



Full wwPDB EM Validation Report ⓘ

May 13, 2025 – 07:22 pm BST

PDB ID : 8Q54 / pdb_00008q54
EMDB ID : EMD-18162
Title : N5-methyl-H4MPT:CoM methyltransferase -coenzyme M complex + CoM
Authors : Aziz, I.; Vonck, J.; Ermler, U.
Deposited on : 2023-08-08
Resolution : 2.39 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.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

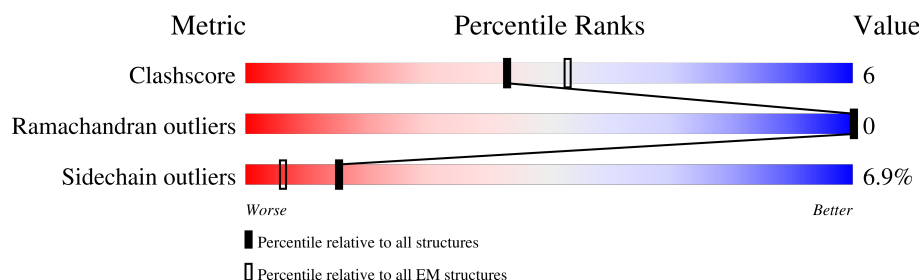
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.39 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.




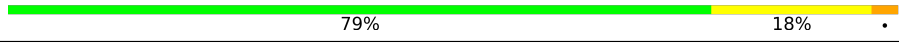
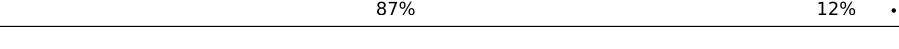




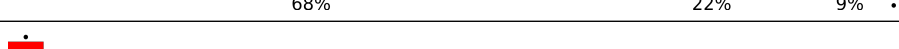





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	238	
1	Q	238	
1	a	238	
2	B	100	
2	R	100	
2	b	100	
3	C	267	
3	S	267	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	c	267	
4	D	233	
4	T	233	
4	d	233	
5	E	295	
5	U	295	
5	e	295	
6	F	68	
6	V	68	
6	f	68	
7	G	86	
7	W	86	
7	g	86	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	COM	E	303[A]	-	X	-	-
11	COM	E	303[B]	-	X	-	-
11	COM	U	303[A]	-	X	-	-
11	COM	U	303[C]	-	X	-	-
11	COM	e	303[A]	-	X	-	-
11	COM	e	303[B]	-	X	-	-
9	JCV	E	304	X	-	-	-
9	JCV	E	306	X	-	-	-
9	JCV	S	301	X	-	-	-
9	JCV	U	305	X	-	-	-
9	JCV	W	101	X	-	-	-
9	JCV	c	301	X	-	-	-

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 48734 atoms, of which 24135 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 Tetrahydromethanopterin S-methyltransferase subunit A 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	61	Total	C	H	N	O	S	0	0
			962	297	499	78	83	5		
1	a	61	Total	C	H	N	O	S	0	0
			962	297	499	78	83	5		
1	Q	61	Total	C	H	N	O	S	0	0
			962	297	499	78	83	5		

- Molecule 2 is a protein called Tetrahydromethanopterin S-methyltransferase subunit B.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	70	Total	C	H	N	O	S	0	0
			1076	346	545	78	106	1		
2	b	70	Total	C	H	N	O	S	0	0
			1076	346	545	78	106	1		
2	R	70	Total	C	H	N	O	S	0	0
			1076	346	545	78	106	1		

- Molecule 3 is a protein called Tetrahydromethanopterin S-methyltransferase subunit C.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	254	Total	C	H	N	O	S	2	0
			3786	1207	1955	296	317	11		
3	c	254	Total	C	H	N	O	S	4	0
			3806	1213	1964	300	318	11		
3	S	254	Total	C	H	N	O	S	2	0
			3786	1207	1955	296	317	11		

- Molecule 4 is a protein called Tetrahydromethanopterin S-methyltransferase subunit D.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	233	Total	C	H	N	O	S	0	0
			3264	1038	1668	257	288	13		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf	Trace
4	d	233	Total	C	H	N	O	S	0	0
			3264	1038	1668	257	288	13		
4	T	233	Total	C	H	N	O	S	0	0
			3264	1038	1668	257	288	13		

- Molecule 5 is a protein called Tetrahydromethanopterin S-methyltransferase subunit E.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	294	Total	C	H	N	O	S	0	0
			4390	1420	2203	363	388	16		
5	e	294	Total	C	H	N	O	S	0	0
			4390	1420	2203	363	388	16		
5	U	294	Total	C	H	N	O	S	0	0
			4390	1420	2203	363	388	16		

- Molecule 6 is a protein called Tetrahydromethanopterin S-methyltransferase subunit F.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	67	Total	C	H	N	O	S	0	0
			1069	329	564	90	84	2		
6	f	67	Total	C	H	N	O	S	0	0
			1069	329	564	90	84	2		
6	V	67	Total	C	H	N	O	S	0	0
			1069	329	564	90	84	2		

- Molecule 7 is a protein called Tetrahydromethanopterin S-methyltransferase subunit G.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	73	Total	C	H	N	O		0	0
			1164	368	598	92	106			
7	g	73	Total	C	H	N	O		0	0
			1164	368	598	92	106			
7	W	73	Total	C	H	N	O		0	0
			1164	368	598	92	106			

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

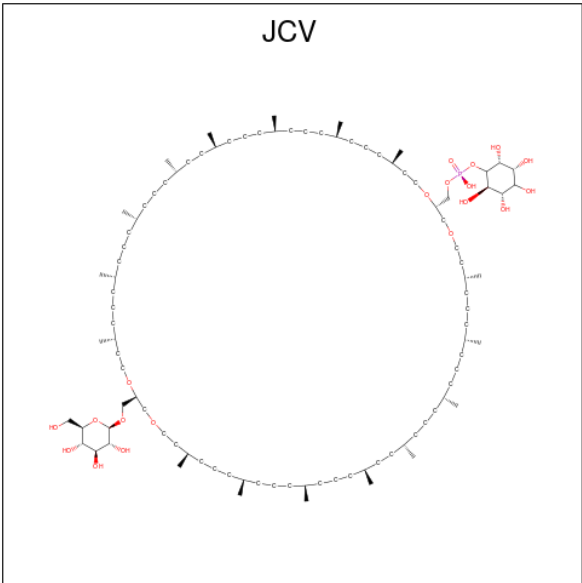
Mol	Chain	Residues	Atoms		AltConf
8	B	1	Total	Mg	0
			1	1	
8	b	1	Total	Mg	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
8	R	1	1	1	0

- Molecule 9 is [(2 {S},7 {R},11 {R},15 {S},19 {S},22 {S},26 {S},30 {R},34 {R},39 {S},43 {R},47 {R},51 {S},55 {S},58 {S},62 {S},66 {R},70 {R})-39-[(2 {R},3 {R},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxymethyl]-7,11,15,19,22,26,30,34,43,47,51,55,58,62,66,70-hexadecamethyl-1,4,37,40-tetraoxacyclodoheptacont-2-yl]methyl [(2 {R},3 {S},5 {R},6 {R})-2,3,4,5,6-pentakis(oxidanyl)cyclohexyl] hydrogen phosphate (CCD ID: JCV) (formula: C₉₈H₁₉₃O₁₉P).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
9	C	1	118	98	19	1	0
9	E	1	118	98	19	1	0
9	E	1	118	98	19	1	0
9	E	1	118	98	19	1	0
9	c	1	118	98	19	1	0
9	e	1	118	98	19	1	0
9	e	1	118	98	19	1	0
9	g	1	118	98	19	1	0

Continued on next page...

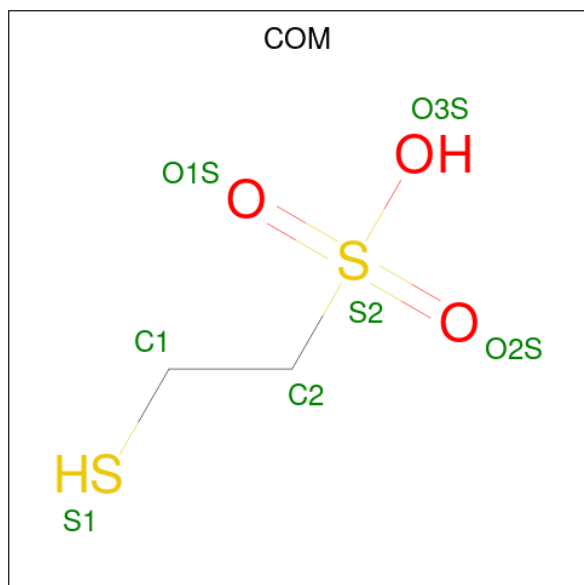
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
9	S	1	Total	C	O	P	0
			118	98	19	1	
9	U	1	Total	C	O	P	0
			114	94	19	1	
9	U	1	Total	C	O	P	0
			118	98	19	1	
9	W	1	Total	C	O	P	0
			118	98	19	1	

- Molecule 10 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
10	E	2	Total	Na	0
			2	2	
10	e	2	Total	Na	0
			2	2	
10	U	2	Total	Na	0
			2	2	

- Molecule 11 is 1-THIOETHANESULFONIC ACID (CCD ID: COM) (formula: C₂H₆O₃S₂).



Mol	Chain	Residues	Atoms					AltConf
11	E	1	Total	C	H	O	S	1
			24	4	10	6	4	
11	e	1	Total	C	H	O	S	1
			24	4	10	6	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
11	U	1	Total	C	H	O	S	1
			24	4	10	6	4	

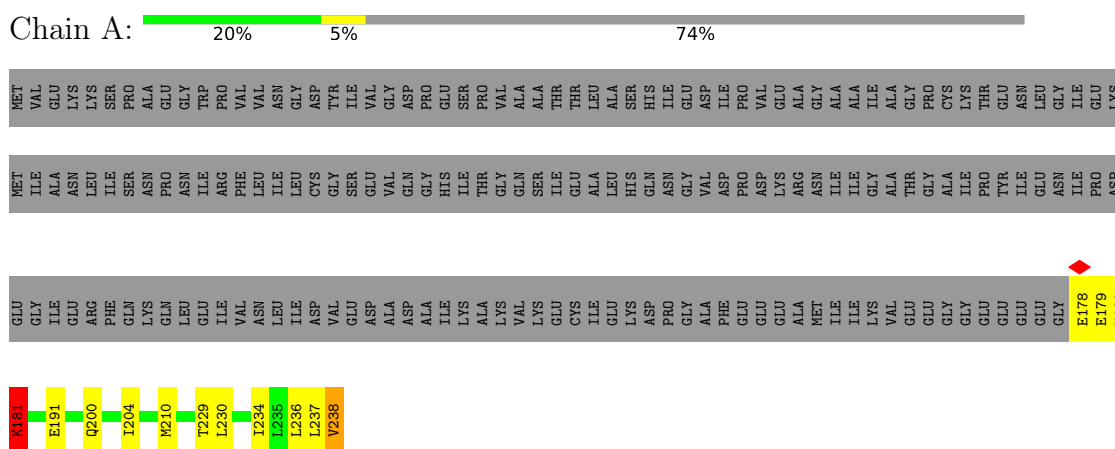
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		AltConf
12	A	2	Total	O	0
			2	2	
12	B	2	Total	O	0
			2	2	
12	C	2	Total	O	0
			2	2	
12	D	2	Total	O	0
			2	2	
12	E	18	Total	O	0
			18	18	
12	F	3	Total	O	0
			3	3	
12	a	1	Total	O	0
			1	1	
12	b	2	Total	O	0
			2	2	
12	c	1	Total	O	0
			1	1	
12	d	4	Total	O	0
			4	4	
12	e	20	Total	O	0
			20	20	
12	f	1	Total	O	0
			1	1	
12	Q	1	Total	O	0
			1	1	
12	R	2	Total	O	0
			2	2	
12	S	1	Total	O	0
			1	1	
12	T	3	Total	O	0
			3	3	
12	U	21	Total	O	0
			21	21	
12	V	2	Total	O	0
			2	2	

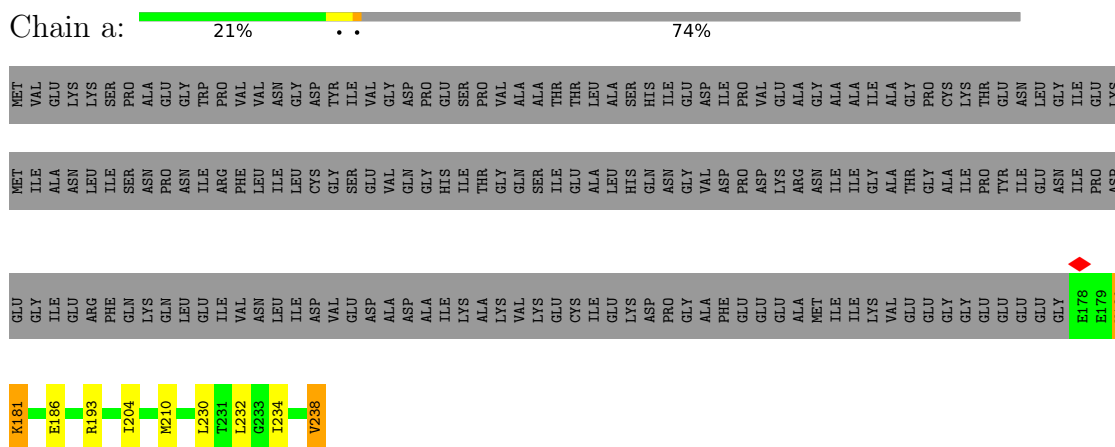
3 Residue-property plots

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.

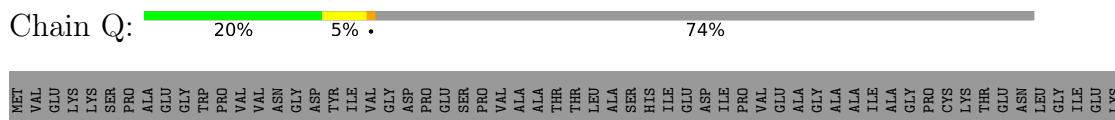
- Molecule 1: Tetrahydromethanopterin S-methyltransferase subunit A 1

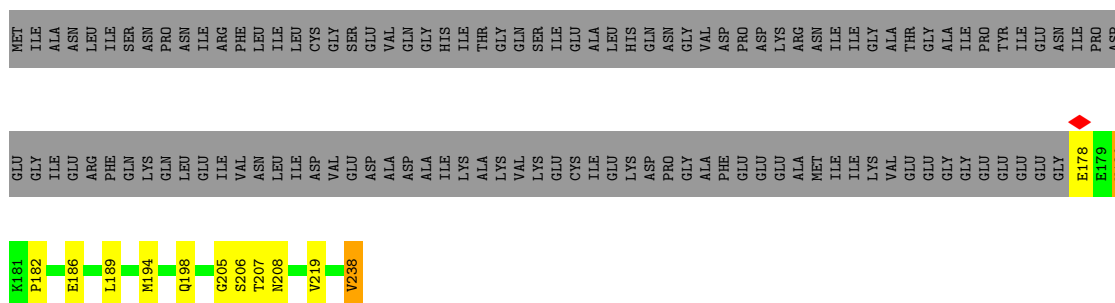


- Molecule 1: Tetrahydromethanopterin S-methyltransferase subunit A 1



- Molecule 1: Tetrahydromethanopterin S-methyltransferase subunit A 1

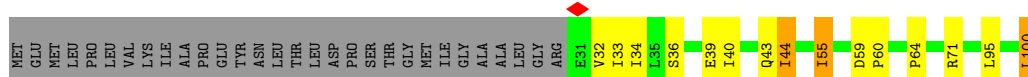




• Molecule 2: Tetrahydromethanopterin S-methyltransferase subunit B



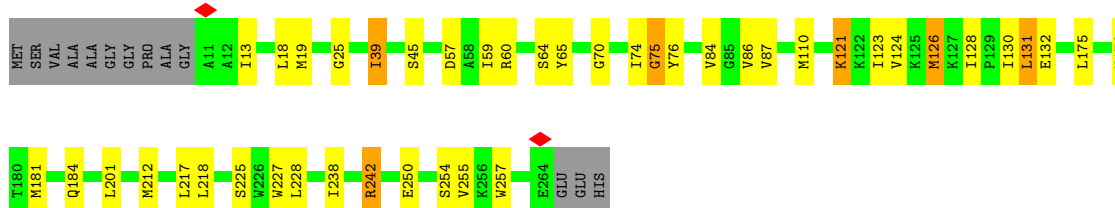
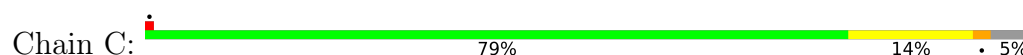
• Molecule 2: Tetrahydromethanopterin S-methyltransferase subunit B



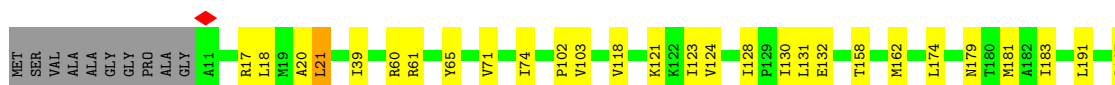
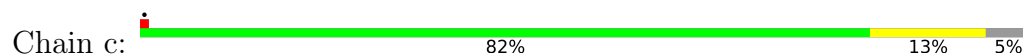
• Molecule 2: Tetrahydromethanopterin S-methyltransferase subunit B

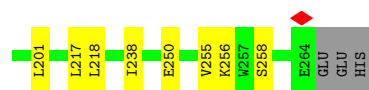


• Molecule 3: Tetrahydromethanopterin S-methyltransferase subunit C



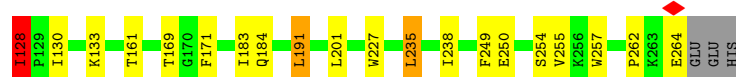
• Molecule 3: Tetrahydromethanopterin S-methyltransferase subunit C





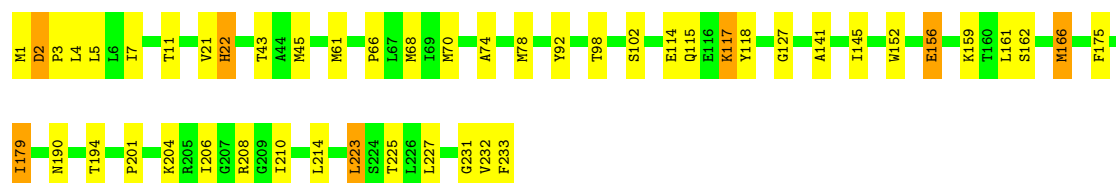
• Molecule 3: Tetrahydromethanopterin S-methyltransferase subunit C

Chain S: 76% 17% 5%



• Molecule 4: Tetrahydromethanopterin S-methyltransferase subunit D

Chain D: 79% 18% 3%



• Molecule 4: Tetrahydromethanopterin S-methyltransferase subunit D

Chain d: 90% 10%



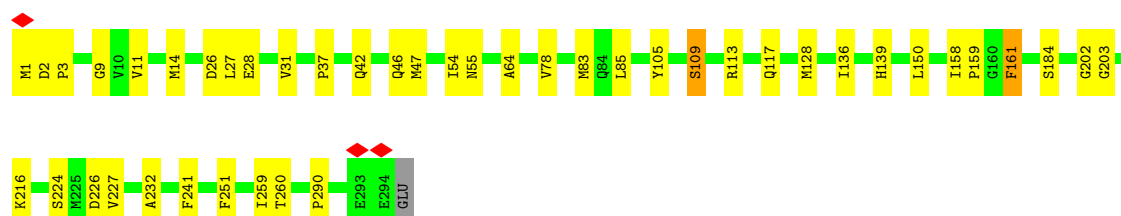
• Molecule 4: Tetrahydromethanopterin S-methyltransferase subunit D

Chain T: 87% 12% 1%

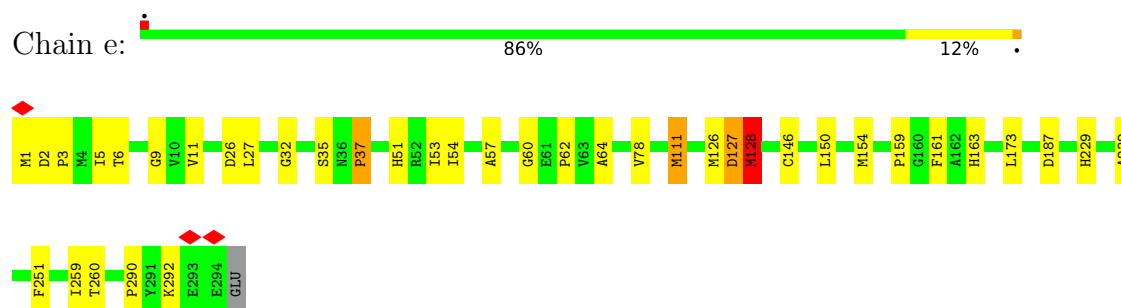


• Molecule 5: Tetrahydromethanopterin S-methyltransferase subunit E

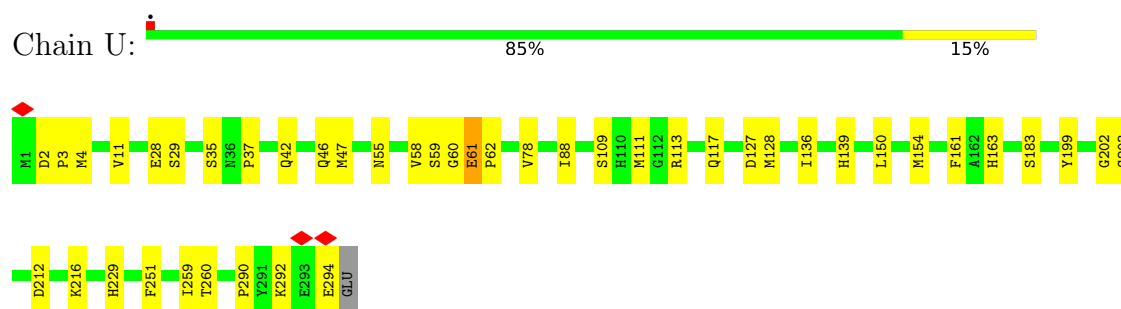
Chain E: 85% 14% 1%



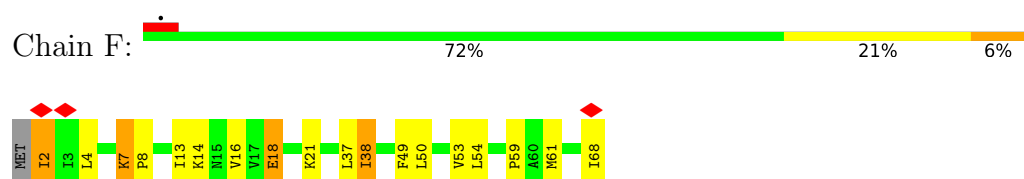
- Molecule 5: Tetrahydromethanopterin S-methyltransferase subunit E



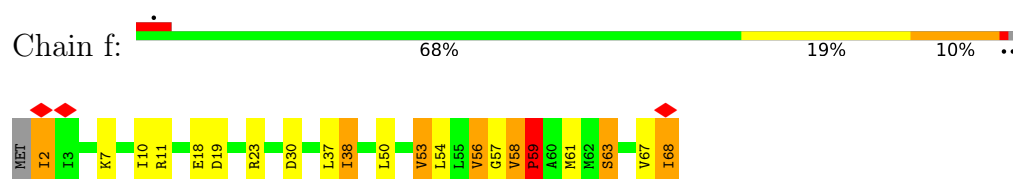
- Molecule 5: Tetrahydromethanopterin S-methyltransferase subunit E



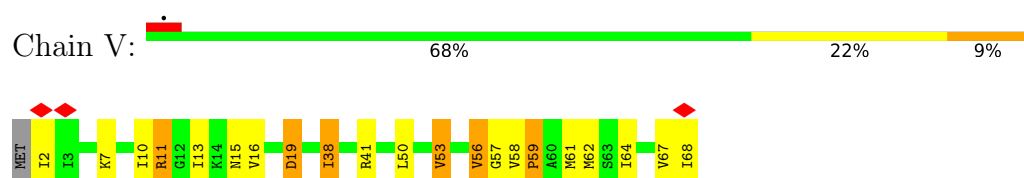
- Molecule 6: Tetrahydromethanopterin S-methyltransferase subunit F



- Molecule 6: Tetrahydromethanopterin S-methyltransferase subunit F



- Molecule 6: Tetrahydromethanopterin S-methyltransferase subunit F

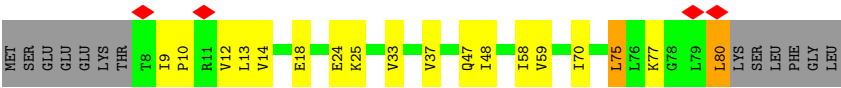


- Molecule 7: Tetrahydromethanopterin S-methyltransferase subunit G

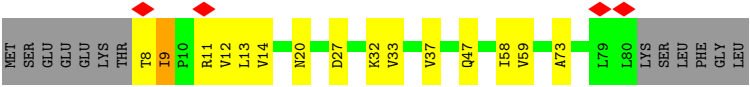




• Molecule 7: Tetrahydromethanopterin S-methyltransferase subunit G



• Molecule 7: Tetrahydromethanopterin S-methyltransferase subunit G



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87173	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 ($e^-/\text{\AA}^2$)	73.9	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.061	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	267.84, 267.84, 267.84	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, COM, MG, JCV

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	1.06	3/467 (0.6%)	0.88	2/626 (0.3%)
1	Q	0.90	6/467 (1.3%)	0.87	0/626
1	a	1.02	2/467 (0.4%)	1.04	3/626 (0.5%)
2	B	0.97	4/538 (0.7%)	1.01	1/733 (0.1%)
2	R	0.92	2/538 (0.4%)	0.99	0/733
2	b	1.04	4/538 (0.7%)	1.13	2/733 (0.3%)
3	C	0.95	6/1878 (0.3%)	1.15	12/2566 (0.5%)
3	S	0.81	4/1878 (0.2%)	1.01	6/2566 (0.2%)
3	c	0.77	3/1894 (0.2%)	0.88	1/2587 (0.0%)
4	D	0.95	5/1624 (0.3%)	1.08	10/2207 (0.5%)
4	T	0.67	1/1624 (0.1%)	0.77	2/2207 (0.1%)
4	d	0.62	0/1624	0.70	3/2207 (0.1%)
5	E	0.66	7/2242 (0.3%)	0.78	6/3055 (0.2%)
5	U	0.79	8/2242 (0.4%)	0.84	8/3055 (0.3%)
5	e	0.77	6/2242 (0.3%)	0.87	10/3055 (0.3%)
6	F	1.20	5/509 (1.0%)	1.27	4/684 (0.6%)
6	V	1.32	7/509 (1.4%)	1.55	10/684 (1.5%)
6	f	1.38	7/509 (1.4%)	1.64	10/684 (1.5%)
7	G	0.59	1/571 (0.2%)	0.75	1/770 (0.1%)
7	W	0.60	1/571 (0.2%)	0.63	0/770
7	g	0.85	2/571 (0.4%)	1.18	6/770 (0.8%)
All	All	0.85	84/23503 (0.4%)	0.97	97/31944 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	e	0	1

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	181	LYS	C-N	17.32	1.54	1.33
6	V	59	PRO	N-CA	16.62	1.69	1.47
6	f	59	PRO	N-CA	16.36	1.69	1.47
1	a	181	LYS	C-N	16.31	1.54	1.33
5	U	61	GLU	C-N	13.67	1.52	1.33
6	f	58	VAL	C-N	7.56	1.44	1.33
6	V	58	VAL	C-O	-7.17	1.18	1.24
5	e	128	MET	C-O	-7.03	1.16	1.24
6	V	58	VAL	C-N	7.00	1.44	1.33
2	B	81	LEU	C-O	-6.90	1.16	1.24
6	F	38	ILE	C-O	-6.88	1.16	1.24
5	U	128	MET	C-O	-6.82	1.16	1.24
3	C	217	LEU	C-O	-6.78	1.16	1.24
4	D	22	HIS	CE1-NE2	-6.76	1.25	1.32
2	b	59	ASP	C-O	-6.74	1.18	1.25
3	S	61	ARG	C-O	-6.68	1.15	1.24
3	C	131	LEU	C-O	-6.47	1.16	1.24
5	E	128	MET	C-O	-6.46	1.16	1.24
4	D	22	HIS	CG-ND1	-6.35	1.31	1.38
3	S	235	LEU	C-O	-6.34	1.16	1.24
3	C	39	ILE	C-O	-6.28	1.17	1.23
7	G	47	GLN	C-O	-6.26	1.16	1.24
1	Q	208	ASN	C-O	-6.24	1.16	1.24
7	W	47	GLN	C-O	-6.22	1.16	1.24
1	Q	219	VAL	C-O	-6.21	1.16	1.24
2	R	69	PRO	C-O	-6.20	1.16	1.23
4	D	210	ILE	C-O	-6.12	1.16	1.24
3	S	102	PRO	C-O	-6.12	1.16	1.24
5	e	62	PRO	C-O	-6.11	1.16	1.24
5	U	202	GLY	C-O	-6.02	1.16	1.24
5	E	26	ASP	C-O	-6.01	1.17	1.24
3	S	262	PRO	C-O	-6.00	1.17	1.23
5	E	202	GLY	C-O	-5.98	1.16	1.24
7	g	47	GLN	C-O	-5.98	1.17	1.24
6	F	37	LEU	C-O	-5.91	1.17	1.24
3	c	102	PRO	C-O	-5.88	1.16	1.24
6	f	37	LEU	C-O	-5.86	1.17	1.24
3	C	238	ILE	C-O	-5.86	1.17	1.24
5	U	203	GLY	CA-C	-5.85	1.45	1.51
2	B	69	PRO	C-O	-5.79	1.17	1.23
4	D	115	GLN	C-O	-5.72	1.15	1.23
5	e	26	ASP	C-O	-5.70	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	16	VAL	C-O	-5.62	1.17	1.24
5	U	55	ASN	C-O	-5.62	1.16	1.23
3	c	20	ALA	C-O	-5.59	1.17	1.24
6	f	57	GLY	C-O	-5.57	1.17	1.23
5	e	146	CYS	C-O	-5.53	1.17	1.24
6	V	57	GLY	C-O	-5.52	1.17	1.23
5	E	31	VAL	C-O	-5.51	1.17	1.24
1	A	210	MET	C-O	-5.50	1.17	1.24
2	b	64	PRO	C-O	-5.49	1.17	1.23
1	Q	182	PRO	C-O	-5.47	1.17	1.23
5	e	37	PRO	C-O	-5.47	1.17	1.24
2	b	71	ARG	C-O	-5.46	1.16	1.24
5	U	62	PRO	C-O	-5.45	1.16	1.24
6	F	53	VAL	C-O	-5.43	1.17	1.24
3	C	75	GLY	C-O	-5.42	1.17	1.23
3	C	76	TYR	C-O	-5.41	1.17	1.24
1	a	210	MET	C-O	-5.40	1.17	1.24
5	e	111	MET	C-O	-5.40	1.17	1.24
6	V	16	VAL	C-O	-5.38	1.17	1.24
2	b	60	PRO	C-O	-5.37	1.17	1.24
2	B	76	LEU	C-O	-5.35	1.17	1.24
5	E	55	ASN	C-O	-5.35	1.16	1.23
4	D	179	ILE	C-O	-5.32	1.17	1.24
1	A	200	GLN	C-O	-5.32	1.17	1.24
5	U	37	PRO	C-O	-5.31	1.17	1.24
4	T	81	ILE	C-O	-5.30	1.17	1.24
2	R	64	PRO	C-O	-5.29	1.17	1.23
6	f	23	ARG	C-O	-5.28	1.18	1.24
1	Q	205	GLY	C-O	-5.28	1.17	1.23
7	g	48	ILE	C-O	-5.28	1.18	1.24
6	V	53	VAL	C-O	-5.27	1.17	1.24
2	B	64	PRO	C-O	-5.26	1.17	1.23
6	f	53	VAL	C-O	-5.26	1.17	1.24
6	V	38	ILE	C-O	-5.24	1.18	1.24
5	U	111	MET	C-O	-5.19	1.18	1.24
6	f	38	ILE	C-O	-5.14	1.17	1.24
6	F	49	PHE	C-O	-5.12	1.18	1.24
5	E	227	VAL	C-O	-5.11	1.18	1.24
1	Q	207	THR	C-O	-5.09	1.18	1.24
3	c	217	LEU	C-O	-5.06	1.18	1.24
5	E	37	PRO	C-O	-5.03	1.17	1.24
1	Q	206	SER	CA-CB	-5.03	1.45	1.53

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	58	VAL	CA-C-N	16.77	136.69	119.24
6	f	58	VAL	C-N-CA	16.77	136.69	119.24
6	V	58	VAL	CA-C-N	14.29	135.61	119.32
6	V	58	VAL	C-N-CA	14.29	135.61	119.32
3	S	67	LEU	N-CA-C	-10.47	99.95	111.36
1	a	181	LYS	CA-C-N	9.27	129.84	119.92
1	a	181	LYS	C-N-CA	9.27	129.84	119.92
6	f	11	ARG	CA-C-N	8.62	129.55	119.98
6	f	11	ARG	C-N-CA	8.62	129.55	119.98
5	e	161	PHE	CA-C-O	-8.48	113.02	117.94
6	V	58	VAL	O-C-N	-8.45	115.01	120.42
5	E	161	PHE	CA-C-O	-8.44	113.01	118.33
3	S	19	MET	CA-C-O	-8.33	111.59	120.42
6	f	59	PRO	CA-N-CD	-8.32	100.36	112.00
1	A	181	LYS	CA-C-N	7.80	129.28	120.85
1	A	181	LYS	C-N-CA	7.80	129.28	120.85
3	C	131	LEU	CA-C-O	-7.74	112.73	120.70
6	f	58	VAL	O-C-N	-7.58	112.46	121.10
3	C	254	SER	O-C-N	-7.50	114.93	123.48
3	S	128	ILE	N-CA-C	-7.31	99.78	107.60
5	U	128	MET	N-CA-C	-7.24	103.32	111.14
6	V	59	PRO	CA-N-CD	-6.98	102.22	112.00
3	C	25	GLY	CA-C-N	6.96	127.53	119.94
3	C	25	GLY	C-N-CA	6.96	127.53	119.94
2	B	44	ILE	CA-C-O	-6.73	112.98	120.25
5	E	251	PHE	CA-CB-CG	-6.66	107.14	113.80
5	U	61	GLU	CA-C-N	6.60	126.11	119.24
5	U	61	GLU	C-N-CA	6.60	126.11	119.24
1	a	232	LEU	CA-C-O	-6.29	114.21	120.82
4	D	22	HIS	CA-CB-CG	-6.25	107.55	113.80
4	D	7	ILE	CA-C-O	-6.23	114.14	121.05
3	C	227	TRP	N-CA-C	-6.19	104.64	111.82
6	V	59	PRO	N-CA-C	-6.14	104.60	113.75
3	C	238	ILE	CA-C-O	-6.08	114.41	120.85
3	C	75	GLY	CA-C-O	-6.06	114.46	121.00
3	S	60	ARG	CA-C-N	6.04	132.29	121.66
3	S	60	ARG	C-N-CA	6.04	132.29	121.66
3	c	131	LEU	CA-C-O	-6.00	114.48	120.90
5	U	161	PHE	CB-CA-C	6.00	122.35	110.42
5	e	127	ASP	CA-CB-CG	5.94	118.54	112.60
4	D	210	ILE	CA-C-O	-5.91	114.20	120.64
7	G	19	PHE	CA-CB-CG	-5.88	107.92	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	61	MET	CA-C-O	-5.84	113.49	120.55
7	g	48	ILE	CA-C-N	5.80	126.42	119.98
7	g	48	ILE	C-N-CA	5.80	126.42	119.98
4	T	46	LEU	N-CA-C	-5.71	104.66	111.69
5	U	163	HIS	CA-CB-CG	-5.70	108.10	113.80
6	V	56	VAL	CA-C-N	5.70	126.26	119.94
6	V	56	VAL	C-N-CA	5.70	126.26	119.94
2	b	44	ILE	N-CA-C	-5.69	104.80	111.00
5	E	202	GLY	CA-C-O	-5.65	113.30	118.95
5	e	127	ASP	CB-CA-C	-5.64	101.79	110.81
5	e	128	MET	N-CA-C	-5.61	105.08	111.14
6	F	59	PRO	CA-C-N	5.59	127.78	120.28
6	F	59	PRO	C-N-CA	5.59	127.78	120.28
4	D	225	THR	CA-C-N	5.54	128.26	120.28
4	D	225	THR	C-N-CA	5.54	128.26	120.28
3	C	70	GLY	CA-C-N	5.47	123.69	120.24
3	C	70	GLY	C-N-CA	5.47	123.69	120.24
4	d	166	MET	CA-C-N	5.44	126.02	119.98
4	d	166	MET	C-N-CA	5.44	126.02	119.98
6	f	30	ASP	CA-C-N	5.42	127.10	120.22
6	f	30	ASP	C-N-CA	5.42	127.10	120.22
5	e	6	THR	CA-C-N	5.41	125.99	119.98
5	e	6	THR	C-N-CA	5.41	125.99	119.98
6	F	8	PRO	N-CA-C	5.41	118.79	111.22
6	f	56	VAL	CA-C-N	5.33	126.00	120.03
6	f	56	VAL	C-N-CA	5.33	126.00	120.03
7	g	24	GLU	CA-C-N	5.33	127.36	120.44
7	g	24	GLU	C-N-CA	5.33	127.36	120.44
5	e	6	THR	N-CA-C	-5.32	105.38	111.07
5	E	26	ASP	CA-CB-CG	-5.31	107.29	112.60
4	D	166	MET	CA-C-N	5.29	125.82	120.00
4	D	166	MET	C-N-CA	5.29	125.82	120.00
5	e	128	MET	CA-C-O	-5.29	115.25	120.70
5	E	226	ASP	CA-C-N	5.27	127.67	120.77
5	E	226	ASP	C-N-CA	5.27	127.67	120.77
3	C	257	TRP	CA-C-O	-5.25	113.40	119.59
5	U	60	GLY	CA-C-N	5.25	126.65	120.09
5	U	60	GLY	C-N-CA	5.25	126.65	120.09
4	T	98	THR	CA-CB-OG1	-5.21	101.78	109.60
5	U	161	PHE	CA-C-O	-5.20	113.08	120.51
2	b	40	ILE	CA-C-O	-5.18	115.36	120.85
7	g	75	LEU	CA-C-N	5.18	127.53	120.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	g	75	LEU	C-N-CA	5.18	127.53	120.54
4	D	175	PHE	N-CA-C	-5.11	105.41	111.69
6	V	64	ILE	N-CA-C	-5.09	105.57	110.72
4	d	98	THR	CA-CB-OG1	-5.09	101.96	109.60
5	e	163	HIS	CA-CB-CG	-5.08	108.72	113.80
4	D	70	MET	CA-C-O	-5.06	115.19	120.55
5	e	60	GLY	O-C-N	-5.05	116.70	122.91
3	C	225	SER	CA-C-N	5.03	127.53	120.28
3	C	225	SER	C-N-CA	5.03	127.53	120.28
6	V	59	PRO	CA-C-N	5.03	127.44	120.29
6	V	59	PRO	C-N-CA	5.03	127.44	120.29
3	S	254	SER	O-C-N	-5.02	117.70	123.42
6	F	14	LYS	CA-C-O	-5.01	115.56	120.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	e	128	MET	Mainchain

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	463	499	499	10	0
1	Q	463	499	499	8	0
1	a	463	499	499	8	0
2	B	531	545	545	13	0
2	R	531	545	545	9	0
2	b	531	545	545	8	0
3	C	1831	1955	1947	26	0
3	S	1831	1955	1947	33	0
3	c	1842	1964	1955	19	0
4	D	1596	1668	1668	33	0
4	T	1596	1668	1668	16	0
4	d	1596	1668	1668	12	0
5	E	2187	2203	2203	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	U	2187	2203	2203	22	0
5	e	2187	2203	2203	21	0
6	F	505	564	564	10	0
6	V	505	564	564	16	0
6	f	505	564	564	13	0
7	G	566	598	598	19	0
7	W	566	598	598	19	0
7	g	566	598	598	15	0
8	B	1	0	0	0	0
8	R	1	0	0	0	0
8	b	1	0	0	0	0
9	C	118	0	0	1	0
9	E	354	0	0	8	0
9	S	118	0	0	10	0
9	U	232	0	0	1	0
9	W	118	0	0	2	0
9	c	118	0	0	1	0
9	e	236	0	0	8	0
9	g	118	0	0	0	0
10	E	2	0	0	0	0
10	U	2	0	0	0	0
10	e	2	0	0	0	0
11	E	14	10	12	1	0
11	U	14	10	12	4	0
11	e	14	10	12	2	0
12	A	2	0	0	0	0
12	B	2	0	0	0	0
12	C	2	0	0	0	0
12	D	2	0	0	0	0
12	E	18	0	0	0	0
12	F	3	0	0	0	0
12	Q	1	0	0	0	0
12	R	2	0	0	0	0
12	S	1	0	0	0	0
12	T	3	0	0	0	0
12	U	21	0	0	0	0
12	V	2	0	0	0	0
12	a	1	0	0	0	0
12	b	2	0	0	0	0
12	c	1	0	0	0	0
12	d	4	0	0	0	0
12	e	20	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	f	1	0	0	0	0
All	All	24599	24135	24116	310	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 (310) 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)
6:V:59:PRO:N	6:V:59:PRO:CA	1.69	1.45
6:f:59:PRO:N	6:f:59:PRO:CA	1.69	1.31
2:B:31:GLU:O	7:g:10:PRO:HB3	1.35	1.24
1:a:238:VAL:HG23	1:a:238:VAL:OXT	1.50	1.04
1:a:238:VAL:OXT	1:a:238:VAL:CG2	2.06	1.02
6:F:68:ILE:HG23	6:F:68:ILE:OXT	1.60	1.01
3:c:118:VAL:HG22	3:c:132:GLU:OE2	1.72	0.90
7:G:11:ARG:HD2	7:W:11:ARG:HD3	1.53	0.89
4:D:66:PRO:HG3	4:D:152:TRP:CZ2	2.12	0.84
6:V:67:VAL:O	6:V:68:ILE:OXT	1.94	0.84
5:E:85:LEU:HD21	9:E:304:JCV:C30M	2.09	0.83
9:S:301:JCV:C61M	9:W:101:JCV:C61M	2.59	0.81
4:T:66:PRO:HG3	4:T:152:TRP:CZ2	2.15	0.81
4:D:66:PRO:HG3	4:D:152:TRP:CE2	2.18	0.78
2:b:39:GLU:HB3	6:f:10:ILE:HD13	1.66	0.78
3:C:13:ILE:HD12	3:C:201:LEU:CD1	2.15	0.76
3:S:191:LEU:HD12	3:S:191:LEU:O	1.86	0.75
6:F:68:ILE:OXT	6:F:68:ILE:CG2	2.30	0.75
2:B:36:SER:O	2:B:39:GLU:OE2	2.05	0.75
2:B:34:ILE:HD13	7:g:13:LEU:HD21	1.68	0.74
4:D:117:LYS:HD3	5:E:290:PRO:HB3	1.68	0.73
3:S:191:LEU:HD12	3:S:191:LEU:C	2.13	0.73
4:D:11:THR:CG2	4:D:214:LEU:HD12	2.19	0.72
5:E:47:MET:HA	5:E:47:MET:HE2	1.73	0.71
5:U:46:GLN:HG2	5:U:47:MET:HE3	1.74	0.70
3:C:75:GLY:HA3	3:C:184[A]:GLN:OE1	1.91	0.70
6:F:61:MET:HA	6:F:61:MET:HE2	1.73	0.69
2:R:43:GLN:HG2	6:V:13:ILE:HG22	1.75	0.69
4:D:156:GLU:OE2	4:D:159:LYS:HE2	1.93	0.69
2:R:72:GLU:OE2	2:R:72:GLU:N	2.25	0.69
4:D:162:SER:HB2	4:D:231:GLY:O	1.94	0.68
3:S:227:TRP:CH2	9:S:301:JCV:C79	2.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:83:MET:HA	5:E:83:MET:HE2	1.74	0.68
9:e:305:JCV:OX5	9:e:305:JCV:O4	2.11	0.66
2:R:39:GLU:HB3	6:V:10:ILE:HD13	1.79	0.64
5:e:5:ILE:CD1	6:f:63:SER:OG	2.46	0.64
3:S:18:LEU:HD12	3:S:57:ASP:OD2	1.97	0.64
3:c:238:ILE:HD11	9:c:301:JCV:C60	2.27	0.64
6:V:59:PRO:N	6:V:59:PRO:C	2.56	0.64
7:W:9:ILE:HG22	7:W:9:ILE:O	1.98	0.63
3:S:257:TRP:O	5:U:127:ASP:HB3	1.98	0.63
1:A:181:LYS:HB3	6:F:7:LYS:O	1.99	0.62
7:G:9:ILE:N	7:G:9:ILE:HD12	2.15	0.61
5:U:42:GLN:O	5:U:117:GLN:NE2	2.33	0.61
4:D:232:VAL:HG23	4:D:232:VAL:O	2.01	0.61
3:c:174:LEU:CD2	3:c:218:LEU:HD11	2.31	0.61
3:S:130:ILE:O	3:S:130:ILE:HG22	2.00	0.61
3:c:130:ILE:HG22	3:c:130:ILE:O	2.01	0.61
6:f:63:SER:HA	6:f:68:ILE:HG22	1.83	0.61
5:U:47:MET:HE2	5:U:47:MET:HA	1.82	0.61
3:c:21:LEU:O	3:c:21:LEU:HD22	1.99	0.61
3:S:90:LEU:HD23	3:S:101:VAL:HG11	1.83	0.61
7:G:17:ASP:OD1	7:G:18:GLU:N	2.34	0.61
5:e:2:ASP:OD1	5:e:3:PRO:HD2	2.01	0.61
5:E:42:GLN:O	5:E:117:GLN:NE2	2.33	0.60
7:G:9:ILE:O	7:G:9:ILE:HG22	1.99	0.60
1:A:238:VAL:HG23	1:A:238:VAL:O	2.01	0.60
9:E:306:JCV:C25	6:F:68:ILE:HD12	2.32	0.60
4:T:2:ASP:OD1	4:T:3:PRO:HD2	2.02	0.60
3:C:181:MET:HE1	5:E:64:ALA:HA	1.82	0.60
5:E:2:ASP:OD1	5:E:3:PRO:HD2	2.00	0.60
5:U:46:GLN:HG2	5:U:47:MET:CE	2.31	0.59
3:S:264:GLU:OE2	3:S:264:GLU:HA	2.01	0.59
5:U:2:ASP:OD1	5:U:3:PRO:HD2	2.01	0.59
6:V:11:ARG:NH1	7:W:20:ASN:CG	2.60	0.59
4:D:2:ASP:OD1	4:D:3:PRO:HD2	2.02	0.59
7:g:9:ILE:HG22	7:g:9:ILE:O	2.02	0.59
5:E:105:TYR:O	5:E:109:SER:OG	2.21	0.59
7:g:13:LEU:H	7:g:13:LEU:HD23	1.68	0.59
3:c:118:VAL:CG2	3:c:132:GLU:OE2	2.49	0.58
7:G:13:LEU:O	7:G:13:LEU:HD23	2.04	0.58
6:V:2:ILE:HG23	6:V:2:ILE:O	2.02	0.58
6:F:18:GLU:OE1	6:F:18:GLU:HA	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:130:ILE:HG22	3:C:130:ILE:O	2.03	0.58
3:c:174:LEU:HD22	3:c:218:LEU:HD11	1.84	0.57
4:D:117:LYS:HD2	4:D:117:LYS:C	2.29	0.57
6:f:67:VAL:HG22	6:f:67:VAL:O	2.03	0.57
1:a:180:VAL:HG12	1:a:180:VAL:O	2.04	0.57
1:A:191:GLU:OE2	1:Q:189:LEU:HD21	2.04	0.57
1:Q:238:VAL:HG23	1:Q:238:VAL:O	2.03	0.57
3:S:169:THR:HG21	3:S:171:PHE:CE2	2.40	0.57
1:A:180:VAL:HG13	6:F:4:LEU:HD23	1.85	0.57
2:B:71:ARG:O	2:B:74:VAL:HG12	2.05	0.57
6:F:2:ILE:O	6:F:2:ILE:HG23	2.04	0.56
3:S:227:TRP:CZ2	9:S:301:JCV:C79	2.87	0.56
5:E:113:ARG:NH1	11:E:303[B]:COM:O1S	2.37	0.56
3:C:13:ILE:HD12	3:C:201:LEU:HD12	1.86	0.56
1:a:186:GLU:N	1:a:186:GLU:OE1	2.39	0.56
1:Q:238:VAL:HG12	7:W:73:ALA:HB3	1.86	0.55
9:E:304:JCV:C66	9:E:304:JCV:C22M	2.85	0.55
4:T:66:PRO:HG3	4:T:152:TRP:CE2	2.41	0.55
6:V:67:VAL:C	6:V:68:ILE:OXT	2.50	0.55
5:e:5:ILE:HD11	6:f:63:SER:OG	2.06	0.55
9:e:305:JCV:C27	9:e:305:JCV:CG8	2.85	0.55
5:E:54:ILE:HG22	5:E:224:SER:OG	2.06	0.54
9:S:301:JCV:C3	9:S:301:JCV:CG3	2.84	0.54
9:e:305:JCV:C4	9:e:305:JCV:C7M	2.85	0.54
9:e:305:JCV:C56	9:e:305:JCV:C60	2.85	0.54
5:U:35:SER:O	11:U:303[A]:COM:C1	2.55	0.54
9:E:304:JCV:C22M	9:E:304:JCV:C65M	2.86	0.54
2:R:98:LEU:C	2:R:98:LEU:HD23	2.32	0.54
9:e:305:JCV:C61M	9:e:305:JCV:C6	2.85	0.54
9:E:304:JCV:C13	9:E:304:JCV:C68M	2.85	0.54
7:G:9:ILE:N	7:G:9:ILE:CD1	2.71	0.54
1:A:204:ILE:HG13	7:g:37:VAL:HG22	1.89	0.53
9:E:304:JCV:C22M	9:E:304:JCV:C67	2.85	0.53
9:e:305:JCV:CG8	9:e:305:JCV:C28	2.85	0.53
5:E:28:GLU:OE1	5:E:136:ILE:HG23	2.08	0.53
9:S:301:JCV:C82	9:S:301:JCV:C78	2.85	0.53
3:C:121:LYS:HD2	3:C:132:GLU:OE2	2.09	0.53
2:b:32:VAL:CG2	7:W:13:LEU:HD22	2.39	0.53
3:c:18:LEU:HD11	3:c:201:LEU:HD11	1.90	0.53
4:T:117:LYS:HD2	5:U:290:PRO:HB3	1.88	0.53
2:R:98:LEU:HD23	2:R:98:LEU:O	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S:301:JCV:C61M	9:W:101:JCV:C61	2.86	0.53
4:T:5:LEU:HD12	4:T:5:LEU:O	2.09	0.53
5:U:29:SER:HB2	5:U:61:GLU:OE2	2.08	0.53
5:e:35:SER:O	11:e:303[B]:COM:H11	2.09	0.53
7:W:9:ILE:N	7:W:9:ILE:CD1	2.72	0.53
6:V:11:ARG:HH11	7:W:20:ASN:CG	2.17	0.53
1:a:204:ILE:HG13	7:W:37:VAL:HG22	1.91	0.53
9:S:301:JCV:C18M	9:S:301:JCV:C21	2.86	0.53
4:D:233:PHE:CD1	4:D:233:PHE:C	2.87	0.52
3:S:124:VAL:HG13	4:T:190:ASN:HA	1.91	0.52
6:V:68:ILE:HG23	6:V:68:ILE:O	2.10	0.52
4:d:52:LEU:HD22	5:e:173:LEU:HD22	1.91	0.52
3:C:65:TYR:CE2	3:C:130:ILE:HB	2.45	0.52
3:S:17:ARG:HH11	3:S:17:ARG:HG2	1.73	0.51
2:B:32:VAL:HG23	2:B:32:VAL:O	2.10	0.51
5:E:85:LEU:CD2	9:E:304:JCV:C30M	2.85	0.51
1:A:237:LEU:C	1:A:238:VAL:OXT	2.52	0.51
3:c:65:TYR:CE2	3:c:130:ILE:HB	2.45	0.51
3:c:181:MET:HE1	5:e:64:ALA:HA	1.93	0.51
4:d:70:MET:HE2	4:d:145:ILE:HG23	1.93	0.51
4:T:49:GLY:C	4:T:80:MET:HE3	2.35	0.51
6:F:61:MET:HA	6:F:61:MET:CE	2.40	0.51
2:B:40:ILE:HD13	6:F:13:ILE:HD13	1.93	0.50
5:e:2:ASP:OD1	5:e:3:PRO:CD	2.58	0.50
9:S:301:JCV:CG3	9:S:301:JCV:C52	2.89	0.50
3:C:60:ARG:HB3	3:C:60:ARG:CZ	2.41	0.50
7:G:13:LEU:HD23	7:G:13:LEU:C	2.34	0.50
4:d:31:ALA:O	4:d:92:TYR:OH	2.28	0.50
5:e:154:MET:HE3	5:e:251:PHE:CZ	2.47	0.50
7:g:13:LEU:HD23	7:g:13:LEU:N	2.27	0.50
7:G:9:ILE:HD12	7:G:9:ILE:H	1.74	0.50
2:b:32:VAL:HG13	2:b:32:VAL:O	2.12	0.50
7:g:33:VAL:O	7:g:37:VAL:HG23	2.12	0.49
3:S:87:VAL:HG12	4:T:227:LEU:HD21	1.94	0.49
4:D:68:MET:HE2	5:E:259:ILE:CG2	2.43	0.49
4:d:74:ALA:HB2	4:d:145:ILE:HG13	1.93	0.49
3:c:39:ILE:C	3:c:39:ILE:HD12	2.38	0.49
3:c:179:ASN:O	3:c:183:ILE:HG13	2.13	0.49
5:e:32:GLY:HA2	5:e:54:ILE:HG21	1.93	0.49
3:C:84:VAL:CG1	4:D:223:LEU:HD23	2.42	0.49
9:e:305:JCV:C57M	9:e:305:JCV:C54	2.84	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:O	1:A:234:ILE:HD12	2.13	0.48
6:f:59:PRO:N	6:f:59:PRO:C	2.60	0.48
3:C:87:VAL:HG12	4:D:227:LEU:HD21	1.94	0.48
4:D:117:LYS:HG2	4:D:117:LYS:O	2.13	0.48
3:c:71:VAL:O	3:c:74:ILE:HG22	2.13	0.48
3:S:95:VAL:HG13	3:S:96:VAL:HG13	1.94	0.48
4:T:31:ALA:O	4:T:92:TYR:OH	2.30	0.48
2:B:43:GLN:OE1	2:B:43:GLN:HA	2.13	0.48
1:Q:238:VAL:HG12	7:W:73:ALA:CB	2.44	0.48
5:U:35:SER:O	11:U:303[A]:COM:H12	2.13	0.48
4:D:74:ALA:HB2	4:D:145:ILE:HG13	1.95	0.48
7:G:58:ILE:HG21	7:W:59:VAL:CG1	2.44	0.48
5:e:111:MET:HE2	5:e:126:MET:HE1	1.96	0.48
4:T:1:MET:HE3	4:T:156:GLU:HB3	1.96	0.48
3:C:175:LEU:O	3:C:179:ASN:OD1	2.31	0.48
6:V:11:ARG:NH1	7:W:20:ASN:ND2	2.62	0.48
3:c:61:ARG:HH11	3:c:61:ARG:HG3	1.78	0.48
9:S:301:JCV:CG3	9:S:301:JCV:C3M	2.91	0.48
4:D:92:TYR:CD2	4:D:127:GLY:HA2	2.49	0.47
5:E:14:MET:SD	5:E:161:PHE:CE1	3.07	0.47
3:S:60:ARG:HB3	3:S:60:ARG:CZ	2.44	0.47
4:d:152:TRP:NE1	4:d:156:GLU:OE1	2.48	0.47
4:d:232:VAL:HG23	4:d:232:VAL:O	2.14	0.47
7:W:8:THR:O	7:W:8:THR:HG22	2.13	0.47
4:D:2:ASP:OD1	4:D:3:PRO:CD	2.62	0.47
4:D:117:LYS:HE3	4:D:118:TYR:CE2	2.50	0.46
3:S:191:LEU:C	3:S:191:LEU:CD1	2.84	0.46
3:c:17:ARG:HG2	3:c:17:ARG:HH11	1.80	0.46
3:c:60:ARG:HB3	3:c:60:ARG:CZ	2.45	0.46
5:e:27:LEU:HD21	5:e:232:ALA:HA	1.97	0.46
7:W:33:VAL:O	7:W:37:VAL:HG23	2.15	0.46
5:E:46:GLN:HG2	5:E:47:MET:HE3	1.97	0.46
4:T:224:SER:O	4:T:227:LEU:HB2	2.15	0.46
5:U:199:TYR:OH	5:U:212:ASP:OD2	2.30	0.46
2:B:100:LEU:HD13	5:E:9:GLY:HA3	1.98	0.46
4:D:11:THR:HG22	4:D:214:LEU:HD12	1.93	0.46
4:D:201:PRO:O	4:D:204:LYS:HD2	2.15	0.46
3:C:18:LEU:HD13	3:C:57:ASP:CB	2.46	0.46
1:A:236:LEU:CD2	2:R:97:ALA:HB2	2.45	0.45
4:T:2:ASP:OD1	4:T:3:PRO:CD	2.65	0.45
7:G:12:VAL:HG12	2:R:33:ILE:HG13	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:60:ARG:HB3	3:S:60:ARG:NH1	2.31	0.45
3:S:71:VAL:O	3:S:74:ILE:HG22	2.16	0.45
4:T:74:ALA:HB2	4:T:145:ILE:HG13	1.99	0.45
1:Q:180:VAL:O	1:Q:180:VAL:HG12	2.17	0.45
3:C:60:ARG:HH11	3:C:60:ARG:HB2	1.80	0.45
3:C:60:ARG:HB2	3:C:60:ARG:NH1	2.32	0.45
2:b:95:LEU:HD13	6:f:56:VAL:HB	1.99	0.45
3:S:126:MET:HB3	3:S:128:ILE:CG1	2.47	0.45
2:B:85:VAL:HG22	5:E:241:PHE:HB2	1.99	0.45
7:G:33:VAL:O	7:G:37:VAL:HG23	2.16	0.44
7:g:59:VAL:CG1	7:W:58:ILE:HG21	2.47	0.44
5:E:83:MET:HE1	9:E:304:JCV:C80	2.47	0.44
6:f:67:VAL:O	6:f:67:VAL:HG13	2.18	0.44
3:C:60:ARG:CZ	3:C:60:ARG:CB	2.95	0.44
6:V:2:ILE:HD13	7:W:13:LEU:HD11	1.99	0.44
3:C:60:ARG:NH1	3:C:60:ARG:CB	2.81	0.44
4:D:1:MET:HE3	4:D:156:GLU:HB3	1.99	0.44
9:C:301:JCV:OX4	9:C:301:JCV:O2	2.36	0.44
1:a:193:ARG:NH2	7:W:27:ASP:OD1	2.49	0.44
3:S:18:LEU:HD11	3:S:201:LEU:HD11	1.99	0.44
5:E:27:LEU:HD21	5:E:232:ALA:HA	2.00	0.43
7:G:13:LEU:N	7:G:13:LEU:CD2	2.80	0.43
2:b:100:LEU:HD13	5:e:9:GLY:HA3	1.99	0.43
3:c:21:LEU:HD22	3:c:21:LEU:C	2.40	0.43
4:d:117:LYS:HE3	5:e:290:PRO:HB3	2.00	0.43
3:S:39:ILE:HD12	3:S:39:ILE:C	2.43	0.43
2:B:76:LEU:HD23	2:B:76:LEU:HA	1.86	0.43
7:G:58:ILE:HG21	7:W:59:VAL:HG11	2.00	0.43
4:T:232:VAL:HG23	4:T:232:VAL:O	2.18	0.43
3:C:45:SER:HB3	3:C:212:MET:HG3	2.01	0.43
4:D:5:LEU:HD12	4:D:5:LEU:O	2.17	0.43
4:d:117:LYS:HG3	5:e:290:PRO:HB3	1.99	0.43
5:U:28:GLU:OE2	5:U:136:ILE:HG23	2.18	0.43
4:D:22:HIS:CG	4:D:206:ILE:HG13	2.53	0.43
7:G:59:VAL:CG1	7:g:58:ILE:HG21	2.48	0.43
3:S:59:ILE:HD12	3:S:183:ILE:HG22	2.01	0.43
4:T:214:LEU:HD23	4:T:214:LEU:C	2.43	0.43
5:e:154:MET:HE3	5:e:251:PHE:HZ	1.83	0.43
3:S:249:PHE:HD2	9:S:301:JCV:CX4	2.31	0.43
5:E:158:ILE:HG23	5:E:159:PRO:HD2	2.01	0.43
7:G:76:LEU:HD11	7:g:75:LEU:HD11	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:124:VAL:HG13	4:D:190:ASN:HA	2.01	0.43
5:e:51:HIS:HB2	5:e:53:ILE:HD12	2.01	0.42
3:S:73:SER:O	3:S:74:ILE:C	2.62	0.42
3:S:126:MET:HB3	3:S:128:ILE:HG13	2.01	0.42
5:U:28:GLU:HG2	5:U:139:HIS:HB2	2.00	0.42
3:C:110:MET:HB3	3:C:110:MET:HE3	1.79	0.42
5:e:37:PRO:HD3	5:e:187:ASP:OD2	2.19	0.42
5:e:150:LEU:O	5:e:154:MET:HG3	2.19	0.42
5:e:128:MET:HE3	5:e:128:MET:HB3	1.97	0.42
3:C:131:LEU:HD12	3:C:131:LEU:HA	1.92	0.42
3:C:242:ARG:HG3	3:C:242:ARG:HH11	1.84	0.42
5:U:154:MET:HE3	5:U:251:PHE:CZ	2.55	0.42
3:c:65:TYR:CZ	3:c:130:ILE:HG13	2.54	0.42
4:d:61:MET:CE	5:e:259:ILE:HG23	2.50	0.42
1:Q:198:GLN:NE2	6:V:19:ASP:OD2	2.53	0.42
5:U:47:MET:HE2	5:U:47:MET:CA	2.49	0.42
2:B:39:GLU:CD	2:B:39:GLU:H	2.27	0.42
4:D:98:THR:HG22	5:E:203:GLY:HA2	2.01	0.42
2:R:32:VAL:O	2:R:32:VAL:HG13	2.20	0.42
3:S:18:LEU:HD13	3:S:57:ASP:CB	2.49	0.42
3:S:235:LEU:O	3:S:238:ILE:HG22	2.20	0.42
5:U:150:LEU:O	5:U:154:MET:HG3	2.20	0.42
1:A:229:THR:HG21	7:G:61:GLY:HA3	2.02	0.42
5:E:28:GLU:HB2	5:E:139:HIS:HB3	2.00	0.42
7:G:12:VAL:O	7:G:12:VAL:HG23	2.19	0.42
4:T:61:MET:HE2	5:U:259:ILE:HD12	2.02	0.42
4:D:78:MET:SD	4:D:141:ALA:HB2	2.60	0.41
4:d:70:MET:HE2	4:d:145:ILE:CG2	2.49	0.41
4:D:156:GLU:OE2	4:D:159:LYS:CE	2.66	0.41
2:b:95:LEU:HD11	6:f:53:VAL:HA	2.01	0.41
4:d:39:VAL:HG12	4:d:128:LEU:HD11	2.03	0.41
4:d:70:MET:HE3	4:d:149:LEU:HB2	2.03	0.41
1:Q:194:MET:SD	6:V:13:ILE:HG23	2.60	0.41
3:S:74:ILE:O	3:S:75:GLY:C	2.63	0.41
3:S:81:ILE:HD11	3:S:116:VAL:HG21	2.03	0.41
5:U:58:VAL:HG13	5:U:59:SER:N	2.35	0.41
1:a:230:LEU:O	1:a:234:ILE:HD12	2.20	0.41
2:R:95:LEU:HD13	6:V:56:VAL:HB	2.01	0.41
5:U:4:MET:HE3	5:U:4:MET:HB2	1.91	0.41
3:C:126:MET:HE3	3:C:126:MET:HB3	1.95	0.41
3:C:74:ILE:HD12	3:C:74:ILE:HA	1.98	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:152:TRP:CZ2	4:D:156:GLU:HG2	2.55	0.41
1:Q:186:GLU:OE1	1:Q:186:GLU:N	2.49	0.41
4:D:21:VAL:HG13	4:D:43:THR:HB	2.02	0.41
2:b:39:GLU:HB3	6:f:10:ILE:CD1	2.44	0.41
7:g:80:LEU:N	7:g:80:LEU:CD1	2.83	0.41
3:S:39:ILE:HD12	3:S:40:GLY:N	2.36	0.41
3:C:19:MET:HE3	3:C:19:MET:HB2	1.92	0.41
4:D:233:PHE:CD1	4:D:233:PHE:O	2.74	0.41
5:U:35:SER:O	11:U:303[A]:COM:H11	2.21	0.41
2:B:43:GLN:OE1	2:B:43:GLN:CA	2.68	0.41
4:D:161:LEU:HD23	4:D:161:LEU:HA	1.87	0.41
3:c:191:LEU:C	3:c:191:LEU:HD12	2.46	0.41
5:e:57:ALA:HB1	11:e:303[A]:COM:H12	2.03	0.41
6:f:54:LEU:HD23	6:f:58:VAL:HG21	2.03	0.41
3:S:238:ILE:HD12	3:S:238:ILE:HA	1.92	0.41
3:S:250:GLU:OE2	3:S:250:GLU:HA	2.21	0.41
5:U:113:ARG:HH22	11:U:303[C]:COM:H22	1.85	0.41
2:B:34:ILE:HD13	7:g:13:LEU:CD2	2.46	0.40
7:G:13:LEU:HD23	7:G:13:LEU:H	1.86	0.40
7:G:59:VAL:HG11	7:g:58:ILE:HG21	2.03	0.40
6:f:2:ILE:O	6:f:2:ILE:HG13	2.21	0.40
3:C:228:LEU:HD12	3:C:228:LEU:HA	1.83	0.40
4:D:117:LYS:O	4:D:117:LYS:CG	2.69	0.40
1:a:238:VAL:HG11	7:g:70:ILE:HG23	2.04	0.40
2:b:55:ILE:HD13	7:W:32:LYS:HG2	2.01	0.40
7:g:59:VAL:HG11	7:W:58:ILE:HG21	2.04	0.40
3:S:18:LEU:HD23	3:S:18:LEU:HA	1.81	0.40
9:U:304:JCV:O2	6:V:41:ARG:NH1	2.53	0.40
1:A:238:VAL:O	1:A:238:VAL:CG2	2.69	0.40
3:C:84:VAL:HG12	4:D:223:LEU:HD23	2.04	0.40
9:e:305:JCV:OG3	9:e:305:JCV:C51	2.70	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	59/238 (25%)	55 (93%)	4 (7%)	0	100	100
1	Q	59/238 (25%)	57 (97%)	2 (3%)	0	100	100
1	a	59/238 (25%)	56 (95%)	3 (5%)	0	100	100
2	B	68/100 (68%)	67 (98%)	1 (2%)	0	100	100
2	R	68/100 (68%)	68 (100%)	0	0	100	100
2	b	68/100 (68%)	68 (100%)	0	0	100	100
3	C	254/267 (95%)	247 (97%)	7 (3%)	0	100	100
3	S	254/267 (95%)	246 (97%)	8 (3%)	0	100	100
3	c	256/267 (96%)	250 (98%)	6 (2%)	0	100	100
4	D	231/233 (99%)	226 (98%)	5 (2%)	0	100	100
4	T	231/233 (99%)	227 (98%)	4 (2%)	0	100	100
4	d	231/233 (99%)	228 (99%)	3 (1%)	0	100	100
5	E	292/295 (99%)	283 (97%)	9 (3%)	0	100	100
5	U	292/295 (99%)	286 (98%)	6 (2%)	0	100	100
5	e	292/295 (99%)	287 (98%)	5 (2%)	0	100	100
6	F	65/68 (96%)	64 (98%)	1 (2%)	0	100	100
6	V	65/68 (96%)	65 (100%)	0	0	100	100
6	f	65/68 (96%)	63 (97%)	2 (3%)	0	100	100
7	G	71/86 (83%)	71 (100%)	0	0	100	100
7	W	71/86 (83%)	71 (100%)	0	0	100	100
7	g	71/86 (83%)	69 (97%)	2 (3%)	0	100	100
All	All	3122/3861 (81%)	3054 (98%)	68 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	50/193 (26%)	46 (92%)	4 (8%)	10	16
1	Q	50/193 (26%)	47 (94%)	3 (6%)	16	27
1	a	50/193 (26%)	47 (94%)	3 (6%)	16	27
2	B	58/82 (71%)	53 (91%)	5 (9%)	8	14
2	R	58/82 (71%)	48 (83%)	10 (17%)	1	2
2	b	58/82 (71%)	51 (88%)	7 (12%)	4	5
3	C	191/196 (97%)	179 (94%)	12 (6%)	15	25
3	S	191/196 (97%)	178 (93%)	13 (7%)	13	22
3	c	192/196 (98%)	179 (93%)	13 (7%)	13	22
4	D	155/155 (100%)	143 (92%)	12 (8%)	10	17
4	T	155/155 (100%)	145 (94%)	10 (6%)	14	24
4	d	155/155 (100%)	146 (94%)	9 (6%)	17	29
5	E	228/229 (100%)	220 (96%)	8 (4%)	31	51
5	U	228/229 (100%)	219 (96%)	9 (4%)	27	46
5	e	228/229 (100%)	220 (96%)	8 (4%)	31	51
6	F	54/55 (98%)	47 (87%)	7 (13%)	3	4
6	V	54/55 (98%)	45 (83%)	9 (17%)	2	2
6	f	54/55 (98%)	44 (82%)	10 (18%)	1	1
7	G	61/73 (84%)	56 (92%)	5 (8%)	9	15
7	W	61/73 (84%)	58 (95%)	3 (5%)	21	36
7	g	61/73 (84%)	55 (90%)	6 (10%)	6	10
All	All	2392/2949 (81%)	2226 (93%)	166 (7%)	15	22

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	GLU
1	A	179	GLU
1	A	181	LYS
1	A	238	VAL
2	B	33	ILE
2	B	34	ILE
2	B	40	ILE
2	B	43	GLN
2	B	65	GLU
3	C	39	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	59	ILE
3	C	64	SER
3	C	86	VAL
3	C	121	LYS
3	C	123	ILE
3	C	126	MET
3	C	128	ILE
3	C	218	LEU
3	C	242	ARG
3	C	250	GLU
3	C	255	VAL
4	D	2	ASP
4	D	4	LEU
4	D	45	MET
4	D	102	SER
4	D	114	GLU
4	D	117	LYS
4	D	156	GLU
4	D	166	MET
4	D	179	ILE
4	D	194	THR
4	D	208	ARG
4	D	223	LEU
5	E	1	MET
5	E	11	VAL
5	E	78	VAL
5	E	109	SER
5	E	150	LEU
5	E	184	SER
5	E	216	LYS
5	E	260	THR
6	F	2	ILE
6	F	7	LYS
6	F	18	GLU
6	F	21	LYS
6	F	38	ILE
6	F	50	LEU
6	F	54	LEU
7	G	8	THR
7	G	9	ILE
7	G	11	ARG
7	G	13	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	14	VAL
1	a	180	VAL
1	a	181	LYS
1	a	238	VAL
2	b	33	ILE
2	b	34	ILE
2	b	36	SER
2	b	43	GLN
2	b	44	ILE
2	b	55	ILE
2	b	100	LEU
3	c	21	LEU
3	c	103	VAL
3	c	121	LYS
3	c	123	ILE
3	c	124	VAL
3	c	128	ILE
3	c	158	THR
3	c	162	MET
3	c	197	GLN
3	c	250	GLU
3	c	255	VAL
3	c	256	LYS
3	c	258	SER
4	d	4	LEU
4	d	64	GLN
4	d	67	LEU
4	d	69	ILE
4	d	116	GLU
4	d	156	GLU
4	d	160	THR
4	d	188	SER
4	d	223	LEU
5	e	1	MET
5	e	11	VAL
5	e	78	VAL
5	e	127	ASP
5	e	159	PRO
5	e	229	HIS
5	e	260	THR
5	e	292	LYS
6	f	2	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	f	7	LYS
6	f	18	GLU
6	f	19	ASP
6	f	38	ILE
6	f	50	LEU
6	f	59	PRO
6	f	61	MET
6	f	63	SER
6	f	68	ILE
7	g	12	VAL
7	g	14	VAL
7	g	18	GLU
7	g	25	LYS
7	g	77	LYS
7	g	80	LEU
1	Q	178	GLU
1	Q	180	VAL
1	Q	238	VAL
2	R	31	GLU
2	R	32	VAL
2	R	33	ILE
2	R	34	ILE
2	R	36	SER
2	R	43	GLN
2	R	48	GLU
2	R	65	GLU
2	R	67	SER
2	R	94	ILE
3	S	36	ASN
3	S	64	SER
3	S	65	TYR
3	S	84	VAL
3	S	121	LYS
3	S	127	LYS
3	S	128	ILE
3	S	133	LYS
3	S	161	THR
3	S	184[A]	GLN
3	S	184[B]	GLN
3	S	191	LEU
3	S	255	VAL
4	T	45	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	T	64	GLN
4	T	67	LEU
4	T	98	THR
4	T	102	SER
4	T	156	GLU
4	T	160	THR
4	T	162	SER
4	T	223	LEU
4	T	228	VAL
5	U	11	VAL
5	U	78	VAL
5	U	88	ILE
5	U	183	SER
5	U	216	LYS
5	U	229	HIS
5	U	260	THR
5	U	292	LYS
5	U	294	GLU
6	V	7	LYS
6	V	11	ARG
6	V	15	ASN
6	V	19	ASP
6	V	38	ILE
6	V	50	LEU
6	V	53	VAL
6	V	61	MET
6	V	62	MET
7	W	9	ILE
7	W	12	VAL
7	W	14	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	208	ASN
4	D	155	ASN
5	E	34	GLN
5	E	40	GLN
1	a	200	GLN
5	e	34	GLN
5	e	49	HIS
5	e	229	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	f	24	ASN
1	Q	200	GLN
2	R	43	GLN
3	S	179	ASN
4	T	64	GLN
7	W	23	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 9 are monoatomic - leaving 18 for Mogul analysis.

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
9	JCV	E	306	-	120,120,120	1.13	10 (8%)	148,154,154	0.68	0
9	JCV	S	301	-	120,120,120	1.10	8 (6%)	148,154,154	1.29	20 (13%)
9	JCV	U	305	-	120,120,120	1.13	11 (9%)	148,154,154	0.67	0
11	COM	U	303[A]	-	6,6,6	1.78	3 (50%)	7,8,8	2.75	4 (57%)
9	JCV	e	305	-	120,120,120	1.15	11 (9%)	148,154,154	1.19	16 (10%)
9	JCV	c	301	-	120,120,120	1.13	10 (8%)	148,154,154	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >
11	COM	E	303[A]	-	6,6,6	1.82	2 (33%)	7,8,8	2.78	4 (57%)
11	COM	E	303[B]	-	6,6,6	1.77	2 (33%)	7,8,8	2.79	4 (57%)
9	JCV	C	301	-	120,120,120	1.13	12 (10%)	148,154,154	0.66	0
9	JCV	e	304	-	120,120,120	1.32	12 (10%)	148,154,154	1.48	26 (17%)
11	COM	e	303[B]	-	6,6,6	1.78	3 (50%)	7,8,8	2.80	4 (57%)
9	JCV	E	304	-	120,120,120	1.25	14 (11%)	148,154,154	1.62	23 (15%)
11	COM	U	303[C]	-	6,6,6	1.84	3 (50%)	7,8,8	2.80	3 (42%)
11	COM	e	303[A]	-	6,6,6	1.31	1 (16%)	7,8,8	3.78	4 (57%)
9	JCV	g	101	-	120,120,120	1.11	10 (8%)	148,154,154	0.71	0
9	JCV	E	305	-	120,120,120	1.32	12 (10%)	148,154,154	1.47	24 (16%)
9	JCV	U	304	-	116,116,120	1.10	9 (7%)	141,146,154	0.73	0
9	JCV	W	101	-	120,120,120	1.13	11 (9%)	148,154,154	0.87	2 (1%)

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
9	JCV	E	306	-	1/1/30/30	55/126/170/170	0/2/2/2
9	JCV	S	301	-	2/2/30/30	51/126/170/170	0/2/2/2
9	JCV	U	305	-	1/1/30/30	72/126/170/170	0/2/2/2
11	COM	U	303[A]	-	-	4/4/4/4	-
9	JCV	e	305	-	-	62/126/170/170	0/2/2/2
9	JCV	c	301	-	2/2/30/30	71/126/170/170	0/2/2/2
11	COM	E	303[A]	-	-	4/4/4/4	-
11	COM	E	303[B]	-	-	2/4/4/4	-
9	JCV	C	301	-	-	71/126/170/170	0/2/2/2
9	JCV	e	304	-	-	44/126/170/170	0/2/2/2
11	COM	e	303[B]	-	-	1/4/4/4	-
9	JCV	E	304	-	1/1/30/30	54/126/170/170	0/2/2/2
11	COM	U	303[C]	-	-	3/4/4/4	-
11	COM	e	303[A]	-	-	3/4/4/4	-
9	JCV	g	101	-	-	51/126/170/170	0/2/2/2
9	JCV	E	305	-	-	29/126/170/170	0/2/2/2
9	JCV	U	304	-	-	34/118/162/170	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	JCV	W	101	-	2/2/30/30	61/126/170/170	0/2/2/2

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	305	JCV	OY1-CG7	-6.30	1.32	1.43
9	e	304	JCV	OY1-CG7	-5.88	1.33	1.43
9	e	305	JCV	OY1-CG7	-5.14	1.34	1.43
9	C	301	JCV	OY1-CG7	-4.27	1.35	1.43
9	g	101	JCV	OY1-CG7	-4.24	1.36	1.43
9	W	101	JCV	OY1-CG7	-4.23	1.36	1.43
9	E	306	JCV	OY1-CG7	-4.21	1.36	1.43
9	U	305	JCV	OY1-CG7	-4.19	1.36	1.43
9	U	304	JCV	OY1-CG7	-4.17	1.36	1.43
9	c	301	JCV	OY1-CG7	-4.14	1.36	1.43
9	S	301	JCV	OY1-CG7	-4.13	1.36	1.43
9	E	304	JCV	OY1-CG7	-4.02	1.36	1.43
9	U	305	JCV	C22M-C22	3.36	1.63	1.52
9	C	301	JCV	C22M-C22	3.35	1.63	1.52
9	c	301	JCV	C22M-C22	3.33	1.63	1.52
9	E	304	JCV	OG3-C1	-3.32	1.27	1.42
9	g	101	JCV	C22M-C22	3.30	1.63	1.52
9	E	306	JCV	C22M-C22	3.29	1.63	1.52
9	e	305	JCV	C22M-C22	3.28	1.63	1.52
9	e	304	JCV	OG3-C1	-3.27	1.27	1.42
9	W	101	JCV	C22M-C22	3.26	1.63	1.52
9	U	304	JCV	C22M-C22	3.25	1.63	1.52
9	E	305	JCV	OG3-C1	-3.24	1.27	1.42
11	E	303[A]	COM	C2-S2	3.19	1.82	1.77
11	U	303[C]	COM	C2-S2	3.17	1.82	1.77
9	E	304	JCV	P-O2	-3.08	1.40	1.50
11	U	303[A]	COM	C2-S2	3.07	1.81	1.77
9	E	305	JCV	C3M-C3	-3.07	1.43	1.52
11	e	303[B]	COM	C2-S2	3.03	1.81	1.77
9	S	301	JCV	C31-C32	3.02	1.61	1.50
9	W	101	JCV	C31-C32	3.01	1.61	1.50
9	U	305	JCV	C31-C32	3.01	1.61	1.50
9	C	301	JCV	C31-C32	3.00	1.61	1.50
9	e	304	JCV	C3M-C3	-3.00	1.43	1.52
9	e	304	JCV	C80M-C80	-2.98	1.43	1.52
9	c	301	JCV	C31-C32	2.98	1.61	1.50
11	E	303[B]	COM	C2-S2	2.97	1.81	1.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	305	JCV	C17-C16	-2.96	1.44	1.53
9	g	101	JCV	C31-C32	2.94	1.61	1.50
9	E	304	JCV	C3M-C3	-2.93	1.43	1.52
9	E	306	JCV	C31-C32	2.93	1.60	1.50
9	E	304	JCV	C22M-C22	2.87	1.61	1.52
9	e	305	JCV	C3M-C3	-2.86	1.43	1.52
9	E	305	JCV	P-O3	-2.84	1.42	1.55
9	U	304	JCV	C31-C32	2.84	1.60	1.50
9	e	305	JCV	OG3-C1	-2.83	1.29	1.42
9	C	301	JCV	C2-C1	2.83	1.60	1.50
9	E	306	JCV	C2-C1	2.82	1.60	1.50
9	c	301	JCV	C2-C1	2.81	1.60	1.50
9	U	304	JCV	C2-C1	2.80	1.60	1.50
9	e	304	JCV	C17-C16	-2.79	1.45	1.53
9	U	305	JCV	C2-C1	2.76	1.60	1.50
9	e	304	JCV	P-O2	-2.74	1.41	1.50
9	E	305	JCV	C80M-C80	-2.73	1.44	1.52
9	e	304	JCV	C22M-C22	2.72	1.61	1.52
9	g	101	JCV	C2-C1	2.72	1.60	1.50
9	W	101	JCV	C2-C1	2.71	1.60	1.50
9	E	306	JCV	C55-C54	2.69	1.63	1.52
9	S	301	JCV	C22M-C22	2.69	1.61	1.52
9	U	305	JCV	C55-C54	2.65	1.63	1.52
9	W	101	JCV	C55-C54	2.65	1.63	1.52
9	C	301	JCV	C55-C54	2.64	1.63	1.52
9	E	305	JCV	C22M-C22	2.63	1.61	1.52
9	c	301	JCV	C55-C54	2.63	1.63	1.52
9	U	304	JCV	C55-C54	2.62	1.63	1.52
9	e	305	JCV	C31-C32	2.62	1.59	1.50
9	E	304	JCV	C31-C32	2.60	1.59	1.50
9	g	101	JCV	C55-C54	2.58	1.63	1.52
9	S	301	JCV	OG3-C1	-2.57	1.30	1.42
9	e	305	JCV	C2-C1	2.57	1.59	1.50
9	S	301	JCV	C3M-C3	-2.56	1.44	1.52
9	E	304	JCV	C17-C16	-2.56	1.45	1.53
9	E	306	JCV	OG3-C1	-2.55	1.31	1.42
9	W	101	JCV	OG3-C1	-2.55	1.31	1.42
9	g	101	JCV	OG3-C1	-2.53	1.31	1.42
9	U	304	JCV	OG3-C1	-2.53	1.31	1.42
9	S	301	JCV	C2-C1	2.53	1.59	1.50
9	U	305	JCV	OG3-C1	-2.52	1.31	1.42
9	e	305	JCV	C80M-C80	-2.51	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	e	304	JCV	P-O3	-2.50	1.43	1.55
9	c	301	JCV	OG3-C1	-2.49	1.31	1.42
9	C	301	JCV	OG3-C1	-2.49	1.31	1.42
9	e	305	JCV	CG8-CG6	2.46	1.58	1.50
9	E	305	JCV	P-O2	-2.43	1.42	1.50
9	E	304	JCV	P-O3	-2.42	1.43	1.55
11	e	303[A]	COM	C2-S2	2.42	1.80	1.77
9	e	304	JCV	C74-C73	-2.36	1.42	1.52
9	c	301	JCV	CG8-CG6	2.31	1.57	1.50
9	W	101	JCV	CG8-CG6	2.28	1.57	1.50
9	E	306	JCV	CG8-CG6	2.27	1.57	1.50
9	E	304	JCV	CX3-CX2	-2.27	1.46	1.52
9	U	305	JCV	CG8-CG6	2.26	1.57	1.50
9	E	304	JCV	C55-C54	2.25	1.61	1.52
9	e	304	JCV	CX3-CX2	-2.23	1.46	1.52
9	e	305	JCV	C55-C54	2.22	1.61	1.52
9	C	301	JCV	CG8-CG6	2.22	1.57	1.50
9	g	101	JCV	CG8-CG6	2.21	1.57	1.50
9	U	304	JCV	C17-C16	-2.21	1.46	1.53
9	E	304	JCV	CX4-CX3	-2.20	1.46	1.52
9	e	304	JCV	C2-C1	2.19	1.58	1.50
9	E	304	JCV	OX2-CX4	-2.19	1.37	1.43
9	U	304	JCV	CG8-CG6	2.16	1.57	1.50
11	U	303[C]	COM	O2S-S2	2.14	1.51	1.45
9	E	304	JCV	CG8-CG6	2.14	1.57	1.50
11	E	303[B]	COM	O2S-S2	2.13	1.51	1.45
9	E	305	JCV	C2-C1	2.13	1.58	1.50
9	E	305	JCV	CX3-CX2	-2.13	1.46	1.52
9	e	305	JCV	C17-C16	-2.11	1.46	1.53
9	g	101	JCV	C17-C16	-2.11	1.47	1.53
9	C	301	JCV	C17-C16	-2.10	1.47	1.53
9	E	304	JCV	OY1-CY1	2.10	1.43	1.40
9	c	301	JCV	C3M-C3	-2.09	1.46	1.52
11	U	303[C]	COM	O1S-S2	2.09	1.51	1.45
9	U	304	JCV	C3M-C3	-2.09	1.46	1.52
9	E	305	JCV	C74-C73	-2.09	1.43	1.52
9	U	305	JCV	C20-C19	2.09	1.61	1.52
9	U	305	JCV	C3M-C3	-2.07	1.46	1.52
9	W	101	JCV	C17-C16	-2.07	1.47	1.53
11	E	303[A]	COM	O1S-S2	2.07	1.51	1.45
9	c	301	JCV	C17-C16	-2.07	1.47	1.53
9	W	101	JCV	C3M-C3	-2.06	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	e	303[B]	COM	O2S-S2	2.06	1.51	1.45
11	e	303[B]	COM	O1S-S2	2.05	1.51	1.45
9	E	306	JCV	C17-C16	-2.05	1.47	1.53
9	U	305	JCV	C17-C16	-2.05	1.47	1.53
9	C	301	JCV	C20-C19	2.05	1.60	1.52
11	U	303[A]	COM	O2S-S2	2.05	1.51	1.45
11	U	303[A]	COM	O1S-S2	2.05	1.51	1.45
9	E	306	JCV	C59-C60	2.05	1.60	1.52
9	U	305	JCV	C59-C60	2.04	1.60	1.52
9	S	301	JCV	C17-C16	-2.04	1.47	1.53
9	g	101	JCV	C3M-C3	-2.03	1.46	1.52
9	W	101	JCV	C59-C60	2.03	1.60	1.52
9	c	301	JCV	OY1-CY1	2.03	1.43	1.40
9	W	101	JCV	C20-C19	2.03	1.60	1.52
9	g	101	JCV	C20-C19	2.03	1.60	1.52
9	C	301	JCV	C3M-C3	-2.02	1.46	1.52
9	S	301	JCV	C80M-C80	-2.02	1.46	1.52
9	e	304	JCV	C55-C54	2.01	1.60	1.52
9	e	305	JCV	C20-C19	2.01	1.60	1.52
9	E	306	JCV	C3M-C3	-2.00	1.46	1.52
9	C	301	JCV	C59-C60	2.00	1.60	1.52
9	C	301	JCV	P-O4	2.00	1.65	1.60
9	E	305	JCV	C55-C54	2.00	1.60	1.52

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	304	JCV	OX4-CX2-CX3	-8.22	91.35	110.35
11	e	303[A]	COM	O3S-S2-C2	6.47	116.24	105.77
9	E	304	JCV	CX6-CX1-CX2	6.09	119.63	110.85
11	e	303[A]	COM	O3S-S2-O1S	-5.50	97.83	111.27
9	e	304	JCV	CX4-CX3-CX2	-5.36	101.46	110.82
9	S	301	JCV	CX5-CX4-CX3	5.34	120.15	110.82
9	E	304	JCV	O4-CX1-CX2	5.27	120.92	108.66
9	E	305	JCV	CX4-CX3-CX2	-4.71	102.60	110.82
9	W	101	JCV	CX6-CX1-CX2	4.66	117.57	110.85
11	e	303[B]	COM	O3S-S2-O1S	-4.44	100.43	111.27
9	S	301	JCV	CX4-CX3-CX2	4.40	118.51	110.82
11	E	303[B]	COM	O3S-S2-O2S	-4.28	100.81	111.27
9	e	305	JCV	OG4-C82-C81	-4.27	99.80	108.77
11	E	303[A]	COM	O3S-S2-O2S	-4.22	100.95	111.27
11	U	303[C]	COM	O3S-S2-O1S	-4.19	101.05	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	E	303[B]	COM	O3S-S2-C2	4.13	112.44	105.77
9	E	305	JCV	CX5-CX4-CX3	-4.12	103.63	110.82
11	U	303[A]	COM	O3S-S2-O1S	-4.05	101.38	111.27
11	E	303[A]	COM	O3S-S2-C2	4.04	112.30	105.77
9	e	304	JCV	CX5-CX4-CX3	-4.01	103.83	110.82
11	e	303[A]	COM	O1S-S2-C2	3.97	111.69	106.92
11	U	303[C]	COM	O1S-S2-C2	3.94	111.66	106.92
9	E	304	JCV	OX2-CX4-CX3	-3.93	101.27	110.35
9	E	305	JCV	C20-C19-C18	-3.88	103.38	115.92
9	E	305	JCV	CY1-CY2-CY3	-3.88	101.92	110.00
9	E	304	JCV	O3-P-O2	-3.81	93.39	112.24
9	e	304	JCV	CG8-CG6-CG7	-3.79	102.82	111.79
11	U	303[C]	COM	O3S-S2-C2	3.79	111.90	105.77
11	U	303[A]	COM	O3S-S2-C2	3.70	111.75	105.77
11	e	303[B]	COM	O1S-S2-C2	3.64	111.30	106.92
11	e	303[B]	COM	O3S-S2-C2	3.60	111.60	105.77
9	E	304	JCV	P-O4-CX1	3.59	132.47	119.41
9	W	101	JCV	CX3-CX2-CX1	3.59	117.88	109.68
9	E	304	JCV	CX5-CX4-CX3	-3.57	104.60	110.82
11	E	303[B]	COM	O2S-S2-C2	3.42	111.03	106.92
11	U	303[A]	COM	O1S-S2-C2	3.41	111.02	106.92
9	e	305	JCV	CY1-OY5-CY5	-3.26	107.29	113.69
9	E	304	JCV	OX2-CX4-CX5	-3.22	102.91	110.35
9	e	305	JCV	OX5-CX5-CX6	-3.16	103.03	110.35
9	e	304	JCV	CX3-CX2-CX1	-3.16	102.47	109.68
9	S	301	JCV	C55-C56-C57	-3.15	105.74	115.92
9	E	304	JCV	O3-P-O4	3.14	119.18	106.78
9	e	304	JCV	OY5-CY1-CY2	-3.12	103.74	110.35
9	e	304	JCV	OY5-CY1-OY1	-3.07	102.71	109.97
9	E	305	JCV	C63-C64-C65	-3.06	106.03	115.92
11	E	303[A]	COM	O1S-S2-C2	3.00	110.53	106.92
9	S	301	JCV	CX6-CX1-CX2	2.99	115.17	110.85
11	U	303[A]	COM	O2S-S2-C2	2.95	110.47	106.92
9	e	304	JCV	C20-C19-C18	-2.95	106.39	115.92
11	E	303[A]	COM	O2S-S2-C2	2.89	110.40	106.92
9	S	301	JCV	C5-C6-C7	-2.87	106.66	115.92
9	E	305	JCV	CX3-CX2-CX1	-2.86	103.15	109.68
9	e	305	JCV	C51-OG2-CG2	-2.80	108.95	115.40
9	E	305	JCV	CX6-CX5-CX4	-2.79	105.96	110.82
9	E	305	JCV	OX5-CX5-CX4	-2.78	103.91	110.35
9	S	301	JCV	C28-C29-C30	-2.78	106.94	115.92
9	E	305	JCV	CG8-CG6-CG7	-2.76	105.27	111.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	305	JCV	CY4-CY3-CY2	-2.74	106.03	110.82
9	e	304	JCV	OX5-CX5-CX4	-2.74	104.02	110.35
9	e	304	JCV	CX6-CX5-CX4	-2.73	106.05	110.82
9	E	305	JCV	OY1-CG7-CG6	-2.66	104.48	110.90
11	e	303[B]	COM	O2S-S2-C2	2.66	110.11	106.92
9	E	304	JCV	CX3-CX2-CX1	2.64	115.71	109.68
9	e	304	JCV	C28-C29-C30	-2.59	107.54	115.92
9	e	304	JCV	C53M-C53-C54	-2.59	101.91	111.29
9	e	305	JCV	C55-C56-C57	-2.59	107.56	115.92
9	e	304	JCV	CY1-CY2-CY3	-2.57	104.64	110.00
9	e	305	JCV	CG7-OY1-CY1	-2.57	108.71	113.74
9	E	305	JCV	OY5-CY1-CY2	-2.57	104.90	110.35
9	E	305	JCV	OG6-CG8-CG6	-2.56	103.42	109.44
9	e	304	JCV	C61M-C61-C60	-2.51	102.19	111.29
9	e	305	JCV	C78-C77-C76	-2.51	107.81	115.92
9	e	305	JCV	CX5-CX6-CX1	-2.51	103.96	109.68
9	e	304	JCV	OG4-CG6-CG7	2.51	116.95	109.06
9	S	301	JCV	CG3-CG2-CG1	-2.49	105.89	111.79
9	E	304	JCV	OY1-CY1-CY2	2.47	112.17	108.30
9	S	301	JCV	C7M-C7-C6	-2.46	102.39	111.29
9	E	304	JCV	C9-C10-C11	-2.44	108.05	115.92
9	e	305	JCV	OY1-CG7-CG6	-2.43	105.04	110.90
9	S	301	JCV	CX6-CX5-CX4	2.41	115.04	110.82
9	e	305	JCV	CY3-CY4-CY5	2.39	114.50	110.24
9	S	301	JCV	C57M-C57-C56	-2.39	102.65	111.29
9	E	304	JCV	O4-P-O2	-2.38	100.55	109.47
9	e	304	JCV	C78-C77-C76	-2.37	108.26	115.92
9	e	304	JCV	OX2-CX4-CX5	-2.37	104.87	110.35
9	S	301	JCV	C63-C62-C61	-2.37	108.27	115.92
9	e	304	JCV	C9-C10-C11	-2.36	108.30	115.92
9	E	304	JCV	C9-C8-C7	-2.34	108.34	115.92
9	e	305	JCV	C5-C6-C7	-2.34	108.36	115.92
9	S	301	JCV	CX3-CX2-CX1	2.33	115.00	109.68
9	e	304	JCV	C72M-C72-C73	-2.33	102.86	111.29
9	E	305	JCV	OG4-C82-C81	-2.33	103.88	108.77
9	e	304	JCV	C63-C64-C65	-2.33	108.40	115.92
9	S	301	JCV	C5-C4-C3	-2.32	108.42	115.92
9	E	305	JCV	C78-C77-C76	-2.32	108.43	115.92
9	E	305	JCV	C9-C8-C7	-2.32	108.43	115.92
9	e	304	JCV	C59-C58-C57	-2.31	108.44	115.92
9	E	304	JCV	C59-C58-C57	-2.31	108.47	115.92
11	E	303[B]	COM	O1S-S2-C2	2.30	109.69	106.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	e	305	JCV	C55-C54-C53	-2.30	108.47	115.92
9	E	304	JCV	C28-C27-C26	-2.26	108.61	115.92
9	E	305	JCV	CY1-OY5-CY5	-2.26	109.25	113.69
9	e	304	JCV	OY2-CY2-CY1	2.25	115.51	110.05
9	E	304	JCV	O4-CX1-CX6	2.25	113.89	108.66
9	S	301	JCV	O4-CX1-CX2	-2.25	103.44	108.66
9	E	305	JCV	CX6-CX1-CX2	-2.24	107.63	110.85
11	e	303[A]	COM	O3S-S2-O2S	2.23	116.72	111.27
9	e	305	JCV	C59-C60-C61	-2.21	108.79	115.92
9	E	305	JCV	C53M-C53-C54	-2.20	103.32	111.29
9	E	304	JCV	CX5-CX6-CX1	2.20	114.71	109.68
9	S	301	JCV	C15M-C15-C14	-2.20	103.33	111.29
9	e	304	JCV	C9-C8-C7	-2.20	108.81	115.92
9	E	304	JCV	O1-P-O2	2.19	117.61	109.07
9	e	305	JCV	CX4-CX3-CX2	-2.19	107.01	110.82
9	E	304	JCV	OX4-CX2-CX1	-2.18	104.17	109.94
9	S	301	JCV	C59-C60-C61	-2.17	108.91	115.92
9	E	305	JCV	CY3-CY4-CY5	2.16	114.09	110.24
9	e	304	JCV	CX6-CX1-CX2	-2.14	107.77	110.85
9	S	301	JCV	C74-C75-C76	-2.14	109.01	115.92
9	E	304	JCV	C28-C29-C30	-2.13	109.03	115.92
9	e	304	JCV	CY3-CY4-CY5	2.09	113.97	110.24
9	e	305	JCV	C63-C62-C61	-2.08	109.19	115.92
9	e	304	JCV	C74-C75-C76	-2.08	109.19	115.92
9	E	304	JCV	C20-C21-C22	-2.07	109.22	115.92
9	E	305	JCV	C80M-C80-C79	-2.07	103.80	111.29
9	E	305	JCV	C20-C21-C22	-2.06	109.25	115.92
9	E	304	JCV	CG7-OY1-CY1	2.06	117.77	113.74
9	S	301	JCV	P-O4-CX1	-2.05	111.96	119.41
9	e	305	JCV	OY1-CY1-CY2	2.03	111.48	108.30
9	S	301	JCV	OX2-CX4-CX5	2.01	115.00	110.35
9	E	305	JCV	C28-C29-C30	-2.01	109.42	115.92
9	S	301	JCV	C63-C64-C65	-2.00	109.44	115.92
9	e	304	JCV	C3M-C3-C4	-2.00	104.04	111.29
9	E	305	JCV	C61M-C61-C60	-2.00	104.04	111.29

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	E	304	JCV	CY4
9	E	306	JCV	CG6
9	c	301	JCV	C80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
9	c	301	JCV	C68
9	S	301	JCV	C61
9	S	301	JCV	CY4
9	U	305	JCV	C22
9	W	101	JCV	CG2
9	W	101	JCV	C26

All (672) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	301	JCV	C52-C51-OG2-CG2
9	C	301	JCV	C30M-C30-C31-C32
9	C	301	JCV	C55-C56-C57-C57M
9	C	301	JCV	C80M-C80-C81-C82
9	C	301	JCV	CG1-O1-P-O2
9	C	301	JCV	CG1-O1-P-O3
9	E	304	JCV	C1-C2-C3-C3M
9	E	304	JCV	C21-C22-C23-C24
9	E	304	JCV	C30M-C30-C31-C32
9	E	304	JCV	CX2-CX1-O4-P
9	E	304	JCV	CY2-CY1-OY1-CG7
9	E	304	JCV	OY5-CY1-OY1-CG7
9	E	304	JCV	CX1-O4-P-O3
9	E	305	JCV	CX1-O4-P-O3
9	E	306	JCV	C1-C2-C3-C3M
9	E	306	JCV	C51-C52-C53-C53M
9	E	306	JCV	C65-C66-C67-C68
9	c	301	JCV	CG1-CG2-OG2-C51
9	c	301	JCV	C16-C17-C18-C18M
9	c	301	JCV	C51-C52-C53-C53M
9	c	301	JCV	C80M-C80-C81-C82
9	c	301	JCV	C81-C82-OG4-CG6
9	c	301	JCV	CX6-CX1-O4-P
9	c	301	JCV	CY2-CY1-OY1-CG7
9	c	301	JCV	OY5-CY1-OY1-CG7
9	e	304	JCV	C80M-C80-C81-C82
9	e	304	JCV	CG6-CG8-OG6-C32
9	e	304	JCV	OY5-CY1-OY1-CG7
9	e	304	JCV	CX1-O4-P-O2
9	e	304	JCV	CX1-O4-P-O3
9	e	305	JCV	C30M-C30-C31-C32
9	e	305	JCV	C51-C52-C53-C53M

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	e	305	JCV	C65-C66-C67-C68
9	e	305	JCV	C74-C75-C76-C76M
9	g	101	JCV	C30M-C30-C31-C32
9	S	301	JCV	C1-C2-C3-C3M
9	S	301	JCV	C53M-C53-C54-C55
9	S	301	JCV	CG1-O1-P-O2
9	S	301	JCV	CX1-O4-P-O1
9	U	304	JCV	C30M-C30-C31-C32
9	U	304	JCV	OG4-CG6-CG8-OG6
9	U	304	JCV	OY5-CY1-OY1-CG7
9	U	304	JCV	CX1-O4-P-O2
9	U	304	JCV	CX1-O4-P-O3
9	U	305	JCV	C52-C51-OG2-CG2
9	U	305	JCV	C1-C2-C3-C3M
9	U	305	JCV	C51-C52-C53-C53M
9	U	305	JCV	C80M-C80-C81-C82
9	U	305	JCV	CY2-CY1-OY1-CG7
9	W	101	JCV	CG3-CG2-OG2-C51
9	W	101	JCV	C51-C52-C53-C53M
9	W	101	JCV	C59-C60-C61-C61M
9	W	101	JCV	CG8-CG6-OG4-C82
9	W	101	JCV	CY2-CY1-OY1-CG7
9	W	101	JCV	OY5-CY1-OY1-CG7
9	W	101	JCV	CG1-O1-P-O2
11	E	303[A]	COM	C1-C2-S2-O1S
11	E	303[A]	COM	C1-C2-S2-O2S
11	e	303[A]	COM	C1-C2-S2-O1S
11	e	303[A]	COM	C1-C2-S2-O2S
11	e	303[A]	COM	C1-C2-S2-O3S
11	U	303[A]	COM	C1-C2-S2-O2S
11	U	303[C]	COM	C1-C2-S2-O1S
11	U	303[C]	COM	C1-C2-S2-O2S
11	U	303[C]	COM	C1-C2-S2-O3S
9	W	101	JCV	CY4-CY5-CY6-OY6
9	e	305	JCV	CY4-CY5-CY6-OY6
9	E	305	JCV	CG6-CG8-OG6-C32
9	c	301	JCV	CG2-CG3-OG3-C1
9	W	101	JCV	CG6-CG8-OG6-C32
9	C	301	JCV	C31-C32-OG6-CG8
9	e	305	JCV	C31-C32-OG6-CG8
9	U	304	JCV	OY5-CY5-CY6-OY6
9	E	306	JCV	C19-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	e	305	JCV	OY5-CY5-CY6-OY6
9	W	101	JCV	OY5-CY5-CY6-OY6
9	S	301	JCV	CY4-CY5-CY6-OY6
9	C	301	JCV	OY5-CY1-OY1-CG7
9	g	101	JCV	OY5-CY1-OY1-CG7
9	U	305	JCV	OY5-CY1-OY1-CG7
9	C	301	JCV	C2-C1-OG3-CG3
9	E	304	JCV	C31-C32-OG6-CG8
9	U	304	JCV	C66-C67-C68-C69
9	E	304	JCV	OG2-C51-C52-C53
9	S	301	JCV	OG2-C51-C52-C53
9	U	304	JCV	CY4-CY5-CY6-OY6
9	W	101	JCV	C27-C28-C29-C30
9	U	304	JCV	CY2-CY1-OY1-CG7
9	S	301	JCV	OY5-CY5-CY6-OY6
9	C	301	JCV	C13-C14-C15-C15M
9	C	301	JCV	C20-C21-C22-C22M
9	C	301	JCV	C22M-C22-C23-C24
9	C	301	JCV	C26M-C26-C27-C28
9	C	301	JCV	C28-C29-C30-C30M
9	C	301	JCV	C57M-C57-C58-C59
9	C	301	JCV	C5-C6-C7-C7M
9	C	301	JCV	C66-C67-C68-C68M
9	C	301	JCV	C76M-C76-C77-C78
9	E	304	JCV	C11M-C11-C12-C13
9	E	304	JCV	C66-C67-C68-C68M
9	E	304	JCV	C76M-C76-C77-C78
9	E	306	JCV	C15M-C15-C16-C17
9	E	306	JCV	C72M-C72-C73-C74
9	E	306	JCV	C74-C75-C76-C76M
9	c	301	JCV	C53M-C53-C54-C55
9	c	301	JCV	C55-C56-C57-C57M
9	c	301	JCV	C59-C60-C61-C61M
9	c	301	JCV	C65M-C65-C66-C67
9	e	304	JCV	C66-C67-C68-C68M
9	e	304	JCV	C78-C79-C80-C80M
9	e	305	JCV	C11M-C11-C12-C13
9	e	305	JCV	C22M-C22-C23-C24
9	e	305	JCV	C78-C79-C80-C80M
9	g	101	JCV	C15M-C15-C16-C17
9	g	101	JCV	C16-C17-C18-C18M
9	g	101	JCV	C63-C64-C65-C65M

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	g	101	JCV	C72M-C72-C73-C74
9	g	101	JCV	C76M-C76-C77-C78
9	g	101	JCV	C78-C79-C80-C80M
9	S	301	JCV	C18M-C18-C19-C20
9	S	301	JCV	C20-C21-C22-C22M
9	S	301	JCV	C65M-C65-C66-C67
9	U	304	JCV	C28-C29-C30-C30M
9	U	305	JCV	C55-C56-C57-C57M
9	U	305	JCV	C61M-C61-C62-C63
9	U	305	JCV	C63-C64-C65-C65M
9	U	305	JCV	C72M-C72-C73-C74
9	U	305	JCV	C76M-C76-C77-C78
9	W	101	JCV	C16-C17-C18-C18M
9	W	101	JCV	C22M-C22-C23-C24
9	W	101	JCV	C65M-C65-C66-C67
9	E	306	JCV	C53-C54-C55-C56
9	e	305	JCV	C26-C27-C28-C29
9	S	301	JCV	C11-C12-C13-C14
9	W	101	JCV	C18-C19-C20-C21
9	g	101	JCV	C61-C62-C63-C64
9	C	301	JCV	C62-C63-C64-C65
9	e	305	JCV	C18-C19-C20-C21
9	e	305	JCV	C27-C28-C29-C30
9	e	305	JCV	C58-C59-C60-C61
9	S	301	JCV	C76-C77-C78-C79
9	U	304	JCV	C19-C20-C21-C22
9	E	304	JCV	C29-C30-C31-C32
9	g	101	JCV	C29-C30-C31-C32
9	C	301	JCV	C27-C28-C29-C30
9	C	301	JCV	C57-C58-C59-C60
9	c	301	JCV	C19-C20-C21-C22
9	g	101	JCV	C57-C58-C59-C60
9	U	304	JCV	C70-C71-C72-C73
9	E	304	JCV	C58-C59-C60-C61
9	W	101	JCV	C76-C77-C78-C79
9	W	101	JCV	C7-C8-C9-C10
9	e	304	JCV	OY5-CY5-CY6-OY6
9	C	301	JCV	C69-C70-C71-C72
9	S	301	JCV	C26-C27-C28-C29
9	E	306	JCV	C54-C55-C56-C57
9	E	304	JCV	C5-C6-C7-C8
9	E	304	JCV	C60-C61-C62-C63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	E	305	JCV	C59-C60-C61-C62
9	E	306	JCV	C21-C22-C23-C24
9	c	301	JCV	C78-C79-C80-C81
9	e	305	JCV	C2-C3-C4-C5
9	e	305	JCV	C56-C57-C58-C59
9	e	305	JCV	C67-C68-C69-C70
9	g	101	JCV	C55-C56-C57-C58
9	S	301	JCV	C71-C72-C73-C74
9	U	304	JCV	C17-C18-C19-C20
9	U	305	JCV	C10-C11-C12-C13
9	U	305	JCV	C13-C14-C15-C16
9	U	305	JCV	C20-C21-C22-C23
9	U	305	JCV	C2-C3-C4-C5
9	W	101	JCV	C9-C10-C11-C12
9	W	101	JCV	C70-C71-C72-C73
9	e	304	JCV	C76-C77-C78-C79
9	S	301	JCV	C54-C55-C56-C57
9	U	305	JCV	C62-C63-C64-C65
9	E	306	JCV	C77-C78-C79-C80
9	e	305	JCV	C73-C74-C75-C76
9	C	301	JCV	C19-C20-C21-C22
9	E	305	JCV	C73-C74-C75-C76
9	c	301	JCV	C3-C4-C5-C6
9	W	101	JCV	C23-C24-C25-C26
9	W	101	JCV	C26-C27-C28-C29
9	C	301	JCV	C54-C55-C56-C57
9	c	301	JCV	C23-C24-C25-C26
9	c	301	JCV	C62-C63-C64-C65
9	c	301	JCV	C69-C70-C71-C72
9	e	305	JCV	C69-C70-C71-C72
9	g	101	JCV	C22-C23-C24-C25
9	W	101	JCV	C62-C63-C64-C65
9	C	301	JCV	CG1-O1-P-O4
9	C	301	JCV	C68-C69-C70-C71
9	E	304	JCV	C30-C31-C32-OG6
9	E	306	JCV	C80-C81-C82-OG4
9	U	304	JCV	C30-C31-C32-OG6
9	E	306	JCV	CY2-CY1-OY1-CG7
9	e	304	JCV	CY2-CY1-OY1-CG7
9	E	304	JCV	C22-C23-C24-C25
9	C	301	JCV	C70-C71-C72-C72M
9	c	301	JCV	C15M-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	c	301	JCV	C24-C25-C26-C26M
9	c	301	JCV	C78-C79-C80-C80M
9	e	305	JCV	C65M-C65-C66-C67
9	S	301	JCV	C72M-C72-C73-C74
9	U	304	JCV	C18M-C18-C19-C20
9	U	305	JCV	C11M-C11-C12-C13
9	W	101	JCV	C24-C25-C26-C26M
9	W	101	JCV	C78-C79-C80-C80M
9	g	101	JCV	C19-C20-C21-C22
9	U	304	JCV	C76-C77-C78-C79
9	S	301	JCV	C53-C54-C55-C56
9	U	305	JCV	CG6-CG8-OG6-C32
9	E	306	JCV	OY5-CY1-OY1-CG7
9	e	305	JCV	C62-C63-C64-C65
9	E	304	JCV	C18-C19-C20-C21
9	S	301	JCV	C57-C58-C59-C60
9	S	301	JCV	C61-C62-C63-C64
9	c	301	JCV	C29-C30-C31-C32
9	S	301	JCV	C79-C80-C81-C82
9	C	301	JCV	C26-C27-C28-C29
9	e	305	JCV	C72-C73-C74-C75
9	E	304	JCV	C26-C27-C28-C29
9	E	306	JCV	C18-C19-C20-C21
9	e	304	JCV	C19-C20-C21-C22
9	W	101	JCV	C53-C54-C55-C56
9	E	305	JCV	C30-C31-C32-OG6
9	W	101	JCV	C30-C31-C32-OG6
9	W	101	JCV	C80-C81-C82-OG4
9	E	305	JCV	C19-C20-C21-C22
9	C	301	JCV	C16-C17-C18-C19
9	C	301	JCV	C21-C22-C23-C24
9	C	301	JCV	C56-C57-C58-C59
9	C	301	JCV	C75-C76-C77-C78
9	E	304	JCV	C10-C11-C12-C13
9	c	301	JCV	C14-C15-C16-C17
9	c	301	JCV	C2-C3-C4-C5
9	e	304	JCV	C24-C25-C26-C27
9	e	304	JCV	C64-C65-C66-C67
9	e	304	JCV	C71-C72-C73-C74
9	e	305	JCV	C52-C53-C54-C55
9	e	305	JCV	C59-C60-C61-C62
9	g	101	JCV	C28-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	g	101	JCV	C63-C64-C65-C66
9	g	101	JCV	C75-C76-C77-C78
9	S	301	JCV	C16-C17-C18-C19
9	U	305	JCV	C5-C6-C7-C8
9	W	101	JCV	C78-C79-C80-C81
9	U	304	JCV	C26-C27-C28-C29
9	U	305	JCV	C19-C20-C21-C22
9	C	301	JCV	C4-C5-C6-C7
9	U	305	JCV	C26-C27-C28-C29
9	C	301	JCV	C58-C59-C60-C61
9	E	304	JCV	C62-C63-C64-C65
9	g	101	JCV	OG2-CG2-CG3-OG3
9	E	305	JCV	OY5-CY5-CY6-OY6
9	C	301	JCV	C16-C17-C18-C18M
9	E	304	JCV	C65M-C65-C66-C67
9	E	305	JCV	C72M-C72-C73-C74
9	E	306	JCV	C66-C67-C68-C68M
9	c	301	JCV	C11M-C11-C12-C13
9	c	301	JCV	C13-C14-C15-C15M
9	c	301	JCV	C3M-C3-C4-C5
9	e	305	JCV	C68M-C68-C69-C70
9	g	101	JCV	C20-C21-C22-C22M
9	g	101	JCV	C28-C29-C30-C30M
9	U	305	JCV	C18M-C18-C19-C20
9	U	305	JCV	C24-C25-C26-C26M
9	U	305	JCV	C53M-C53-C54-C55
9	W	101	JCV	C9-C10-C11-C11M
9	W	101	JCV	C13-C14-C15-C15M
9	W	101	JCV	C70-C71-C72-C72M
9	U	305	JCV	C76-C77-C78-C79
9	E	306	JCV	OY5-CY5-CY6-OY6
9	E	304	JCV	C19-C20-C21-C22
9	E	306	JCV	C11-C12-C13-C14
9	e	305	JCV	C54-C55-C56-C57
9	U	305	JCV	C68-C69-C70-C71
9	c	301	JCV	CG1-O1-P-O4
9	g	101	JCV	C68-C69-C70-C71
11	E	303[A]	COM	S1-C1-C2-S2
9	E	306	JCV	C1-C2-C3-C4
9	E	306	JCV	C51-C52-C53-C54
9	e	304	JCV	C79-C80-C81-C82
9	U	305	JCV	C51-C52-C53-C54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	U	305	JCV	C79-C80-C81-C82
9	E	304	JCV	CG1-CG2-CG3-OG3
9	E	306	JCV	CG8-CG6-CG7-OY1
9	c	301	JCV	CG1-CG2-CG3-OG3
9	c	301	JCV	CG8-CG6-CG7-OY1
9	e	305	JCV	CG7-CG6-CG8-OG6
9	g	101	JCV	CG7-CG6-CG8-OG6
9	S	301	JCV	CG7-CG6-CG8-OG6
9	U	304	JCV	CG8-CG6-CG7-OY1
9	U	304	JCV	CG7-CG6-CG8-OG6
9	U	305	JCV	CG8-CG6-CG7-OY1
9	e	304	JCV	C73-C74-C75-C76
9	c	301	JCV	CG6-CG7-OY1-CY1
9	E	305	JCV	C68-C69-C70-C71
9	E	305	JCV	CX1-O4-P-O1
9	e	304	JCV	CX1-O4-P-O1
9	U	304	JCV	CX1-O4-P-O1
9	C	301	JCV	OY5-CY5-CY6-OY6
9	U	305	JCV	C3-C4-C5-C6
9	E	306	JCV	C61-C62-C63-C64
9	e	304	JCV	C68-C69-C70-C71
9	c	301	JCV	C61-C62-C63-C64
9	E	306	JCV	OG4-CG6-CG8-OG6
9	e	304	JCV	OG4-CG6-CG7-OY1
9	W	101	JCV	OG4-CG6-CG7-OY1
9	U	305	JCV	C72-C73-C74-C75
9	c	301	JCV	CX2-CX1-O4-P
9	C	301	JCV	C5-C6-C7-C8
9	E	304	JCV	C28-C29-C30-C31
9	E	305	JCV	C17-C18-C19-C20
9	E	306	JCV	C52-C53-C54-C55
9	E	306	JCV	C56-C57-C58-C59
9	E	306	JCV	C66-C67-C68-C69
9	E	306	JCV	C71-C72-C73-C74
9	c	301	JCV	C13-C14-C15-C16
9	c	301	JCV	C52-C53-C54-C55
9	c	301	JCV	C56-C57-C58-C59
9	e	304	JCV	C17-C18-C19-C20
9	e	304	JCV	C63-C64-C65-C66
9	e	304	JCV	C66-C67-C68-C69
9	e	305	JCV	C9-C10-C11-C12
9	e	305	JCV	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	e	305	JCV	C74-C75-C76-C77
9	g	101	JCV	C20-C21-C22-C23
9	g	101	JCV	C78-C79-C80-C81
9	S	301	JCV	C17-C18-C19-C20
9	S	301	JCV	C64-C65-C66-C67
9	U	305	JCV	C17-C18-C19-C20
9	U	305	JCV	C52-C53-C54-C55
9	U	305	JCV	C55-C56-C57-C58
9	W	101	JCV	C20-C21-C22-C23
9	W	101	JCV	C59-C60-C61-C62
9	W	101	JCV	C66-C67-C68-C69
9	C	301	JCV	C18M-C18-C19-C20
9	C	301	JCV	C65M-C65-C66-C67
9	E	304	JCV	C26M-C26-C27-C28
9	E	304	JCV	C28-C29-C30-C30M
9	E	305	JCV	C18M-C18-C19-C20
9	E	305	JCV	C59-C60-C61-C61M
9	E	306	JCV	C16-C17-C18-C18M
9	E	306	JCV	C53M-C53-C54-C55
9	c	301	JCV	C61M-C61-C62-C63
9	e	304	JCV	C18M-C18-C19-C20
9	e	305	JCV	C9-C10-C11-C11M
9	e	305	JCV	C57M-C57-C58-C59
9	e	305	JCV	C7M-C7-C8-C9
9	g	101	JCV	C26M-C26-C27-C28
9	g	101	JCV	C59-C60-C61-C61M
9	S	301	JCV	C7M-C7-C8-C9
9	U	305	JCV	C13-C14-C15-C15M
9	U	305	JCV	C22M-C22-C23-C24
9	U	305	JCV	C28-C29-C30-C30M
9	U	305	JCV	C3M-C3-C4-C5
9	U	305	JCV	C57M-C57-C58-C59
11	E	303[B]	COM	C1-C2-S2-O2S
11	U	303[A]	COM	C1-C2-S2-O1S
9	c	301	JCV	C72-C73-C74-C75
9	U	305	JCV	C18-C19-C20-C21
9	W	101	JCV	C68-C69-C70-C71
9	U	305	JCV	O1-CG1-CG2-CG3
11	E	303[A]	COM	C1-C2-S2-O3S
11	U	303[A]	COM	C1-C2-S2-O3S
9	e	305	JCV	C4-C5-C6-C7
9	e	305	JCV	C30-C31-C32-OG6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	c	301	JCV	C53-C54-C55-C56
9	E	304	JCV	CX1-O4-P-O1
9	C	301	JCV	C29-C30-C31-C32
9	e	305	JCV	C29-C30-C31-C32
9	e	305	JCV	C51-C52-C53-C54
9	U	304	JCV	C29-C30-C31-C32
9	E	304	JCV	C77-C78-C79-C80
9	E	306	JCV	CG7-CG6-CG8-OG6
9	g	101	JCV	CG1-CG2-CG3-OG3
9	U	304	JCV	CG7-CG6-OG4-C82
9	U	305	JCV	CG1-CG2-CG3-OG3
9	U	305	JCV	CG7-CG6-CG8-OG6
9	E	305	JCV	CX1-O4-P-O2
9	E	306	JCV	CX1-O4-P-O2
9	S	301	JCV	CX1-O4-P-O2
9	C	301	JCV	C18-C19-C20-C21
9	C	301	JCV	CG6-CG8-OG6-C32
9	W	101	JCV	CG1-O1-P-O4
9	S	301	JCV	C23-C24-C25-C26
9	E	304	JCV	OG2-CG2-CG3-OG3
9	E	304	JCV	OG4-CG6-CG8-OG6
9	E	306	JCV	OG4-CG6-CG7-OY1
9	S	301	JCV	OG4-CG6-CG8-OG6
9	E	304	JCV	C7-C8-C9-C10
9	C	301	JCV	C53M-C53-C54-C55
9	C	301	JCV	C63-C64-C65-C65M
9	E	304	JCV	C5-C6-C7-C7M
9	E	306	JCV	C5-C6-C7-C7M
9	e	304	JCV	C68M-C68-C69-C70
9	e	305	JCV	C15M-C15-C16-C17
9	e	305	JCV	C3M-C3-C4-C5
9	g	101	JCV	C55-C56-C57-C57M
9	W	101	JCV	C20-C21-C22-C22M
9	W	101	JCV	C7M-C7-C8-C9
9	W	101	JCV	C72M-C72-C73-C74
9	e	305	JCV	C19-C20-C21-C22
9	E	304	JCV	OY5-CY5-CY6-OY6
9	e	305	JCV	C3-C4-C5-C6
9	c	301	JCV	C2-C1-OG3-CG3
9	e	305	JCV	O1-CG1-CG2-CG3
9	C	301	JCV	C25-C26-C27-C28
9	C	301	JCV	C52-C53-C54-C55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	C	301	JCV	C55-C56-C57-C58
9	C	301	JCV	C64-C65-C66-C67
9	C	301	JCV	C66-C67-C68-C69
9	E	305	JCV	C75-C76-C77-C78
9	E	306	JCV	C16-C17-C18-C19
9	c	301	JCV	C16-C17-C18-C19
9	c	301	JCV	C55-C56-C57-C58
9	c	301	JCV	C64-C65-C66-C67
9	c	301	JCV	C71-C72-C73-C74
9	e	304	JCV	C67-C68-C69-C70
9	e	305	JCV	C21-C22-C23-C24
9	e	305	JCV	C60-C61-C62-C63
9	g	101	JCV	C25-C26-C27-C28
9	g	101	JCV	C67-C68-C69-C70
9	S	301	JCV	C20-C21-C22-C23
9	S	301	JCV	C52-C53-C54-C55
9	S	301	JCV	C63-C64-C65-C66
9	S	301	JCV	C6-C7-C8-C9
9	U	304	JCV	C28-C29-C30-C31
9	U	305	JCV	C21-C22-C23-C24
9	U	305	JCV	C28-C29-C30-C31
9	U	305	JCV	C63-C64-C65-C66
9	U	305	JCV	C64-C65-C66-C67
9	U	305	JCV	C71-C72-C73-C74
9	W	101	JCV	C60-C61-C62-C63
9	W	101	JCV	C63-C64-C65-C66
9	C	301	JCV	CX1-O4-P-O1
9	c	301	JCV	CX1-O4-P-O1
9	S	301	JCV	C73-C74-C75-C76
9	S	301	JCV	C12-C13-C14-C15
9	C	301	JCV	C79-C80-C81-C82
9	E	304	JCV	C1-C2-C3-C4
9	c	301	JCV	C79-C80-C81-C82
9	U	305	JCV	C1-C2-C3-C4
9	C	301	JCV	CG8-CG6-CG7-OY1
9	E	304	JCV	CG7-CG6-CG8-OG6
9	W	101	JCV	CG8-CG6-CG7-OY1
9	C	301	JCV	O1-CG1-CG2-OG2
9	E	304	JCV	O1-CG1-CG2-OG2
9	E	306	JCV	O1-CG1-CG2-OG2
9	c	301	JCV	C26-C27-C28-C29
9	C	301	JCV	OG4-CG6-CG7-OY1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	c	301	JCV	OG4-CG6-CG7-OY1
9	E	304	JCV	C65-C66-C67-C68
9	E	304	JCV	C63-C64-C65-C65M
9	E	305	JCV	C76M-C76-C77-C78
9	E	306	JCV	C22M-C22-C23-C24
9	e	304	JCV	C63-C64-C65-C65M
9	g	101	JCV	C68M-C68-C69-C70
9	U	305	JCV	C20-C21-C22-C22M
9	U	305	JCV	C65M-C65-C66-C67
9	W	101	JCV	C61M-C61-C62-C63
9	c	301	JCV	C31-C32-OG6-CG8
9	e	305	JCV	C2-C1-OG3-CG3
9	U	305	JCV	C30-C31-C32-OG6
9	S	301	JCV	C27-C28-C29-C30
9	S	301	JCV	CG1-O1-P-O4
9	c	301	JCV	CG2-CG1-O1-P
9	g	101	JCV	CG2-CG1-O1-P
9	c	301	JCV	CG1-O1-P-O3
9	W	101	JCV	CG1-O1-P-O3
9	C	301	JCV	O1-CG1-CG2-CG3
9	E	304	JCV	O1-CG1-CG2-CG3
9	E	306	JCV	O1-CG1-CG2-CG3
9	c	301	JCV	O1-CG1-CG2-CG3
9	U	304	JCV	C71-C72-C73-C74
9	U	304	JCV	C79-C80-C81-C82
9	E	304	JCV	C56-C57-C58-C59
9	E	304	JCV	C63-C64-C65-C66
9	E	304	JCV	C66-C67-C68-C69
9	E	304	JCV	C6-C7-C8-C9
9	E	304	JCV	C75-C76-C77-C78
9	E	305	JCV	C24-C25-C26-C27
9	c	301	JCV	O1-CG1-CG2-OG2
9	c	301	JCV	C59-C60-C61-C62
9	c	301	JCV	C60-C61-C62-C63
9	c	301	JCV	C74-C75-C76-C77
9	e	304	JCV	C74-C75-C76-C77
9	e	305	JCV	C10-C11-C12-C13
9	e	305	JCV	C14-C15-C16-C17
9	e	305	JCV	C78-C79-C80-C81
9	g	101	JCV	C14-C15-C16-C17
9	g	101	JCV	C71-C72-C73-C74
9	S	301	JCV	C66-C67-C68-C69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	U	304	JCV	C24-C25-C26-C27
9	U	305	JCV	O1-CG1-CG2-OG2
9	U	305	JCV	C6-C7-C8-C9
9	U	305	JCV	C70-C71-C72-C73
9	W	101	JCV	C21-C22-C23-C24
9	W	101	JCV	C25-C26-C27-C28
9	W	101	JCV	C64-C65-C66-C67
9	W	101	JCV	C6-C7-C8-C9
11	e	303[B]	COM	S1-C1-C2-S2
11	U	303[A]	COM	S1-C1-C2-S2
9	C	301	JCV	C23-C24-C25-C26
9	c	301	JCV	C51-C52-C53-C54
9	W	101	JCV	C51-C52-C53-C54
9	E	305	JCV	CG8-CG6-OG4-C82
9	e	304	JCV	CG8-CG6-CG7-OY1
9	g	101	JCV	C51-C52-C53-C53M
9	S	301	JCV	C51-C52-C53-C53M
9	U	305	JCV	C30M-C30-C31-C32
9	c	301	JCV	OG2-CG2-CG3-OG3
9	e	304	JCV	OG4-CG6-CG8-OG6
9	g	101	JCV	OG4-CG6-CG8-OG6
9	U	304	JCV	OG4-CG6-CG7-OY1
9	U	305	JCV	OG2-CG2-CG3-OG3
9	U	305	JCV	OG4-CG6-CG7-OY1
9	U	305	JCV	OG4-CG6-CG8-OG6
9	e	305	JCV	CG6-CG7-OY1-CY1
9	E	305	JCV	C76-C77-C78-C79
9	C	301	JCV	C15M-C15-C16-C17
9	C	301	JCV	C61M-C61-C62-C63
9	E	304	JCV	C22M-C22-C23-C24
9	E	304	JCV	C57M-C57-C58-C59
9	E	304	JCV	C7M-C7-C8-C9
9	E	305	JCV	C26M-C26-C27-C28
9	E	306	JCV	C11M-C11-C12-C13
9	E	306	JCV	C57M-C57-C58-C59
9	c	301	JCV	C20-C21-C22-C22M
9	c	301	JCV	C57M-C57-C58-C59
9	c	301	JCV	C72M-C72-C73-C74
9	e	304	JCV	C24-C25-C26-C26M
9	e	304	JCV	C72M-C72-C73-C74
9	e	305	JCV	C26M-C26-C27-C28
9	e	305	JCV	C61M-C61-C62-C63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	S	301	JCV	C28-C29-C30-C30M
9	S	301	JCV	C63-C64-C65-C65M
9	W	101	JCV	C63-C64-C65-C65M
9	e	304	JCV	C31-C32-OG6-CG8
9	W	101	JCV	C57-C58-C59-C60
9	C	301	JCV	CG2-CG3-OG3-C1
9	S	301	JCV	CG2-CG3-OG3-C1
9	U	305	JCV	CG2-CG3-OG3-C1
9	U	304	JCV	C78-C79-C80-C81
9	e	305	JCV	O1-CG1-CG2-OG2
9	g	101	JCV	C27-C28-C29-C30
9	S	301	JCV	C62-C63-C64-C65
9	C	301	JCV	OG4-CG6-CG8-OG6
9	e	305	JCV	OG4-CG6-CG8-OG6
9	e	305	JCV	C1-C2-C3-C4
9	C	301	JCV	CG7-CG6-CG8-OG6
9	C	301	JCV	C13-C14-C15-C16
9	C	301	JCV	C28-C29-C30-C31
9	C	301	JCV	C60-C61-C62-C63
9	E	305	JCV	C56-C57-C58-C59
9	E	306	JCV	C63-C64-C65-C66
9	c	301	JCV	C66-C67-C68-C69
9	e	304	JCV	C13-C14-C15-C16
9	e	304	JCV	C59-C60-C61-C62
9	S	301	JCV	C14-C15-C16-C17
9	U	304	JCV	C59-C60-C61-C62
9	W	101	JCV	C16-C17-C18-C19
9	E	306	JCV	CX1-O4-P-O1
9	c	301	JCV	C74-C75-C76-C76M
9	e	304	JCV	C74-C75-C76-C76M
9	S	301	JCV	C22M-C22-C23-C24
9	S	301	JCV	C66-C67-C68-C68M
9	U	305	JCV	C7M-C7-C8-C9
9	U	305	JCV	C70-C71-C72-C72M
9	W	101	JCV	C26M-C26-C27-C28
9	g	101	JCV	C31-C32-OG6-CG8
9	g	101	JCV	C81-C82-OG4-CG6
9	E	305	JCV	C26-C27-C28-C29
9	g	101	JCV	C23-C24-C25-C26
9	E	306	JCV	C31-C32-OG6-CG8
9	C	301	JCV	C11M-C11-C12-C13
9	E	304	JCV	C3M-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	E	306	JCV	C63-C64-C65-C65M
9	c	301	JCV	C66-C67-C68-C68M
9	e	304	JCV	C26M-C26-C27-C28
9	U	305	JCV	C5-C6-C7-C7M
9	C	301	JCV	C53-C54-C55-C56
9	C	301	JCV	C73-C74-C75-C76
9	c	301	JCV	CG7-CG6-CG8-OG6
9	e	305	JCV	CG8-CG6-CG7-OY1
9	E	305	JCV	C3-C4-C5-C6
9	E	306	JCV	CX1-O4-P-O3
9	C	301	JCV	C20-C21-C22-C23
9	E	306	JCV	C74-C75-C76-C77
9	g	101	JCV	C21-C22-C23-C24
9	g	101	JCV	C6-C7-C8-C9
9	U	304	JCV	C2-C3-C4-C5
9	U	305	JCV	C75-C76-C77-C78
9	e	305	JCV	CG2-CG3-OG3-C1
9	C	301	JCV	C3-C4-C5-C6
9	c	301	JCV	C11-C12-C13-C14
9	W	101	JCV	C12-C13-C14-C15
9	W	101	JCV	C31-C32-OG6-CG8
9	c	301	JCV	C65-C66-C67-C68
11	E	303[B]	COM	S1-C1-C2-S2
9	E	305	JCV	C57M-C57-C58-C59
9	E	306	JCV	C59-C60-C61-C61M
9	S	301	JCV	C58-C59-C60-C61
9	e	304	JCV	CY4-CY5-CY6-OY6
9	U	305	JCV	C27-C28-C29-C30
9	U	305	JCV	C4-C5-C6-C7
9	E	306	JCV	C52-C51-OG2-CG2
9	S	301	JCV	C52-C51-OG2-CG2
9	U	305	JCV	CG6-CG7-OY1-CY1
9	e	305	JCV	C76-C77-C78-C79
9	U	304	JCV	C3-C4-C5-C6
9	g	101	JCV	C2-C1-OG3-CG3
9	W	101	JCV	C4-C5-C6-C7
9	E	306	JCV	C75-C76-C77-C78
9	e	304	JCV	C78-C79-C80-C81
9	e	305	JCV	C66-C67-C68-C69
9	S	301	JCV	C10-C11-C12-C13
9	U	304	JCV	C20-C21-C22-C23
9	W	101	JCV	C55-C56-C57-C58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	E	306	JCV	C73-C74-C75-C76
9	E	304	JCV	C61M-C61-C62-C63
9	e	304	JCV	C65M-C65-C66-C67
9	g	101	JCV	C7M-C7-C8-C9
9	W	101	JCV	C28-C29-C30-C30M
9	g	101	JCV	C79-C80-C81-C82
9	E	306	JCV	CG1-CG2-CG3-OG3
9	e	304	JCV	CG7-CG6-CG8-OG6
9	C	301	JCV	C77-C78-C79-C80
9	e	304	JCV	C22-C23-C24-C25
9	E	305	JCV	OG4-CG6-CG8-OG6
9	E	306	JCV	OG2-CG2-CG3-OG3
9	e	305	JCV	OG2-CG2-CG3-OG3
9	g	101	JCV	C24-C25-C26-C27
9	U	305	JCV	C60-C61-C62-C63
9	C	301	JCV	C9-C10-C11-C11M
9	E	305	JCV	C24-C25-C26-C26M
9	c	301	JCV	C22M-C22-C23-C24
9	e	304	JCV	C59-C60-C61-C61M
9	e	305	JCV	C53M-C53-C54-C55
9	e	305	JCV	C59-C60-C61-C61M
9	g	101	JCV	C24-C25-C26-C26M
9	g	101	JCV	C74-C75-C76-C76M
9	S	301	JCV	C16-C17-C18-C18M
9	U	304	JCV	C59-C60-C61-C61M
9	U	305	JCV	C74-C75-C76-C76M
9	c	301	JCV	C30-C31-C32-OG6
9	e	304	JCV	C30-C31-C32-OG6
9	e	304	JCV	C61-C62-C63-C64
9	e	305	JCV	OG3-C1-C2-C3
9	g	101	JCV	C80-C81-C82-OG4
9	E	304	JCV	C78-C79-C80-C80M
9	E	306	JCV	C7M-C7-C8-C9
9	E	306	JCV	C76M-C76-C77-C78
9	S	301	JCV	C70-C71-C72-C72M
9	U	304	JCV	C61M-C61-C62-C63
9	W	101	JCV	C18M-C18-C19-C20
9	S	301	JCV	C72-C73-C74-C75
9	E	304	JCV	C12-C13-C14-C15
9	E	304	JCV	C78-C79-C80-C81
9	E	305	JCV	C13-C14-C15-C16
9	E	305	JCV	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

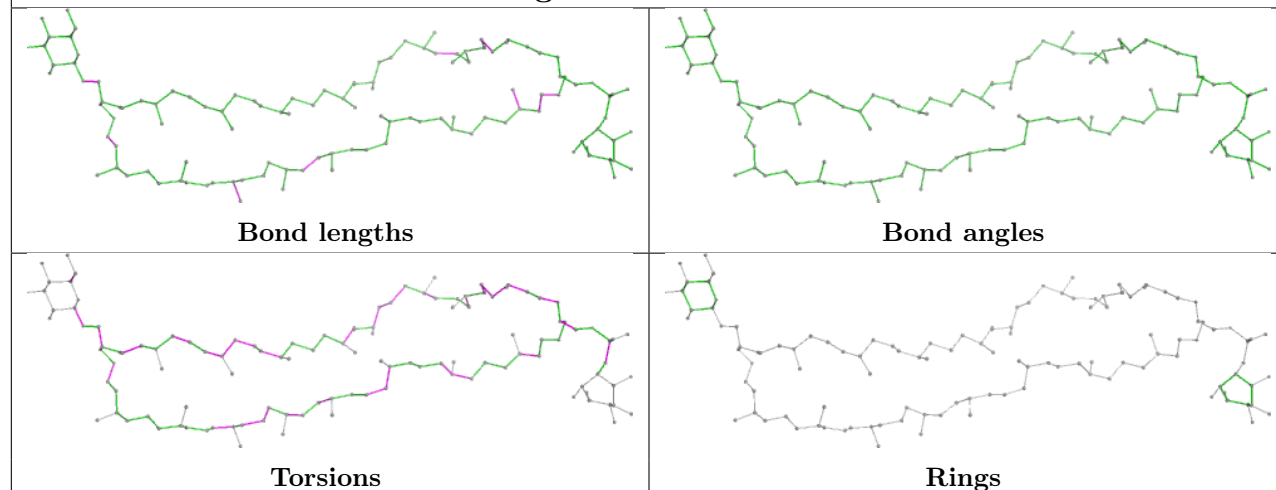
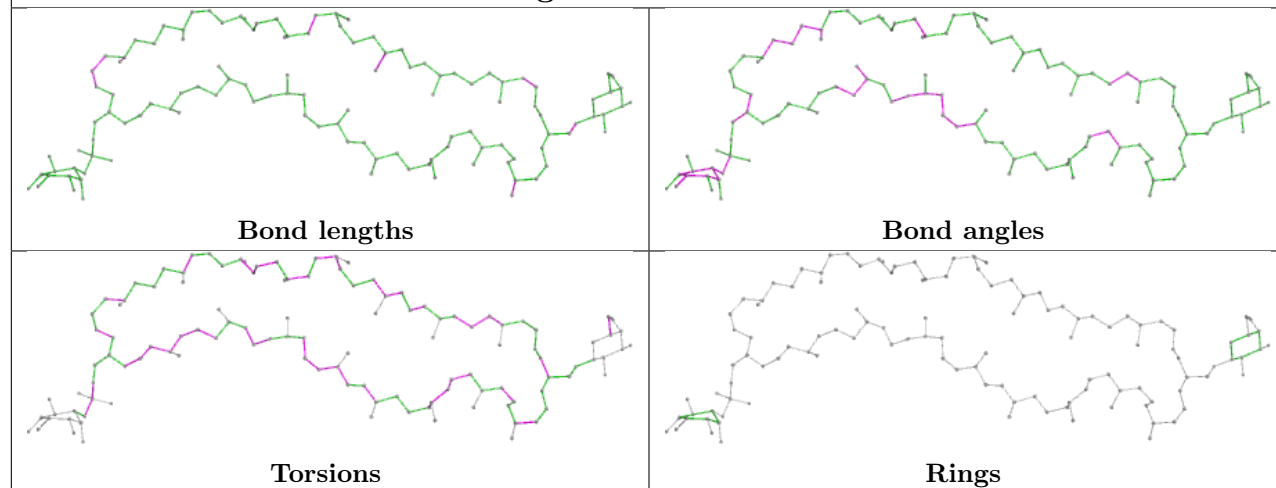
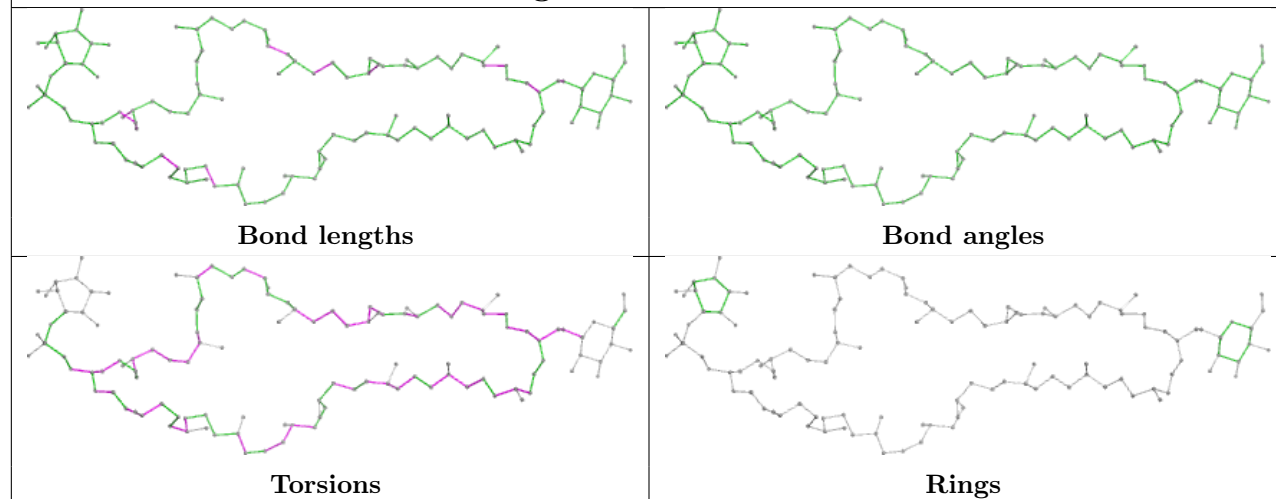
Mol	Chain	Res	Type	Atoms
9	E	306	JCV	C14-C15-C16-C17
9	c	301	JCV	C21-C22-C23-C24
9	g	101	JCV	C16-C17-C18-C19
9	g	101	JCV	C70-C71-C72-C73
9	U	305	JCV	C74-C75-C76-C77
9	U	305	JCV	C78-C79-C80-C81
9	W	101	JCV	C28-C29-C30-C31
9	E	305	JCV	OY5-CY1-OY1-CG7
9	U	305	JCV	C22-C23-C24-C25
9	E	306	JCV	C62-C63-C64-C65

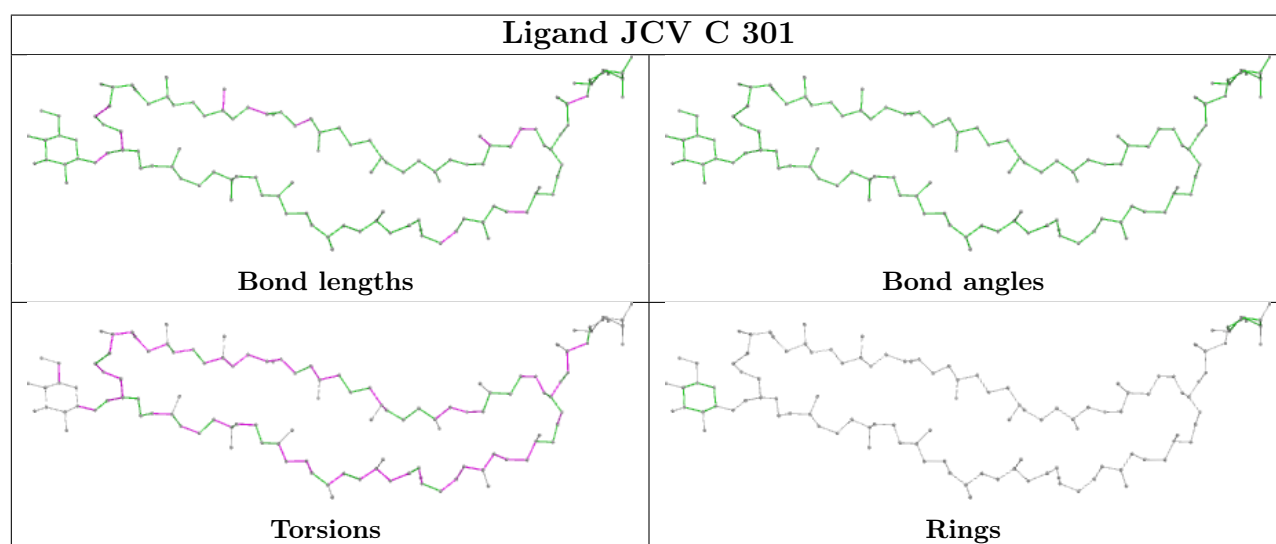
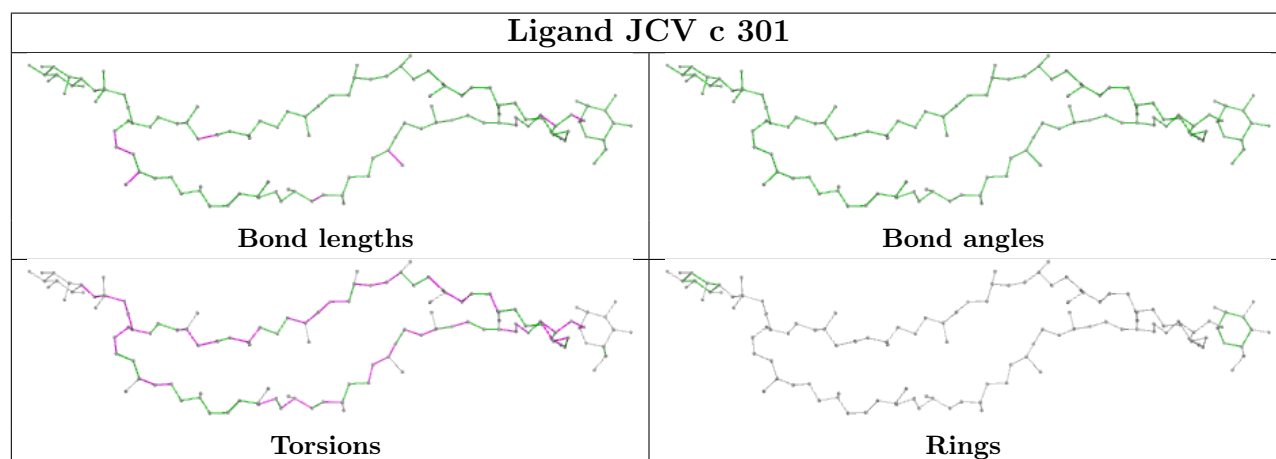
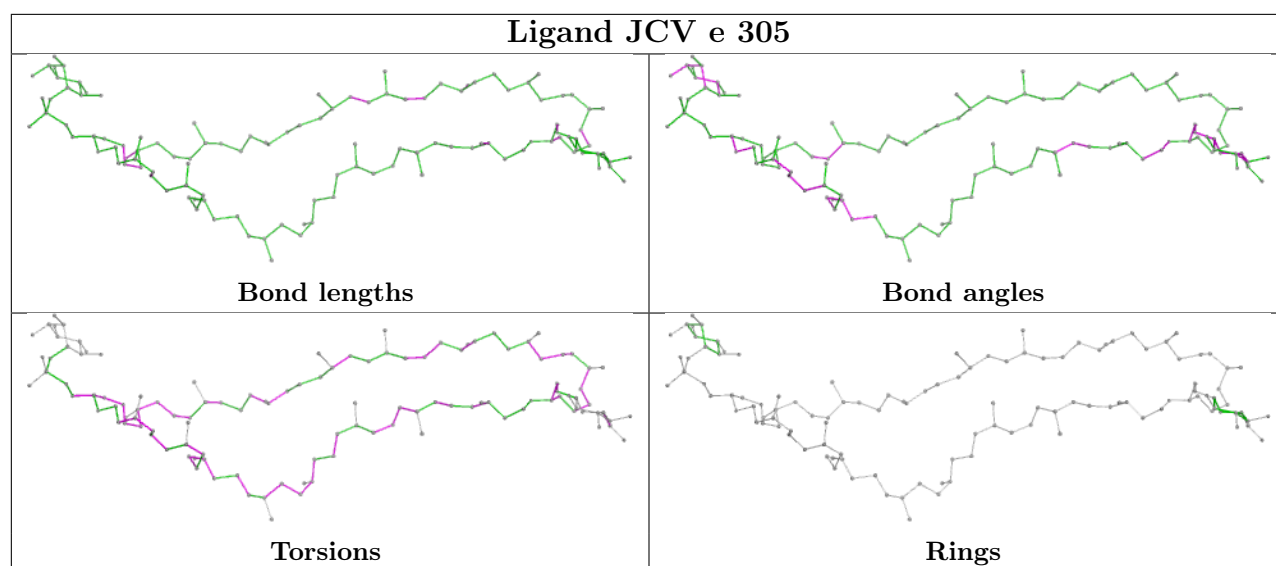
There are no ring outliers.

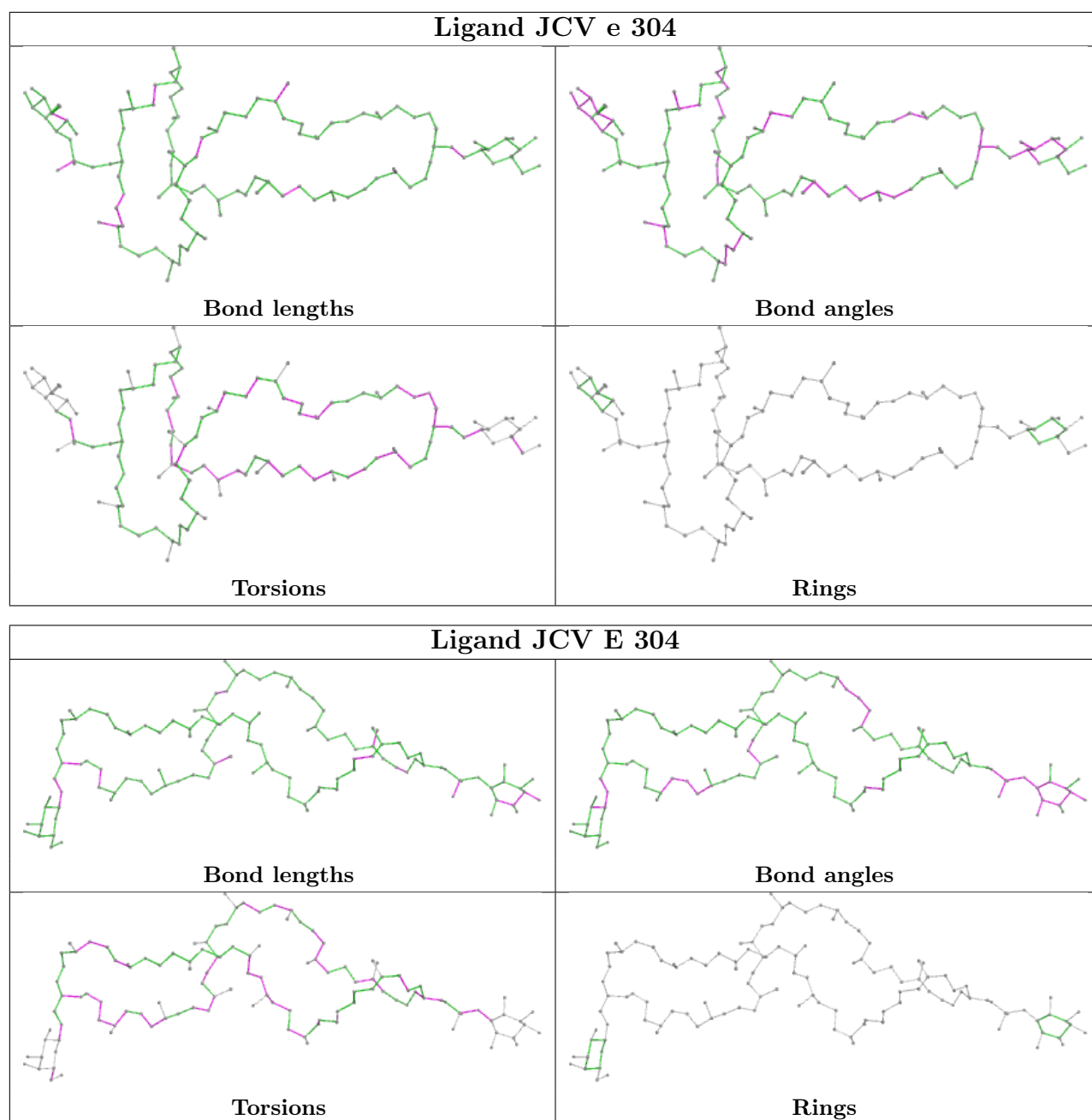
13 monomers are involved in 36 short contacts:

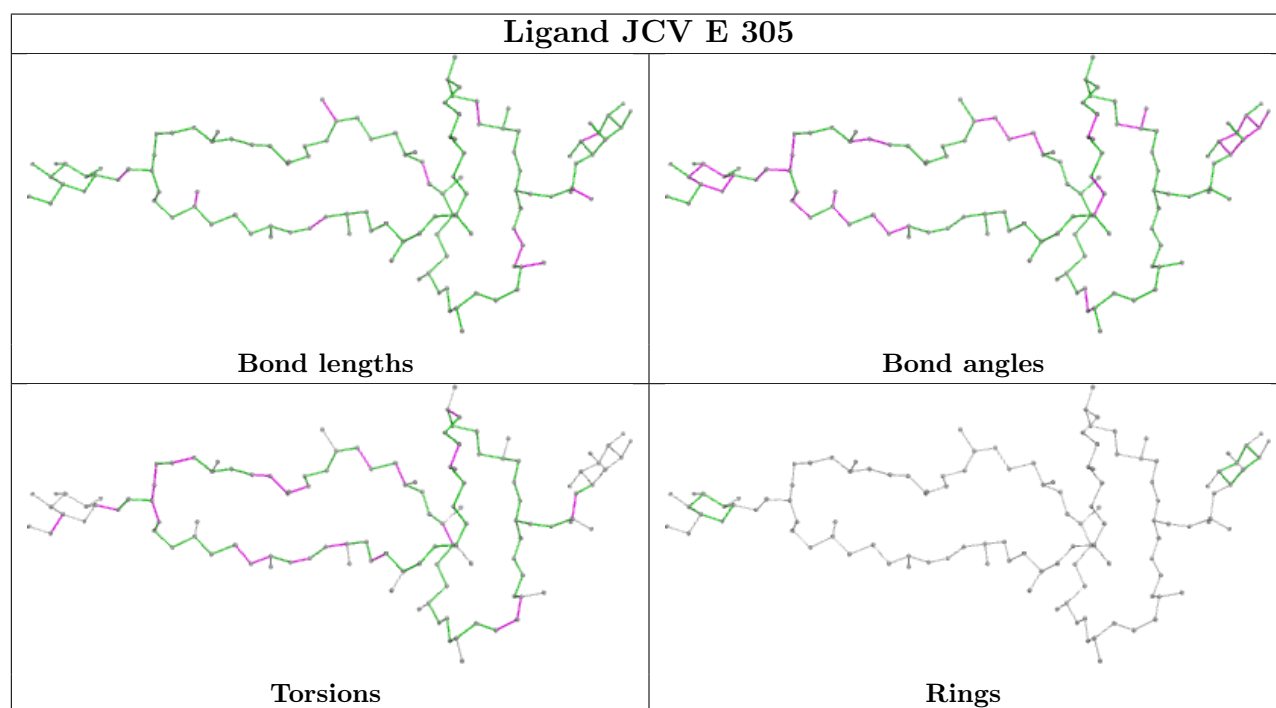
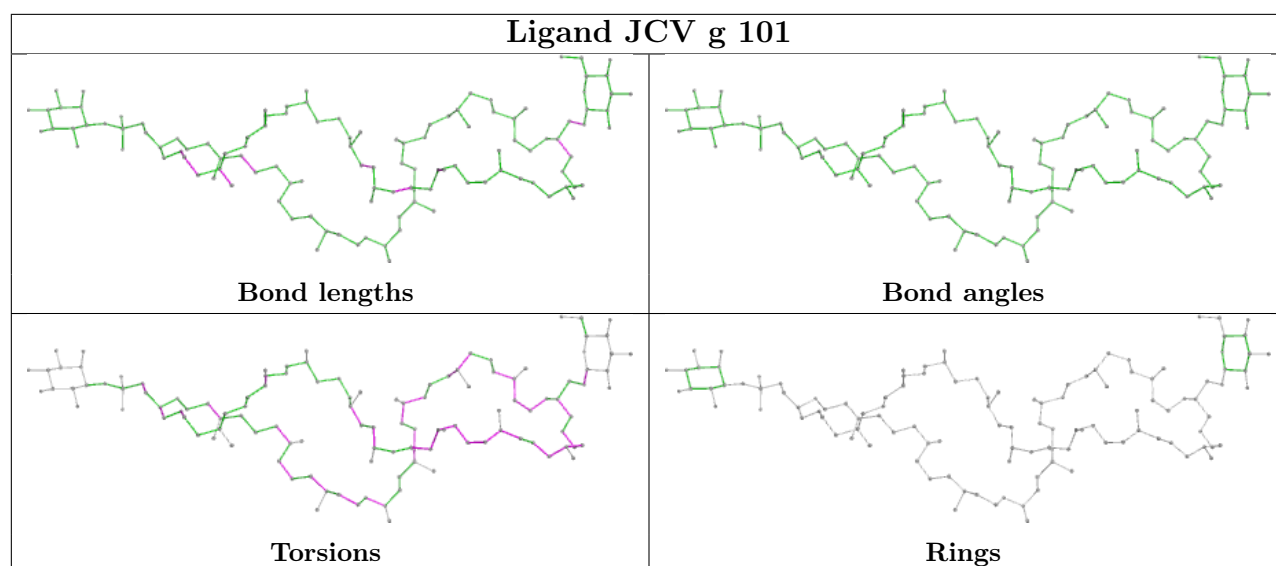
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E	306	JCV	1	0
9	S	301	JCV	10	0
11	U	303[A]	COM	3	0
9	e	305	JCV	8	0
9	c	301	JCV	1	0
11	E	303[B]	COM	1	0
9	C	301	JCV	1	0
11	e	303[B]	COM	1	0
9	E	304	JCV	7	0
11	U	303[C]	COM	1	0
11	e	303[A]	COM	1	0
9	U	304	JCV	1	0
9	W	101	JCV	2	0

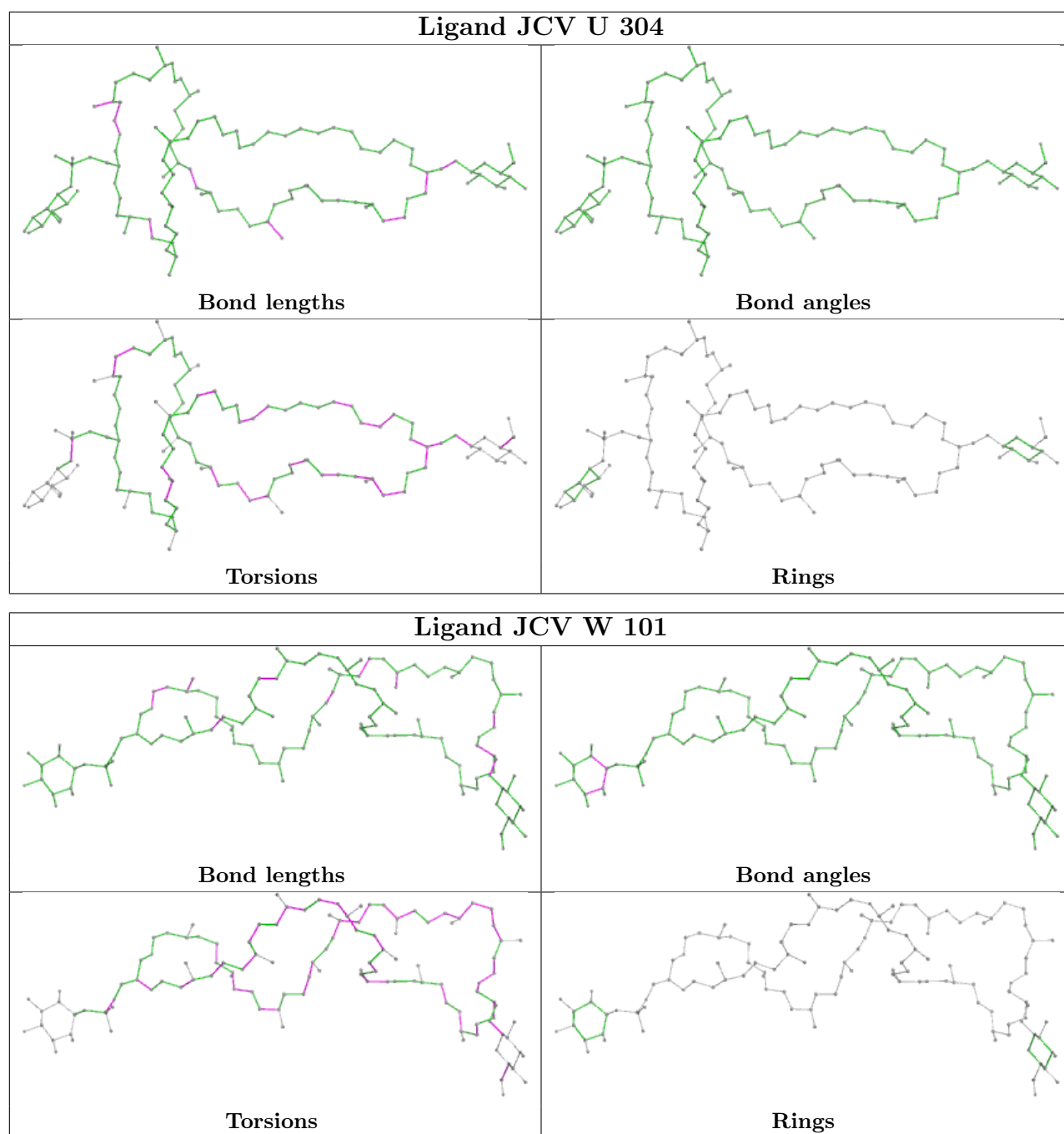
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand JCV E 306**Ligand JCV S 301****Ligand JCV U 305**









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.

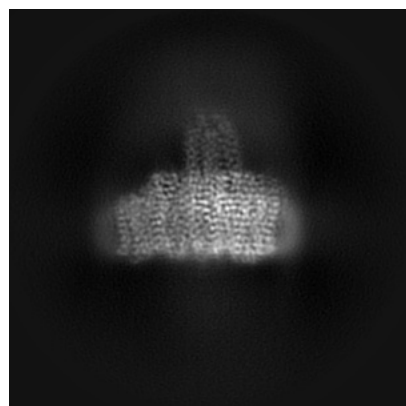
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18162. These allow visual inspection of the internal detail of the map and identification of artifacts.

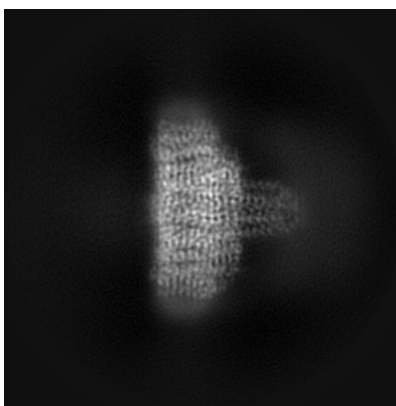
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

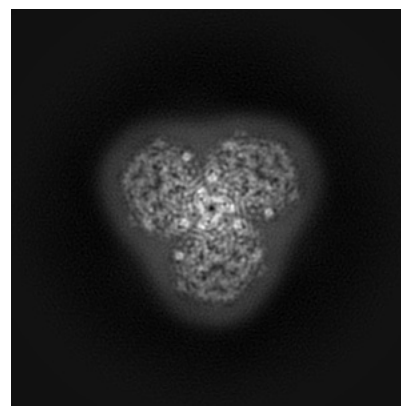
6.1.1 Primary map



X

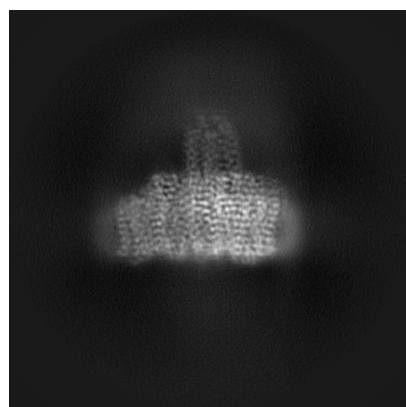


Y

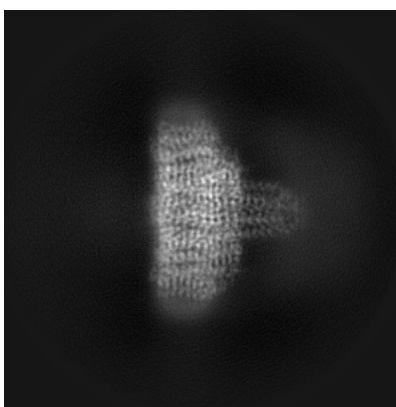


Z

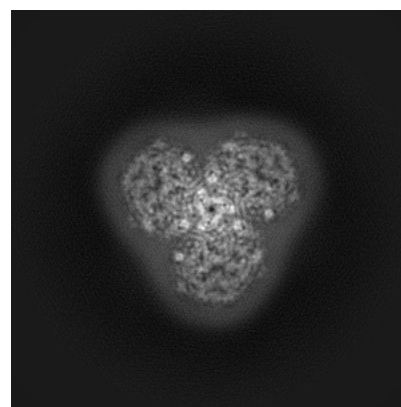
6.1.2 Raw map



X



Y

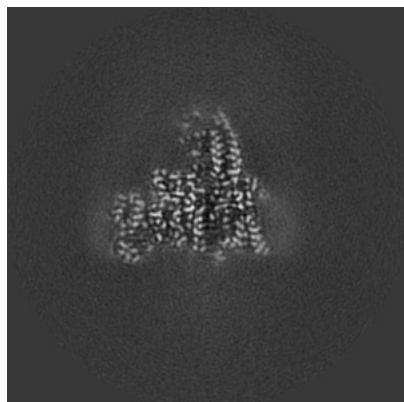


Z

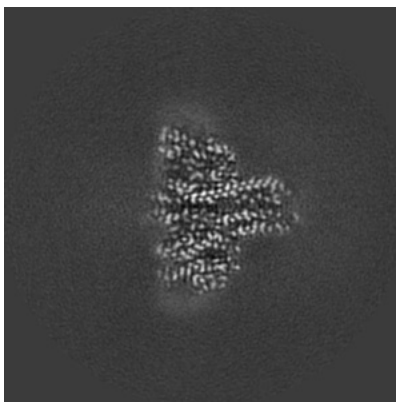
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

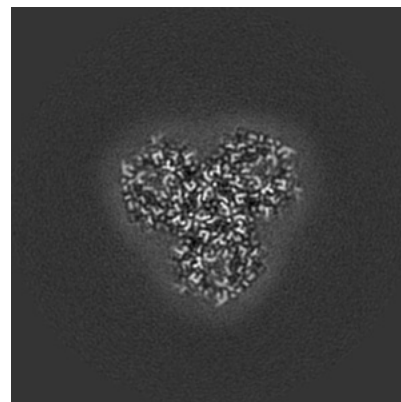
6.2.1 Primary map



X Index: 160

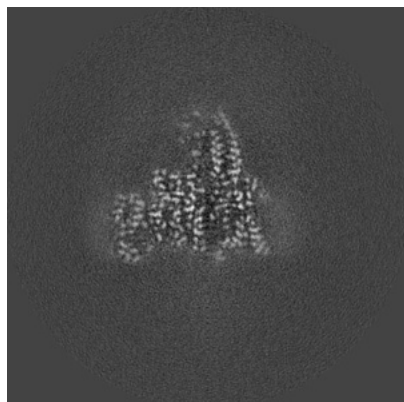


Y Index: 160

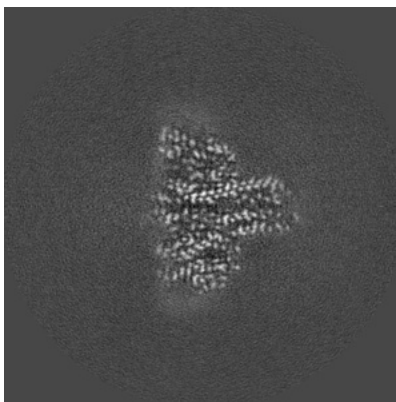


Z Index: 160

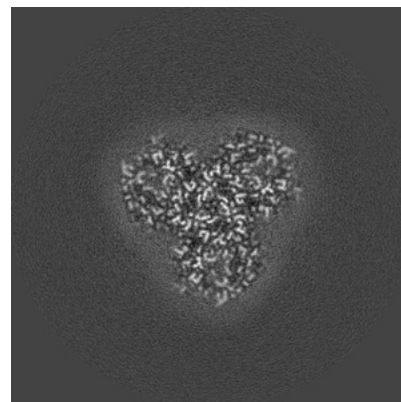
6.2.2 Raw map



X Index: 160



Y Index: 160

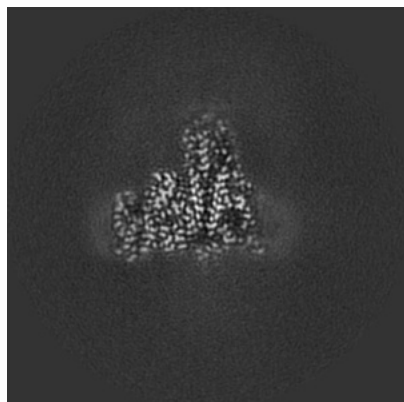


Z Index: 160

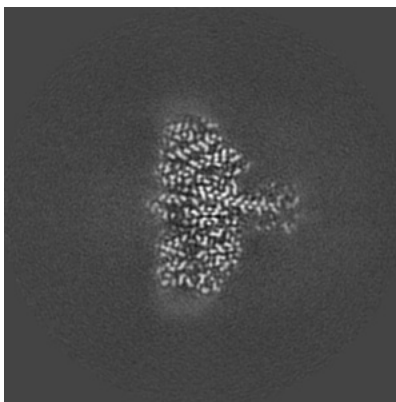
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

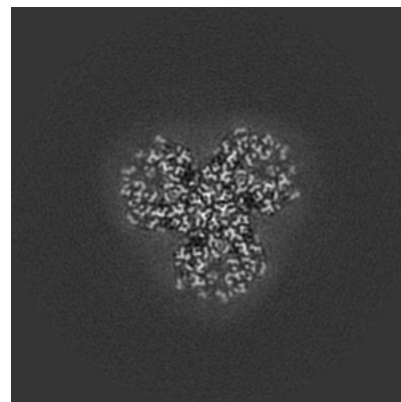
6.3.1 Primary map



X Index: 155

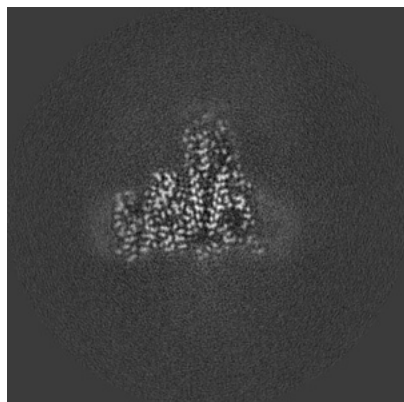


Y Index: 167

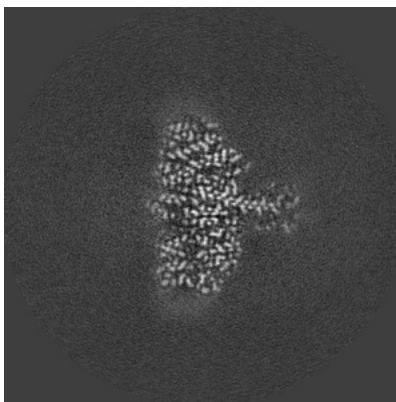


Z Index: 165

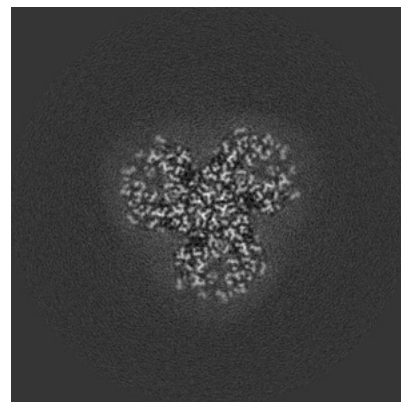
6.3.2 Raw map



X Index: 155



Y Index: 167

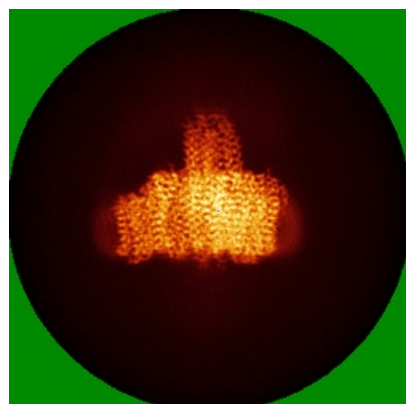


Z Index: 165

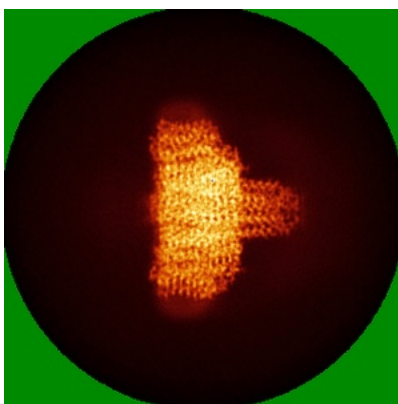
The images above show the largest variance slices of the map in three orthogonal directions.

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

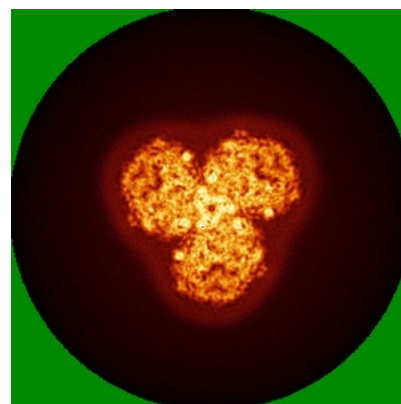
6.4.1 Primary map



X

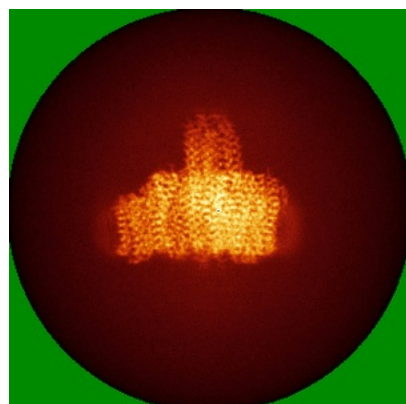


Y

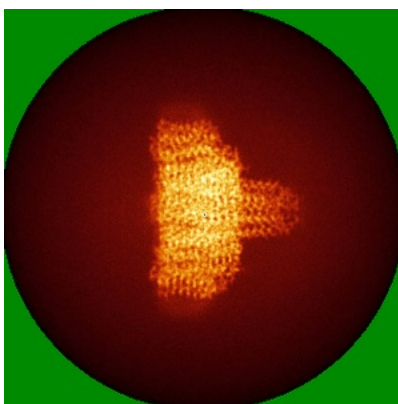


Z

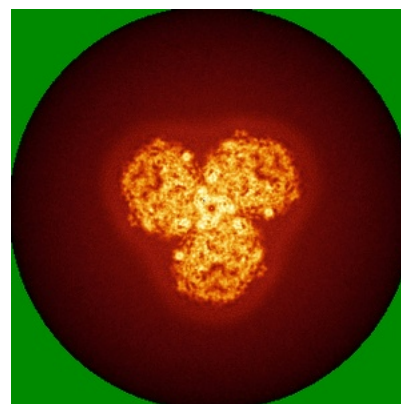
6.4.2 Raw map



X



Y

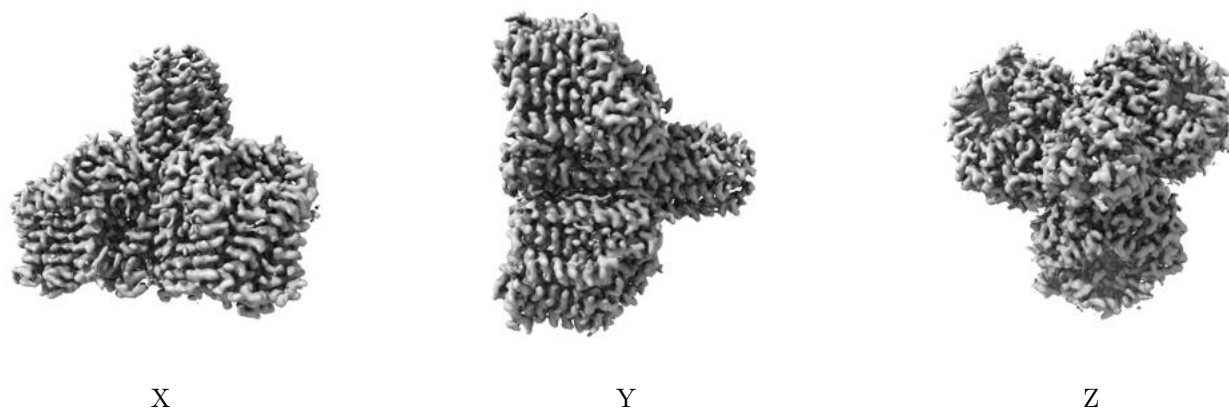


Z

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

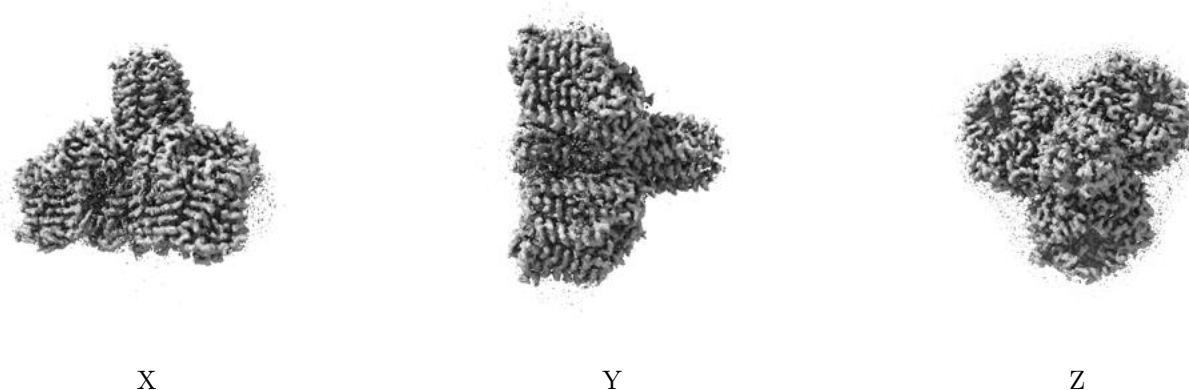
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

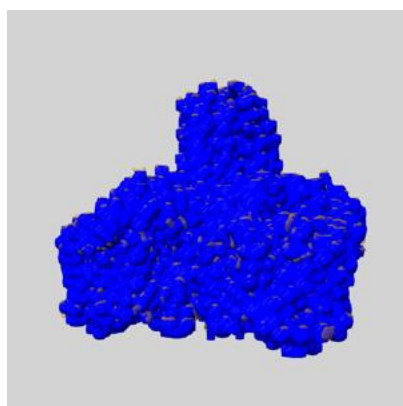
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

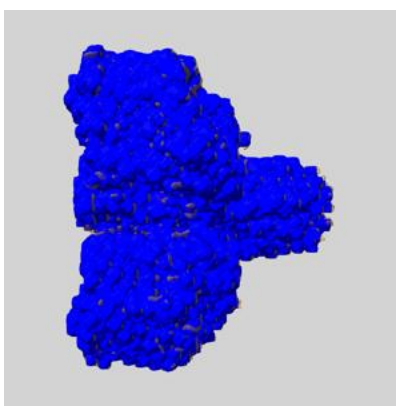
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

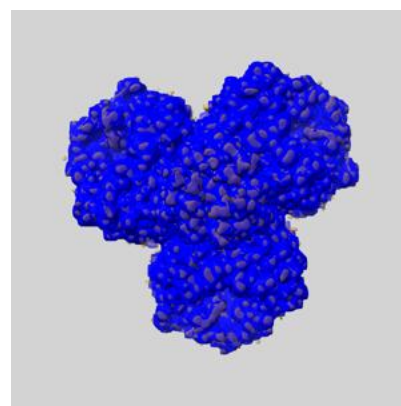
6.6.1 emd_18162_msk_1.map [i](#)



X



Y

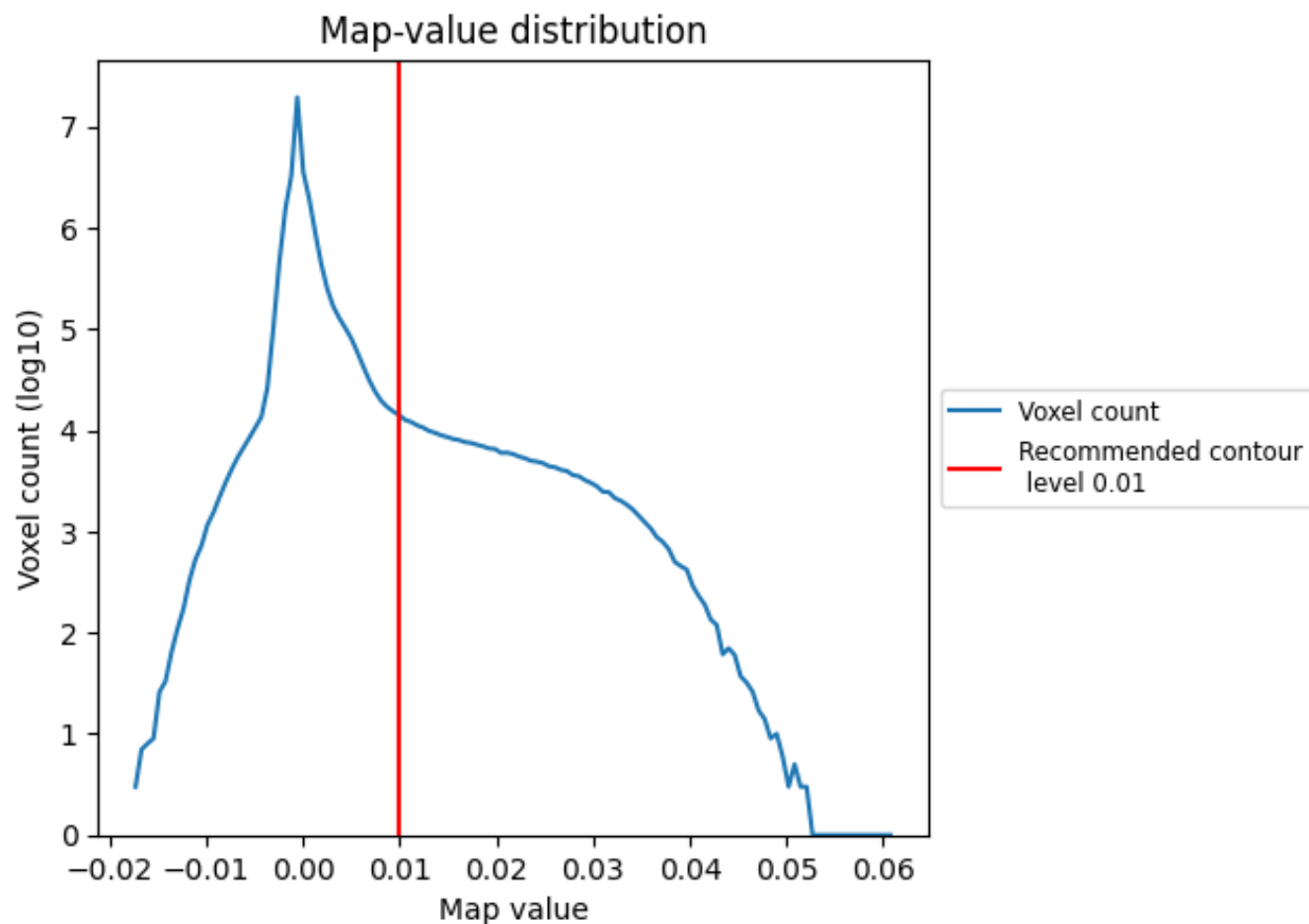


Z

7 Map analysis [i](#)

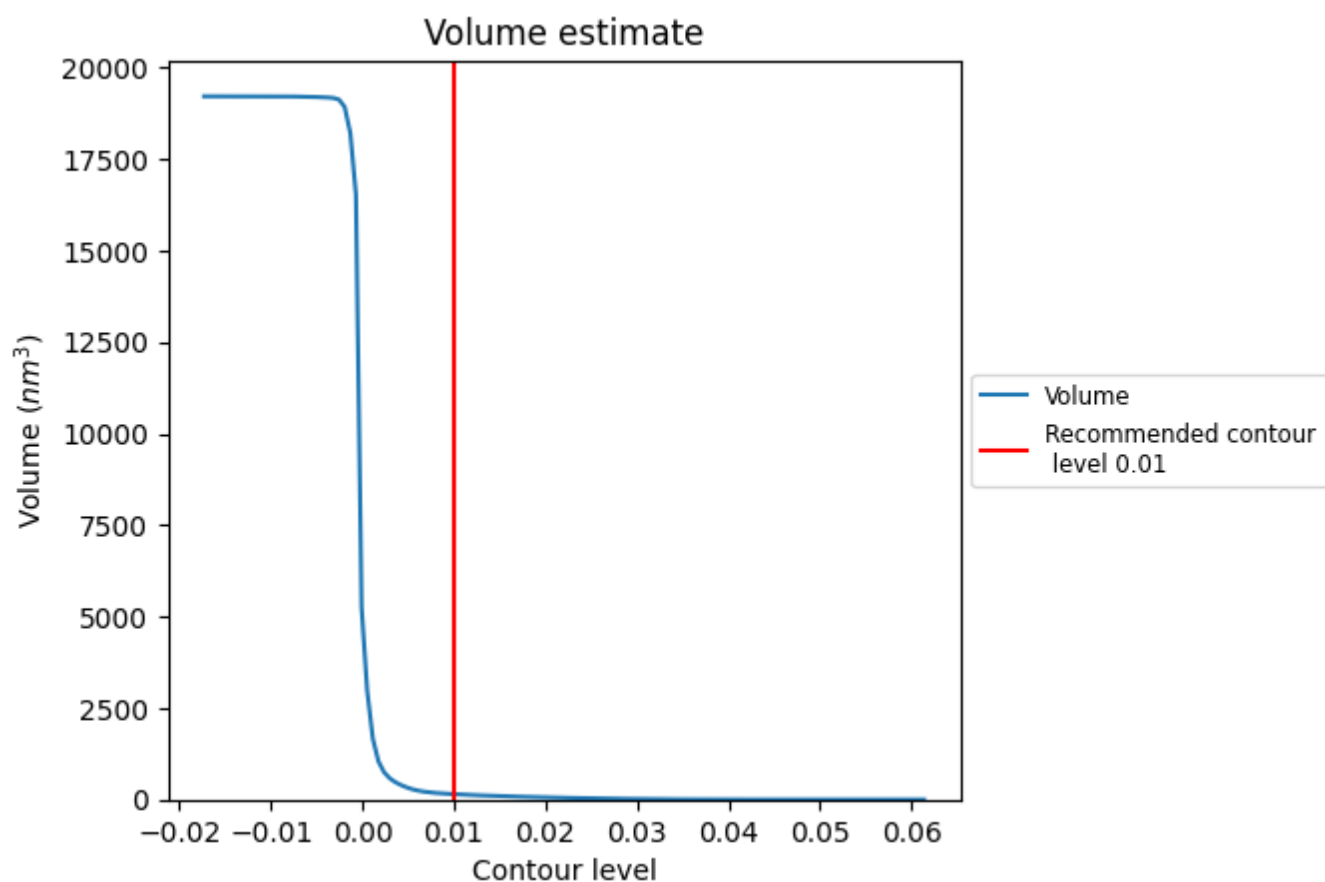
This section contains the results of statistical analysis of the map.

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.

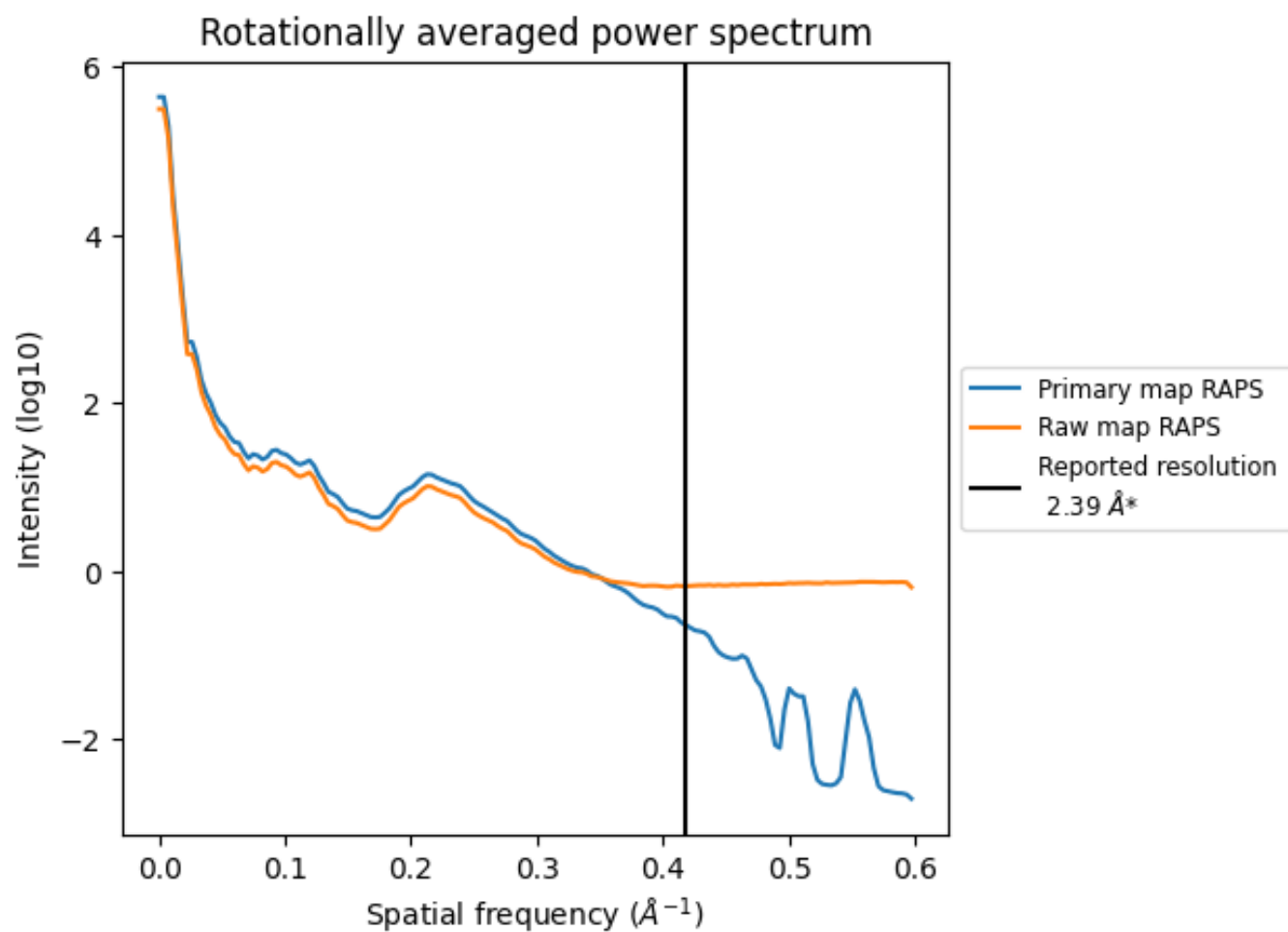
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 148 nm³; this corresponds to an approximate mass of 133 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 ⓘ

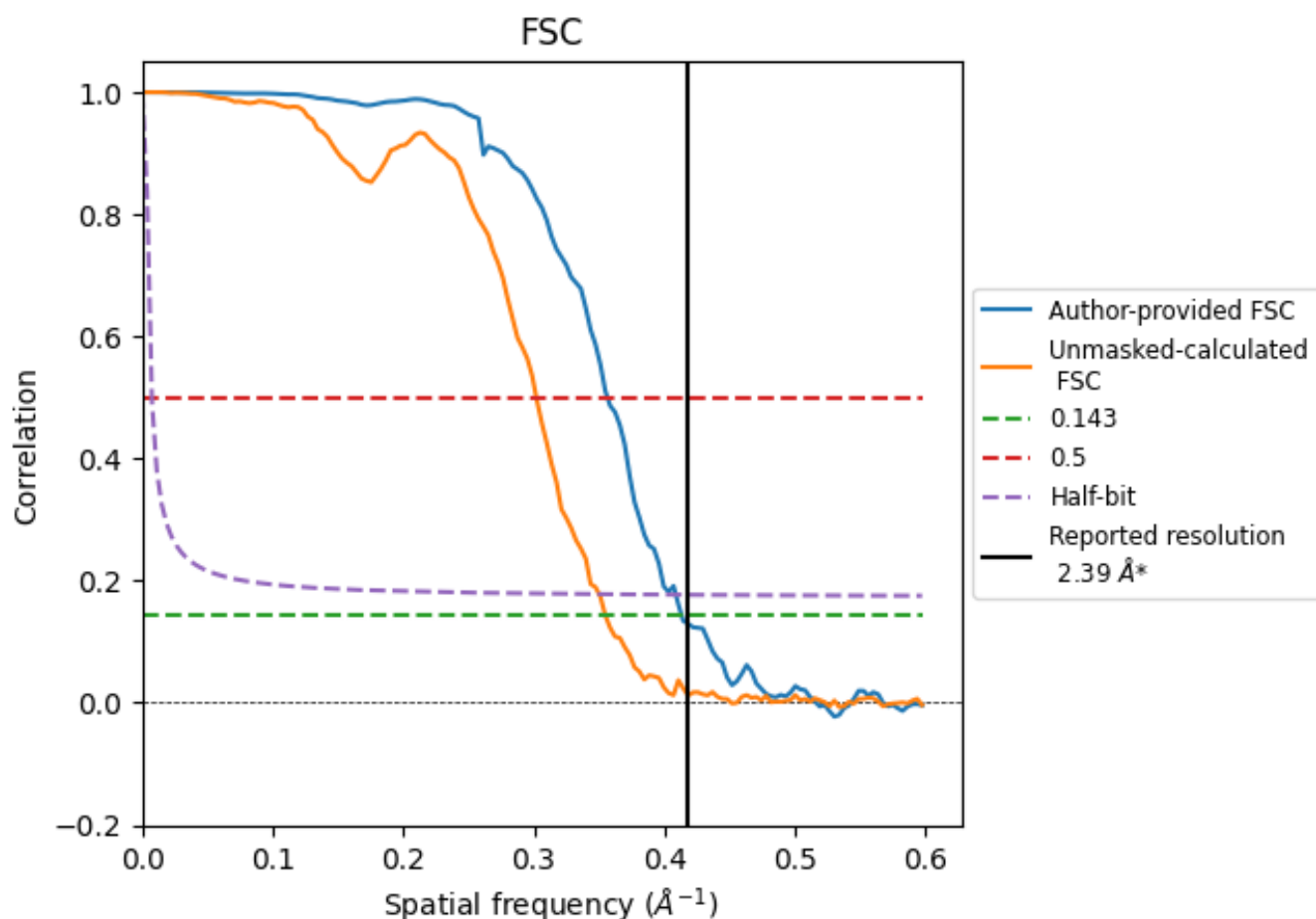


*Reported resolution corresponds to spatial frequency of 0.418 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.418 \AA^{-1}

8.2 Resolution estimates [i](#)

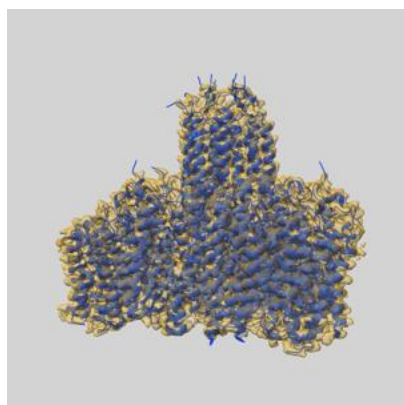
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.39	-	-
Author-provided FSC curve	2.42	2.81	2.45
Unmasked-calculated*	2.82	3.31	2.86

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.82 differs from the reported value 2.39 by more than 10 %

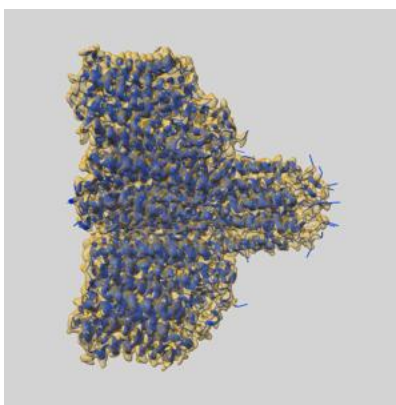
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18162 and PDB model 8Q54. Per-residue inclusion information can be found in section [3](#) on page [9](#).

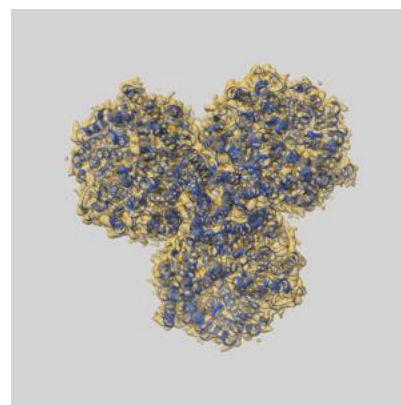
9.1 Map-model overlay [i](#)



X



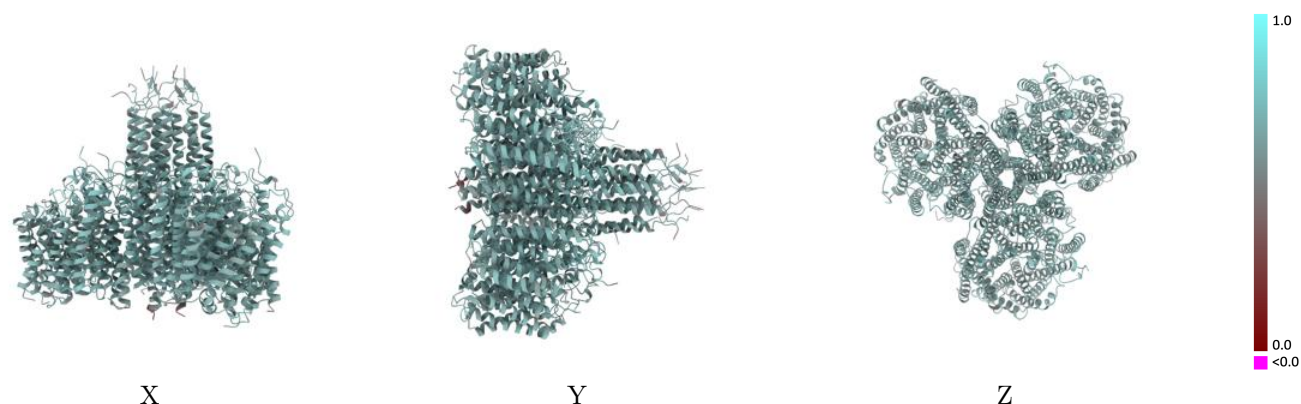
Y



Z

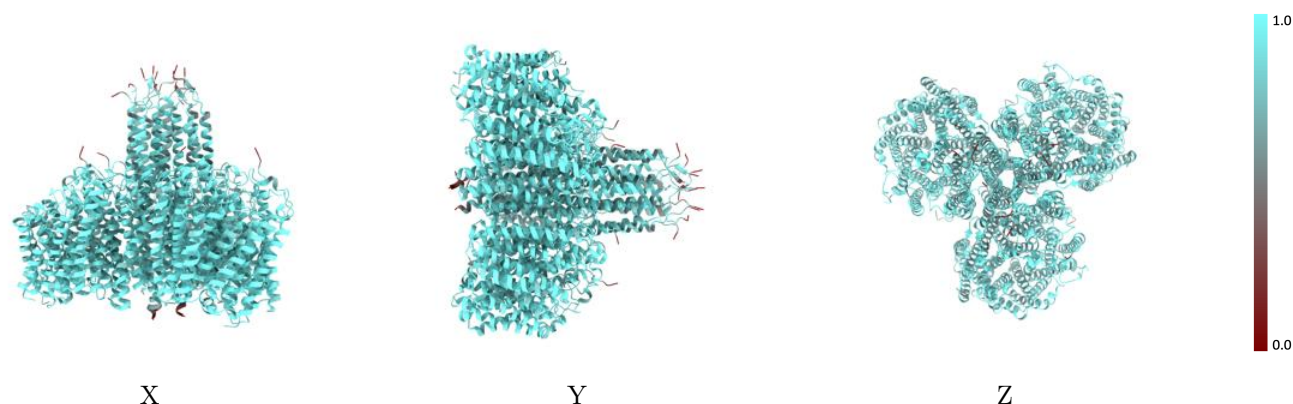
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



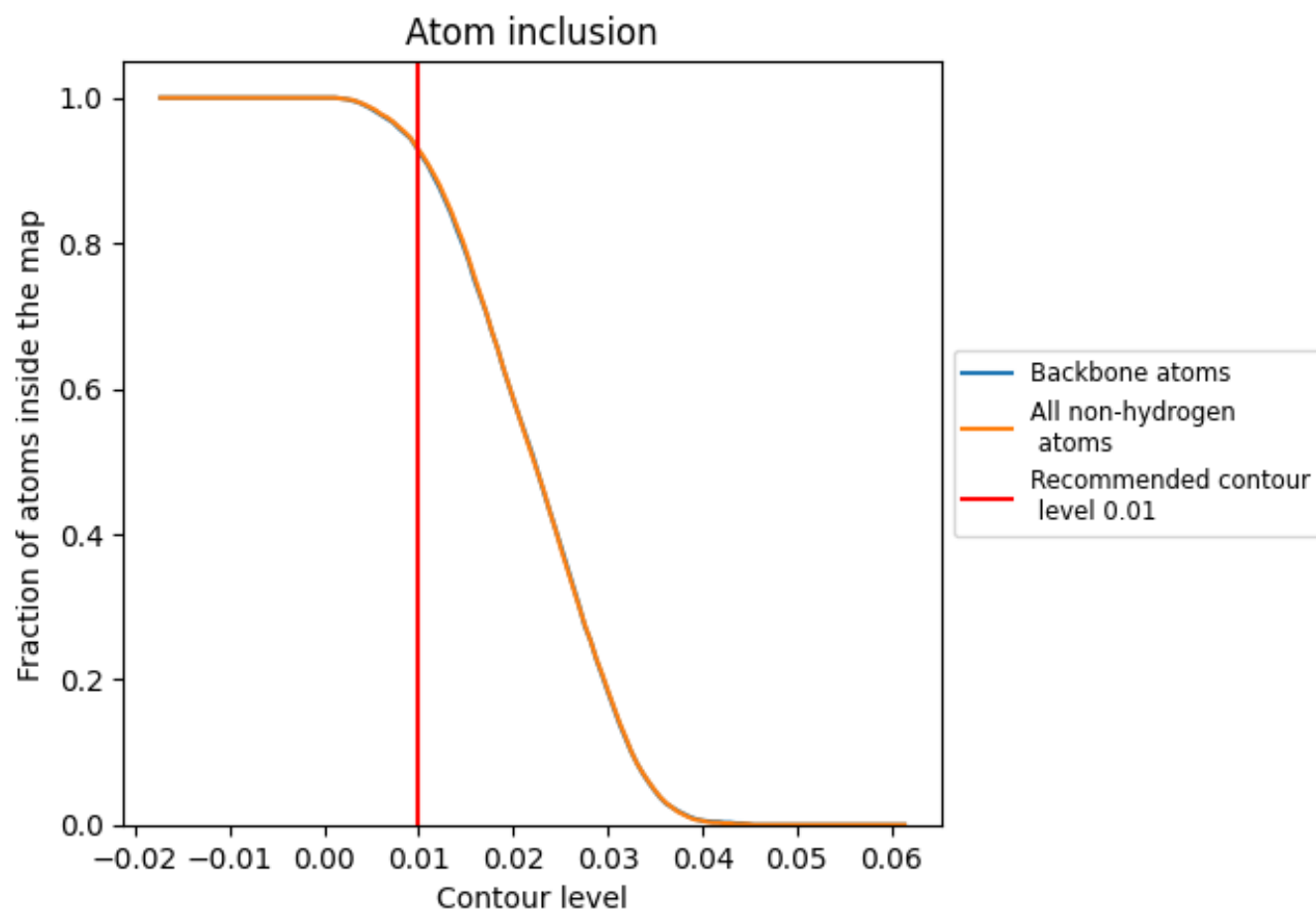
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.01).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 93% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9280	 0.6320
A	 0.9250	 0.6360
B	 0.9090	 0.6340
C	 0.9110	 0.6160
D	 0.9600	 0.6290
E	 0.9270	 0.6430
F	 0.8970	 0.6350
G	 0.8500	 0.6140
Q	 0.9190	 0.6440
R	 0.9130	 0.6370
S	 0.9210	 0.6130
T	 0.9630	 0.6370
U	 0.9380	 0.6490
V	 0.8990	 0.6270
W	 0.8170	 0.6080
a	 0.9230	 0.6420
b	 0.9180	 0.6350
c	 0.9130	 0.6180
d	 0.9670	 0.6370
e	 0.9410	 0.6490
f	 0.8950	 0.6300
g	 0.8140	 0.6100

