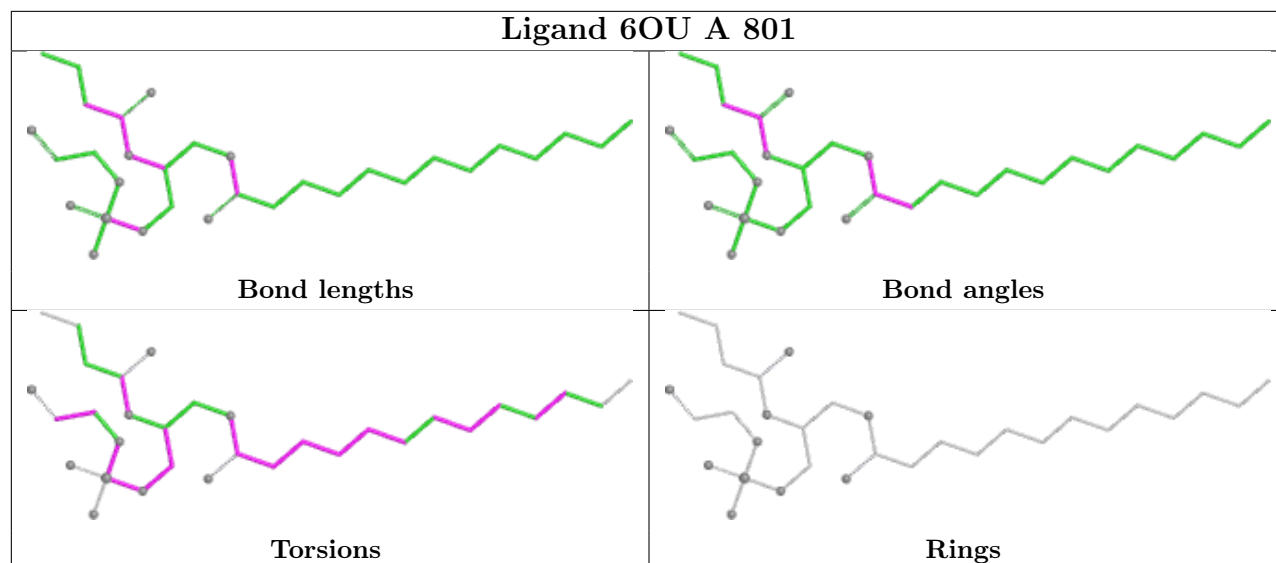


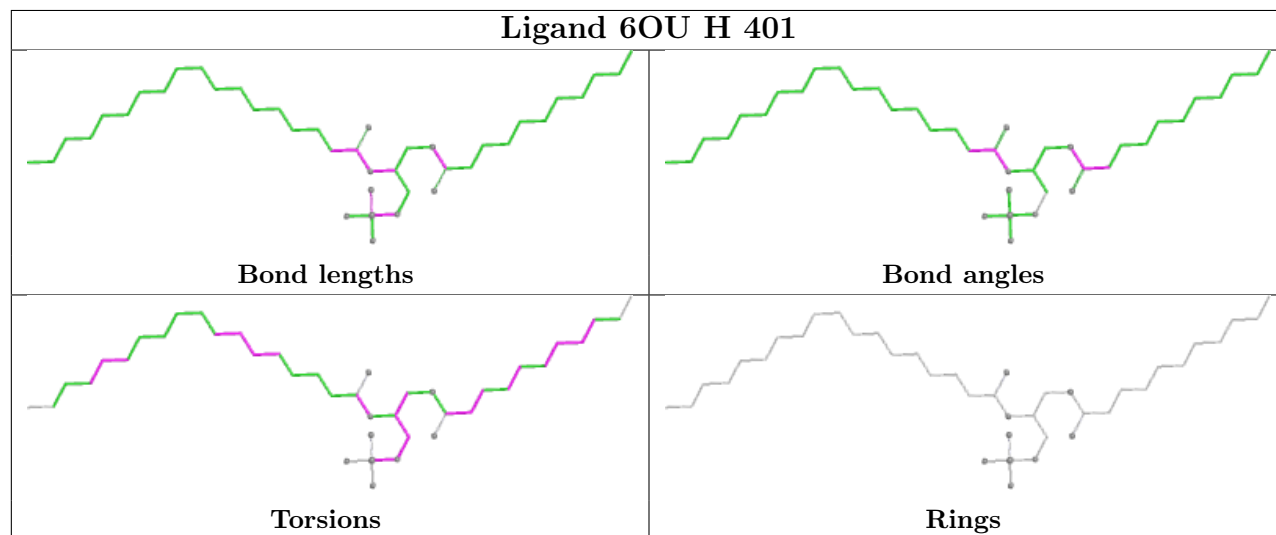
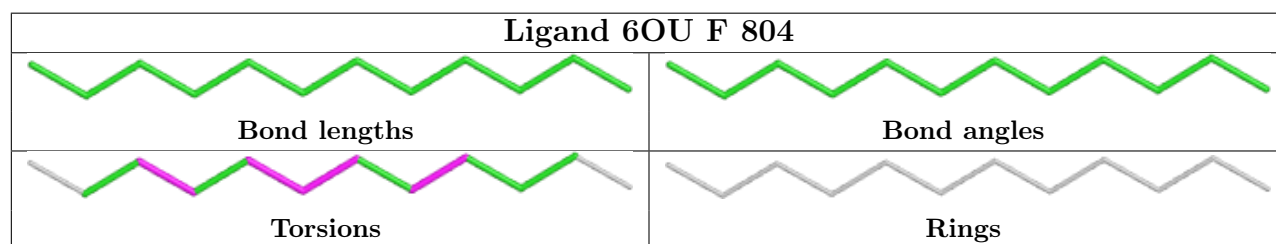
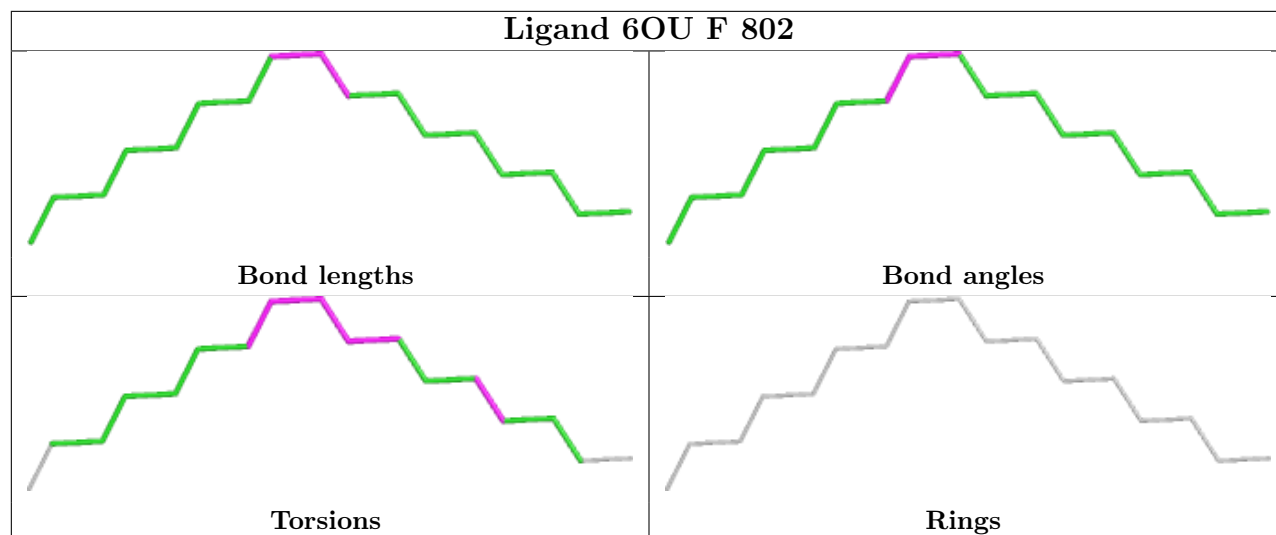


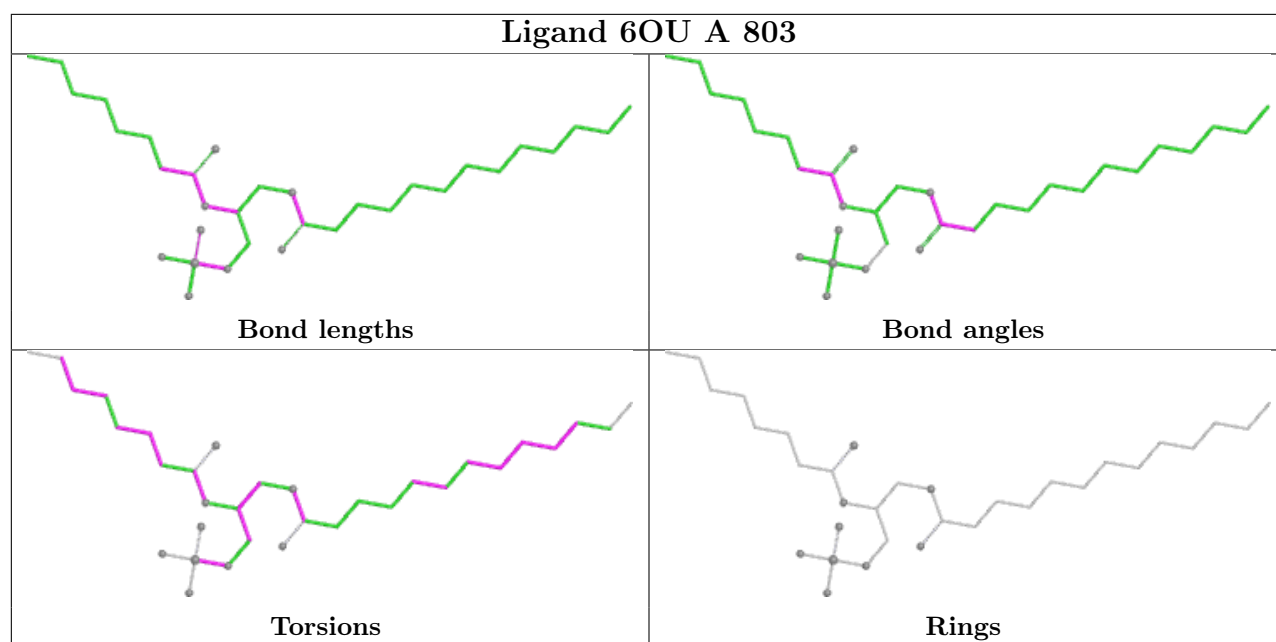












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

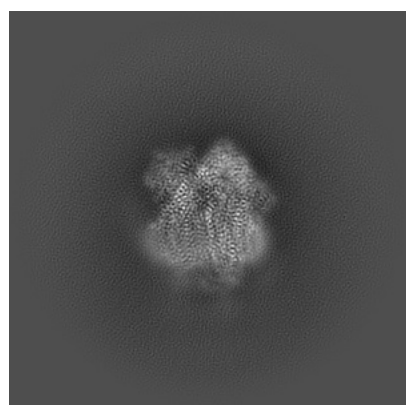
6 Map visualisation [i](#)

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

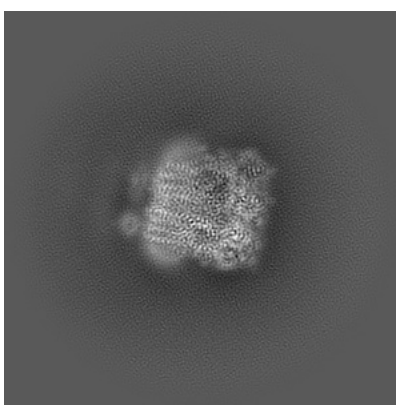
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

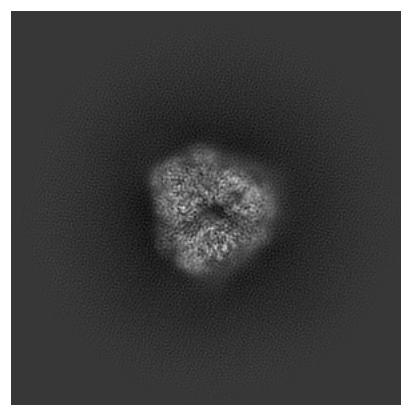
6.1.1 Primary map



X



Y

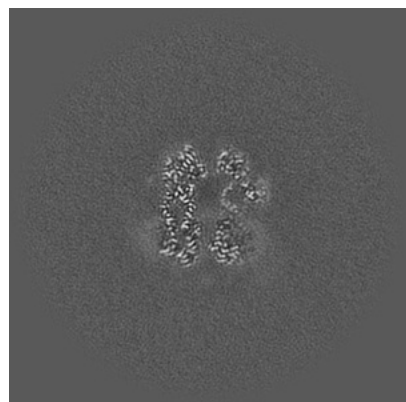


Z

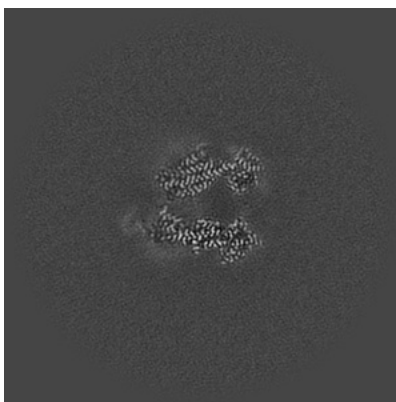
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

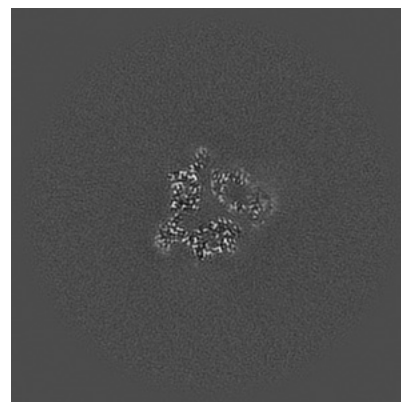
6.2.1 Primary map



X Index: 192



Y Index: 192

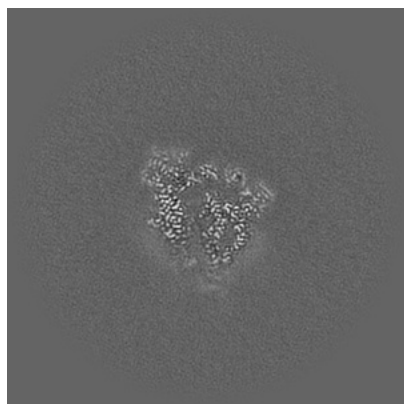


Z Index: 192

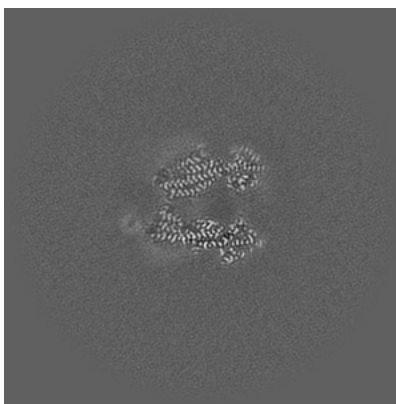
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

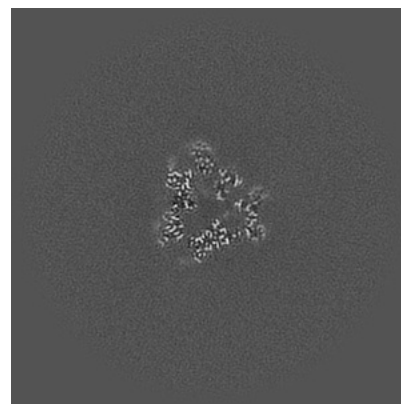
6.3.1 Primary map



X Index: 177



Y Index: 193

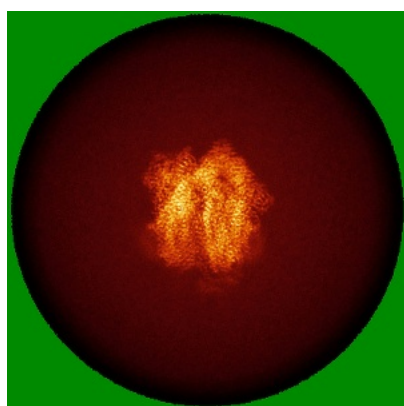


Z Index: 201

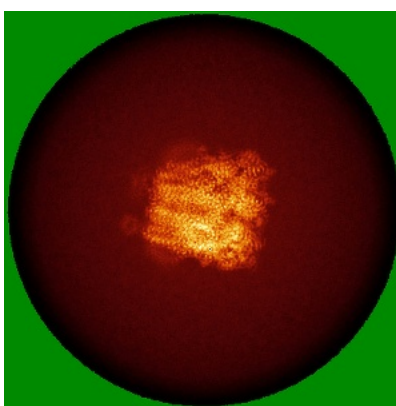
The images above show the largest variance slices of the map in three orthogonal directions.

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

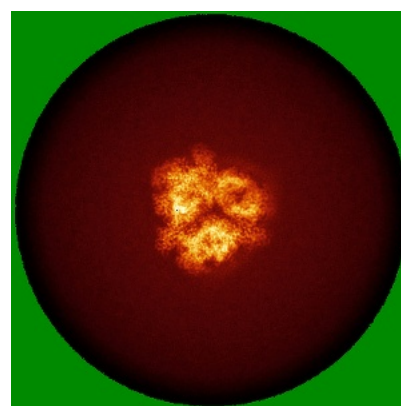
6.4.1 Primary map



X



Y

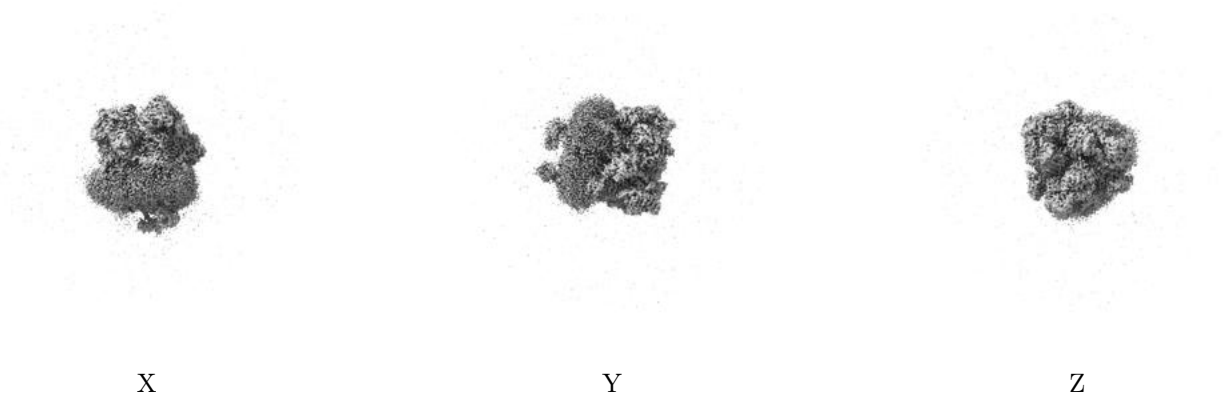


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

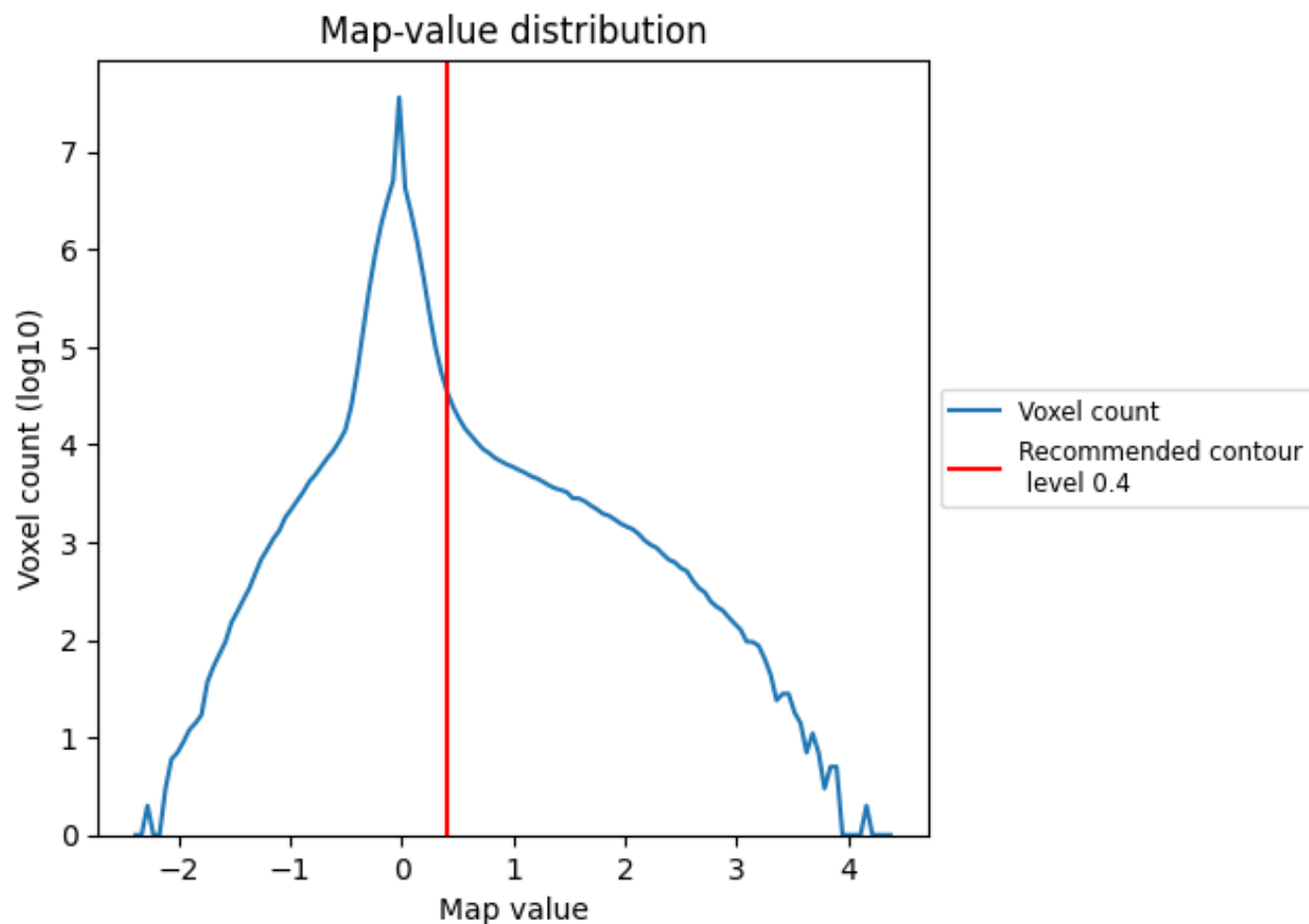
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

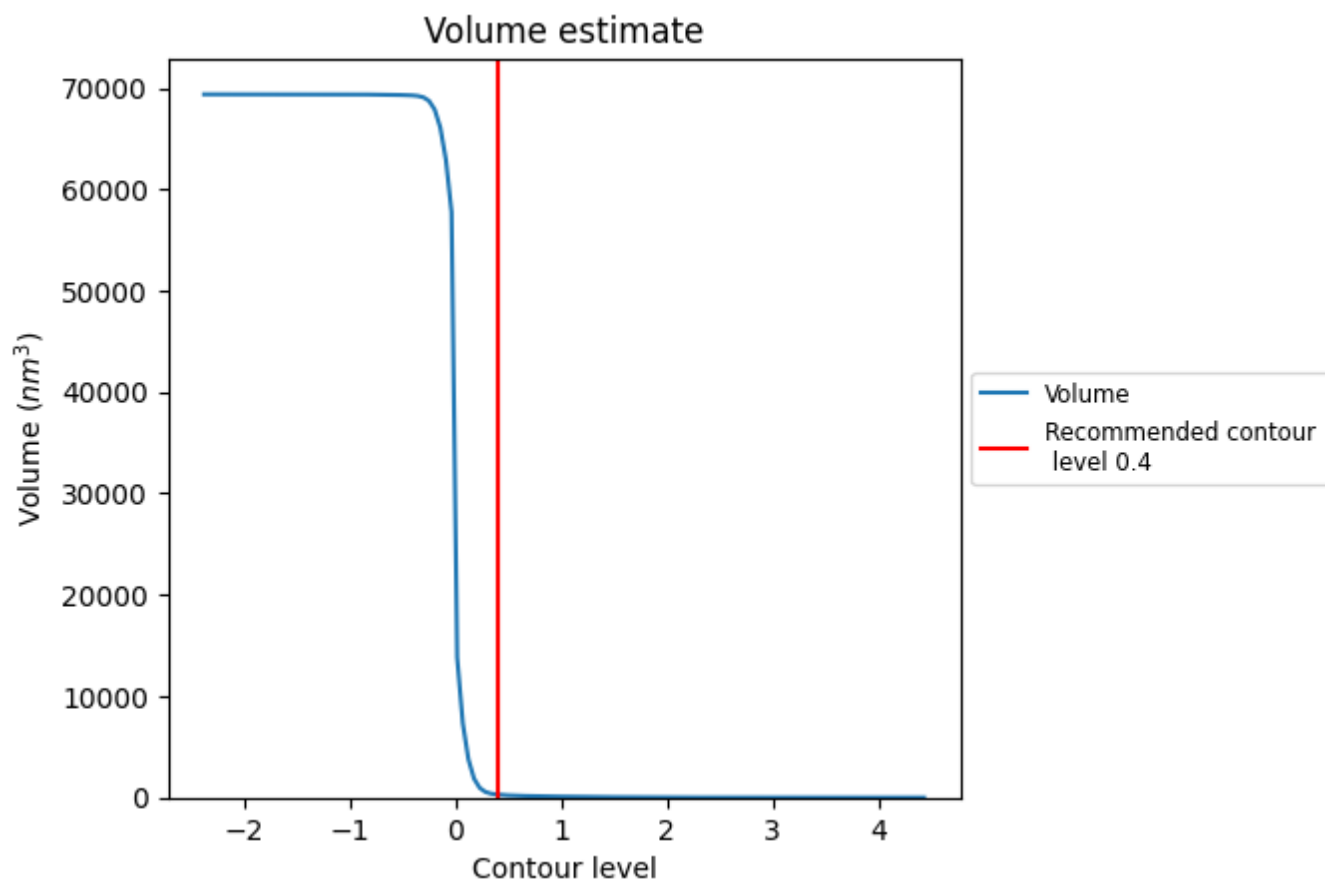
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

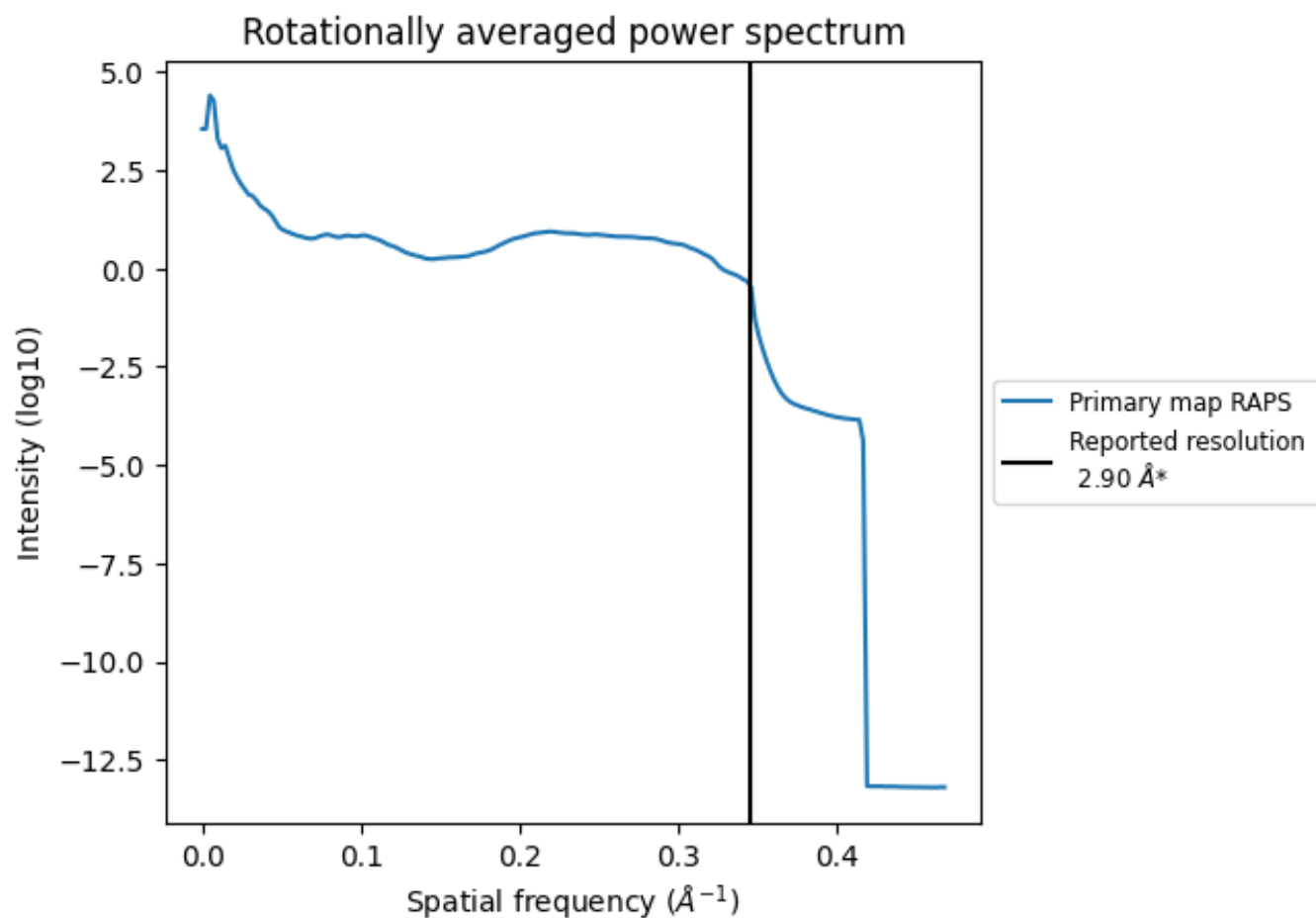
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 291 nm³; 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 ⓘ



*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.

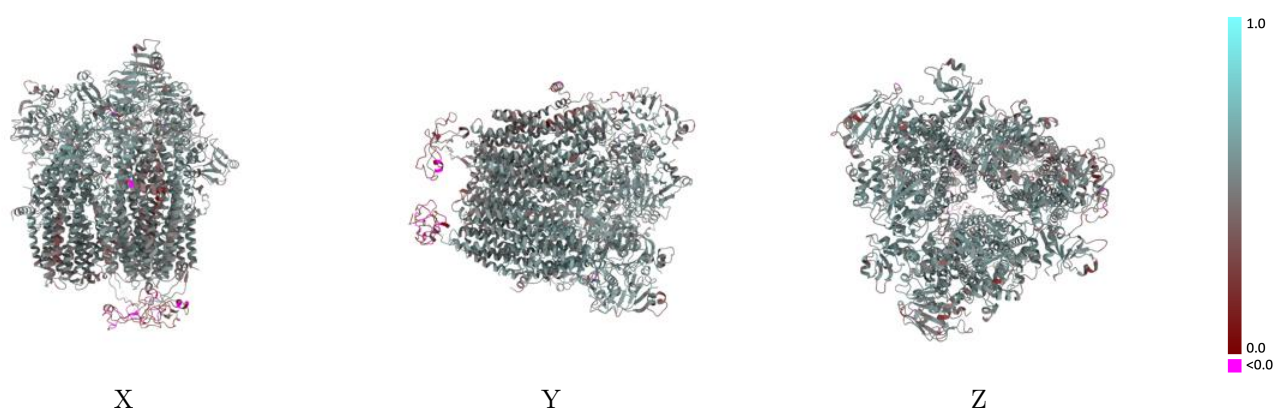
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD 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 [i](#)

This section was not generated.

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

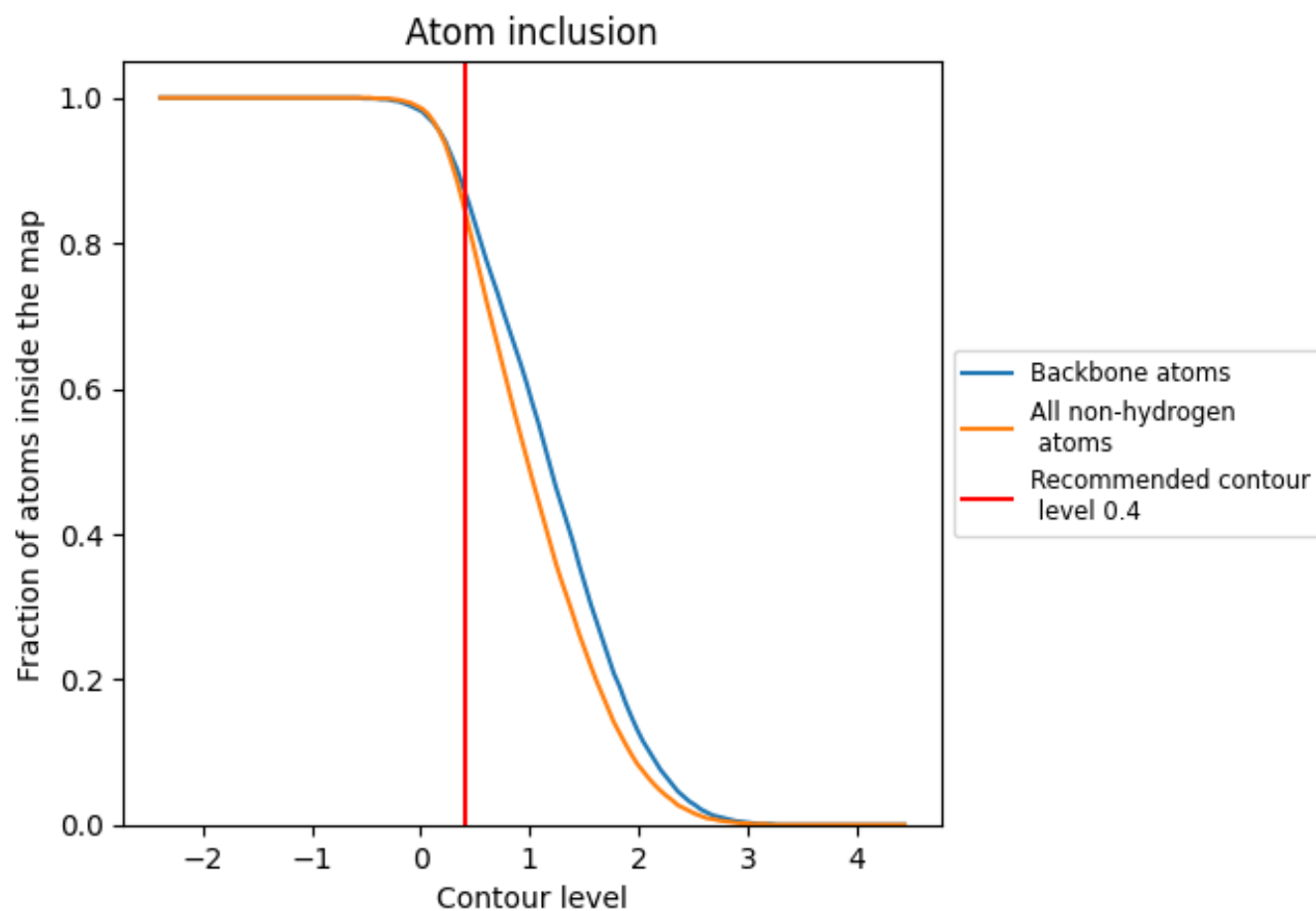


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

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	0.8480	0.5180
A	0.8550	0.5260
B	0.8280	0.4990
C	0.6360	0.4040
D	0.6970	0.4320
E	0.8930	0.5530
F	0.8790	0.5330
G	0.5800	0.3200
H	0.8410	0.5200
I	0.8780	0.5420
J	0.8740	0.5280
K	0.7190	0.4620
L	0.8470	0.5010

