



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:45 AM UTC

PDB ID : 3J9F / pdb_00003j9f
EMDB ID : EMD-6243
Title : Poliovirus complexed with soluble, deglycosylated poliovirus receptor (Pvr) at 4 degrees C
Authors : Strauss, M.; Filman, D.J.; Belnap, D.M.; Cheng, N.; Noel, R.T.; Hogle, J.M.
Deposited on : 2015-01-15
Resolution : 9.00 Å(reported)
Based on initial model : 1HXS

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

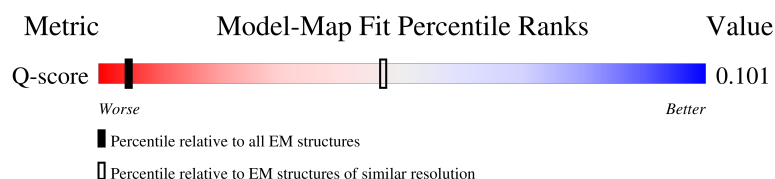
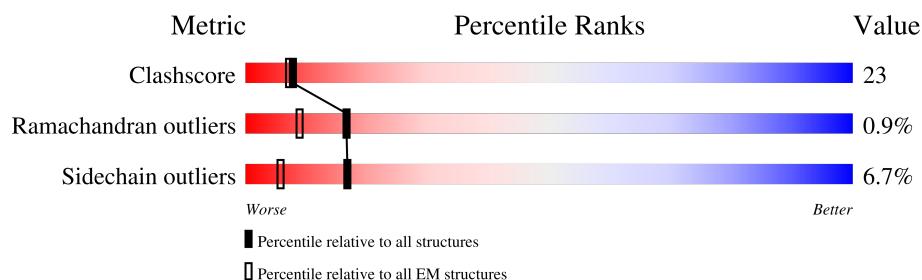
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



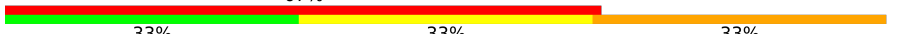
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	257 (8.50 - 9.50)

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	1	302	
2	2	272	
3	3	238	
4	4	69	

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Mol	Chain	Length	Quality of chain
5	7	116	
6	8	102	
7	9	92	
8	A	3	
8	E	3	
9	B	5	
10	C	2	
10	D	2	
11	F	4	

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	NAG	F	1	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 9313 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	283	Total	C	N	O	S	0	0
			2221	1416	378	422	5		

- Molecule 2 is a protein called Protein VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	267	Total	C	N	O	S	0	0
			2075	1312	357	392	14		

- Molecule 3 is a protein called Protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	235	Total	C	N	O	S	0	0
			1834	1169	299	349	17		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	123	SER	PHE	conflict	UNP P03300

- Molecule 4 is a protein called Protein VP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	69	Total	C	N	O	S	0	0
			534	333	91	109	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	1	MYR	-	modified residue	UNP P03300

- Molecule 5 is a protein called Poliovirus receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	7	116	Total	C	N	O	S	2	0
			904	572	159	168	5		

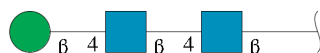
- Molecule 6 is a protein called Poliovirus receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	8	102	Total	C	N	O	S	4	0
			771	489	130	148	4		

- Molecule 7 is a protein called Poliovirus receptor.

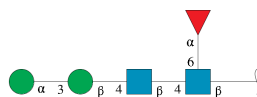
Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	92	Total	C	N	O	S	2	0
			699	440	118	138	3		

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
8	A	3	Total	C	N	O	0	0
			39	22	2	15		
8	E	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



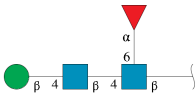
Mol	Chain	Residues	Atoms				AltConf	Trace
9	B	5	Total	C	N	O	0	0
			60	34	2	24		

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



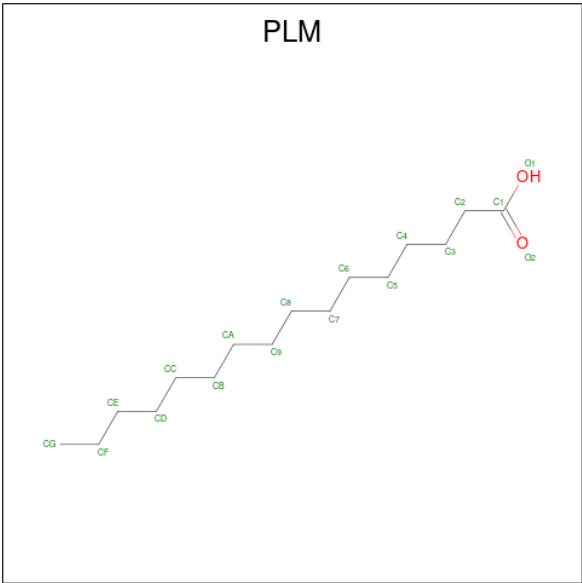
Mol	Chain	Residues	Atoms				AltConf	Trace
10	C	2	Total	C	N	O	0	0
			28	16	2	10		
10	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 11 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
11	F	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 12 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			AltConf
12	1	1	Total	C	O	0
			18	16	2	

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
13	9	1	14	8	1	5	0

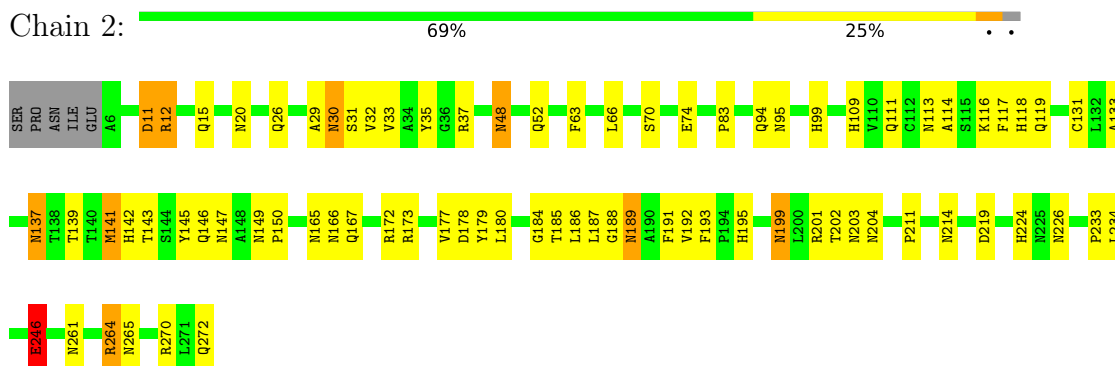
3 Residue-property plots

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.

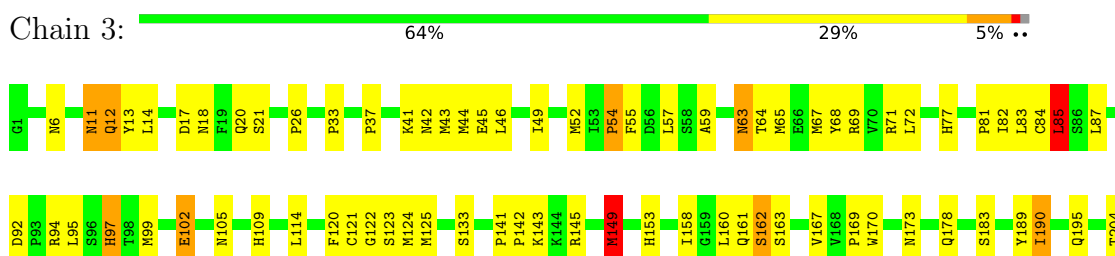
• Molecule 1: Protein VP1

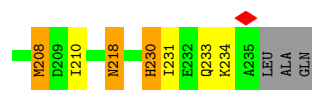


• Molecule 2: Protein VP2



• Molecule 3: Protein VP3

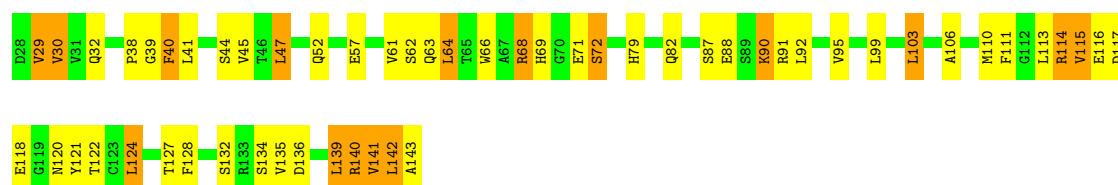




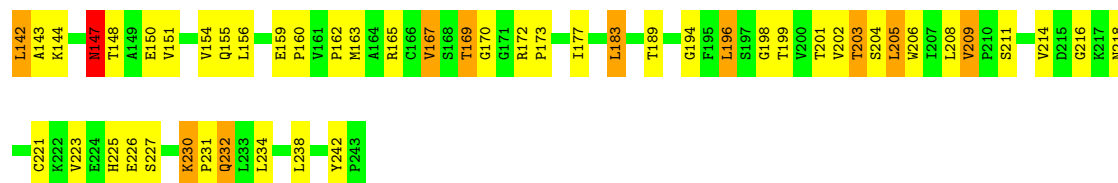
- Molecule 4: Protein VP4



- Molecule 5: Poliovirus receptor



- Molecule 6: Poliovirus receptor



- Molecule 7: Poliovirus receptor



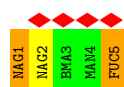
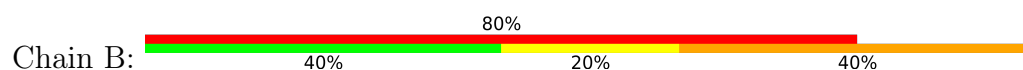
- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	3822	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	318.570	Depositor
Minimum map value	-109.877	Depositor
Average map value	15.762	Depositor
Map value standard deviation	57.866	Depositor
Recommended contour level	59	Depositor
Map size ($\text{\AA}$)	508.51233, 508.51233, 508.51233	wwPDB
Map dimensions	287, 287, 287	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.77182, 1.77182, 1.77182	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, BMA, NAG, FUC, MYR, PLM

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	1	0.97	7/2284 (0.3%)	1.74	49/3124 (1.6%)
2	2	0.95	7/2132 (0.3%)	1.76	51/2916 (1.7%)
3	3	1.07	10/1881 (0.5%)	1.97	39/2562 (1.5%)
4	4	1.12	1/528 (0.2%)	2.08	21/714 (2.9%)
5	7	0.98	0/925	0.84	1/1258 (0.1%)
6	8	0.98	0/790	0.79	2/1083 (0.2%)
7	9	0.77	0/717	0.72	0/987
All	All	0.98	25/9257 (0.3%)	1.63	163/12644 (1.3%)

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
2	2	0	1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	42	ASN	C-N	15.84	1.55	1.33
3	3	230	HIS	CD2-NE2	-7.11	1.30	1.37
3	3	109	HIS	CD2-NE2	-6.98	1.30	1.37
3	3	97	HIS	CD2-NE2	-6.83	1.30	1.37
3	3	12	GLN	C-N	6.81	1.42	1.33
3	3	153	HIS	CD2-NE2	-6.71	1.30	1.37
2	2	118	HIS	CD2-NE2	-6.67	1.30	1.37
2	2	109	HIS	CD2-NE2	-6.54	1.30	1.37
1	1	65	HIS	CD2-NE2	-6.52	1.30	1.37
3	3	77	HIS	CD2-NE2	-6.49	1.30	1.37
1	1	69	HIS	CD2-NE2	-6.46	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	224	HIS	CD2-NE2	-6.40	1.30	1.37
1	1	207	HIS	CD2-NE2	-6.20	1.31	1.37
1	1	37	HIS	CD2-NE2	-6.13	1.31	1.37
1	1	265	HIS	CD2-NE2	-6.08	1.31	1.37
2	2	195	HIS	CD2-NE2	-6.05	1.31	1.37
3	3	153	HIS	CG-ND1	-5.99	1.31	1.38
2	2	99	HIS	CD2-NE2	-5.73	1.31	1.37
1	1	248	HIS	CD2-NE2	-5.56	1.31	1.37
2	2	142	HIS	CD2-NE2	-5.46	1.31	1.37
3	3	71	ARG	NE-CZ	5.42	1.39	1.33
2	2	118	HIS	CG-ND1	-5.32	1.32	1.38
1	1	248	HIS	CG-ND1	-5.20	1.32	1.38
3	3	102	GLU	CB-CG	5.14	1.67	1.52
4	4	20	TYR	CA-CB	5.07	1.62	1.53

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	12	GLN	O-C-N	33.52	163.54	122.65
3	3	12	GLN	CA-C-N	-33.40	74.85	122.95
3	3	12	GLN	C-N-CA	-33.40	74.85	122.95
3	3	218	ASN	OD1-CG-ND2	-11.67	110.93	122.60
1	1	83	ARG	NE-CZ-NH2	-10.33	109.90	119.20
2	2	26	GLN	OE1-CD-NE2	-9.95	112.65	122.60
4	4	44	GLN	OE1-CD-NE2	-9.19	113.41	122.60
2	2	165	ASN	CA-CB-CG	-8.89	103.71	112.60
4	4	46	PHE	CA-CB-CG	-8.51	105.29	113.80
2	2	137	ASN	OD1-CG-ND2	-8.24	114.36	122.60
1	1	117	GLN	OE1-CD-NE2	-8.19	114.41	122.60
4	4	31	ASN	OD1-CG-ND2	-8.14	114.45	122.60
3	3	97	HIS	CB-CG-CD2	-8.12	120.64	131.20
4	4	48	GLN	OE1-CD-NE2	-8.01	114.59	122.60
4	4	8	GLN	OE1-CD-NE2	-7.92	114.68	122.60
1	1	266	ILE	N-CA-C	7.92	120.50	108.71
1	1	83	ARG	NE-CZ-NH1	7.91	129.41	121.50
1	1	232	ALA	O-C-N	-7.86	114.68	123.48
3	3	149	MET	CA-CB-CG	7.84	129.77	114.10
4	4	4	GLN	OE1-CD-NE2	-7.82	114.78	122.60
1	1	235	ASN	OD1-CG-ND2	-7.71	114.89	122.60
2	2	261	ASN	OD1-CG-ND2	-7.67	114.93	122.60
3	3	105	ASN	OD1-CG-ND2	-7.61	114.99	122.60
3	3	173	ASN	OD1-CG-ND2	-7.55	115.05	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	48	ASN	OD1-CG-ND2	-7.48	115.12	122.60
1	1	215	VAL	CB-CA-C	-7.45	102.74	110.71
4	4	51	SER	N-CA-C	7.41	121.23	111.75
2	2	219	ASP	CA-CB-CG	7.38	119.98	112.60
1	1	235	ASN	CA-CB-CG	-7.33	105.27	112.60
1	1	53	ASN	OD1-CG-ND2	-7.30	115.30	122.60
1	1	263	PRO	N-CA-CB	7.21	106.96	102.92
2	2	95	ASN	OD1-CG-ND2	-7.20	115.40	122.60
1	1	147	ASN	OD1-CG-ND2	-7.19	115.41	122.60
2	2	20	ASN	OD1-CG-ND2	-7.09	115.51	122.60
1	1	220	GLN	OE1-CD-NE2	-7.08	115.52	122.60
2	2	165	ASN	OD1-CG-ND2	-7.03	115.57	122.60
4	4	39	ASN	OD1-CG-ND2	-6.96	115.64	122.60
4	4	49	ASP	CA-CB-CG	6.86	119.46	112.60
3	3	162	SER	N-CA-C	6.85	120.74	112.38
2	2	204	ASN	OD1-CG-ND2	-6.75	115.85	122.60
1	1	149	HIS	CB-CG-CD2	-6.75	122.43	131.20
2	2	214	ASN	OD1-CG-ND2	-6.74	115.86	122.60
1	1	100	ASN	OD1-CG-ND2	-6.74	115.86	122.60
2	2	147	ASN	OD1-CG-ND2	-6.72	115.88	122.60
1	1	116	VAL	N-CA-C	6.69	119.65	112.96
6	8	242[A]	TYR	N-CA-C	6.68	114.23	108.22
4	4	18	ARG	N-CA-C	-6.63	103.35	112.03
3	3	17	ASP	CA-CB-CG	6.62	119.22	112.60
2	2	167	GLN	CA-CB-CG	-6.62	100.86	114.10
2	2	178	ASP	N-CA-C	6.61	119.05	111.11
2	2	113	ASN	OD1-CG-ND2	-6.61	115.99	122.60
2	2	226	ASN	OD1-CG-ND2	-6.61	115.99	122.60
3	3	161	GLN	OE1-CD-NE2	-6.61	115.99	122.60
1	1	69	HIS	CB-CG-CD2	-6.57	122.66	131.20
2	2	146	GLN	OE1-CD-NE2	-6.57	116.03	122.60
2	2	264	ARG	NE-CZ-NH2	-6.55	113.31	119.20
3	3	183	SER	N-CA-C	6.53	118.40	111.28
2	2	224	HIS	CA-CB-CG	6.47	120.28	113.80
1	1	83	ARG	CG-CD-NE	-6.46	97.78	112.00
1	1	141	ASN	OD1-CG-ND2	-6.42	116.18	122.60
2	2	15	GLN	OE1-CD-NE2	-6.42	116.18	122.60
1	1	149	HIS	CA-CB-CG	-6.38	107.42	113.80
3	3	218	ASN	CB-CG-ND2	6.35	125.93	116.40
2	2	142	HIS	CB-CG-CD2	-6.34	122.96	131.20
2	2	94	GLN	OE1-CD-NE2	-6.30	116.30	122.60
3	3	6	ASN	OD1-CG-ND2	-6.27	116.33	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	10	VAL	N-CA-C	6.26	117.81	108.54
4	4	69	ASN	OD1-CG-ND2	-6.25	116.35	122.60
3	3	11	ASN	OD1-CG-ND2	-6.25	116.36	122.60
3	3	54	PRO	N-CA-CB	6.23	106.77	102.35
4	4	24	THR	CA-C-N	-6.19	114.98	122.90
4	4	24	THR	C-N-CA	-6.19	114.98	122.90
4	4	17	ASN	CA-C-O	6.16	126.56	121.02
4	4	13	HIS	CB-CG-CD2	-6.15	123.20	131.20
1	1	68	GLN	OE1-CD-NE2	-6.14	116.45	122.60
1	1	263	PRO	O-C-N	-6.08	118.41	122.73
1	1	172	ASP	CA-CB-CG	6.07	118.67	112.60
1	1	246	ASN	OD1-CG-ND2	-6.06	116.54	122.60
2	2	52	GLN	OE1-CD-NE2	-6.06	116.54	122.60
2	2	63	PHE	N-CA-C	6.00	118.42	109.59
2	2	178	ASP	CA-CB-CG	5.99	118.59	112.60
2	2	199	ASN	OD1-CG-ND2	-5.99	116.61	122.60
3	3	149	MET	N-CA-CB	-5.97	100.48	110.39
3	3	63	ASN	OD1-CG-ND2	-5.93	116.67	122.60
1	1	94	ASN	OD1-CG-ND2	-5.93	116.67	122.60
1	1	153	GLN	OE1-CD-NE2	-5.92	116.68	122.60
1	1	93	ASP	CA-CB-CG	5.92	118.52	112.60
2	2	99	HIS	CB-CG-CD2	-5.91	123.51	131.20
1	1	256	LYS	CA-CB-CG	-5.88	102.35	114.10
3	3	85	LEU	CD1-CG-CD2	-5.85	97.92	110.80
2	2	119	GLN	OE1-CD-NE2	-5.85	116.75	122.60
1	1	237	PHE	CA-CB-CG	-5.84	107.96	113.80
3	3	97	HIS	CB-CG-ND1	5.80	131.41	122.70
2	2	246	GLU	CA-CB-CG	5.78	125.66	114.10
2	2	137	ASN	CA-CB-CG	-5.74	106.86	112.60
2	2	272	GLN	OE1-CD-NE2	-5.72	116.88	122.60
4	4	67	MET	CG-SD-CE	-5.72	88.32	100.90
2	2	111	GLN	OE1-CD-NE2	-5.69	116.91	122.60
2	2	265	ASN	OD1-CG-ND2	-5.69	116.91	122.60
3	3	102	GLU	CG-CD-OE1	-5.68	105.33	118.40
2	2	203	ASN	OD1-CG-ND2	-5.67	116.92	122.60
3	3	18	ASN	OD1-CG-ND2	-5.65	116.95	122.60
4	4	18	ARG	CA-CB-CG	5.64	125.38	114.10
2	2	137	ASN	CB-CG-ND2	5.63	124.85	116.40
3	3	170	TRP	CG-CD2-CE3	5.62	139.53	133.90
3	3	21	SER	O-C-N	-5.62	117.92	121.85
2	2	141	MET	CG-SD-CE	-5.61	88.55	100.90
3	3	133	SER	N-CA-C	5.60	118.60	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	177	THR	CB-CA-C	-5.59	99.30	110.42
3	3	26	PRO	N-CA-CB	5.58	108.21	103.35
1	1	144	GLU	CB-CG-CD	5.58	122.09	112.60
3	3	33	PRO	N-CA-CB	5.58	109.23	103.38
2	2	109	HIS	CB-CG-CD2	-5.57	123.95	131.20
1	1	177	THR	OG1-CB-CG2	5.56	120.42	109.30
1	1	153	GLN	N-CA-C	5.56	118.71	110.48
1	1	104	LEU	N-CA-C	5.53	117.25	108.67
3	3	195	GLN	OE1-CD-NE2	-5.53	117.07	122.60
1	1	203	ASN	OD1-CG-ND2	-5.51	117.09	122.60
1	1	248	HIS	CB-CG-CD2	-5.50	124.05	131.20
3	3	153	HIS	CB-CG-CD2	-5.49	124.07	131.20
2	2	12	ARG	CB-CG-CD	-5.42	98.82	111.30
2	2	95	ASN	CB-CG-ND2	5.42	124.53	116.40
4	4	66	PRO	N-CA-CB	5.42	108.15	103.27
2	2	118	HIS	CB-CG-CD2	-5.40	124.18	131.20
4	4	18	ARG	CA-C-O	5.40	125.04	119.97
2	2	189	ASN	OD1-CG-ND2	-5.39	117.21	122.60
2	2	30	ASN	OD1-CG-ND2	-5.38	117.22	122.60
2	2	149	ASN	OD1-CG-ND2	-5.37	117.23	122.60
2	2	246	GLU	CB-CG-CD	5.37	121.73	112.60
1	1	83	ARG	CA-CB-CG	5.35	124.81	114.10
2	2	83	PRO	N-CA-CB	5.33	108.47	102.60
1	1	102	ASP	N-CA-C	5.33	117.75	110.24
1	1	156	GLN	OE1-CD-NE2	-5.32	117.28	122.60
1	1	29	ASN	OD1-CG-ND2	-5.31	117.29	122.60
2	2	26	GLN	CG-CD-NE2	5.29	124.34	116.40
5	7	40	PHE	N-CA-C	5.28	117.13	108.52
1	1	111	THR	O-C-N	-5.28	118.24	123.46
3	3	102	GLU	CB-CG-CD	5.28	121.57	112.60
1	1	152	ASN	OD1-CG-ND2	-5.27	117.33	122.60
1	1	216	PRO	N-CA-CB	5.26	107.99	103.36
1	1	146	ASN	N-CA-CB	-5.24	103.13	111.62
2	2	211	PRO	N-CA-CB	5.24	108.88	103.38
3	3	102	GLU	CG-CD-OE2	5.23	130.44	118.40
3	3	170	TRP	CB-CG-CD1	-5.23	119.06	126.90
2	2	48	ASN	CB-CG-ND2	5.22	124.23	116.40
1	1	175	TRP	CG-CD2-CE3	5.19	139.09	133.90
4	4	69	ASN	CA-CB-CG	-5.19	107.41	112.60
3	3	170	TRP	CE2-CD2-CG	-5.17	100.99	107.20
2	2	166	ASN	OD1-CG-ND2	-5.14	117.46	122.60
3	3	12	GLN	OE1-CD-NE2	-5.14	117.46	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	37	HIS	CA-CB-CG	5.13	118.93	113.80
3	3	55	PHE	N-CA-C	5.13	116.88	111.28
2	2	150	PRO	N-CA-CB	5.12	108.07	103.20
3	3	109	HIS	CB-CG-CD2	-5.11	124.56	131.20
6	8	147	ASN	N-CA-C	5.10	116.95	109.24
1	1	73	SER	N-CA-C	5.10	116.84	111.28
1	1	117	GLN	N-CA-C	5.10	116.65	111.14
2	2	264	ARG	CB-CG-CD	5.07	122.95	111.30
3	3	105	ASN	CA-CB-CG	-5.05	107.55	112.60
3	3	92	ASP	CA-C-N	5.04	124.83	119.28
3	3	92	ASP	C-N-CA	5.04	124.83	119.28
1	1	35	PRO	N-CA-CB	5.03	108.12	103.39
1	1	175	TRP	CE2-CD2-CG	-5.01	101.19	107.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	11	ASP	Mainchain

5.2 Too-close contacts [i](#)

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	1	2221	0	2173	136	0
2	2	2075	0	1994	110	0
3	3	1834	0	1816	132	0
4	4	534	0	524	45	0
5	7	904	0	877	135	0
6	8	771	0	766	107	0
7	9	699	0	674	20	0
8	A	39	0	34	1	0
8	E	39	0	34	2	0
9	B	60	0	52	2	0
10	C	28	0	25	0	0
10	D	28	0	25	3	0
11	F	49	0	43	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	1	18	0	31	6	0
13	9	14	0	13	1	0
All	All	9313	0	9081	415	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 23.

All (415) 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)
5:7:140:ARG:HG2	6:8:142[B]:LEU:CD2	1.39	1.53
5:7:115:VAL:CG1	6:8:198:GLY:HA3	1.07	1.51
5:7:115:VAL:HG11	6:8:198:GLY:CA	1.01	1.46
5:7:140:ARG:CG	6:8:142[B]:LEU:HD23	1.46	1.43
5:7:41:LEU:CG	6:8:143[B]:ALA:HB2	1.51	1.37
5:7:142[A]:LEU:HD13	6:8:227:SER:CB	1.62	1.29
1:1:297:LYS:NZ	5:7:87:SER:O	1.66	1.26
5:7:41:LEU:HG	6:8:143[B]:ALA:CB	1.72	1.19
5:7:140:ARG:NH2	6:8:173:PRO:HG3	1.58	1.17
5:7:40:PHE:CE2	6:8:144:LYS:HB2	1.77	1.17
3:3:59:ALA:HB3	5:7:116:GLU:OE1	1.43	1.16
3:3:59:ALA:CB	5:7:116:GLU:CD	2.18	1.16
5:7:142[A]:LEU:HD13	6:8:227:SER:HB3	1.27	1.14
5:7:140:ARG:HD3	6:8:226:GLU:OE1	1.42	1.13
5:7:41:LEU:CG	6:8:143[B]:ALA:CB	2.25	1.13
1:1:292:THR:HB	3:3:63:ASN:ND2	1.62	1.13
5:7:41:LEU:HD11	6:8:199:THR:CG2	1.79	1.12
5:7:40:PHE:HE2	6:8:144:LYS:HB2	0.95	1.11
3:3:59:ALA:HB3	5:7:116:GLU:CD	1.75	1.11
3:3:97:HIS:CE1	5:7:72:SER:HB3	1.87	1.09
5:7:115:VAL:HG11	6:8:198:GLY:C	1.78	1.09
5:7:140:ARG:C	6:8:142[B]:LEU:HG	1.77	1.08
5:7:140:ARG:CD	6:8:226:GLU:OE1	1.93	1.07
7:9:283:MET:CE	7:9:308:THR:HG22	1.82	1.07
5:7:142[A]:LEU:HD13	6:8:227:SER:HB2	1.34	1.06
5:7:41:LEU:HD13	6:8:196:LEU:CD1	1.86	1.06
1:1:220:GLN:O	2:2:270:ARG:NH2	1.88	1.05
9:B:1:NAG:H4	9:B:5:FUC:H5	1.39	1.05
3:3:59:ALA:HB2	5:7:116:GLU:OE2	1.55	1.05
5:7:115:VAL:CB	6:8:198:GLY:HA3	1.90	1.02
5:7:140:ARG:O	6:8:142[B]:LEU:HG	1.60	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:7:41:LEU:CD1	6:8:196:LEU:HD13	1.89	1.02
5:7:140:ARG:HG3	5:7:140:ARG:HH11	1.21	1.02
5:7:40:PHE:HE2	6:8:144:LYS:CB	1.73	1.01
5:7:41:LEU:CD1	6:8:143[B]:ALA:CB	2.38	0.99
5:7:41:LEU:HD12	6:8:143[B]:ALA:CB	1.93	0.99
5:7:41:LEU:CD1	6:8:199:THR:CG2	2.42	0.98
5:7:140:ARG:HH22	6:8:173:PRO:HG3	1.18	0.98
1:1:294:LEU:HD13	3:3:67:MET:SD	2.03	0.96
5:7:141:VAL:HG23	6:8:142[B]:LEU:O	1.66	0.96
1:1:292:THR:HA	3:3:63:ASN:CG	1.92	0.95
1:1:24:ARG:NH2	4:4:7:SER:O	2.00	0.93
1:1:297:LYS:HG2	3:3:94:ARG:CZ	1.99	0.93
5:7:39:GLY:O	6:8:142[B]:LEU:HD12	1.69	0.93
3:3:97:HIS:HE1	5:7:72:SER:HB3	1.24	0.93
5:7:41:LEU:HD11	6:8:199:THR:HG23	1.52	0.92
5:7:68:ARG:HB3	5:7:71:GLU:HG3	1.51	0.92
7:9:283:MET:HE2	7:9:308:THR:HG22	1.49	0.91
2:2:33:VAL:N	4:4:56:PRO:O	2.04	0.91
6:8:183:LEU:HD12	6:8:183:LEU:H	1.33	0.91
1:1:226:ASP:OD2	2:2:172:ARG:NH1	2.04	0.89
3:3:97:HIS:CE1	5:7:72:SER:CB	2.56	0.89
1:1:22:THR:HA	4:4:45:ASP:O	1.72	0.89
1:1:296:THR:HA	3:3:57:LEU:O	1.71	0.89
1:1:302:TYR:CE1	3:3:189:TYR:HB3	2.08	0.88
5:7:115:VAL:HG13	6:8:172:ARG:HD3	1.56	0.88
5:7:41:LEU:HD12	6:8:143[B]:ALA:HB1	1.56	0.88
5:7:142[A]:LEU:HA	6:8:172:ARG:O	1.73	0.88
3:3:59:ALA:CB	5:7:116:GLU:OE2	2.18	0.87
6:8:147:ASN:ND2	6:8:223:VAL:HG11	1.88	0.87
2:2:116:LYS:HD3	3:3:125:MET:HE2	1.56	0.87
1:1:295:SER:HB3	5:7:71:GLU:HB3	1.57	0.87
5:7:142[A]:LEU:CD1	6:8:227:SER:HB3	2.05	0.87
2:2:35:TYR:C	4:4:52:LYS:HB2	1.99	0.86
2:2:116:LYS:HE3	3:3:124:MET:SD	2.16	0.85
1:1:295:SER:O	3:3:57:LEU:HB3	1.76	0.85
2:2:31:SER:O	4:4:57:ILE:HA	1.76	0.85
1:1:24:ARG:O	4:4:9:LYS:NZ	2.09	0.85
1:1:272:ARG:O	3:3:99:MET:HE1	1.77	0.84
1:1:299:LEU:O	3:3:84:CYS:N	2.11	0.84
1:1:292:THR:CA	3:3:63:ASN:CG	2.50	0.83
5:7:41:LEU:CD1	6:8:199:THR:HG21	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:7:141:VAL:O	6:8:172:ARG:HG3	1.79	0.83
1:1:49:THR:HA	2:2:29:ALA:O	1.78	0.82
6:8:162:PRO:HB3	6:8:205:LEU:HD12	1.60	0.82
1:1:292:THR:HA	3:3:63:ASN:OD1	1.80	0.81
7:9:305:PRO:HB2	11:F:1:NAG:H82	1.63	0.81
6:8:216:GLY:O	8:E:1:NAG:H82	1.81	0.81
2:2:35:TYR:O	4:4:52:LYS:HB2	1.81	0.81
1:1:48:GLU:OE2	2:2:202:THR:HG21	1.81	0.80
5:7:141:VAL:CG2	6:8:142[B]:LEU:O	2.30	0.80
5:7:41:LEU:HD13	6:8:196:LEU:HD13	0.92	0.80
2:2:11:ASP:HB2	4:4:68:LEU:HA	1.62	0.80
1:1:291:LEU:HD22	2:2:180:LEU:CD1	2.11	0.80
1:1:299:LEU:O	3:3:83:LEU:HA	1.80	0.80
1:1:158:MET:SD	1:1:177:THR:HG23	2.23	0.79
1:1:276:ALA:CB	2:2:186:LEU:HG	2.12	0.79
5:7:140:ARG:HG3	5:7:140:ARG:NH1	1.95	0.78
2:2:12:ARG:NH2	3:3:160:LEU:HB3	1.98	0.78
5:7:38:PRO:HB3	6:8:142[B]:LEU:HD11	1.66	0.78
6:8:170:GLY:H	6:8:201:THR:HG22	1.48	0.78
1:1:226:ASP:OD1	2:2:172:ARG:NH2	2.16	0.78
5:7:143[A]:ALA:HB1	6:8:144:LYS:O	1.82	0.77
1:1:299:LEU:HG	3:3:82:ILE:O	1.84	0.76
2:2:199:ASN:ND2	3:3:120:PHE:O	2.18	0.76
5:7:140:ARG:CD	6:8:142[B]:LEU:HD23	2.16	0.76
2:2:116:LYS:HB3	3:3:125:MET:HG2	1.66	0.76
5:7:40:PHE:CE2	6:8:144:LYS:CB	2.58	0.75
1:1:132:MET:HE1	12:1:901:PLM:H82	1.68	0.75
1:1:292:THR:CB	3:3:63:ASN:ND2	2.46	0.75
1:1:294:LEU:HB3	3:3:57:LEU:HD22	1.69	0.75
1:1:297:LYS:HE2	3:3:94:ARG:NH2	2.01	0.75
5:7:140:ARG:HG2	6:8:142[B]:LEU:CG	2.16	0.75
1:1:276:ALA:HB1	2:2:186:LEU:HG	1.69	0.74
5:7:41:LEU:CD1	6:8:143[B]:ALA:HB2	2.10	0.74
5:7:68:ARG:CB	5:7:71:GLU:HG3	2.18	0.74
1:1:273:PRO:HD3	2:2:192:VAL:CG2	2.17	0.74
3:3:97:HIS:NE2	5:7:72:SER:CB	2.51	0.74
5:7:39:GLY:O	6:8:142[B]:LEU:O	2.06	0.74
1:1:294:LEU:HD22	3:3:57:LEU:HD21	1.68	0.74
3:3:20:GLN:NE2	4:4:32:TYR:CD2	2.56	0.73
5:7:115:VAL:CG1	6:8:198:GLY:CA	1.97	0.73
1:1:120:ARG:NH2	3:3:102:GLU:OE1	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:7:41:LEU:HG	6:8:143[B]:ALA:HB2	0.78	0.72
5:7:141:VAL:O	6:8:172:ARG:CG	2.37	0.72
1:1:20:ALA:HA	4:4:46:PHE:CE1	2.25	0.72
1:1:291:LEU:HD22	2:2:180:LEU:HD11	1.69	0.72
5:7:90:LYS:H	5:7:90:LYS:HD2	1.55	0.72
5:7:68:ARG:HB3	5:7:71:GLU:CG	2.21	0.71
5:7:141:VAL:CG2	6:8:142[B]:LEU:C	2.63	0.71
2:2:30:ASN:ND2	4:4:57:ILE:HD12	2.05	0.71
1:1:226:ASP:CG	2:2:172:ARG:HH12	1.98	0.71
1:1:159:TYR:HB2	12:1:901:PLM:HE2	1.72	0.70
5:7:41:LEU:HB2	6:8:143[B]:ALA:HB1	1.74	0.69
5:7:140:ARG:NH2	6:8:173:PRO:CG	2.48	0.69
11:F:1:NAG:H62	11:F:2:NAG:C1	2.22	0.69
1:1:48:GLU:HB2	2:2:29:ALA:HB1	1.75	0.69
1:1:293:PRO:HD2	3:3:63:ASN:OD1	1.91	0.69
2:2:117:PHE:CD2	3:3:204:THR:OG1	2.46	0.68
5:7:140:ARG:CG	6:8:142[B]:LEU:CD2	2.28	0.68
1:1:48:GLU:CD	2:2:202:THR:HG21	2.19	0.67
6:8:163:MET:HE2	6:8:238:LEU:HD22	1.75	0.67
5:7:124:LEU:CB	5:7:134:SER:HB3	2.24	0.67
6:8:183:LEU:HD12	6:8:183:LEU:N	2.06	0.67
1:1:273:PRO:HB3	2:2:189:ASN:CB	2.25	0.67
5:7:142[A]:LEU:HB2	6:8:225:HIS:HE1	1.60	0.67
5:7:61:VAL:HG11	5:7:103:LEU:O	1.94	0.66
5:7:124:LEU:HB3	5:7:134:SER:HB3	1.78	0.66
1:1:291:LEU:HB3	2:2:179:TYR:OH	1.97	0.65
6:8:167:VAL:HB	6:8:203:THR:HG23	1.79	0.65
1:1:292:THR:C	3:3:63:ASN:OD1	2.40	0.65
1:1:286:TYR:HH	2:2:177:VAL:H	1.43	0.65
1:1:292:THR:CA	3:3:63:ASN:OD1	2.42	0.65
2:2:187:LEU:HD22	3:3:65:MET:SD	2.37	0.65
2:2:12:ARG:CZ	4:4:68:LEU:HD13	2.26	0.64
1:1:273:PRO:HD3	2:2:192:VAL:HG22	1.77	0.64
1:1:293:PRO:HG2	2:2:186:LEU:HD21	1.78	0.64
1:1:237:PHE:CE2	12:1:901:PLM:H21	2.32	0.64
2:2:234:LEU:HD22	3:3:52:MET:HE1	1.78	0.64
1:1:286:TYR:OH	2:2:177:VAL:N	2.23	0.64
1:1:299:LEU:O	3:3:83:LEU:CA	2.46	0.64
2:2:35:TYR:CD1	4:4:53:PHE:HE1	2.15	0.64
5:7:44:SER:HB3	5:7:111:PHE:HA	1.78	0.64
1:1:292:THR:CB	3:3:63:ASN:CG	2.70	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:8:169:THR:HA	6:8:201:THR:HB	1.79	0.64
6:8:218:ASN:ND2	10:D:1:NAG:O7	2.29	0.64
1:1:20:ALA:HA	4:4:46:PHE:HE1	1.61	0.64
1:1:177:THR:HG22	1:1:180:ASN:HB2	1.79	0.64
11:F:1:NAG:C6	11:F:2:NAG:C1	2.76	0.64
11:F:1:NAG:C6	11:F:4:FUC:O2	2.46	0.63
5:7:141:VAL:HG22	6:8:142[B]:LEU:C	2.22	0.63
6:8:189:THR:HG23	6:8:204:SER:HB2	1.80	0.63
1:1:216:PRO:HB2	2:2:270:ARG:HB3	1.79	0.63
4:4:14:GLU:HB3	4:4:20:TYR:CD2	2.33	0.62
1:1:107:VAL:HG13	1:1:239:ILE:HD13	1.80	0.62
2:2:11:ASP:HB3	4:4:68:LEU:HD23	1.81	0.62
5:7:39:GLY:H	5:7:45:VAL:HG11	1.65	0.62
5:7:41:LEU:CB	6:8:143[B]:ALA:CB	2.77	0.62
1:1:21:ALA:O	4:4:46:PHE:HA	1.99	0.62
11:F:1:NAG:H61	11:F:4:FUC:O2	1.97	0.62
1:1:292:THR:HB	3:3:63:ASN:CG	2.25	0.62
2:2:12:ARG:HG2	4:4:68:LEU:HD22	1.81	0.62
5:7:118:GLU:HB3	6:8:172:ARG:NH2	2.15	0.62
6:8:147:ASN:OD1	6:8:232:GLN:NE2	2.30	0.62
1:1:131:ASP:OD2	4:4:37:ALA:HA	2.00	0.61
2:2:35:TYR:CD1	4:4:53:PHE:CE1	2.88	0.61
2:2:35:TYR:HD1	4:4:53:PHE:CE1	2.19	0.61
2:2:201:ARG:NH1	3:3:120:PHE:CE2	2.68	0.61
1:1:265:HIS:CE1	4:4:39:ASN:O	2.53	0.61
1:1:291:LEU:CB	2:2:179:TYR:OH	2.49	0.61
1:1:300:THR:O	3:3:143:LYS:NZ	2.33	0.61
2:2:30:ASN:HD21	4:4:57:ILE:HD12	1.65	0.61
3:3:72:LEU:HB2	3:3:208:MET:CE	2.30	0.61
2:2:12:ARG:HG3	4:4:68:LEU:HB3	1.81	0.61
7:9:251:TYR:CE1	7:9:327:VAL:HG23	2.35	0.61
5:7:92:LEU:HD23	5:7:110:MET:HB3	1.81	0.60
2:2:201:ARG:CD	3:3:120:PHE:HD2	2.15	0.60
5:7:41:LEU:CG	6:8:143[B]:ALA:HB1	2.27	0.60
7:9:322:GLN:HE22	13:9:405:NAG:H82	1.66	0.60
2:2:201:ARG:HB3	3:3:122:GLY:O	2.02	0.60
1:1:177:THR:HG21	1:1:182:SER:OG	2.01	0.60
1:1:302:TYR:HE2	3:3:142:PRO:O	1.85	0.59
5:7:118:GLU:HB2	5:7:141:VAL:CG1	2.32	0.59
6:8:154:VAL:HG21	6:8:163:MET:HG2	1.85	0.59
1:1:300:THR:HG21	3:3:81:PRO:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:273:PRO:HB3	2:2:189:ASN:HB3	1.85	0.59
1:1:302:TYR:CD2	3:3:141:PRO:HB2	2.37	0.59
3:3:97:HIS:HA	3:3:102:GLU:HG2	1.85	0.59
7:9:283:MET:CE	7:9:308:THR:CG2	2.71	0.59
2:2:201:ARG:NH1	3:3:120:PHE:HE2	2.01	0.58
1:1:48:GLU:CB	2:2:29:ALA:CB	2.82	0.58
5:7:142[A]:LEU:CA	6:8:172:ARG:O	2.50	0.58
1:1:48:GLU:HB3	2:2:29:ALA:CB	2.33	0.58
1:1:273:PRO:HB3	2:2:189:ASN:HB2	1.86	0.58
1:1:235:ASN:HA	1:1:237:PHE:CZ	2.39	0.57
1:1:120:ARG:HH22	3:3:102:GLU:CD	2.08	0.57
1:1:297:LYS:CG	3:3:94:ARG:CZ	2.78	0.57
1:1:299:LEU:HD11	3:3:83:LEU:HB3	1.85	0.57
5:7:140:ARG:CG	5:7:140:ARG:HH11	2.06	0.57
2:2:30:ASN:OD1	4:4:57:ILE:HB	2.04	0.57
3:3:72:LEU:HB2	3:3:208:MET:HE2	1.85	0.57
5:7:115:VAL:CG1	6:8:198:GLY:C	2.54	0.57
2:2:116:LYS:HG2	3:3:124:MET:HB3	1.86	0.57
7:9:283:MET:HE1	7:9:308:THR:HG22	1.80	0.57
1:1:226:ASP:CG	2:2:172:ARG:HH22	2.09	0.57
1:1:293:PRO:CD	3:3:63:ASN:OD1	2.53	0.56
1:1:190:ALA:HB2	3:3:11:ASN:HB3	1.86	0.56
3:3:20:GLN:NE2	4:4:32:TYR:CE2	2.73	0.56
5:7:41:LEU:HB2	6:8:143[B]:ALA:CB	2.35	0.56
5:7:120:ASN:ND2	9:B:5:FUC:H61	2.19	0.56
1:1:300:THR:O	3:3:84:CYS:SG	2.63	0.56
1:1:271:PRO:HB3	3:3:46:LEU:HD22	1.87	0.56
1:1:300:THR:HG22	3:3:81:PRO:HB2	1.86	0.56
3:3:97:HIS:NE2	5:7:72:SER:HB2	2.19	0.56
1:1:302:TYR:CE2	3:3:142:PRO:O	2.59	0.56
2:2:12:ARG:CG	4:4:68:LEU:HB3	2.35	0.56
5:7:140:ARG:HG2	6:8:142[B]:LEU:HD23	0.61	0.56
7:9:306:ILE:H	7:9:329:VAL:HG23	1.69	0.56
1:1:265:HIS:NE2	4:4:39:ASN:O	2.39	0.56
5:7:41:LEU:CB	6:8:143[B]:ALA:HB1	2.36	0.56
7:9:274:PRO:HA	7:9:316:ASN:HB2	1.87	0.56
1:1:294:LEU:HB3	3:3:57:LEU:CD2	2.35	0.56
1:1:300:THR:C	3:3:84:CYS:SG	2.89	0.56
2:2:33:VAL:O	4:4:56:PRO:HB3	2.06	0.56
1:1:191:PRO:HG2	3:3:13:TYR:HB2	1.88	0.55
1:1:275:ARG:NH1	2:2:184:GLY:HA3	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:8:216:GLY:O	8:E:1:NAG:C8	2.54	0.55
5:7:142[A]:LEU:CD1	6:8:227:SER:CB	2.57	0.55
5:7:142[A]:LEU:CB	6:8:225:HIS:HE1	2.18	0.55
5:7:142[A]:LEU:HD22	6:8:227:SER:HB3	1.88	0.55
6:8:170:GLY:N	6:8:201:THR:HG22	2.20	0.55
7:9:309:THR:OG1	7:9:326:THR:HG22	2.07	0.55
5:7:114:ARG:NH1	5:7:117:ASP:OD1	2.39	0.55
5:7:118:GLU:CB	6:8:172:ARG:NH2	2.70	0.55
1:1:300:THR:C	3:3:84:CYS:HB2	2.32	0.55
1:1:301:THR:N	3:3:84:CYS:HB2	2.22	0.55
1:1:275:ARG:HA	2:2:185:THR:HG22	1.89	0.54
2:2:117:PHE:HD2	3:3:204:THR:HG1	1.48	0.54
2:2:201:ARG:NE	3:3:120:PHE:HD2	2.04	0.54
1:1:274:PRO:HD3	3:3:99:MET:SD	2.47	0.54
2:2:201:ARG:CD	3:3:120:PHE:CD2	2.91	0.54
11:F:1:NAG:H62	11:F:2:NAG:HN2	1.73	0.54
5:7:63:GLN:HB3	5:7:79:HIS:HD2	1.72	0.54
2:2:191:PHE:CE2	3:3:52:MET:HB2	2.43	0.53
5:7:115:VAL:CG1	6:8:172:ARG:HD3	2.33	0.53
2:2:192:VAL:HA	3:3:49:ILE:HG21	1.89	0.53
6:8:218:ASN:ND2	10:D:1:NAG:C7	2.72	0.53
1:1:48:GLU:CB	2:2:29:ALA:HB1	2.38	0.53
2:2:12:ARG:HH22	3:3:160:LEU:HB3	1.71	0.53
2:2:29:ALA:HA	4:4:68:LEU:HD21	1.90	0.53
5:7:64:LEU:CD1	5:7:106:ALA:HA	2.40	0.52
1:1:297:LYS:CG	3:3:94:ARG:NH1	2.73	0.52
5:7:39:GLY:N	5:7:45:VAL:HG11	2.24	0.52
1:1:299:LEU:CG	3:3:82:ILE:O	2.56	0.52
2:2:37:ARG:HG3	3:3:37:PRO:HB3	1.92	0.52
5:7:110:MET:HE1	5:7:117:ASP:CG	2.34	0.52
5:7:142[A]:LEU:CG	6:8:227:SER:HB3	2.40	0.52
1:1:299:LEU:CD1	3:3:83:LEU:HB3	2.40	0.52
5:7:124:LEU:HB2	5:7:134:SER:HB3	1.92	0.52
1:1:271:PRO:CB	3:3:46:LEU:HD22	2.40	0.52
1:1:297:LYS:HG3	3:3:94:ARG:NH1	2.25	0.52
1:1:51:ALA:HA	4:4:54:THR:O	2.10	0.52
5:7:124:LEU:HB3	5:7:134:SER:CB	2.40	0.52
5:7:32:GLN:HG2	5:7:52:GLN:HE21	1.74	0.51
5:7:90:LYS:H	5:7:90:LYS:CD	2.22	0.51
1:1:49:THR:HG22	2:2:30:ASN:HB2	1.91	0.51
1:1:271:PRO:HB3	3:3:46:LEU:CD2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:8:154:VAL:HG12	6:8:155:GLN:O	2.10	0.51
1:1:273:PRO:HD2	2:2:193:PHE:CZ	2.45	0.51
5:7:41:LEU:CD1	6:8:143[B]:ALA:HB1	2.21	0.51
1:1:237:PHE:HE2	12:1:901:PLM:H21	1.76	0.51
1:1:280:TYR:OH	2:2:137:ASN:HA	2.10	0.51
2:2:201:ARG:HH11	3:3:120:PHE:HE2	1.57	0.51
7:9:287:PRO:HG2	7:9:308:THR:HG21	1.94	0.50
2:2:33:VAL:O	4:4:56:PRO:CB	2.60	0.50
1:1:190:ALA:HB2	3:3:11:ASN:CB	2.41	0.50
3:3:85:LEU:HD21	3:3:95:LEU:HD11	1.94	0.50
2:2:116:LYS:O	3:3:123:SER:HB2	2.11	0.50
2:2:116:LYS:HE3	3:3:124:MET:CE	2.41	0.50
1:1:299:LEU:HG	3:3:83:LEU:HA	1.93	0.50
7:9:287:PRO:CG	7:9:308:THR:HG21	2.42	0.50
5:7:64:LEU:HD12	5:7:106:ALA:CB	2.42	0.50
1:1:217:LEU:C	2:2:270:ARG:HB2	2.37	0.49
6:8:211:SER:O	6:8:214:VAL:HG22	2.11	0.49
2:2:199:ASN:OD1	3:3:121:CYS:HA	2.12	0.49
5:7:142[A]:LEU:HB3	6:8:172:ARG:O	2.12	0.49
1:1:132:MET:SD	12:1:901:PLM:H62	2.52	0.49
2:2:188:GLY:HA3	3:3:68:TYR:CE1	2.48	0.49
2:2:11:ASP:CB	4:4:68:LEU:HA	2.37	0.49
3:3:87:LEU:HD13	3:3:190:ILE:HD11	1.94	0.49
2:2:201:ARG:HD3	3:3:120:PHE:CD2	2.48	0.49
3:3:12:GLN:HG3	3:3:14:LEU:N	2.27	0.49
3:3:167:VAL:O	3:3:169:PRO:HD3	2.12	0.49
5:7:115:VAL:HG12	6:8:172:ARG:NH1	2.26	0.49
1:1:293:PRO:N	3:3:63:ASN:OD1	2.46	0.49
5:7:95:VAL:CG1	8:A:1:NAG:H62	2.43	0.49
6:8:143[B]:ALA:HB3	6:8:172:ARG:HB3	1.95	0.49
5:7:30:VAL:HG13	5:7:52:GLN:HB2	1.95	0.48
1:1:237:PHE:CE2	12:1:901:PLM:H52	2.48	0.48
2:2:117:PHE:HD2	3:3:204:THR:OG1	1.91	0.48
5:7:135:VAL:HG22	5:7:136:ASP:N	2.27	0.48
6:8:218:ASN:HD22	10:D:1:NAG:C7	2.24	0.48
3:3:97:HIS:ND1	3:3:102:GLU:OE2	2.43	0.48
4:4:22:GLY:O	4:4:24:THR:N	2.47	0.48
7:9:244:PRO:HG3	7:9:316:ASN:HB3	1.95	0.48
5:7:41:LEU:HD11	6:8:199:THR:HG22	1.83	0.48
5:7:140:ARG:CG	5:7:140:ARG:NH1	2.69	0.48
7:9:252:ASP:O	7:9:254:ASN:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:44:MET:HA	3:3:44:MET:HE2	1.96	0.47
3:3:234:LYS:HA	3:3:234:LYS:HD3	1.66	0.47
1:1:292:THR:HG22	3:3:63:ASN:CB	2.44	0.47
1:1:47:VAL:HG22	3:3:163:SER:OG	2.13	0.47
5:7:39:GLY:HA3	5:7:140:ARG:O	2.13	0.47
5:7:114:ARG:O	5:7:117:ASP:HB2	2.15	0.47
1:1:299:LEU:CD2	3:3:82:ILE:O	2.63	0.46
2:2:35:TYR:HD1	4:4:53:PHE:CD1	2.33	0.46
7:9:300:ARG:HB3	7:9:301:PRO:HD2	1.98	0.46
1:1:96:ALA:HA	1:1:249:ASN:O	2.16	0.46
2:2:199:ASN:HD21	3:3:121:CYS:HA	1.81	0.46
3:3:102:GLU:OE2	3:3:230:HIS:ND1	2.46	0.46
5:7:63:GLN:HB3	5:7:79:HIS:CD2	2.50	0.46
5:7:141:VAL:O	6:8:172:ARG:HG2	2.14	0.46
2:2:31:SER:O	4:4:57:ILE:HG22	2.16	0.46
2:2:201:ARG:NH2	3:3:158:ILE:HG22	2.31	0.46
11:F:1:NAG:H61	11:F:4:FUC:H3	1.98	0.46
2:2:12:ARG:CZ	4:4:68:LEU:CD1	2.94	0.46
2:2:201:ARG:HD3	3:3:120:PHE:HD2	1.79	0.46
1:1:116:VAL:HB	3:3:231:ILE:HG12	1.96	0.45
7:9:254:ASN:N	7:9:254:ASN:OD1	2.48	0.45
1:1:229:TYR:OH	2:2:131:CYS:HA	2.17	0.45
1:1:294:LEU:HD22	3:3:54:PRO:HB2	1.98	0.45
5:7:128:PHE:CD1	5:7:128:PHE:C	2.93	0.45
5:7:140:ARG:CD	6:8:142[B]:LEU:CD2	2.87	0.45
11:F:1:NAG:H62	11:F:2:NAG:N2	2.31	0.45
1:1:22:THR:CA	4:4:45:ASP:O	2.56	0.45
1:1:48:GLU:HB2	2:2:29:ALA:CB	2.41	0.45
7:9:245:GLU:OE1	7:9:269:ARG:NH1	2.48	0.45
7:9:255:TRP:CZ3	7:9:299:ILE:HG21	2.51	0.45
1:1:285:ASP:HA	2:2:133:ALA:CB	2.47	0.45
5:7:142[A]:LEU:CD2	6:8:227:SER:HB3	2.47	0.45
1:1:228:LEU:HD22	2:2:141:MET:O	2.16	0.45
2:2:201:ARG:CZ	3:3:120:PHE:CD2	2.99	0.44
3:3:41:LYS:N	3:3:45:GLU:OE2	2.46	0.44
5:7:64:LEU:N	5:7:64:LEU:HD23	2.32	0.44
1:1:218:LYS:HG3	2:2:270:ARG:HA	1.99	0.44
2:2:116:LYS:CE	3:3:124:MET:SD	2.99	0.44
1:1:115:THR:HA	3:3:233:GLN:OE1	2.18	0.44
2:2:11:ASP:HB2	4:4:69:ASN:H	1.82	0.44
2:2:187:LEU:O	2:2:187:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:192:VAL:HG11	3:3:99:MET:HE2	1.99	0.44
5:7:39:GLY:O	5:7:142[A]:LEU:N	2.50	0.44
5:7:88:GLU:CD	5:7:91:ARG:HD3	2.42	0.44
1:1:294:LEU:HD21	3:3:54:PRO:CG	2.48	0.44
7:9:283:MET:HE1	7:9:308:THR:CG2	2.45	0.44
6:8:230:LYS:O	6:8:231:PRO:C	2.60	0.44
5:7:38:PRO:HA	5:7:140:ARG:O	2.18	0.43
1:1:291:LEU:O	2:2:179:TYR:CE2	2.71	0.43
3:3:145:ARG:O	3:3:149:MET:HB3	2.18	0.43
6:8:205:LEU:HD23	6:8:205:LEU:N	2.32	0.43
1:1:216:PRO:HG3	2:2:145:TYR:HB3	1.99	0.43
4:4:6:SER:HB2	4:4:27:TYR:CE1	2.54	0.43
5:7:47:LEU:HB3	5:7:66:TRP:CH2	2.54	0.43
3:3:59:ALA:HB2	5:7:116:GLU:CD	2.05	0.43
6:8:194:GLY:HA2	6:8:201:THR:HG23	2.00	0.43
3:3:120:PHE:HA	3:3:210:ILE:HG22	2.01	0.43
5:7:142[A]:LEU:CB	6:8:172:ARG:O	2.67	0.43
3:3:12:GLN:HG3	3:3:14:LEU:H	1.83	0.42
1:1:273:PRO:HD2	2:2:193:PHE:CE2	2.55	0.42
6:8:206:TRP:CH2	6:8:208:LEU:HD22	2.55	0.42
1:1:51:ALA:CA	4:4:54:THR:O	2.66	0.42
2:2:32:VAL:HG13	4:4:56:PRO:HG2	2.01	0.42
6:8:160:PRO:HG3	6:8:209:VAL:HG22	2.01	0.42
5:7:61:VAL:HA	5:7:127:THR:HA	2.00	0.42
1:1:291:LEU:HB2	2:2:179:TYR:OH	2.19	0.42
1:1:300:THR:HB	3:3:81:PRO:HG2	2.02	0.42
2:2:234:LEU:O	3:3:69:ARG:NE	2.38	0.42
5:7:29:VAL:O	5:7:29:VAL:CG1	2.64	0.42
2:2:12:ARG:NH1	4:4:68:LEU:HD13	2.35	0.42
6:8:177:ILE:HG21	6:8:204:SER:HB3	2.02	0.42
3:3:114:LEU:HD23	3:3:114:LEU:HA	1.85	0.41
5:7:38:PRO:HA	5:7:39:GLY:HA3	1.74	0.41
6:8:221:CYS:N	6:8:234:LEU:O	2.49	0.41
5:7:40:PHE:CE2	6:8:144:LYS:HD2	2.56	0.41
5:7:68:ARG:HG2	5:7:121:TYR:CE2	2.55	0.41
1:1:291:LEU:O	2:2:179:TYR:HE2	2.03	0.41
2:2:201:ARG:HB2	3:3:124:MET:HA	2.03	0.41
3:3:64:THR:O	3:3:67:MET:HG2	2.20	0.41
1:1:48:GLU:OE1	3:3:162:SER:OG	2.36	0.41
2:2:143:THR:HG23	2:2:173:ARG:HA	2.01	0.41
2:2:233:PRO:O	3:3:69:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:7:118:GLU:HG3	5:7:139:LEU:O	2.20	0.41
6:8:142[B]:LEU:HB2	6:8:172:ARG:O	2.21	0.41
6:8:156:LEU:HD23	6:8:156:LEU:HA	1.93	0.41
7:9:281:THR:HG23	7:9:283:MET:H	1.86	0.41
1:1:46:ALA:HB3	4:4:67:MET:HG2	2.03	0.40
1:1:80:PHE:CZ	3:3:43:MET:HE2	2.56	0.40
2:2:188:GLY:N	3:3:68:TYR:OH	2.47	0.40
5:7:142[A]:LEU:CD1	6:8:227:SER:HB2	2.24	0.40
1:1:228:LEU:CD2	2:2:141:MET:O	2.69	0.40
1:1:299:LEU:O	3:3:83:LEU:C	2.64	0.40
4:4:20:TYR:CD2	4:4:21:GLY:N	2.90	0.40
1:1:297:LYS:HE2	3:3:94:ARG:HH22	1.82	0.40
2:2:70:SER:OG	2:2:246:GLU:HG2	2.21	0.40
1:1:297:LYS:CE	3:3:94:ARG:NH2	2.81	0.40
5:7:110:MET:HE2	5:7:113:LEU:HG	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	281/302 (93%)	272 (97%)	8 (3%)	1 (0%)	30	67
2	2	265/272 (97%)	252 (95%)	11 (4%)	2 (1%)	16	54
3	3	233/238 (98%)	223 (96%)	10 (4%)	0	100	100
4	4	66/69 (96%)	54 (82%)	6 (9%)	6 (9%)	0	8
5	7	114/116 (98%)	107 (94%)	7 (6%)	0	100	100
6	8	100/102 (98%)	92 (92%)	8 (8%)	0	100	100
7	9	90/92 (98%)	85 (94%)	4 (4%)	1 (1%)	11	46
All	All	1149/1191 (96%)	1085 (94%)	54 (5%)	10 (1%)	16	51

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	4	15	ASN
4	4	23	SER
4	4	24	THR
4	4	19	ALA
4	4	21	GLY
2	2	48	ASN
1	1	145	THR
2	2	114	ALA
7	9	253	ASN
4	4	60	VAL

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	1	245/261 (94%)	240 (98%)	5 (2%)	48	66
2	2	227/232 (98%)	222 (98%)	5 (2%)	45	64
3	3	210/212 (99%)	204 (97%)	6 (3%)	37	58
4	4	57/57 (100%)	55 (96%)	2 (4%)	32	53
5	7	99/99 (100%)	77 (78%)	22 (22%)	1	6
6	8	90/90 (100%)	73 (81%)	17 (19%)	1	8
7	9	77/77 (100%)	67 (87%)	10 (13%)	4	15
All	All	1005/1028 (98%)	938 (93%)	67 (7%)	17	36

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	83	ARG
1	1	147	ASN
1	1	177	THR
1	1	196	VAL
1	1	224	LEU
2	2	66	LEU

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Mol	Chain	Res	Type
2	2	74	GLU
2	2	139	THR
2	2	246	GLU
2	2	264	ARG
3	3	85	LEU
3	3	149	MET
3	3	178	GLN
3	3	190	ILE
3	3	208	MET
3	3	218	ASN
4	4	18	ARG
4	4	61	LEU
5	7	29	VAL
5	7	30	VAL
5	7	47	LEU
5	7	57	GLU
5	7	62	SER
5	7	64	LEU
5	7	68	ARG
5	7	69	HIS
5	7	72	SER
5	7	82	GLN
5	7	90	LYS
5	7	99	LEU
5	7	103	LEU
5	7	114	ARG
5	7	115	VAL
5	7	122	THR
5	7	124	LEU
5	7	132	SER
5	7	139	LEU
5	7	140	ARG
5	7	141	VAL
5	7	142[A]	LEU
6	8	142[B]	LEU
6	8	147	ASN
6	8	148	THR
6	8	150	GLU
6	8	151	VAL
6	8	159	GLU
6	8	165	ARG
6	8	167	VAL

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Mol	Chain	Res	Type
6	8	169	THR
6	8	183	LEU
6	8	196	LEU
6	8	202	VAL
6	8	203	THR
6	8	205	LEU
6	8	209	VAL
6	8	230	LYS
6	8	232	GLN
7	9	264	LEU
7	9	267	ASP
7	9	297	LEU
7	9	302	VAL
7	9	315	THR
7	9	316	ASN
7	9	327	VAL
7	9	329	VAL
7	9	330	LYS
7	9	331	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	117	GLN
2	2	52	GLN
2	2	95	ASN
2	2	137	ASN
2	2	142	HIS
2	2	261	ASN
3	3	6	ASN
4	4	8	GLN
4	4	31	ASN
4	4	44	GLN
5	7	52	GLN
5	7	63	GLN
5	7	82	GLN
6	8	180	HIS
6	8	191	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

19 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	NAG	A	1	8,5	14,14,15	0.98	0	17,19,21	0.99	1 (5%)
8	NAG	A	2	8	14,14,15	0.54	0	17,19,21	0.90	0
8	BMA	A	3	8	11,11,12	0.64	0	15,15,17	0.99	0
9	NAG	B	1	5,9	14,14,15	1.05	1 (7%)	17,19,21	2.15	4 (23%)
9	NAG	B	2	9	14,14,15	0.77	0	17,19,21	1.36	2 (11%)
9	BMA	B	3	9	11,11,12	0.27	0	15,15,17	0.53	0
9	MAN	B	4	9	11,11,12	0.65	0	15,15,17	0.52	0
9	FUC	B	5	9	10,10,11	0.98	0	14,14,16	1.33	2 (14%)
10	NAG	C	1	6,10	14,14,15	0.83	0	17,19,21	1.49	3 (17%)
10	NAG	C	2	10	14,14,15	0.72	0	17,19,21	0.91	0
10	NAG	D	1	6,10	14,14,15	0.77	0	17,19,21	0.87	0
10	NAG	D	2	10	14,14,15	0.71	0	17,19,21	0.92	0
8	NAG	E	1	8,6	14,14,15	0.75	0	17,19,21	1.11	3 (17%)
8	NAG	E	2	8	14,14,15	0.49	0	17,19,21	1.19	1 (5%)
8	BMA	E	3	8	11,11,12	0.27	0	15,15,17	0.52	0
11	NAG	F	1	7,11	14,14,15	0.56	0	17,19,21	0.62	0
11	NAG	F	2	11	14,14,15	0.58	0	17,19,21	1.11	2 (11%)
11	BMA	F	3	11	11,11,12	0.26	0	15,15,17	0.53	0
11	FUC	F	4	11	10,10,11	0.76	0	14,14,16	0.93	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	1	8,5	-	0/6/23/26	0/1/1/1
8	NAG	A	2	8	-	0/6/23/26	0/1/1/1
8	BMA	A	3	8	-	2/2/19/22	1/1/1/1
9	NAG	B	1	5,9	-	2/6/23/26	0/1/1/1
9	NAG	B	2	9	-	2/6/23/26	0/1/1/1
9	BMA	B	3	9	-	1/2/19/22	0/1/1/1
9	MAN	B	4	9	-	0/2/19/22	0/1/1/1
9	FUC	B	5	9	-	-	0/1/1/1
10	NAG	C	1	6,10	-	0/6/23/26	0/1/1/1
10	NAG	C	2	10	-	1/6/23/26	0/1/1/1
10	NAG	D	1	6,10	-	0/6/23/26	0/1/1/1
10	NAG	D	2	10	-	0/6/23/26	0/1/1/1
8	NAG	E	1	8,6	-	1/6/23/26	0/1/1/1
8	NAG	E	2	8	-	1/6/23/26	0/1/1/1
8	BMA	E	3	8	-	0/2/19/22	0/1/1/1
11	NAG	F	1	7,11	-	3/6/23/26	0/1/1/1
11	NAG	F	2	11	-	0/6/23/26	0/1/1/1
11	BMA	F	3	11	-	0/2/19/22	0/1/1/1
11	FUC	F	4	11	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1	NAG	C1-C2	-2.18	1.49	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1	NAG	O5-C1-C2	5.10	119.17	111.29
10	C	1	NAG	C4-C3-C2	4.00	116.87	111.02
9	B	1	NAG	O6-C6-C5	3.48	123.17	111.33
9	B	1	NAG	C6-C5-C4	3.46	121.52	113.02
9	B	1	NAG	O4-C4-C3	-3.44	102.27	110.38
9	B	2	NAG	C4-C3-C2	3.23	115.75	111.02
10	C	1	NAG	C1-O5-C5	2.82	115.97	112.19
8	E	2	NAG	O5-C5-C6	2.70	112.92	107.66
8	E	1	NAG	C1-O5-C5	2.49	115.53	112.19
8	A	1	NAG	C1-O5-C5	2.45	115.47	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	1	NAG	O5-C5-C6	2.43	112.39	107.66
9	B	5	FUC	O5-C1-C2	-2.42	105.02	110.79
11	F	2	NAG	C4-C3-C2	-2.37	107.55	111.02
9	B	2	NAG	O5-C5-C4	-2.27	105.30	110.83
9	B	5	FUC	O3-C3-C2	2.17	114.48	110.05
8	E	1	NAG	C6-C5-C4	-2.12	107.81	113.02
11	F	2	NAG	C1-O5-C5	2.07	114.96	112.19
10	C	1	NAG	O5-C5-C4	-2.06	105.82	110.83

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	F	1	NAG	C8-C7-N2-C2
11	F	1	NAG	O7-C7-N2-C2
9	B	1	NAG	C4-C5-C6-O6
9	B	1	NAG	O5-C5-C6-O6
8	A	3	BMA	O5-C5-C6-O6
9	B	2	NAG	O5-C5-C6-O6
8	A	3	BMA	C4-C5-C6-O6
9	B	2	NAG	C4-C5-C6-O6
11	F	1	NAG	C3-C2-N2-C7
8	E	2	NAG	O5-C5-C6-O6
9	B	3	BMA	O5-C5-C6-O6
8	E	1	NAG	C1-C2-N2-C7
10	C	2	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	3	BMA	C1-C2-C3-C4-C5-O5

8 monomers are involved in 16 short contacts:

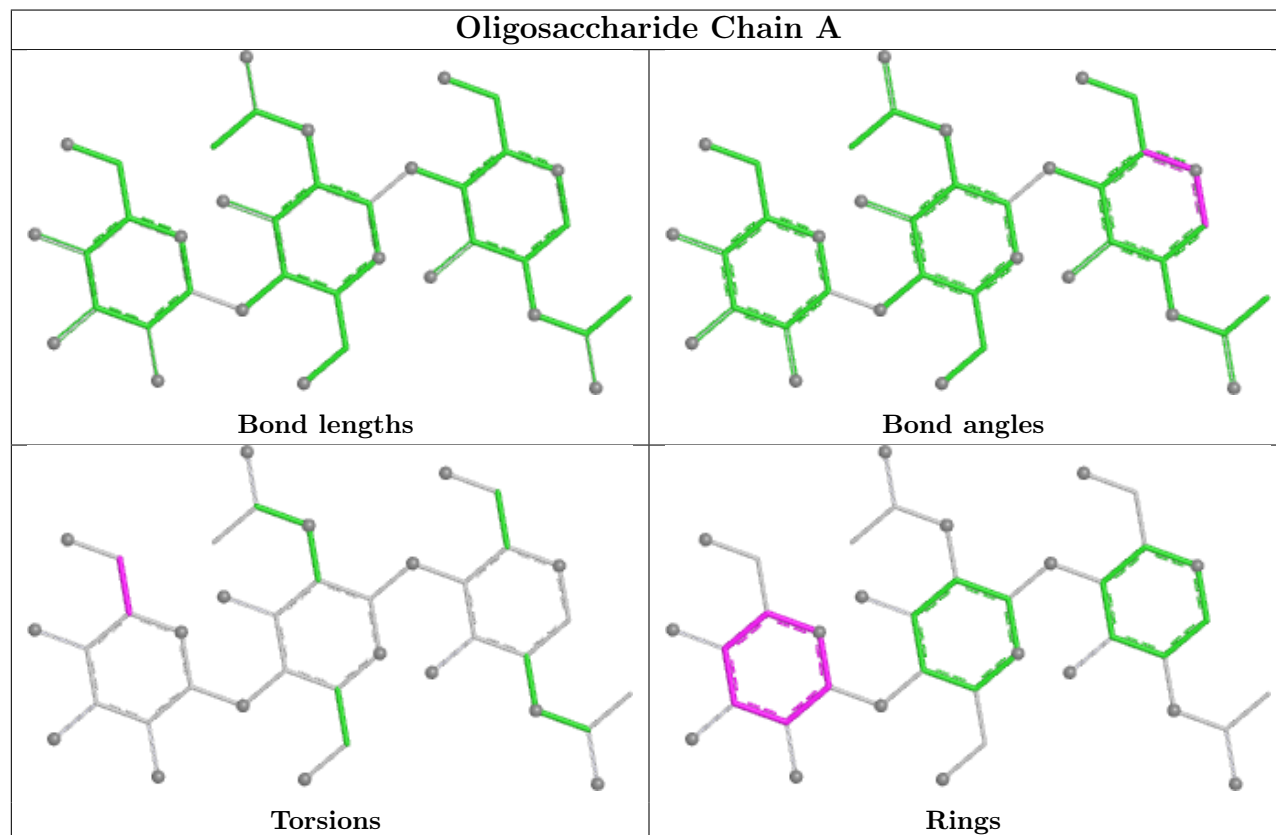
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	2	NAG	4	0
10	D	1	NAG	3	0
8	A	1	NAG	1	0
9	B	1	NAG	1	0
8	E	1	NAG	2	0
11	F	1	NAG	8	0

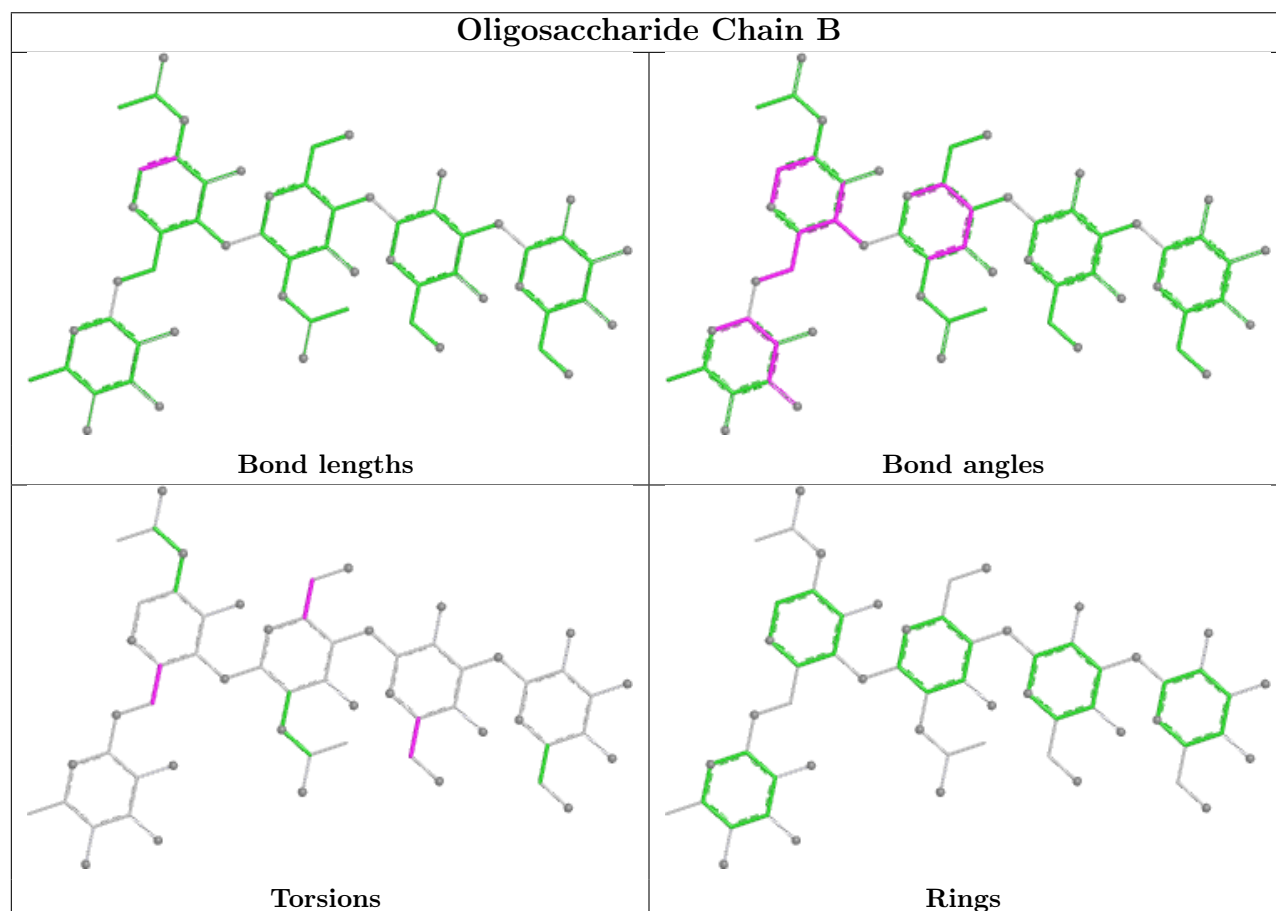
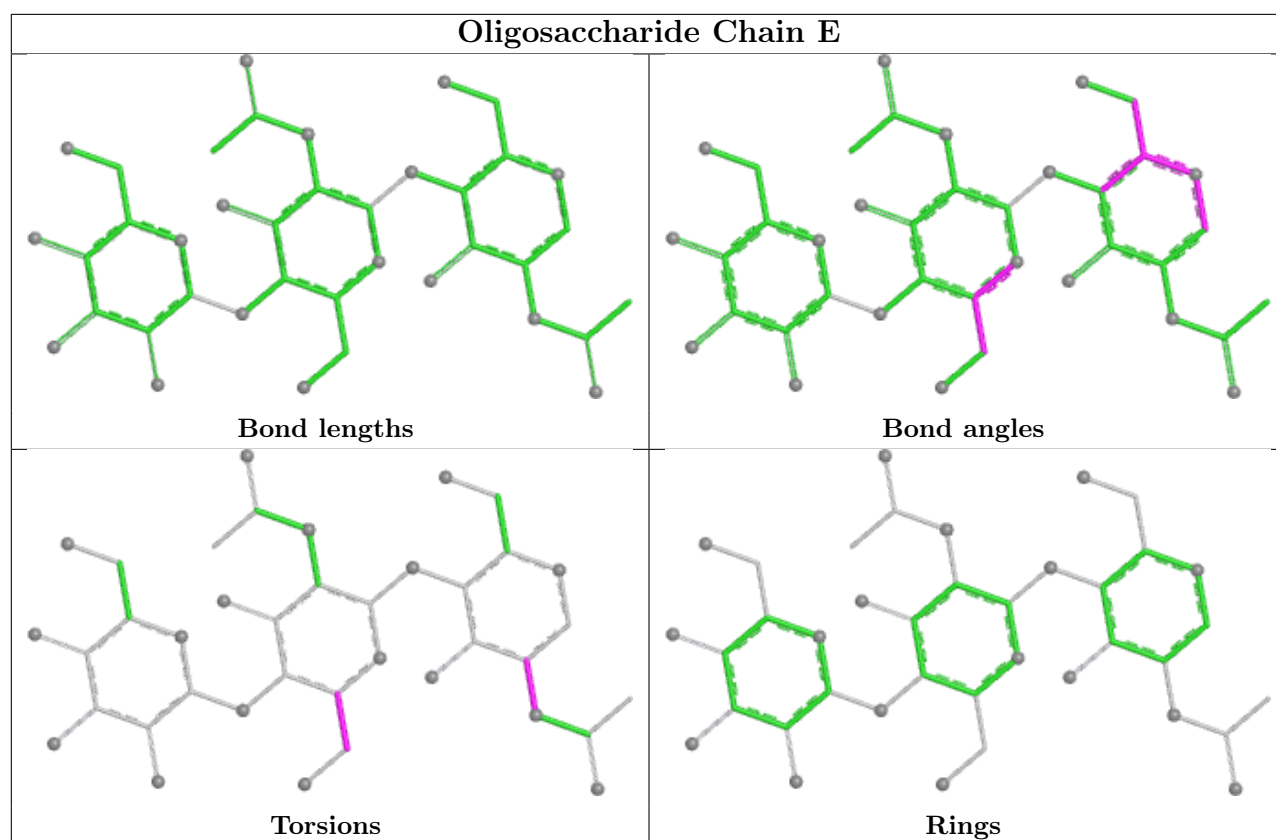
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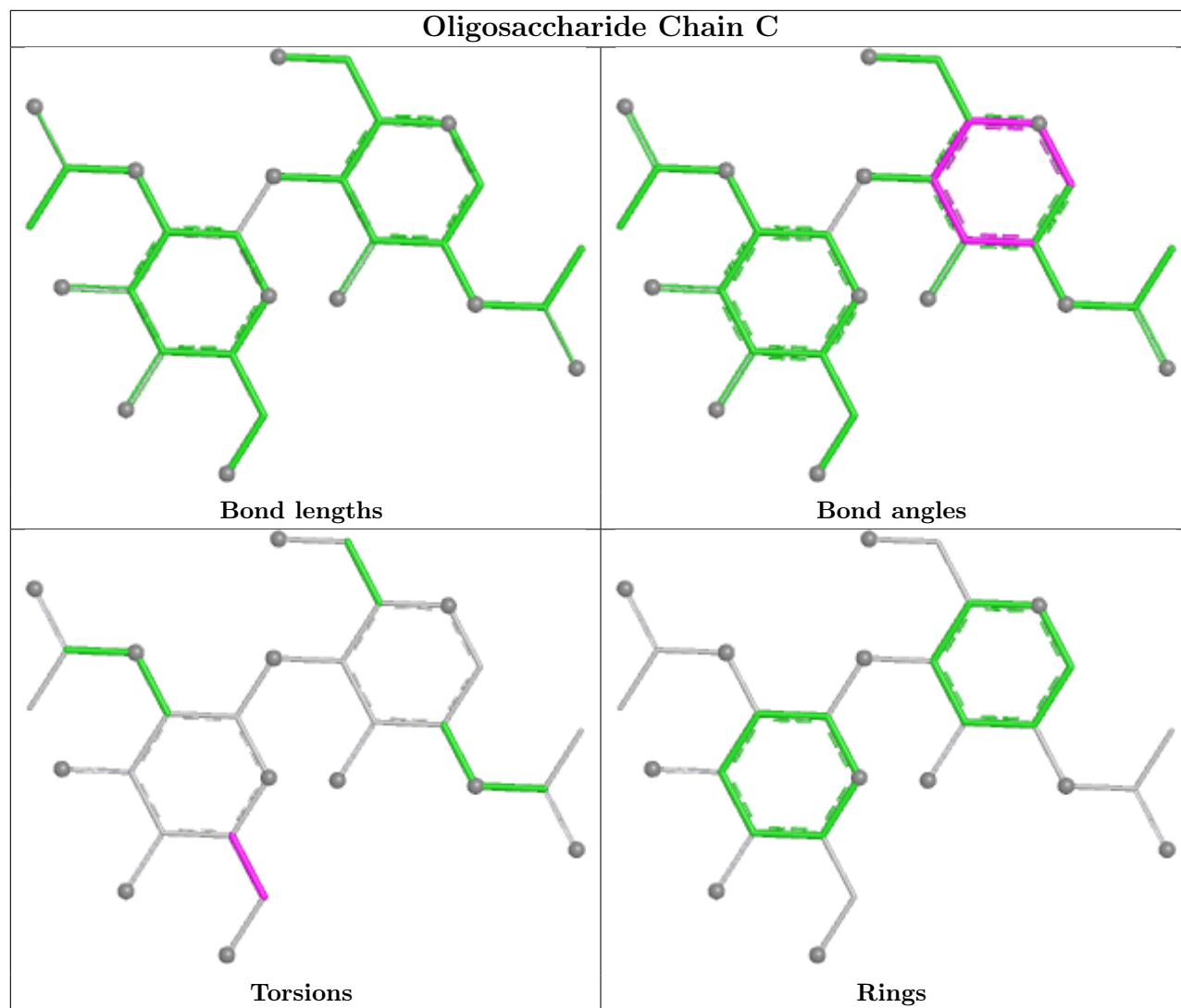
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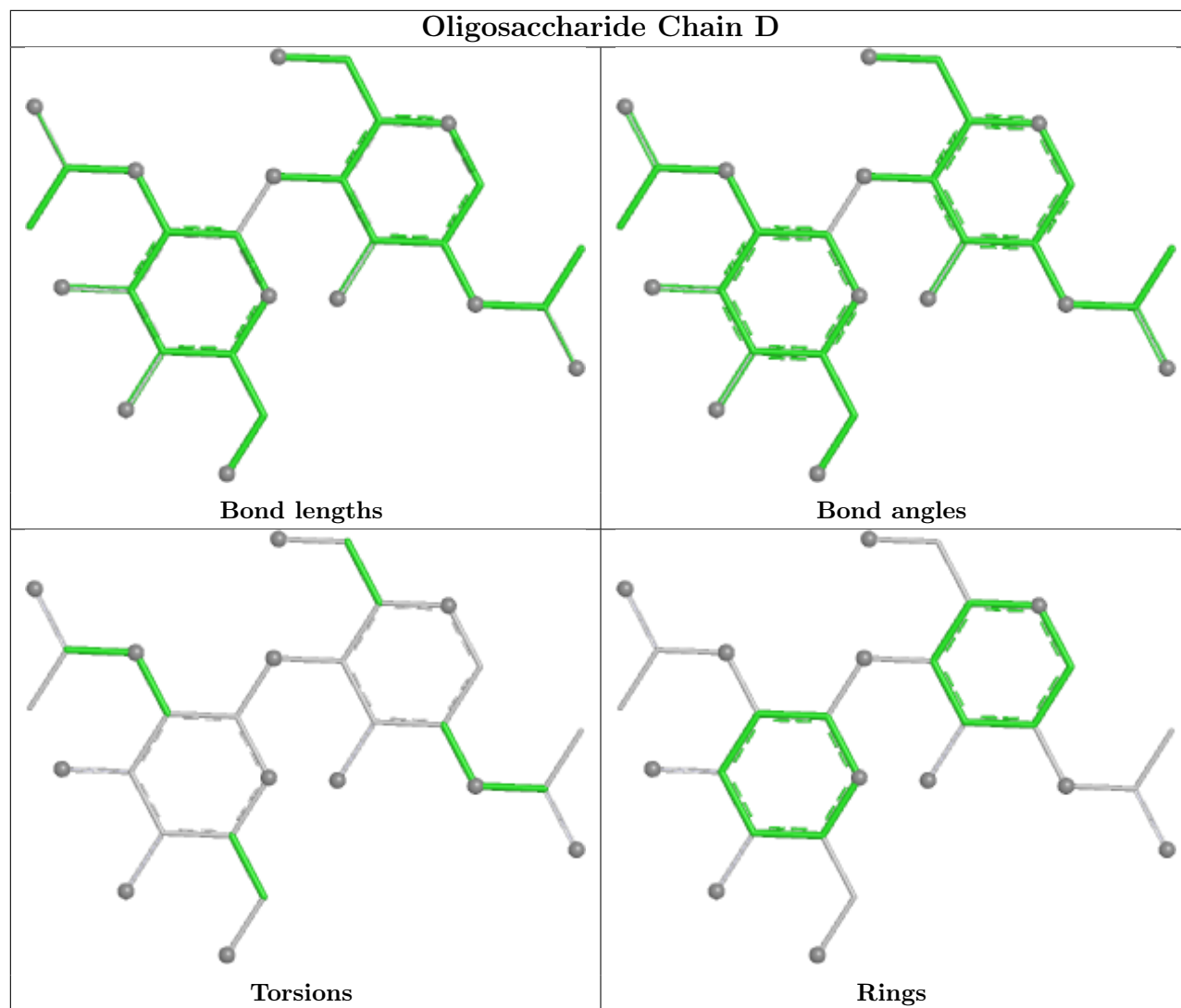
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	4	FUC	3	0
9	B	5	FUC	2	0

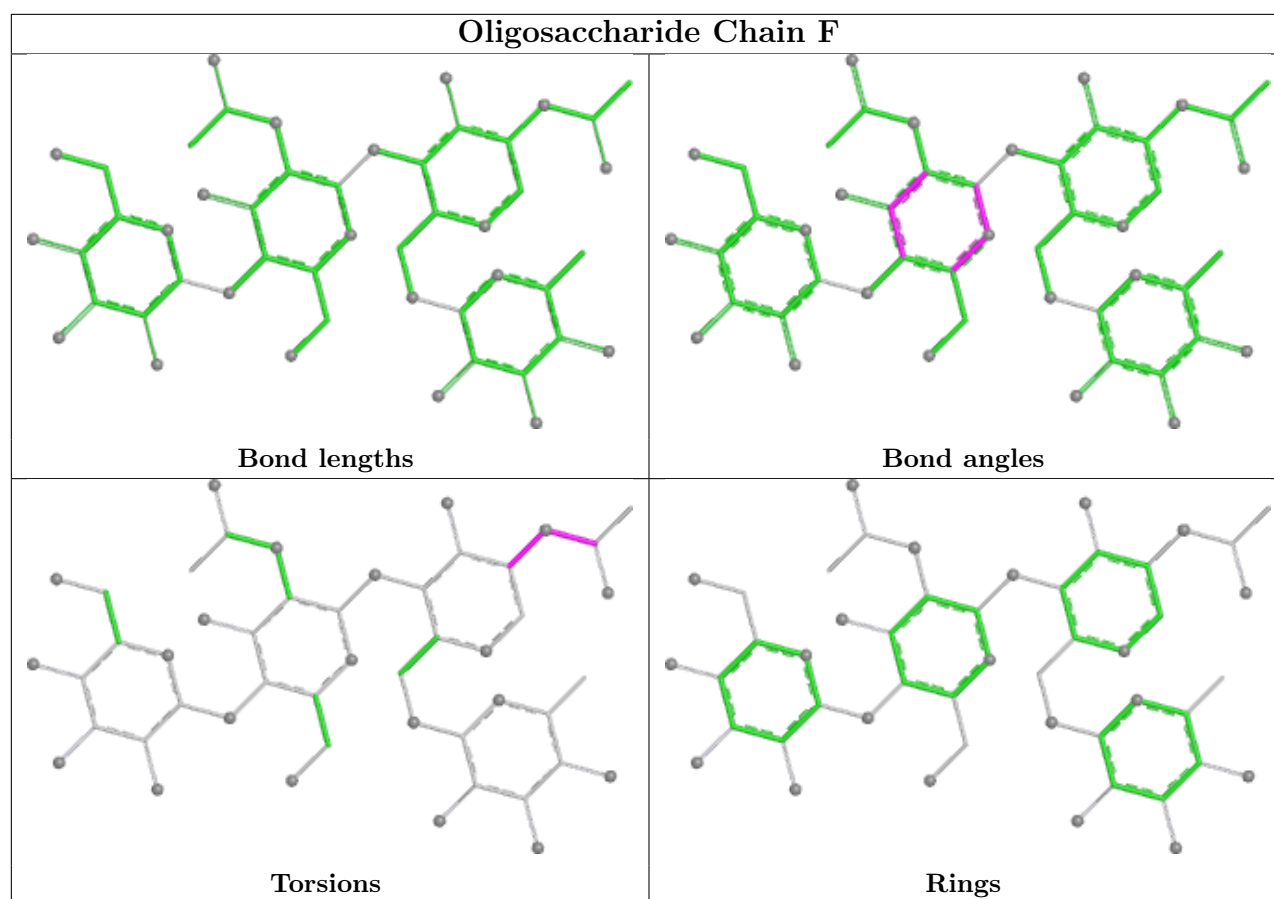
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	PLM	1	901	-	17,17,17	0.90	1 (5%)	17,17,17	1.01	1 (5%)
13	NAG	9	405	7	14,14,15	1.38	1 (7%)	17,19,21	1.57	2 (11%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PLM	1	901	-	-	2/15/15/15	-
13	NAG	9	405	7	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	9	405	NAG	C1-C2	3.82	1.57	1.52
12	1	901	PLM	C2-C1	2.10	1.55	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	9	405	NAG	C1-O5-C5	4.47	118.17	112.19
13	9	405	NAG	C1-C2-N2	2.26	113.99	110.43
12	1	901	PLM	O1-C1-C2	2.07	120.54	114.00

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	9	405	NAG	C4-C5-C6-O6
13	9	405	NAG	O5-C5-C6-O6
12	1	901	PLM	O2-C1-C2-C3
12	1	901	PLM	O1-C1-C2-C3

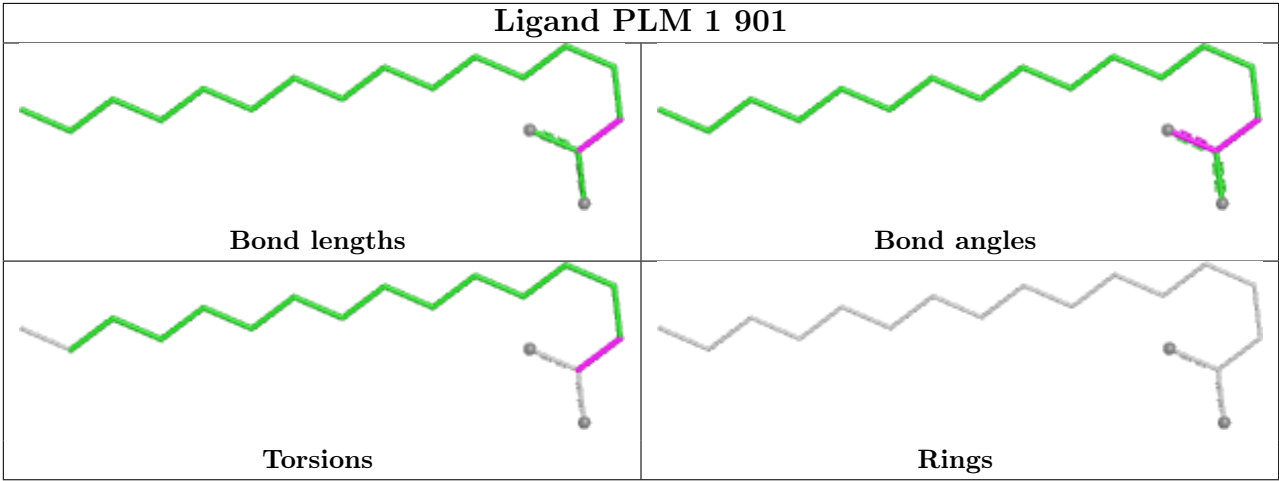
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	1	901	PLM	6	0
13	9	405	NAG	1	0

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

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	1:MYR	C1	2:GLY	N	0.65

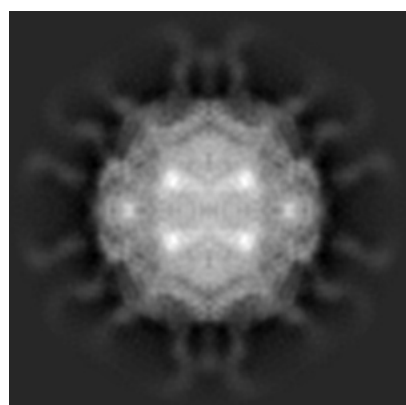
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6243. These allow visual inspection of the internal detail of the map and identification of artifacts.

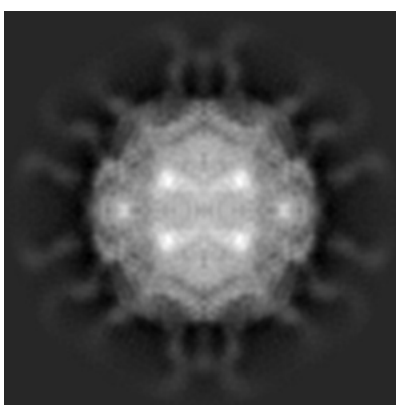
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

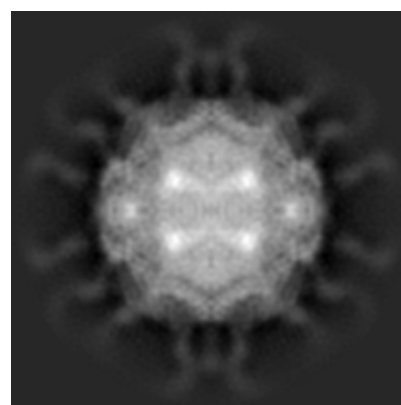
6.1.1 Primary map



X



Y

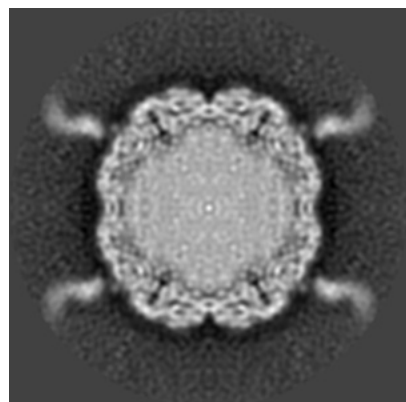


Z

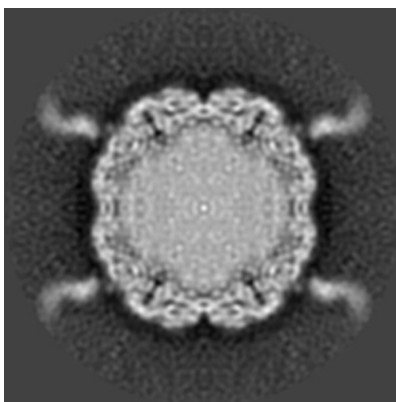
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

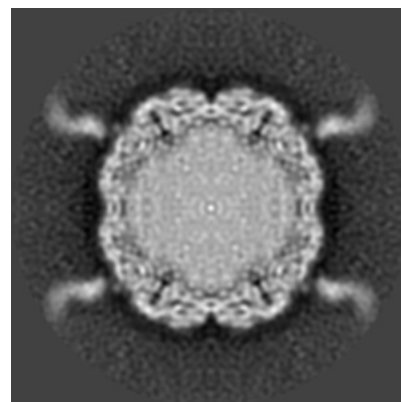
6.2.1 Primary map



X Index: 143



Y Index: 143

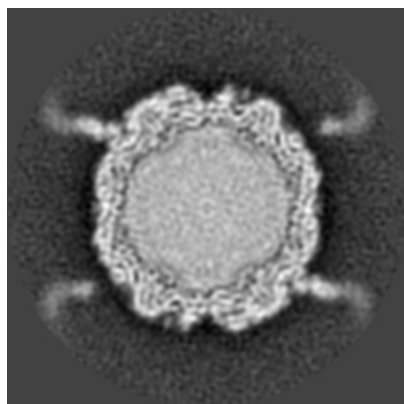


Z Index: 143

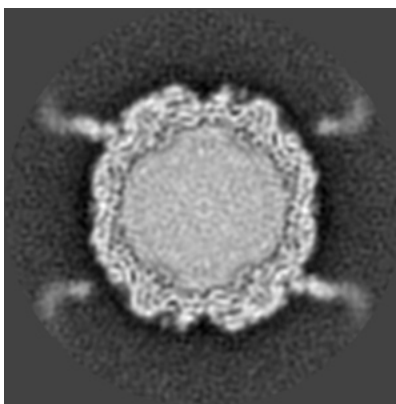
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

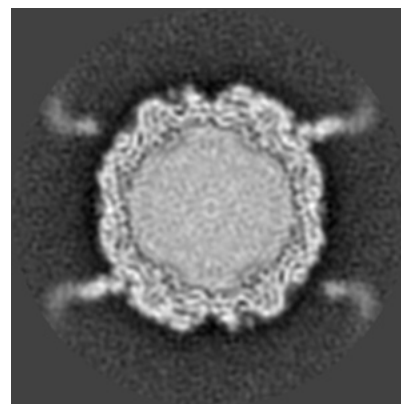
6.3.1 Primary map



X Index: 139



Y Index: 139

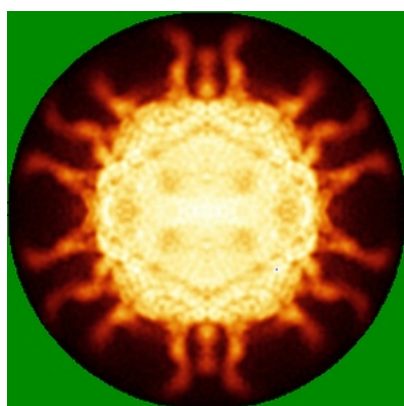


Z Index: 147

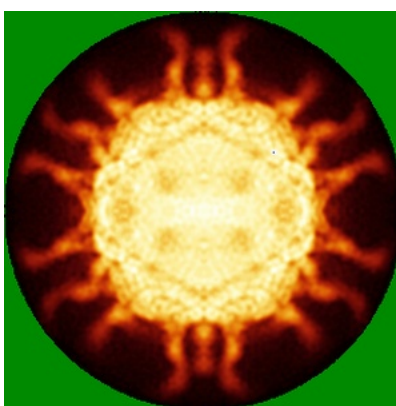
The images above show the largest variance slices of the map in three orthogonal directions.

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

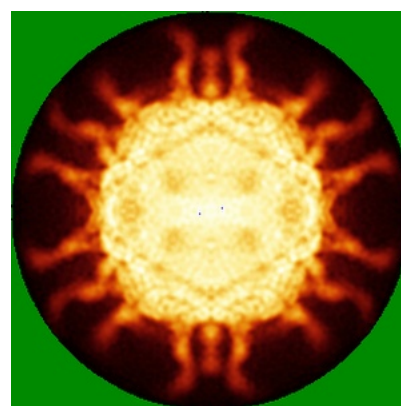
6.4.1 Primary map



X



Y

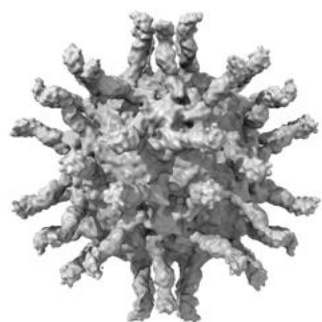


Z

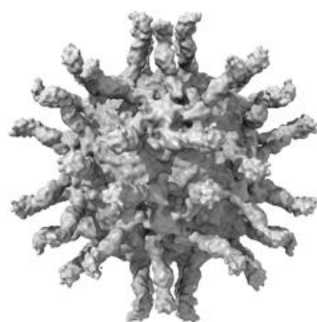
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

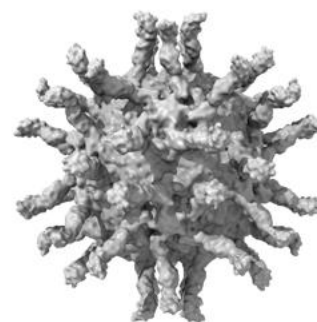
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 59.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

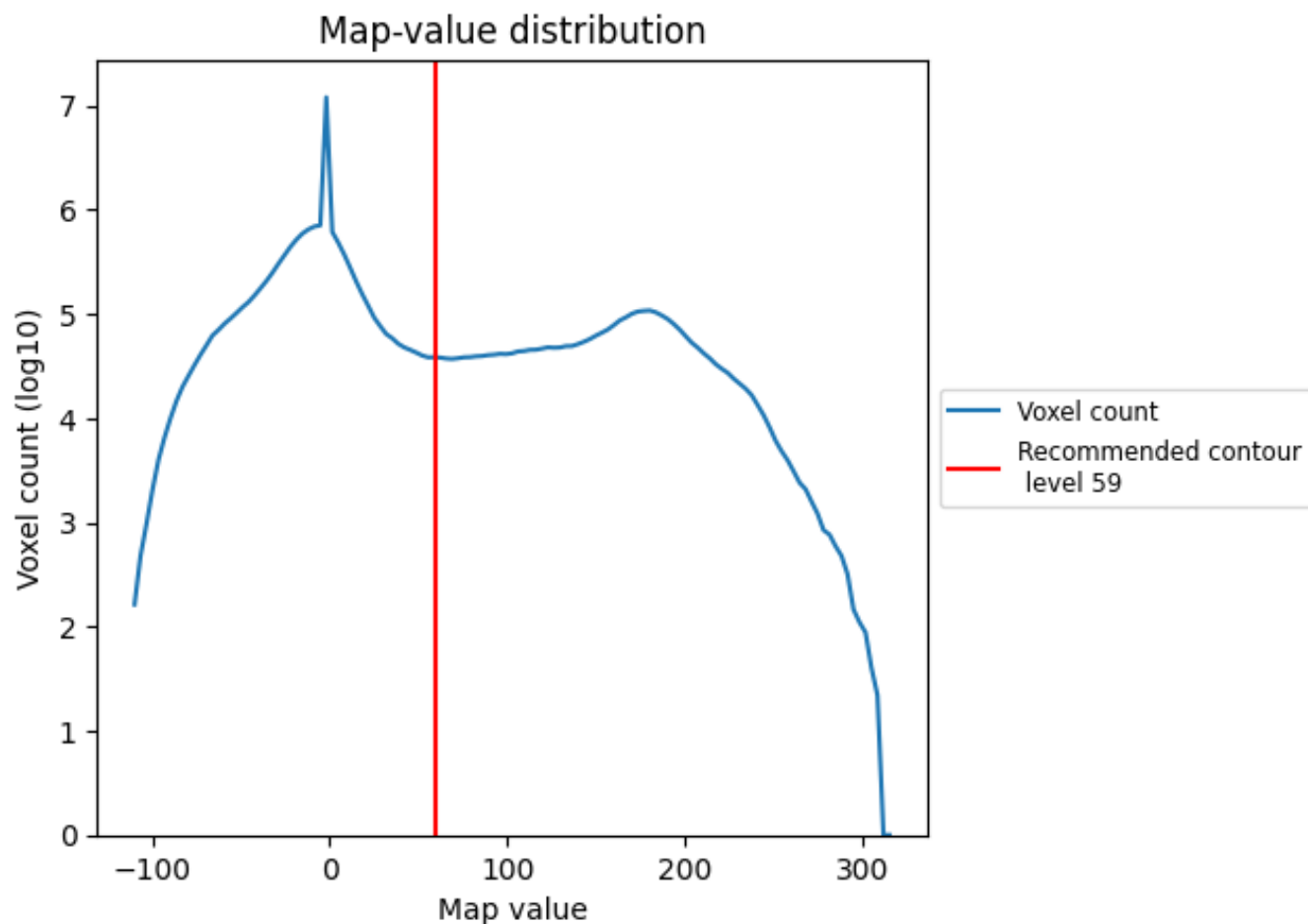
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

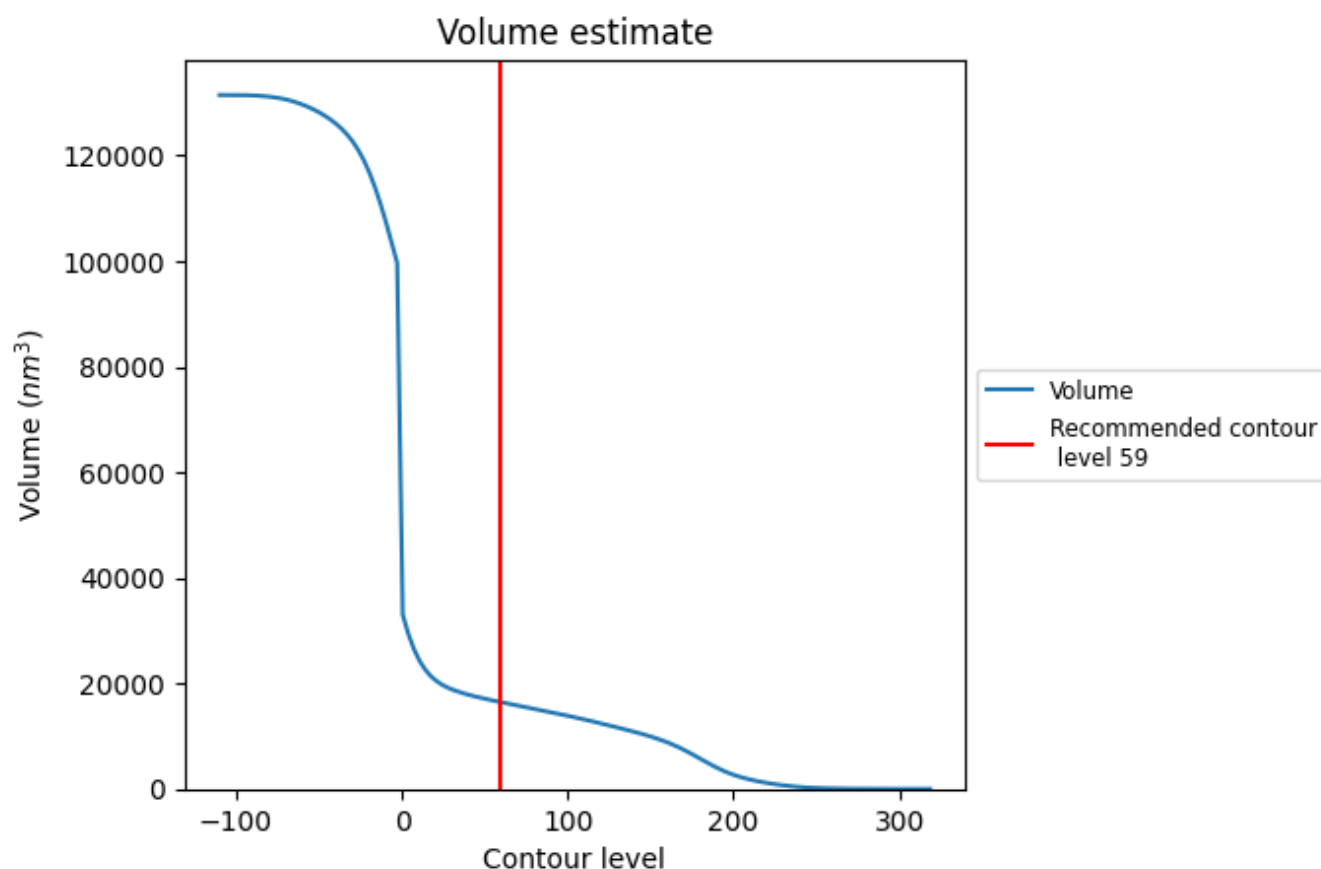
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

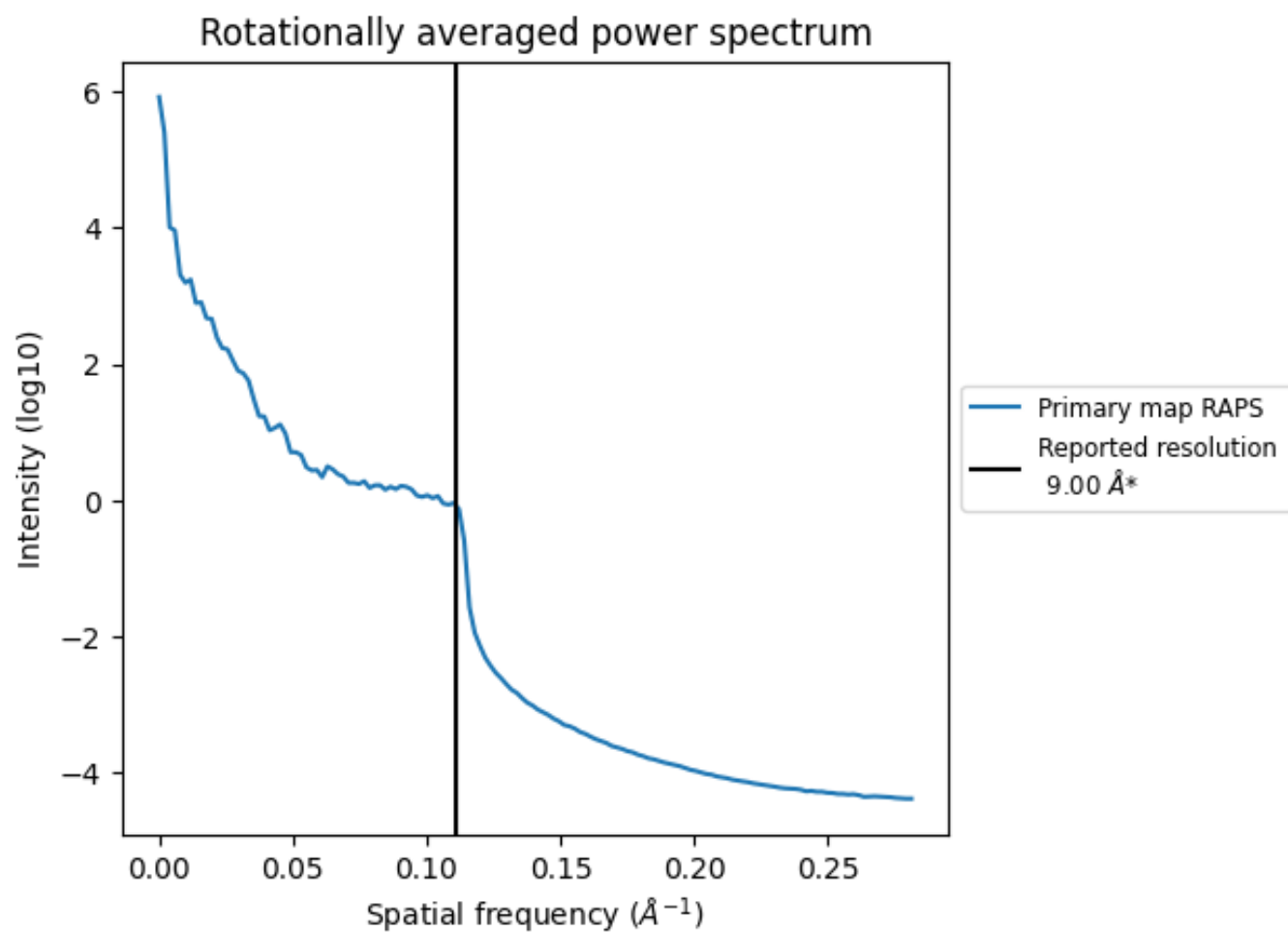
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 16503 nm³; this corresponds to an approximate mass of 14907 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 0.111 Å⁻¹

8 Fourier-Shell correlation

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

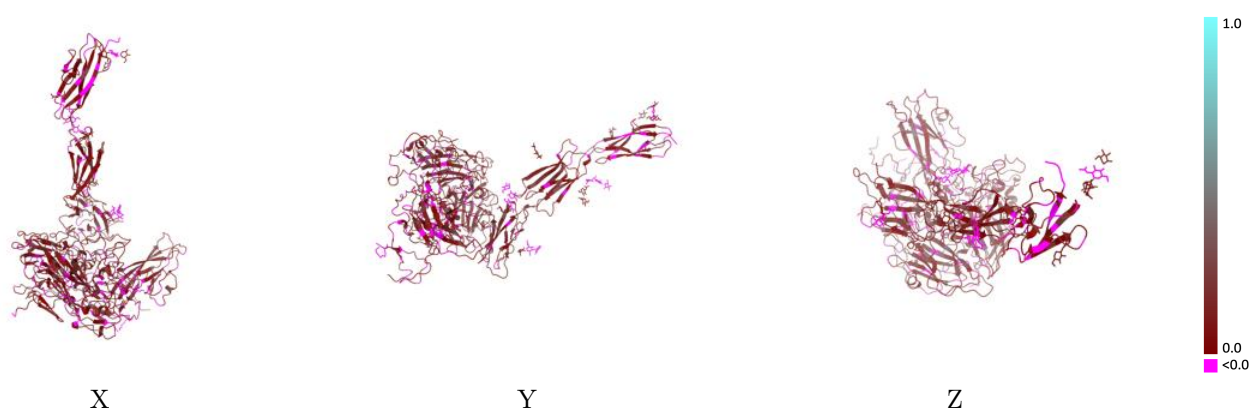
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6243 and PDB model 3J9F. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

This section was not generated.

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

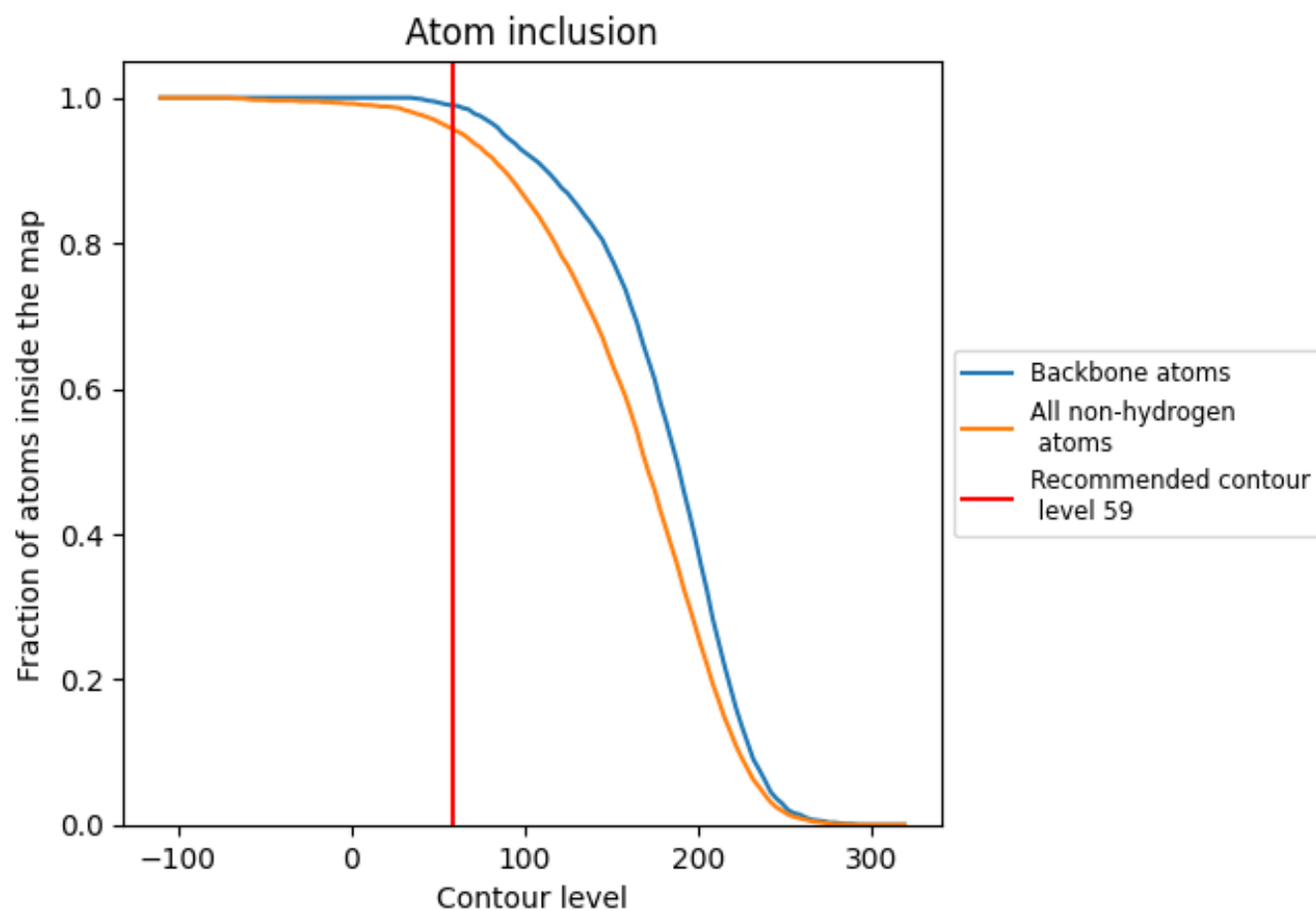


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 96% 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 (59) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9560	 0.1010
1	 0.9840	 0.1000
2	 0.9870	 0.1090
3	 0.9870	 0.0990
4	 0.9810	 0.0760
7	 0.9830	 0.1390
8	 0.9720	 0.1210
9	 0.8490	 0.0690
A	 0.2560	 -0.1570
B	 0.2670	 0.0030
C	 0.2500	 0.0730
D	 0.5000	 0.1060
E	 0.2050	 -0.0390
F	 0.3880	 0.1100

