



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 06:32 AM EDT

PDB ID : 7KYC / pdb_00007kyc
EMDB ID : EMD-23075
Title : Structure of the *S. cerevisiae* phosphatidylcholine flippase Dnf1-Lem3 complex in the E2P state
Authors : Bai, L.; You, Q.; Jain, B.K.; Duan, H.D.; Kovach, A.; Graham, T.R.; Li, H.
Deposited on : 2020-12-07
Resolution : 2.80 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.dev133
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) : 2.50

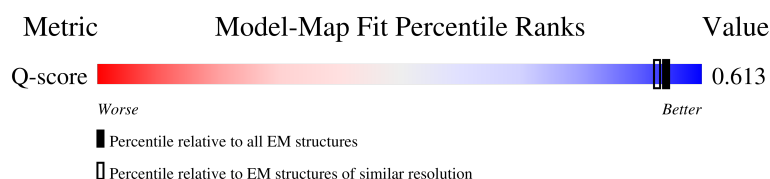
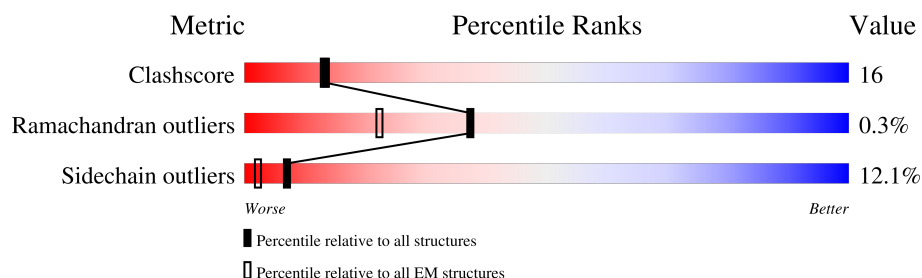
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	11806 (2.30 - 3.30)

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	1571	5% 47% 23% 5% 25%
2	B	414	63% 24% 10%
3	C	3	67% 33%
4	D	2	50% 50%

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Mol	Chain	Length	Quality of chain
4	E	2	50% 50%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12697 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.

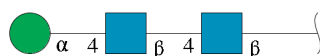
- Molecule 1 is a protein called Phospholipid-transporting ATPase DNF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1178	Total	C	N	O	S	0	0
			9409	6066	1561	1735	47		

- Molecule 2 is a protein called Alkylphosphocholine resistance protein LEM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	374	Total	C	N	O	S	0	0
			3004	1926	508	556	14		

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



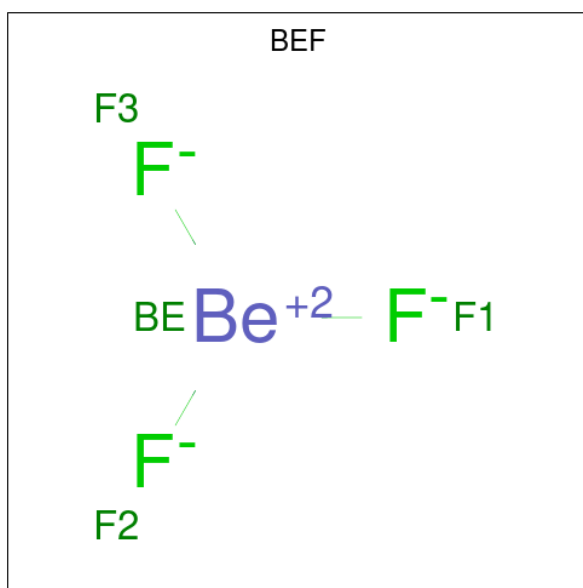
Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 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
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).

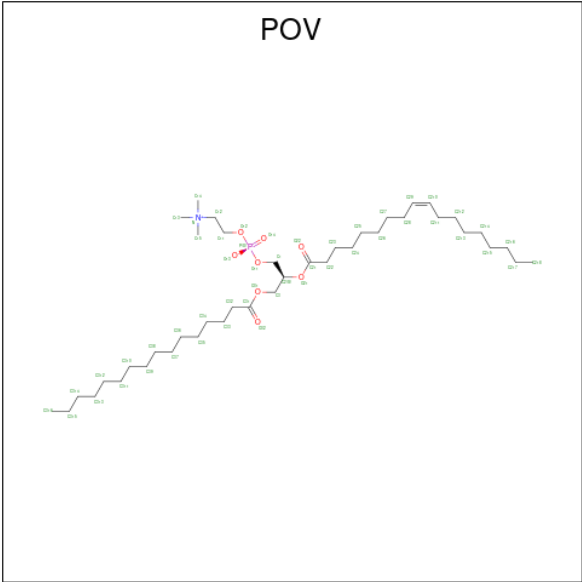


Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	Be	F	0
			4	1	3	

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

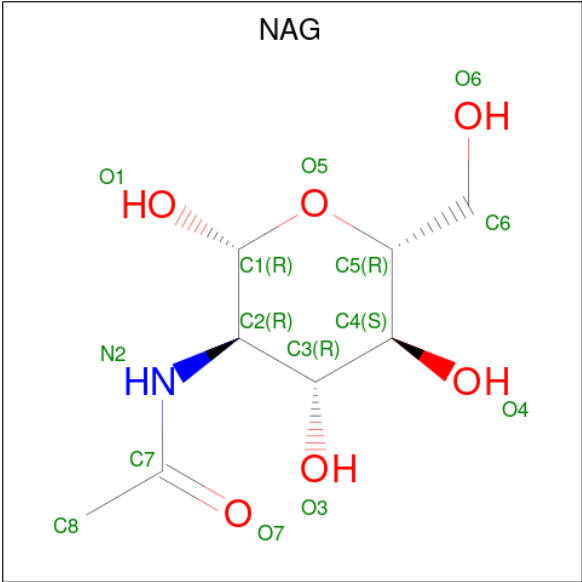
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Mg	0
			1	1	

- Molecule 7 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (CCD ID: POV) (formula: $\text{C}_{42}\text{H}_{82}\text{NO}_8\text{P}$).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
7	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
7	A	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

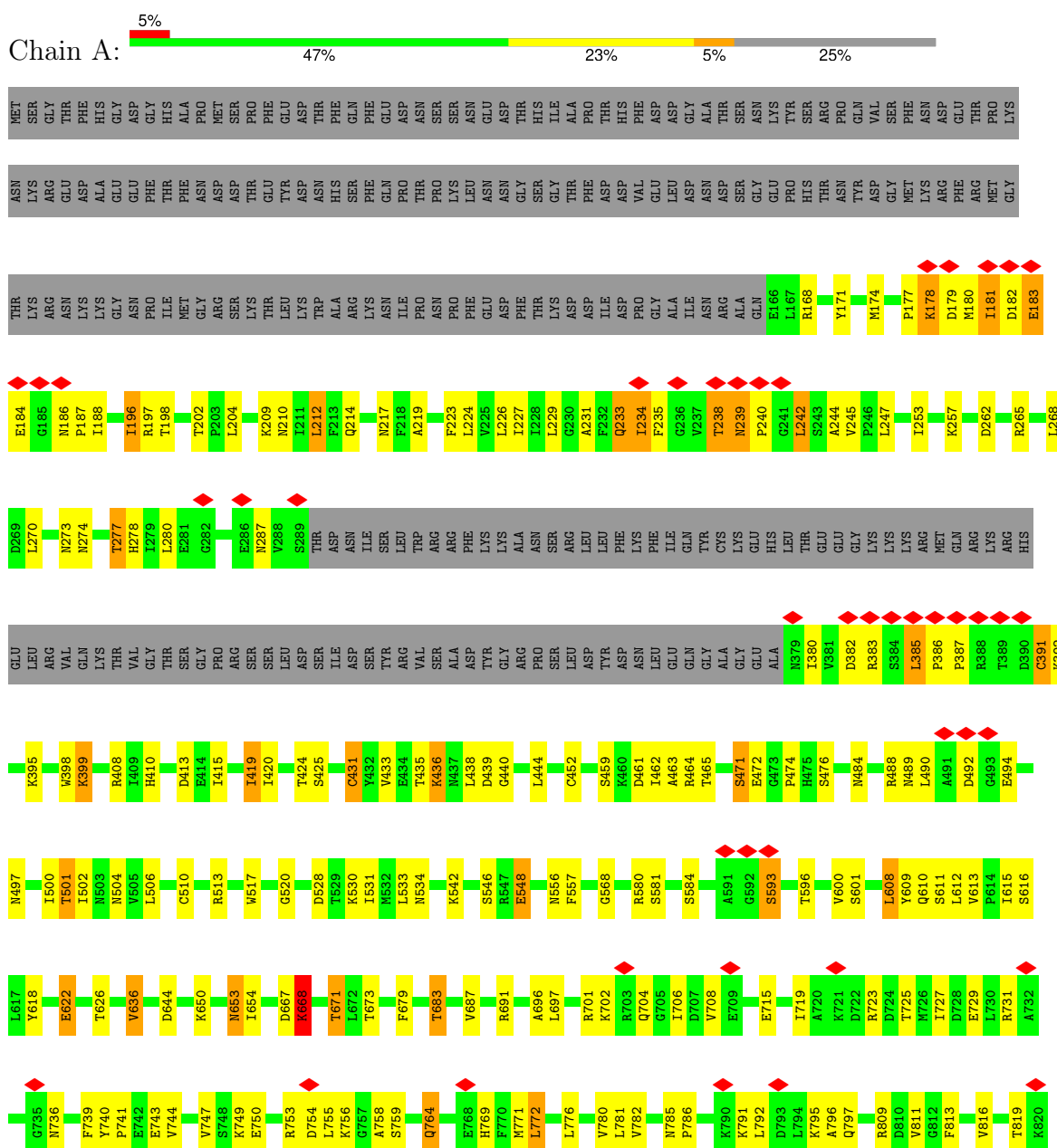


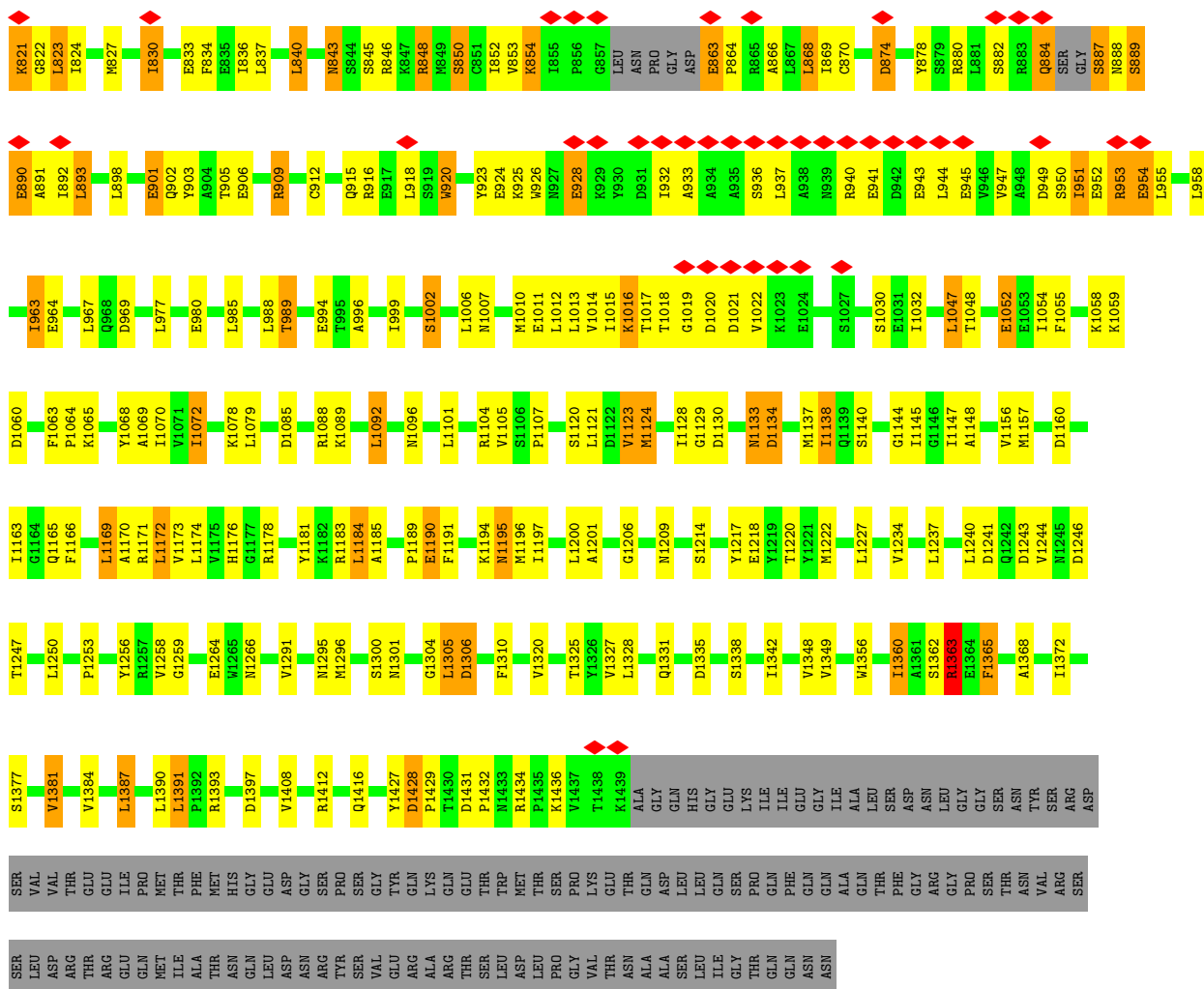
Mol	Chain	Residues	Atoms				AltConf
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	

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.

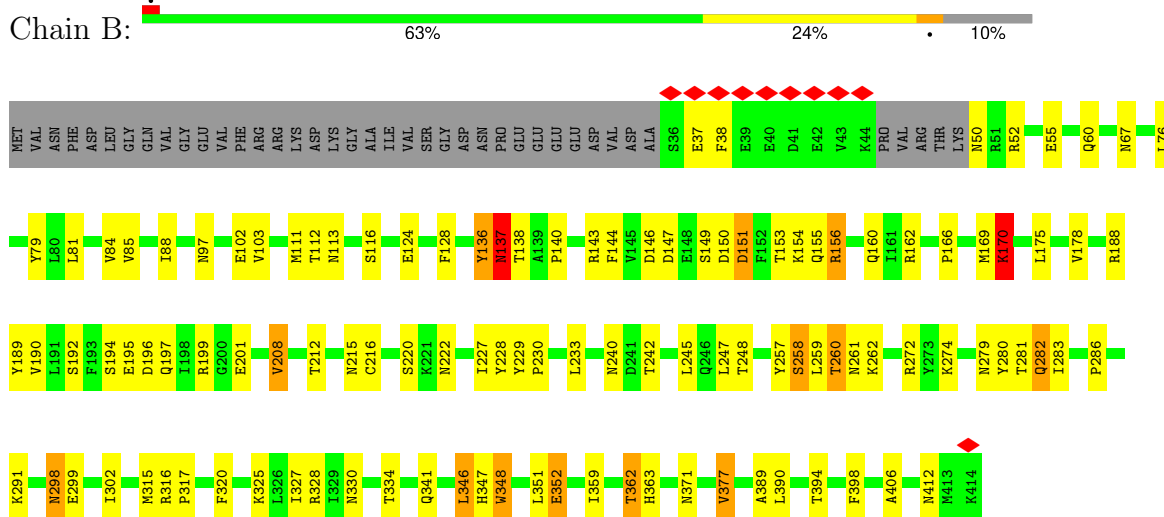
• Molecule 1: Phospholipid-transporting ATPase DNF1





• Molecule 2: Alkylphosphocholine resistance protein LEM3

Chain B:



• Molecule 3: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  67% 33%

HAG1
HAG2
HAG3

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

Chain D:  50% 50%

HAG1
HAG2

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

Chain E:  50% 50%

HAG1
HAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	590043	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.156	Depositor
Minimum map value	-0.097	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.018	Depositor
Map size ($\text{\AA}$)	231.28, 231.28, 231.28	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.826, 0.826, 0.826	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, POV, MAN, BEF, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.48	0/9614	0.61	8/13025 (0.1%)
2	B	0.57	0/3086	0.63	3/4196 (0.1%)
All	All	0.50	0/12700	0.62	11/17221 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	136	TYR	N-CA-C	9.85	121.70	110.97
1	A	1363	ARG	N-CA-C	9.08	120.79	111.07
1	A	1304	GLY	N-CA-C	7.45	121.45	111.03
1	A	668	LYS	N-CA-C	6.43	118.36	111.36
1	A	1306	ASP	N-CA-C	6.31	120.08	112.38
1	A	1365	PHE	N-CA-C	-5.61	105.75	112.59
1	A	1240	LEU	N-CA-C	5.52	120.12	113.17
1	A	233	GLN	N-CA-C	5.17	116.99	111.36
2	B	84	VAL	CA-C-N	-5.15	114.23	121.55
2	B	84	VAL	C-N-CA	-5.15	114.23	121.55
1	A	231	ALA	N-CA-C	5.12	116.87	111.28

There are no chirality outliers.

There are no planarity outliers.

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	A	9409	0	9410	330	0
2	B	3004	0	2883	82	0
3	C	39	0	34	1	0
4	D	28	0	25	0	0
4	E	28	0	25	1	0
5	A	4	0	0	1	0
6	A	1	0	0	0	0
7	A	156	0	246	29	0
8	B	28	0	26	3	0
All	All	12697	0	12649	407	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 16.

All (407) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLU:OE1	1:A:184:GLU:HG3	1.25	1.28
1:A:183:GLU:OE1	1:A:184:GLU:CG	1.82	1.25
1:A:884:GLN:C	1:A:887:SER:HB3	1.60	1.25
1:A:884:GLN:O	1:A:887:SER:HB3	1.36	1.20
1:A:616:SER:HB3	7:A:1603:POV:H25	1.33	1.09
1:A:183:GLU:CD	1:A:184:GLU:HG3	1.78	1.08
1:A:616:SER:HB3	7:A:1603:POV:C25	1.86	1.04
1:A:622:GLU:HB3	7:A:1604:POV:H31G	1.39	1.01
1:A:884:GLN:C	1:A:887:SER:CB	2.36	0.97
1:A:1320:VAL:HG11	1:A:1349:VAL:HG21	1.50	0.93
1:A:408:ARG:HH22	2:B:38:PHE:CB	1.82	0.91
1:A:668:LYS:HB3	1:A:989:THR:HG23	1.53	0.90
1:A:840:LEU:HB3	1:A:846:ARG:HH22	1.39	0.87
1:A:1169:LEU:HD22	1:A:1173:VAL:HG21	1.57	0.86
1:A:1305:LEU:HD22	1:A:1310:PHE:HD1	1.41	0.85
1:A:1047:LEU:O	1:A:1047:LEU:HD23	1.78	0.82
1:A:1058:LYS:HG3	1:A:1121:LEU:HD23	1.62	0.82
1:A:889:SER:C	1:A:891:ALA:H	1.90	0.80
1:A:387:PRO:HB3	1:A:464:ARG:HH11	1.44	0.79
2:B:169:MET:O	2:B:170:LYS:O	2.00	0.79
7:A:1604:POV:H36A	7:A:1605:POV:H35A	1.64	0.79
1:A:1107:PRO:HB3	1:A:1133:ASN:HA	1.66	0.78
1:A:238:THR:HG22	1:A:240:PRO:HD3	1.67	0.77
7:A:1605:POV:O22	7:A:1605:POV:H11A	1.84	0.76
1:A:1169:LEU:HD22	1:A:1173:VAL:CG2	2.14	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:LYS:HB3	1:A:989:THR:CG2	2.17	0.75
1:A:1169:LEU:O	1:A:1173:VAL:HB	1.86	0.75
1:A:183:GLU:OE1	1:A:184:GLU:HG2	1.82	0.74
1:A:616:SER:HB3	7:A:1603:POV:H25A	1.69	0.74
1:A:743:GLU:OE2	1:A:809:ARG:NH1	2.20	0.74
2:B:146:ASP:OD2	2:B:156:ARG:HD2	1.87	0.74
1:A:822:GLY:HA2	1:A:836:ILE:HG12	1.67	0.74
1:A:1181:TYR:CE2	1:A:1264:GLU:HB2	2.23	0.74
1:A:202:THR:HG22	1:A:204:LEU:H	1.52	0.74
2:B:52:ARG:NH2	2:B:55:GLU:OE2	2.20	0.73
1:A:1305:LEU:HD22	1:A:1310:PHE:CD1	2.24	0.73
1:A:1055:PHE:CE2	1:A:1059:LYS:NZ	2.56	0.73
2:B:150:ASP:O	2:B:156:ARG:NH2	2.21	0.73
7:A:1604:POV:H3A	7:A:1604:POV:H34A	1.70	0.73
2:B:170:LYS:HB2	2:B:363:HIS:CD2	2.23	0.73
2:B:299:GLU:OE2	8:B:1001:NAG:H82	1.89	0.73
1:A:474:PRO:HB2	1:A:533:LEU:HD11	1.71	0.73
1:A:616:SER:CB	7:A:1603:POV:H25	2.14	0.72
1:A:1178:ARG:NH2	1:A:1243:ASP:OD2	2.22	0.72
7:A:1603:POV:H14B	7:A:1603:POV:O14	1.89	0.72
1:A:415:ILE:HD13	1:A:506:LEU:HB3	1.72	0.71
1:A:1022:VAL:HG22	1:A:1032:ILE:HD12	1.73	0.71
2:B:136:TYR:CZ	2:B:166:PRO:HD3	2.25	0.71
1:A:622:GLU:HB3	7:A:1604:POV:C316	2.20	0.71
1:A:408:ARG:NH2	2:B:38:PHE:CB	2.55	0.70
1:A:239:ASN:N	1:A:240:PRO:HD3	2.07	0.70
1:A:691:ARG:NH2	1:A:715:GLU:OE1	2.23	0.70
1:A:889:SER:O	1:A:891:ALA:N	2.24	0.69
1:A:168:ARG:NH2	1:A:528:ASP:OD2	2.23	0.69
2:B:394:THR:O	2:B:398:PHE:HD2	1.75	0.69
1:A:234:ILE:HB	1:A:238:THR:HG23	1.72	0.69
1:A:1377:SER:O	1:A:1381:VAL:HG23	1.92	0.69
1:A:1363:ARG:HB3	2:B:195:GLU:OE2	1.94	0.68
1:A:408:ARG:HH22	2:B:38:PHE:CA	2.07	0.67
1:A:196:ILE:H	1:A:273:ASN:HD21	1.42	0.67
1:A:667:ASP:HB3	1:A:671:THR:HG21	1.76	0.67
1:A:408:ARG:NH2	2:B:38:PHE:HA	2.09	0.66
1:A:719:ILE:HG23	1:A:747:VAL:HG11	1.78	0.66
1:A:1363:ARG:HG2	2:B:195:GLU:HG3	1.77	0.66
1:A:824:ILE:HG22	1:A:833:GLU:HB3	1.76	0.65
1:A:750:GLU:O	1:A:754:ASP:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1006:LEU:HD11	1:A:1101:LEU:HD11	1.78	0.65
1:A:1291:VAL:HG21	1:A:1381:VAL:HG22	1.78	0.65
1:A:933:ALA:HB1	1:A:943:GLU:HB3	1.78	0.65
1:A:420:ILE:HD13	1:A:500:ILE:HD13	1.79	0.65
2:B:155:GLN:NE2	2:B:346:LEU:HB3	2.11	0.65
7:A:1604:POV:C36	7:A:1605:POV:H35A	2.26	0.64
1:A:874:ASP:OD1	1:A:874:ASP:N	2.30	0.64
1:A:915:GLN:HG2	1:A:958:LEU:HD22	1.79	0.64
1:A:1170:ALA:O	1:A:1174:LEU:HB2	1.96	0.64
7:A:1605:POV:H14A	7:A:1605:POV:O12	1.96	0.64
2:B:154:LYS:NZ	2:B:352:GLU:OE2	2.30	0.64
1:A:1058:LYS:HG2	1:A:1121:LEU:HA	1.79	0.64
1:A:1408:VAL:O	1:A:1412:ARG:HG3	1.97	0.64
1:A:1047:LEU:HD22	1:A:1047:LEU:H	1.63	0.64
1:A:1306:ASP:OD2	2:B:316:ARG:HD2	1.98	0.63
1:A:177:PRO:HD2	1:A:180:MET:HG3	1.81	0.63
1:A:415:ILE:HD12	1:A:510:CYS:HB2	1.80	0.63
1:A:1363:ARG:HB3	2:B:195:GLU:CD	2.24	0.63
1:A:1185:ALA:O	1:A:1189:PRO:HD2	1.98	0.63
1:A:776:LEU:HD13	1:A:853:VAL:HG21	1.79	0.63
1:A:696:ALA:HB2	1:A:1002:SER:O	1.99	0.62
1:A:1134:ASP:O	1:A:1138:ILE:HB	1.98	0.62
7:A:1604:POV:H36A	7:A:1605:POV:C35	2.29	0.62
2:B:151:ASP:OD1	2:B:151:ASP:N	2.33	0.62
1:A:1412:ARG:HH21	2:B:67:ASN:HD22	1.48	0.62
1:A:771:MET:HG3	1:A:811:VAL:HG21	1.82	0.61
1:A:848:ARG:NH2	1:A:952:GLU:OE2	2.32	0.61
2:B:406:ALA:O	2:B:412:ASN:ND2	2.23	0.61
2:B:279:ASN:HB2	2:B:282:GLN:HE21	1.66	0.60
7:A:1603:POV:H39A	7:A:1603:POV:H24	1.84	0.60
2:B:128:PHE:CZ	2:B:140:PRO:HG3	2.36	0.60
1:A:408:ARG:NH2	2:B:38:PHE:CA	2.65	0.60
1:A:274:ASN:OD1	1:A:399:LYS:NZ	2.34	0.60
1:A:419:ILE:HD12	1:A:520:GLY:HA3	1.84	0.60
1:A:866:ALA:HB3	1:A:918:LEU:HB3	1.84	0.60
1:A:889:SER:C	1:A:891:ALA:N	2.55	0.59
2:B:162:ARG:HE	2:B:341:GLN:HE21	1.49	0.59
1:A:653:ASN:HD22	1:A:654:ILE:HG23	1.67	0.59
1:A:954:GLU:OE2	1:A:955:LEU:N	2.36	0.59
1:A:1181:TYR:CE2	1:A:1259:GLY:HA2	2.39	0.58
1:A:1306:ASP:OD1	2:B:325:LYS:NZ	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:889:SER:HB3	1:A:892:ILE:HG12	1.85	0.58
1:A:1019:GLY:HA2	1:A:1022:VAL:HB	1.85	0.58
1:A:257:LYS:HD2	7:A:1604:POV:H31H	1.85	0.57
1:A:1169:LEU:CD2	1:A:1173:VAL:CG2	2.83	0.57
1:A:755:LEU:O	1:A:764:GLN:NE2	2.21	0.57
1:A:1054:ILE:HG13	1:A:1088:ARG:HG2	1.86	0.57
1:A:1178:ARG:NH2	1:A:1243:ASP:CG	2.63	0.57
2:B:137:ASN:O	2:B:138:THR:C	2.48	0.57
1:A:819:THR:OG1	1:A:821:LYS:O	2.23	0.56
1:A:1393:ARG:NH1	1:A:1397:ASP:OD1	2.38	0.56
2:B:175:LEU:HB3	2:B:328:ARG:HB2	1.87	0.56
7:A:1603:POV:H32	7:A:1603:POV:H36	1.87	0.56
1:A:1296:MET:HE1	2:B:320:PHE:HD2	1.69	0.56
1:A:171:TYR:H	1:A:287:ASN:HD21	1.54	0.56
1:A:636:VAL:H	2:B:60:GLN:HE22	1.53	0.56
1:A:1169:LEU:CD2	1:A:1173:VAL:HG21	2.32	0.56
1:A:182:ASP:HB2	1:A:188:ILE:HG13	1.87	0.56
1:A:769:HIS:NE2	1:A:915:GLN:OE1	2.31	0.56
1:A:926:TRP:NE1	1:A:951:ILE:HB	2.21	0.56
1:A:1183:ARG:NE	1:A:1241:ASP:O	2.32	0.56
1:A:1016:LYS:HE3	1:A:1018:THR:HG21	1.88	0.55
1:A:1291:VAL:HG21	1:A:1381:VAL:CG2	2.36	0.55
2:B:260:THR:OG1	4:E:1:NAG:H83	2.06	0.55
1:A:1428:ASP:HB3	1:A:1431:ASP:HB2	1.88	0.55
1:A:1138:ILE:HG23	1:A:1144:GLY:HA3	1.89	0.55
1:A:994:GLU:CD	1:A:994:GLU:H	2.15	0.55
1:A:380:ILE:HG12	1:A:465:THR:HG23	1.89	0.55
1:A:727:ILE:HG23	1:A:739:PHE:HZ	1.71	0.54
1:A:772:LEU:HD21	1:A:827:MET:HE2	1.89	0.54
1:A:1015:ILE:HB	1:A:1072:ILE:HG23	1.90	0.54
2:B:79:TYR:HB3	2:B:389:ALA:HB2	1.90	0.54
1:A:184:GLU:O	1:A:186:ASN:ND2	2.40	0.54
1:A:1133:ASN:OD1	1:A:1133:ASN:N	2.41	0.54
1:A:1178:ARG:HB3	1:A:1178:ARG:CZ	2.37	0.54
1:A:596:THR:O	1:A:600:VAL:HG23	2.08	0.54
1:A:1328:LEU:HB2	1:A:1342:ILE:HD13	1.90	0.54
1:A:880:ARG:HG2	1:A:953:ARG:HA	1.90	0.54
1:A:1178:ARG:NH2	1:A:1243:ASP:OD1	2.39	0.54
1:A:265:ARG:NH2	1:A:1157:MET:O	2.40	0.54
1:A:1174:LEU:HD23	1:A:1256:TYR:CD2	2.43	0.53
1:A:242:LEU:N	1:A:242:LEU:HD22	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:TYR:CZ	1:A:791:LYS:HD2	2.43	0.53
1:A:471:SER:OG	1:A:472:GLU:O	2.27	0.53
1:A:593:SER:HB2	1:A:596:THR:HG22	1.90	0.53
1:A:947:VAL:O	1:A:950:SER:OG	2.25	0.53
1:A:1246:ASP:OD1	1:A:1246:ASP:N	2.41	0.53
2:B:259:LEU:HB3	2:B:328:ARG:HB3	1.90	0.53
1:A:1227:LEU:HB2	7:A:1603:POV:H22A	1.91	0.53
2:B:258:SER:O	2:B:330:ASN:ND2	2.40	0.53
1:A:792:LEU:HD11	1:A:816:VAL:HG13	1.90	0.52
1:A:888:ASN:HB3	1:A:893:LEU:CD2	2.38	0.52
1:A:772:LEU:HD23	1:A:813:PHE:HD1	1.73	0.52
1:A:171:TYR:HE2	1:A:180:MET:HE2	1.74	0.52
1:A:943:GLU:O	1:A:947:VAL:HG23	2.09	0.52
1:A:1169:LEU:O	1:A:1173:VAL:N	2.36	0.52
2:B:199:ARG:HH21	2:B:274:LYS:HZ2	1.58	0.52
2:B:208:VAL:HG13	2:B:216:CYS:SG	2.50	0.52
1:A:888:ASN:HB3	1:A:893:LEU:HD21	1.92	0.52
1:A:1218:GLU:OE1	1:A:1220:THR:OG1	2.27	0.52
1:A:219:ALA:HB3	1:A:618:TYR:CE2	2.45	0.52
1:A:489:ASN:HD22	1:A:490:LEU:H	1.58	0.52
1:A:928:GLU:O	1:A:932:ILE:HD12	2.10	0.51
1:A:226:LEU:HD13	1:A:610:GLN:HG2	1.91	0.51
1:A:1387:LEU:O	1:A:1391:LEU:HB2	2.10	0.51
2:B:143:ARG:NH2	2:B:160:GLN:OE1	2.43	0.51
1:A:843:ASN:HB2	1:A:846:ARG:HB2	1.92	0.51
1:A:1006:LEU:CD2	1:A:1010:MET:HE2	2.40	0.51
1:A:1121:LEU:O	1:A:1123:VAL:HB	2.09	0.51
1:A:754:ASP:HA	1:A:758:ALA:HB3	1.93	0.51
2:B:315:MET:O	2:B:317:PRO:HD3	2.11	0.50
1:A:1014:VAL:HG12	1:A:1016:LYS:H	1.77	0.50
1:A:697:LEU:HD11	1:A:701:ARG:NH2	2.26	0.50
1:A:179:ASP:OD1	1:A:179:ASP:N	2.40	0.50
1:A:489:ASN:HD22	1:A:490:LEU:N	2.09	0.50
1:A:840:LEU:HB3	1:A:846:ARG:NH2	2.18	0.50
1:A:501:THR:H	1:A:504:ASN:HD22	1.60	0.50
1:A:673:THR:HA	1:A:967:LEU:HA	1.92	0.50
1:A:1052:GLU:CD	1:A:1052:GLU:H	2.20	0.50
1:A:902:GLN:NE2	1:A:906:GLU:OE2	2.44	0.50
1:A:920:TRP:O	1:A:924:GLU:HG2	2.12	0.50
1:A:1006:LEU:HD22	1:A:1010:MET:HE2	1.94	0.50
2:B:150:ASP:OD1	2:B:291:LYS:NZ	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:VAL:HG21	2:B:55:GLU:HG3	1.94	0.49
1:A:785:ASN:OD1	1:A:786:PRO:HD2	2.12	0.49
1:A:824:ILE:HA	1:A:833:GLU:HA	1.93	0.49
2:B:242:THR:HG23	2:B:347:HIS:CD2	2.47	0.49
1:A:1047:LEU:H	1:A:1047:LEU:CD2	2.24	0.49
7:A:1605:POV:H22A	7:A:1605:POV:C26	2.42	0.49
2:B:85:VAL:HA	2:B:88:ILE:HG13	1.94	0.49
1:A:1325:THR:HB	1:A:1390:LEU:HD11	1.95	0.49
1:A:902:GLN:O	1:A:905:THR:OG1	2.28	0.49
1:A:1320:VAL:HG11	1:A:1349:VAL:CG2	2.32	0.49
1:A:1412:ARG:NH2	2:B:67:ASN:HD22	2.10	0.49
7:A:1604:POV:H3A	7:A:1604:POV:C34	2.42	0.49
1:A:679:PHE:HA	1:A:963:ILE:HG13	1.95	0.48
1:A:1362:SER:HB2	1:A:1365:PHE:HB3	1.94	0.48
1:A:459:SER:OG	2:B:37:GLU:CB	2.61	0.48
1:A:626:THR:HG22	7:A:1604:POV:H37A	1.96	0.48
1:A:668:LYS:HD2	1:A:996:ALA:HA	1.93	0.48
1:A:671:THR:HB	1:A:1147:ILE:HD12	1.96	0.48
2:B:170:LYS:HB2	2:B:363:HIS:CG	2.48	0.48
1:A:227:ILE:HD13	1:A:244:ALA:HA	1.95	0.48
1:A:542:LYS:HE2	1:A:546:SER:HB3	1.96	0.48
1:A:749:LYS:HD3	1:A:753:ARG:CZ	2.43	0.48
1:A:1047:LEU:HD23	1:A:1047:LEU:C	2.31	0.48
1:A:749:LYS:HD3	1:A:753:ARG:NH1	2.28	0.48
2:B:291:LYS:HE3	3:C:1:NAG:H83	1.96	0.48
1:A:1190:GLU:HG2	1:A:1327:VAL:HG22	1.95	0.48
1:A:1363:ARG:HG2	2:B:195:GLU:CG	2.42	0.48
1:A:168:ARG:HG3	1:A:168:ARG:O	2.14	0.48
7:A:1605:POV:C36	7:A:1605:POV:H24A	2.44	0.48
2:B:283:ILE:HD11	2:B:302:ILE:HD13	1.96	0.48
2:B:327:ILE:O	2:B:328:ARG:NH2	2.44	0.48
2:B:102:GLU:HB3	2:B:362:THR:HG23	1.96	0.48
2:B:103:VAL:HG13	2:B:128:PHE:CE1	2.48	0.48
1:A:736:ASN:HB3	1:A:739:PHE:HB2	1.95	0.48
1:A:1022:VAL:HA	1:A:1032:ILE:CD1	2.44	0.48
7:A:1605:POV:H22A	7:A:1605:POV:H26	1.96	0.48
2:B:188:ARG:NH2	2:B:215:ASN:O	2.47	0.48
2:B:227:ILE:O	2:B:283:ILE:HA	2.14	0.48
1:A:239:ASN:N	1:A:239:ASN:HD22	2.11	0.47
1:A:233:GLN:HB3	1:A:235:PHE:CD1	2.49	0.47
1:A:608:LEU:HD13	1:A:609:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:ILE:HG12	1:A:868:LEU:HD23	1.97	0.47
1:A:1194:LYS:HG3	1:A:1195:ASN:H	1.79	0.47
1:A:1250:LEU:HD13	1:A:1429:PRO:HD2	1.96	0.47
2:B:169:MET:C	2:B:170:LYS:O	2.57	0.47
1:A:863:GLU:HG2	1:A:920:TRP:HD1	1.80	0.47
7:A:1603:POV:H39A	7:A:1603:POV:C24	2.44	0.47
2:B:170:LYS:HD2	2:B:170:LYS:HA	1.36	0.47
2:B:279:ASN:C	2:B:281:THR:H	2.23	0.47
1:A:217:ASN:HB3	1:A:618:TYR:CZ	2.49	0.47
1:A:548:GLU:H	1:A:548:GLU:HG2	1.52	0.47
1:A:725:THR:O	1:A:729:GLU:HG3	2.15	0.47
1:A:926:TRP:NE1	1:A:947:VAL:HG12	2.29	0.47
1:A:1384:VAL:HG21	2:B:377:VAL:HG13	1.96	0.47
1:A:440:GLY:HA3	5:A:1601:BEF:F3	2.04	0.47
1:A:977:LEU:HD11	1:A:1429:PRO:HG2	1.97	0.47
1:A:1140:SER:O	1:A:1140:SER:OG	2.30	0.47
1:A:1306:ASP:OD2	2:B:316:ARG:CD	2.63	0.47
7:A:1603:POV:H32	7:A:1603:POV:C36	2.43	0.47
2:B:229:TYR:CD1	2:B:229:TYR:C	2.88	0.47
1:A:593:SER:O	1:A:596:THR:HG22	2.15	0.47
1:A:1130:ASP:OD1	1:A:1130:ASP:O	2.33	0.47
1:A:239:ASN:N	1:A:239:ASN:ND2	2.60	0.46
1:A:568:GLY:HA2	1:A:601:SER:HB2	1.95	0.46
1:A:277:THR:HG1	1:A:398:TRP:CD1	2.33	0.46
1:A:382:ASP:OD1	1:A:385:LEU:HD13	2.16	0.46
1:A:1201:ALA:HB3	1:A:1217:TYR:OH	2.16	0.46
1:A:1206:GLY:HA2	1:A:1209:ASN:OD1	2.14	0.46
1:A:1247:THR:HG23	1:A:1427:TYR:HB3	1.97	0.46
1:A:926:TRP:CE2	1:A:947:VAL:HG12	2.51	0.46
1:A:1018:THR:O	1:A:1022:VAL:N	2.44	0.46
1:A:1436:LYS:HB3	1:A:1436:LYS:HE3	1.64	0.46
1:A:226:LEU:CD1	1:A:610:GLN:HG2	2.44	0.46
1:A:242:LEU:N	1:A:242:LEU:CD2	2.79	0.46
2:B:298:ASN:OD1	8:B:1001:NAG:C2	2.63	0.46
1:A:223:PHE:CZ	1:A:615:ILE:HA	2.51	0.46
1:A:461:ASP:O	1:A:465:THR:OG1	2.33	0.46
1:A:1356:TRP:CE2	1:A:1362:SER:HB3	2.51	0.46
2:B:240:ASN:HB2	2:B:348:TRP:HD1	1.80	0.46
1:A:391:CYS:SG	1:A:463:ALA:HB2	2.55	0.46
1:A:484:ASN:OD1	1:A:497:ASN:HB2	2.16	0.46
1:A:1184:LEU:HD23	1:A:1184:LEU:HA	1.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:261:ASN:HB3	2:B:328:ARG:NH2	2.31	0.46
1:A:884:GLN:C	1:A:887:SER:CA	2.89	0.45
1:A:671:THR:HG21	1:A:1129:GLY:HA2	1.99	0.45
1:A:1172:LEU:HA	1:A:1176:HIS:HD2	1.81	0.45
1:A:476:SER:HB2	1:A:533:LEU:HB3	1.98	0.45
1:A:925:LYS:HD3	1:A:925:LYS:N	2.32	0.45
1:A:1092:LEU:O	1:A:1096:ASN:ND2	2.50	0.45
1:A:1191:PHE:O	1:A:1194:LYS:HG3	2.17	0.45
2:B:196:ASP:O	2:B:201:GLU:HB2	2.17	0.45
1:A:918:LEU:HD12	1:A:918:LEU:HA	1.79	0.45
2:B:240:ASN:HB3	2:B:347:HIS:HB2	1.99	0.45
2:B:247:LEU:HB2	2:B:257:TYR:HB3	1.97	0.45
1:A:702:LYS:HB2	1:A:708:VAL:HG21	1.99	0.45
1:A:780:VAL:HG22	1:A:796:ALA:HB2	1.99	0.45
1:A:644:ASP:OD2	2:B:50:ASN:HB2	2.17	0.45
1:A:827:MET:O	1:A:830:ILE:HG23	2.17	0.45
1:A:1063:PHE:CG	1:A:1064:PRO:HD2	2.52	0.45
1:A:1431:ASP:O	1:A:1434:ARG:HB2	2.17	0.45
1:A:781:LEU:O	1:A:795:LYS:N	2.50	0.44
1:A:837:LEU:HD21	1:A:854:LYS:HB2	1.99	0.44
1:A:949:ASP:O	1:A:953:ARG:HD3	2.18	0.44
1:A:383:ARG:HA	1:A:383:ARG:HH11	1.82	0.44
1:A:747:VAL:HG12	1:A:747:VAL:O	2.17	0.44
1:A:268:LEU:HD11	1:A:650:LYS:HZ1	1.83	0.44
1:A:683:THR:HG22	1:A:903:TYR:HE2	1.81	0.44
1:A:444:LEU:HB2	1:A:797:GLN:HG2	2.00	0.44
1:A:1010:MET:HE3	1:A:1069:ALA:HB2	1.98	0.44
1:A:1237:LEU:HD12	1:A:1331:GLN:HG3	1.98	0.44
1:A:1335:ASP:OD2	1:A:1338:SER:HB2	2.17	0.44
1:A:1030:SER:HB2	1:A:1079:LEU:HD22	1.99	0.44
1:A:178:LYS:HD3	1:A:178:LYS:HA	1.68	0.44
1:A:837:LEU:HB3	1:A:923:TYR:OH	2.18	0.44
1:A:1058:LYS:CG	1:A:1121:LEU:HD23	2.39	0.44
1:A:1243:ASP:OD2	1:A:1244:VAL:N	2.46	0.44
1:A:212:LEU:HD23	1:A:212:LEU:HA	1.85	0.43
1:A:874:ASP:HA	1:A:912:CYS:SG	2.58	0.43
1:A:969:ASP:HB3	1:A:1432:PRO:HG2	1.99	0.43
1:A:980:GLU:HB3	1:A:1253:PRO:HG2	2.00	0.43
2:B:222:ASN:HB3	2:B:228:TYR:CE1	2.52	0.43
1:A:1163:ILE:HD12	1:A:1165:GLN:O	2.18	0.43
1:A:234:ILE:HB	1:A:238:THR:CG2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:LEU:HD12	1:A:510:CYS:SG	2.58	0.43
1:A:580:ARG:HA	1:A:580:ARG:HD3	1.84	0.43
1:A:1169:LEU:CD2	1:A:1173:VAL:HG23	2.48	0.43
1:A:706:ILE:H	1:A:706:ILE:HG13	1.67	0.43
1:A:878:TYR:OH	1:A:893:LEU:O	2.37	0.43
2:B:111:MET:HE2	2:B:111:MET:HB3	1.79	0.43
2:B:248:THR:HB	2:B:341:GLN:HB3	2.00	0.43
1:A:424:THR:HG21	1:A:431:CYS:HB2	2.01	0.43
1:A:436:LYS:HB2	1:A:436:LYS:HE3	1.79	0.43
1:A:776:LEU:HD23	1:A:823:LEU:HD12	2.00	0.43
1:A:916:ARG:NE	1:A:954:GLU:HB3	2.34	0.43
1:A:941:GLU:O	1:A:945:GLU:HG2	2.19	0.43
1:A:198:THR:HG21	1:A:1157:MET:HE2	2.01	0.43
1:A:1007:ASN:ND2	1:A:1010:MET:HB2	2.34	0.43
1:A:864:PRO:HG2	1:A:920:TRP:NE1	2.33	0.43
1:A:1011:GLU:HB3	1:A:1068:TYR:HD1	1.83	0.43
1:A:1148:ALA:HA	1:A:1156:VAL:HG21	2.01	0.43
1:A:1368:ALA:O	1:A:1372:ILE:HB	2.19	0.43
1:A:1169:LEU:O	1:A:1173:VAL:CB	2.60	0.43
2:B:298:ASN:HB2	2:B:299:GLU:OE1	2.19	0.43
1:A:1047:LEU:CD2	1:A:1047:LEU:N	2.80	0.42
1:A:1089:LYS:HB2	1:A:1089:LYS:HE2	1.89	0.42
1:A:1363:ARG:HG2	2:B:195:GLU:CD	2.44	0.42
2:B:291:LYS:HE3	2:B:291:LYS:HB3	1.83	0.42
1:A:901:GLU:O	1:A:905:THR:HG23	2.19	0.42
1:A:1197:ILE:HG21	1:A:1197:ILE:HD13	1.76	0.42
1:A:1222:MET:HB3	1:A:1222:MET:HE2	1.82	0.42
1:A:425:SER:HB3	1:A:517:TRP:CD1	2.55	0.42
7:A:1603:POV:H11A	7:A:1603:POV:H15A	1.78	0.42
2:B:194:SER:HB3	2:B:197:GLN:HB2	2.01	0.42
1:A:1016:LYS:HE3	1:A:1018:THR:CG2	2.50	0.42
1:A:183:GLU:OE1	1:A:184:GLU:CD	2.55	0.42
1:A:988:LEU:HD12	1:A:1137:MET:SD	2.58	0.42
1:A:408:ARG:HH21	2:B:38:PHE:HA	1.83	0.42
1:A:489:ASN:HB3	1:A:492:ASP:O	2.20	0.42
1:A:840:LEU:HB2	1:A:850:SER:OG	2.20	0.42
1:A:880:ARG:NH2	1:A:949:ASP:OD1	2.37	0.42
1:A:884:GLN:H	1:A:884:GLN:CD	2.27	0.42
1:A:1124:MET:HE3	1:A:1124:MET:HB3	1.63	0.42
1:A:501:THR:HG22	1:A:502:ILE:H	1.85	0.42
1:A:880:ARG:HD3	1:A:952:GLU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1012:LEU:HD23	1:A:1069:ALA:HB3	2.01	0.42
1:A:1412:ARG:NH2	2:B:67:ASN:HB3	2.35	0.42
2:B:230:PRO:HD2	2:B:286:PRO:HD3	2.00	0.42
1:A:410:HIS:O	1:A:413:ASP:HB2	2.20	0.42
1:A:1169:LEU:HD23	1:A:1169:LEU:HA	1.90	0.42
1:A:530:LYS:O	1:A:534:ASN:ND2	2.53	0.42
1:A:1013:LEU:HB2	1:A:1070:ILE:HD13	2.02	0.42
1:A:392:LYS:HB2	1:A:392:LYS:HE3	1.87	0.41
1:A:822:GLY:HA3	1:A:834:PHE:O	2.20	0.41
1:A:1222:MET:O	7:A:1603:POV:O13	2.37	0.41
1:A:754:ASP:OD2	1:A:759:SER:HB2	2.20	0.41
1:A:936:SER:O	1:A:940:ARG:HB3	2.20	0.41
1:A:1128:ILE:HA	1:A:1145:ILE:O	2.20	0.41
1:A:223:PHE:HB2	1:A:247:LEU:HD13	2.01	0.41
1:A:239:ASN:N	1:A:240:PRO:CD	2.80	0.41
1:A:557:PHE:CE1	1:A:613:VAL:HG21	2.55	0.41
1:A:1012:LEU:HD23	1:A:1012:LEU:HA	1.88	0.41
1:A:1181:TYR:CZ	1:A:1264:GLU:HB2	2.55	0.41
2:B:111:MET:HG2	2:B:144:PHE:CE2	2.56	0.41
1:A:1166:PHE:O	1:A:1169:LEU:HB2	2.20	0.41
2:B:189:TYR:HA	2:B:233:LEU:HD12	2.01	0.41
1:A:1196:MET:O	1:A:1197:ILE:C	2.64	0.41
2:B:97:ASN:HD21	2:B:371:ASN:H	1.69	0.41
8:B:1001:NAG:O7	8:B:1001:NAG:O3	2.31	0.41
1:A:1063:PHE:CD1	1:A:1064:PRO:HD2	2.56	0.41
2:B:169:MET:O	2:B:334:THR:HG23	2.20	0.41
1:A:210:ASN:O	1:A:214:GLN:HG3	2.21	0.41
1:A:435:THR:HG22	1:A:510:CYS:SG	2.60	0.41
1:A:888:ASN:O	1:A:890:GLU:N	2.54	0.41
1:A:1078:LYS:HE2	1:A:1078:LYS:HB2	1.71	0.41
1:A:1200:LEU:HD23	1:A:1200:LEU:HA	1.91	0.41
1:A:209:LYS:HB3	1:A:209:LYS:HE3	1.74	0.41
1:A:731:ARG:HH21	1:A:741:PRO:HG3	1.86	0.41
1:A:909:ARG:H	1:A:909:ARG:HG3	1.59	0.41
1:A:1018:THR:HG23	1:A:1021:ASP:HB2	2.02	0.41
1:A:1092:LEU:HA	1:A:1092:LEU:HD23	1.82	0.41
1:A:612:LEU:HD23	1:A:612:LEU:HA	1.78	0.41
1:A:701:ARG:HG2	1:A:706:ILE:HD12	2.02	0.41
1:A:848:ARG:HG3	1:A:870:CYS:SG	2.61	0.41
1:A:863:GLU:HG2	1:A:920:TRP:CD1	2.56	0.41
1:A:926:TRP:CD1	1:A:951:ILE:HB	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ILE:HA	1:A:187:PRO:HA	2.03	0.40
1:A:399:LYS:H	1:A:399:LYS:HG3	1.47	0.40
1:A:940:ARG:O	1:A:943:GLU:HB2	2.22	0.40
7:A:1604:POV:H35A	7:A:1604:POV:H38A	1.84	0.40
2:B:146:ASP:OD2	2:B:147:ASP:N	2.54	0.40
1:A:257:LYS:CD	7:A:1604:POV:H31H	2.49	0.40
1:A:278:HIS:HE1	1:A:395:LYS:NZ	2.20	0.40
1:A:884:GLN:C	1:A:887:SER:HA	2.46	0.40
1:A:171:TYR:HD1	1:A:174:MET:HE2	1.87	0.40
1:A:386:PRO:HA	1:A:387:PRO:HD3	1.95	0.40
7:A:1604:POV:H211	7:A:1604:POV:H214	1.81	0.40
1:A:654:ILE:HD11	1:A:1160:ASP:HB3	2.03	0.40
1:A:1360:ILE:CD1	2:B:272:ARG:HG3	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1170/1571 (74%)	1121 (96%)	47 (4%)	2 (0%)	43	72
2	B	370/414 (89%)	353 (95%)	15 (4%)	2 (0%)	24	55
All	All	1540/1985 (78%)	1474 (96%)	62 (4%)	4 (0%)	37	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	890	GLU
2	B	170	LYS
1	A	889	SER
2	B	137	ASN

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	1023/1367 (75%)	894 (87%)	129 (13%)	4	15
2	B	321/364 (88%)	288 (90%)	33 (10%)	7	23
All	All	1344/1731 (78%)	1182 (88%)	162 (12%)	7	16

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	LYS
1	A	181	ILE
1	A	183	GLU
1	A	196	ILE
1	A	197	ARG
1	A	212	LEU
1	A	224	LEU
1	A	229	LEU
1	A	234	ILE
1	A	238	THR
1	A	239	ASN
1	A	242	LEU
1	A	245	VAL
1	A	253	ILE
1	A	262	ASP
1	A	270	LEU
1	A	277	THR
1	A	280	LEU
1	A	385	LEU
1	A	391	CYS
1	A	399	LYS
1	A	419	ILE
1	A	431	CYS
1	A	433	VAL
1	A	436	LYS
1	A	439	ASP
1	A	452	CYS

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Mol	Chain	Res	Type
1	A	462	ILE
1	A	471	SER
1	A	488	ARG
1	A	494	GLU
1	A	501	THR
1	A	513	ARG
1	A	531	ILE
1	A	548	GLU
1	A	556	ASN
1	A	581	SER
1	A	584	SER
1	A	593	SER
1	A	608	LEU
1	A	611	SER
1	A	622	GLU
1	A	636	VAL
1	A	653	ASN
1	A	668	LYS
1	A	671	THR
1	A	683	THR
1	A	687	VAL
1	A	704	GLN
1	A	723	ARG
1	A	744	VAL
1	A	756	LYS
1	A	764	GLN
1	A	772	LEU
1	A	782	VAL
1	A	821	LYS
1	A	823	LEU
1	A	830	ILE
1	A	840	LEU
1	A	843	ASN
1	A	845	SER
1	A	848	ARG
1	A	850	SER
1	A	854	LYS
1	A	863	GLU
1	A	868	LEU
1	A	869	ILE
1	A	874	ASP
1	A	882	SER

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Mol	Chain	Res	Type
1	A	884	GLN
1	A	887	SER
1	A	893	LEU
1	A	898	LEU
1	A	901	GLU
1	A	909	ARG
1	A	920	TRP
1	A	928	GLU
1	A	937	LEU
1	A	944	LEU
1	A	951	ILE
1	A	953	ARG
1	A	954	GLU
1	A	963	ILE
1	A	964	GLU
1	A	985	LEU
1	A	989	THR
1	A	999	ILE
1	A	1002	SER
1	A	1016	LYS
1	A	1017	THR
1	A	1020	ASP
1	A	1047	LEU
1	A	1048	THR
1	A	1052	GLU
1	A	1060	ASP
1	A	1065	LYS
1	A	1072	ILE
1	A	1085	ASP
1	A	1092	LEU
1	A	1104	ARG
1	A	1105	VAL
1	A	1120	SER
1	A	1123	VAL
1	A	1124	MET
1	A	1133	ASN
1	A	1134	ASP
1	A	1138	ILE
1	A	1169	LEU
1	A	1171	ARG
1	A	1172	LEU
1	A	1184	LEU

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Mol	Chain	Res	Type
1	A	1190	GLU
1	A	1195	ASN
1	A	1214	SER
1	A	1234	VAL
1	A	1258	VAL
1	A	1266	ASN
1	A	1295	ASN
1	A	1300	SER
1	A	1301	ASN
1	A	1305	LEU
1	A	1348	VAL
1	A	1360	ILE
1	A	1363	ARG
1	A	1381	VAL
1	A	1387	LEU
1	A	1391	LEU
1	A	1416	GLN
1	A	1428	ASP
2	B	76	LEU
2	B	81	LEU
2	B	112	THR
2	B	113	ASN
2	B	116	SER
2	B	124	GLU
2	B	137	ASN
2	B	149	SER
2	B	151	ASP
2	B	153	THR
2	B	156	ARG
2	B	170	LYS
2	B	178	VAL
2	B	190	VAL
2	B	192	SER
2	B	208	VAL
2	B	212	THR
2	B	220	SER
2	B	245	LEU
2	B	258	SER
2	B	260	THR
2	B	262	LYS
2	B	280	TYR
2	B	282	GLN

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Mol	Chain	Res	Type
2	B	298	ASN
2	B	346	LEU
2	B	348	TRP
2	B	351	LEU
2	B	352	GLU
2	B	359	ILE
2	B	362	THR
2	B	377	VAL
2	B	390	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	ASN
1	A	239	ASN
1	A	273	ASN
1	A	278	HIS
1	A	285	ASN
1	A	287	ASN
1	A	379	ASN
1	A	410	HIS
1	A	443	ASN
1	A	448	GLN
1	A	454	ASN
1	A	504	ASN
1	A	571	ASN
1	A	597	ASN
1	A	653	ASN
1	A	888	ASN
1	A	902	GLN
1	A	939	ASN
1	A	1004	ASN
1	A	1096	ASN
1	A	1139	GLN
1	A	1154	GLN
1	A	1176	HIS
1	A	1195	ASN
1	A	1324	ASN
2	B	60	GLN
2	B	67	ASN
2	B	97	ASN
2	B	155	GLN

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Mol	Chain	Res	Type
2	B	172	ASN
2	B	176	ASN
2	B	186	HIS
2	B	246	GLN
2	B	282	GLN
2	B	341	GLN
2	B	347	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

7 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	$\# Z > 2$
3	NAG	C	1	2,3	14,14,15	0.76	1 (7%)	17,19,21	0.64	0
3	NAG	C	2	3	14,14,15	0.87	1 (7%)	17,19,21	0.53	0
3	MAN	C	3	3	11,11,12	1.13	2 (18%)	15,15,17	1.55	2 (13%)
4	NAG	D	1	2,4	14,14,15	0.61	1 (7%)	17,19,21	0.51	0
4	NAG	D	2	4	14,14,15	0.34	0	17,19,21	0.53	0
4	NAG	E	1	2,4	14,14,15	0.45	0	17,19,21	0.42	0
4	NAG	E	2	4	14,14,15	0.41	0	17,19,21	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	MAN	C	3	3	-	2/2/19/22	1/1/1/1
4	NAG	D	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	O5-C1	-2.98	1.38	1.43
3	C	3	MAN	O5-C5	2.81	1.48	1.43
3	C	1	NAG	O5-C1	-2.55	1.39	1.43
4	D	1	NAG	O5-C1	-2.20	1.40	1.43
3	C	3	MAN	C2-C3	-2.03	1.49	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	MAN	C1-O5-C5	4.00	117.54	112.19
3	C	3	MAN	O2-C2-C3	-2.75	104.45	110.15

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	C	3	MAN	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
3	C	3	MAN	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6

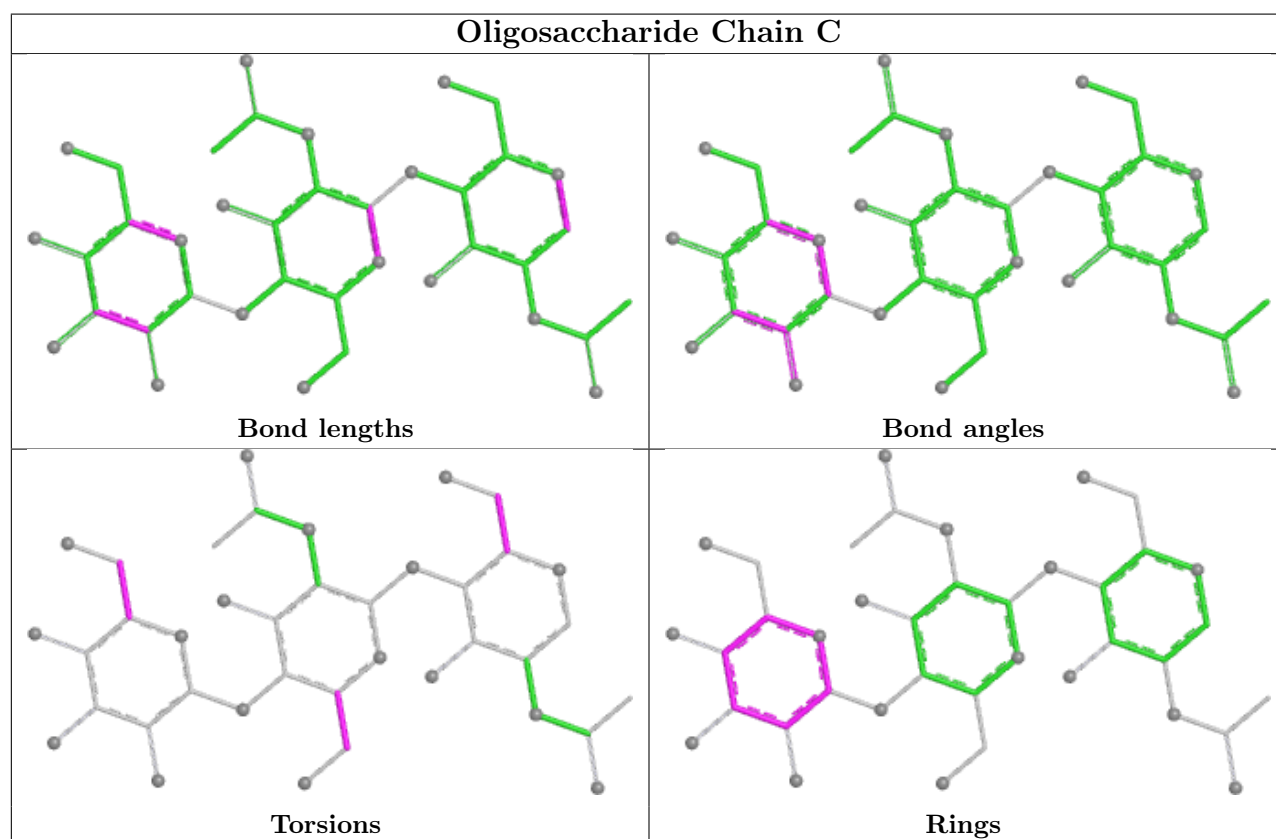
All (1) ring outliers are listed below:

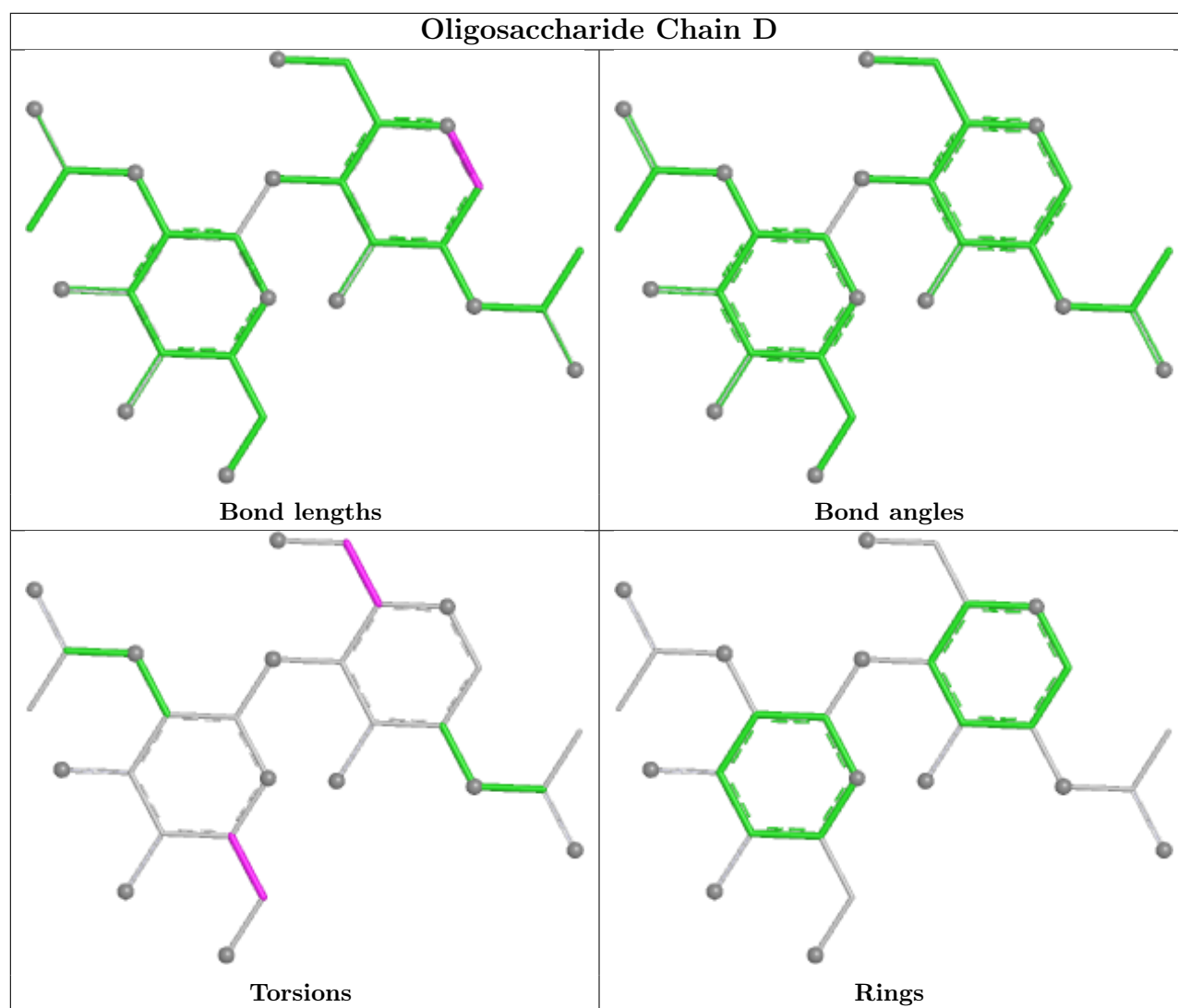
Mol	Chain	Res	Type	Atoms
3	C	3	MAN	C1-C2-C3-C4-C5-O5

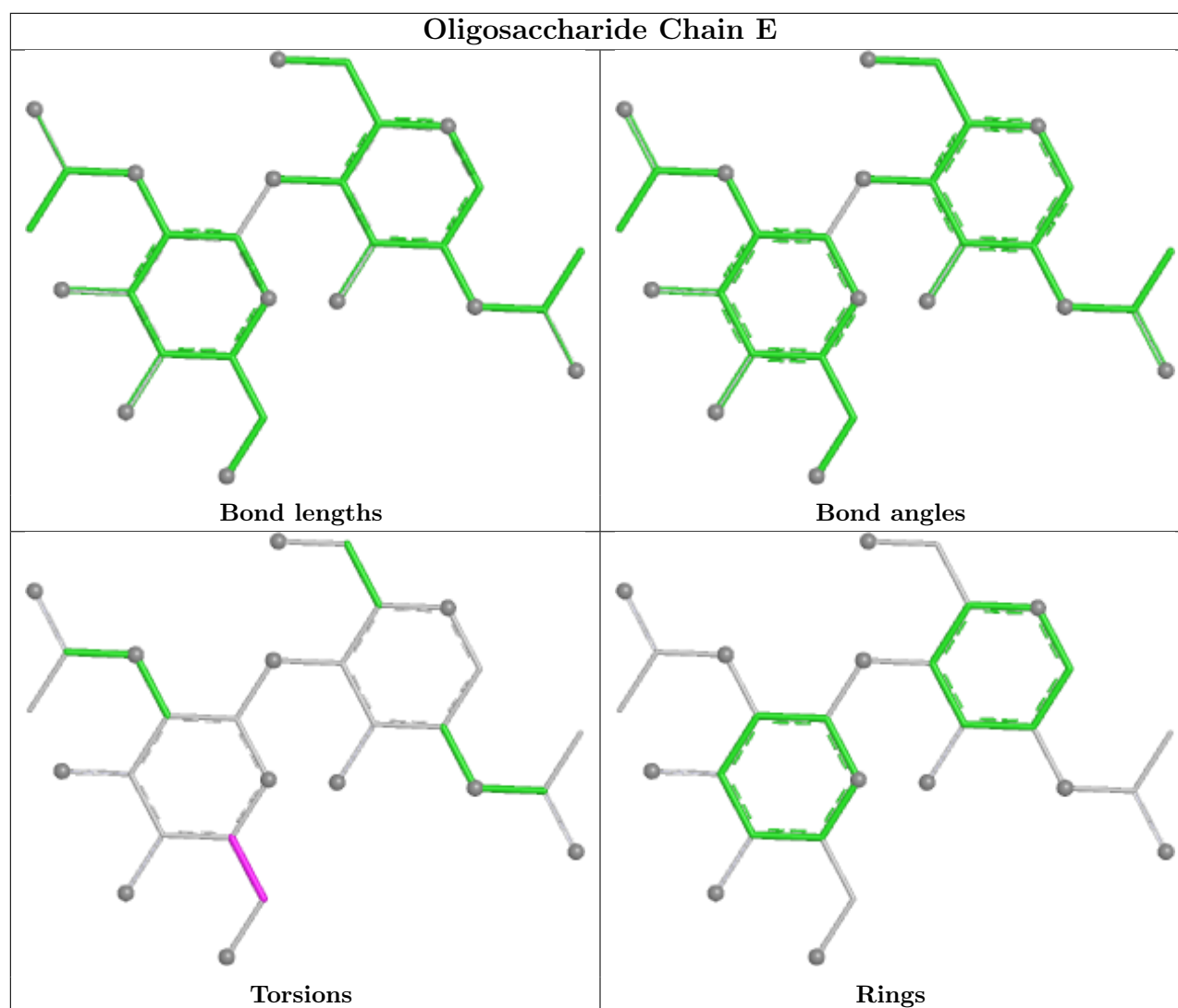
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	1	0
3	C	1	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 oligosaccharide.







5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	$\# Z > 2$
8	NAG	B	1002	2	14,14,15	0.56	1 (7%)	17,19,21	0.41	0
7	POV	A	1603	-	51,51,51	1.26	6 (11%)	57,59,59	1.04	2 (3%)
5	BEF	A	1601	1	0,3,3	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	POV	A	1605	-	51,51,51	1.25	5 (9%)	57,59,59	1.11	3 (5%)
8	NAG	B	1001	2	14,14,15	0.30	0	17,19,21	0.56	0
7	POV	A	1604	-	51,51,51	1.26	6 (11%)	57,59,59	1.05	2 (3%)

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	B	1002	2	-	2/6/23/26	0/1/1/1
7	POV	A	1603	-	-	25/55/55/55	-
7	POV	A	1605	-	-	25/55/55/55	-
8	NAG	B	1001	2	-	2/6/23/26	0/1/1/1
7	POV	A	1604	-	-	30/55/55/55	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1603	POV	O31-C31	3.42	1.43	1.33
7	A	1604	POV	O31-C31	3.38	1.43	1.33
7	A	1605	POV	O31-C31	3.22	1.42	1.33
7	A	1603	POV	O21-C21	2.92	1.42	1.34
7	A	1604	POV	O21-C21	2.89	1.42	1.34
7	A	1605	POV	O21-C21	2.88	1.42	1.34
7	A	1605	POV	O21-C2	-2.72	1.40	1.46
7	A	1603	POV	O21-C2	-2.65	1.40	1.46
7	A	1604	POV	O21-C2	-2.64	1.40	1.46
7	A	1603	POV	C14-N	-2.28	1.43	1.50
7	A	1604	POV	C14-N	-2.26	1.43	1.50
7	A	1605	POV	C14-N	-2.24	1.43	1.50
7	A	1605	POV	C13-N	-2.07	1.44	1.50
7	A	1603	POV	C13-N	-2.06	1.44	1.50
7	A	1604	POV	C13-N	-2.05	1.44	1.50
8	B	1002	NAG	O5-C1	-2.03	1.40	1.43
7	A	1604	POV	P-O12	2.03	1.67	1.59
7	A	1603	POV	P-O11	2.03	1.67	1.59

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1604	POV	O21-C21-C22	3.93	119.97	111.48
7	A	1603	POV	O21-C21-C22	3.83	119.77	111.48
7	A	1605	POV	O21-C21-C22	3.77	119.64	111.48
7	A	1605	POV	C214-C213-C212	3.46	131.87	114.37
7	A	1605	POV	O31-C31-C32	2.87	120.59	111.83
7	A	1604	POV	O31-C31-C32	2.68	120.02	111.83
7	A	1603	POV	O31-C31-C32	2.66	119.96	111.83

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1603	POV	C11-O12-P-O11
7	A	1603	POV	C11-O12-P-O13
7	A	1603	POV	C11-O12-P-O14
7	A	1603	POV	O12-C11-C12-N
7	A	1604	POV	C1-O11-P-O12
7	A	1604	POV	C1-O11-P-O13
7	A	1604	POV	C11-O12-P-O14
7	A	1604	POV	C22-C21-O21-C2
7	A	1604	POV	C32-C31-O31-C3
7	A	1604	POV	O32-C31-O31-C3
7	A	1605	POV	C1-O11-P-O12
7	A	1605	POV	C1-O11-P-O13
7	A	1605	POV	C11-O12-P-O11
7	A	1605	POV	C11-O12-P-O14
7	A	1604	POV	O22-C21-O21-C2
8	B	1002	NAG	O5-C5-C6-O6
8	B	1002	NAG	C4-C5-C6-O6
7	A	1605	POV	C32-C31-O31-C3
7	A	1605	POV	O32-C31-O31-C3
7	A	1604	POV	C31-C32-C33-C34
7	A	1605	POV	C210-C211-C212-C213
7	A	1605	POV	C31-C32-C33-C34
7	A	1605	POV	C22-C23-C24-C25
7	A	1604	POV	C39-C310-C311-C312
7	A	1605	POV	C212-C213-C214-C215
7	A	1604	POV	C311-C310-C39-C38
7	A	1603	POV	C24-C25-C26-C27
7	A	1603	POV	C33-C34-C35-C36
7	A	1604	POV	C25-C26-C27-C28
7	A	1603	POV	C31-C32-C33-C34
7	A	1605	POV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
7	A	1604	POV	C23-C24-C25-C26
7	A	1605	POV	C21-C22-C23-C24
7	A	1605	POV	C213-C214-C215-C216
7	A	1603	POV	C35-C36-C37-C38
7	A	1603	POV	C210-C211-C212-C213
7	A	1605	POV	C312-C313-C314-C315
7	A	1604	POV	C26-C27-C28-C29
7	A	1604	POV	C310-C311-C312-C313
7	A	1604	POV	C37-C38-C39-C310
7	A	1604	POV	C35-C36-C37-C38
7	A	1605	POV	C310-C311-C312-C313
8	B	1001	NAG	O5-C5-C6-O6
7	A	1603	POV	C214-C215-C216-C217
7	A	1604	POV	C33-C34-C35-C36
7	A	1603	POV	C36-C37-C38-C39
7	A	1604	POV	C34-C35-C36-C37
7	A	1605	POV	C25-C26-C27-C28
7	A	1603	POV	C311-C312-C313-C314
7	A	1603	POV	O11-C1-C2-C3
7	A	1604	POV	C212-C213-C214-C215
7	A	1604	POV	C213-C214-C215-C216
7	A	1604	POV	C21-C22-C23-C24
7	A	1605	POV	C36-C37-C38-C39
7	A	1605	POV	C214-C215-C216-C217
7	A	1603	POV	C23-C24-C25-C26
7	A	1605	POV	C24-C25-C26-C27
7	A	1605	POV	C211-C212-C213-C214
7	A	1604	POV	O12-C11-C12-N
7	A	1605	POV	C32-C33-C34-C35
7	A	1603	POV	C2-C1-O11-P
7	A	1605	POV	C37-C38-C39-C310
7	A	1603	POV	O11-C1-C2-O21
7	A	1604	POV	C1-O11-P-O14
7	A	1604	POV	C29-C210-C211-C212
7	A	1605	POV	C215-C216-C217-C218
7	A	1603	POV	C212-C213-C214-C215
7	A	1604	POV	C27-C28-C29-C210
7	A	1604	POV	C32-C33-C34-C35
7	A	1603	POV	C215-C216-C217-C218
7	A	1605	POV	C34-C35-C36-C37
7	A	1603	POV	C313-C314-C315-C316
7	A	1605	POV	O11-C1-C2-O21

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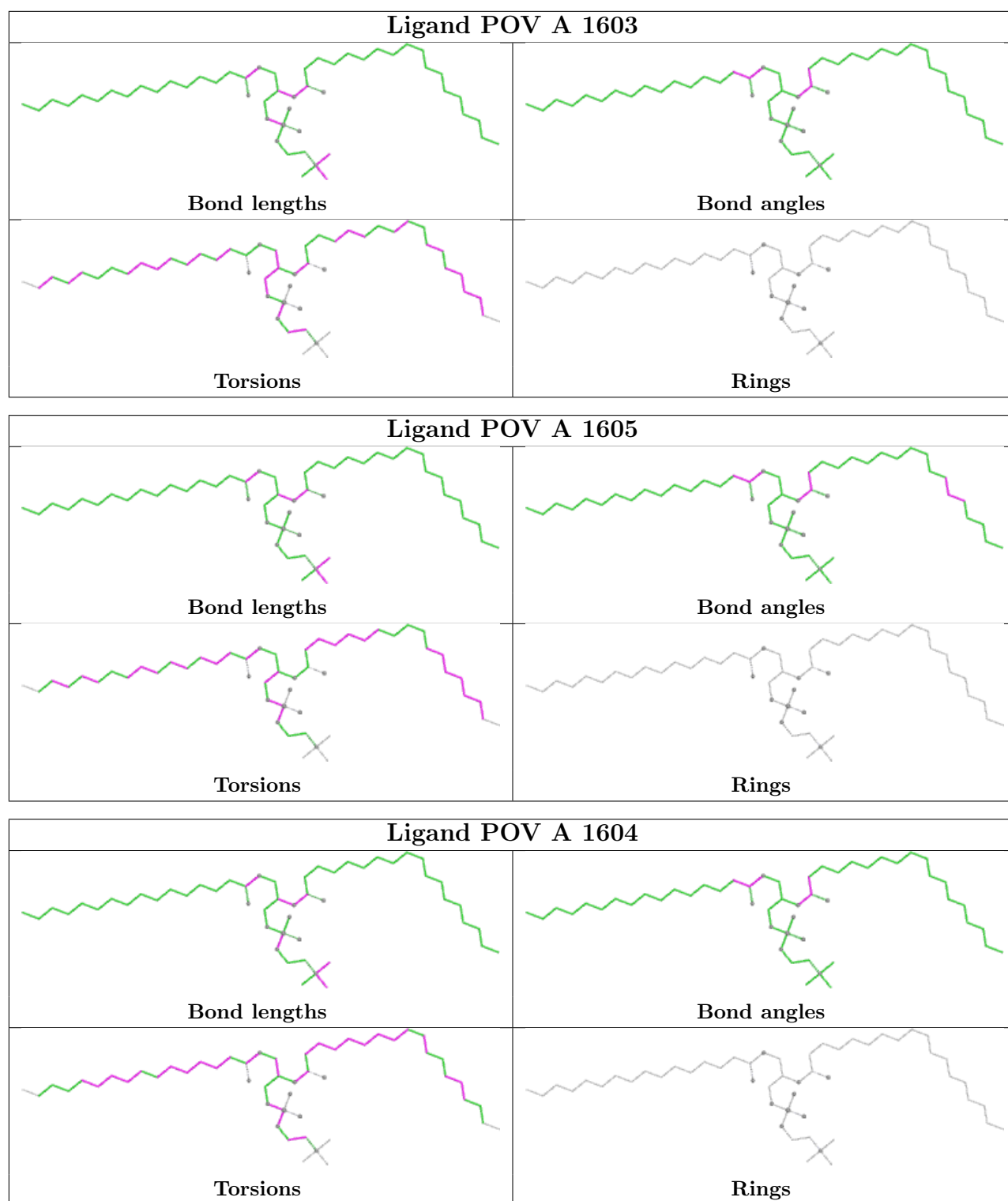
Mol	Chain	Res	Type	Atoms
7	A	1603	POV	C213-C214-C215-C216
7	A	1603	POV	O22-C21-O21-C2
7	A	1604	POV	C22-C23-C24-C25
8	B	1001	NAG	C3-C2-N2-C7
7	A	1603	POV	O21-C2-C3-O31
7	A	1604	POV	O21-C2-C3-O31
7	A	1603	POV	C37-C38-C39-C310
7	A	1603	POV	C27-C28-C29-C210
7	A	1603	POV	C22-C21-O21-C2
7	A	1604	POV	C24-C25-C26-C27
7	A	1604	POV	C1-C2-C3-O31

There are no ring outliers.

5 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1603	POV	12	0
5	A	1601	BEF	1	0
7	A	1605	POV	8	0
8	B	1001	NAG	3	0
7	A	1604	POV	12	0

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



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

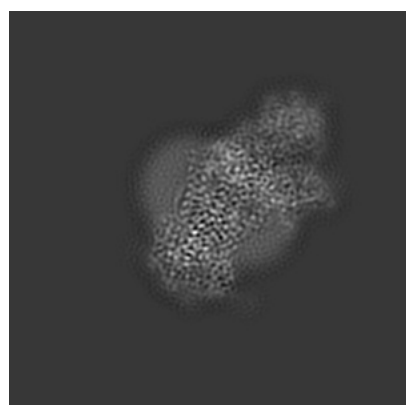
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23075. These allow visual inspection of the internal detail of the map and identification of artifacts.

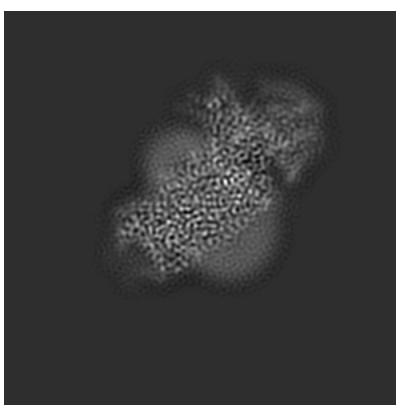
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

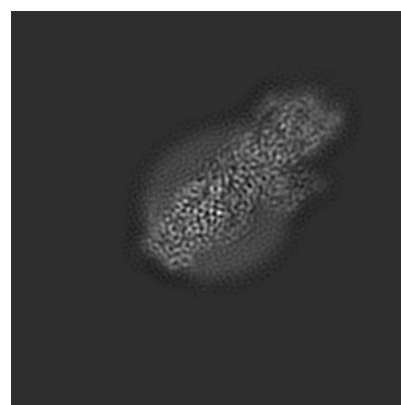
6.1.1 Primary map



X



Y

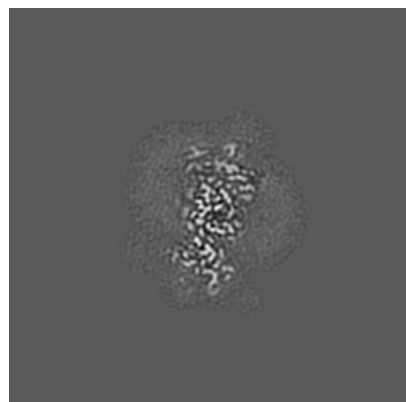


Z

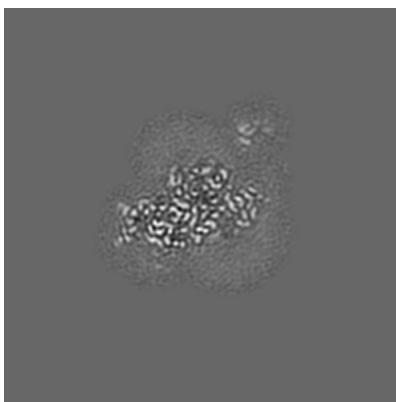
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

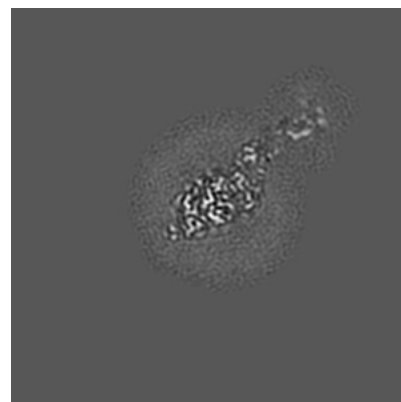
6.2.1 Primary map



X Index: 140



Y Index: 140

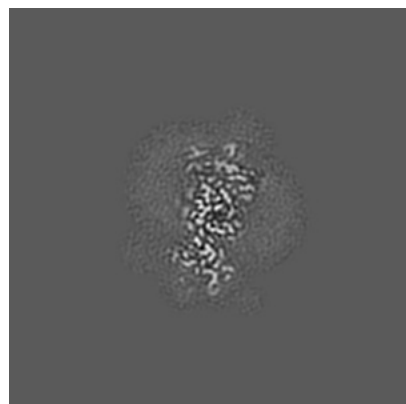


Z Index: 140

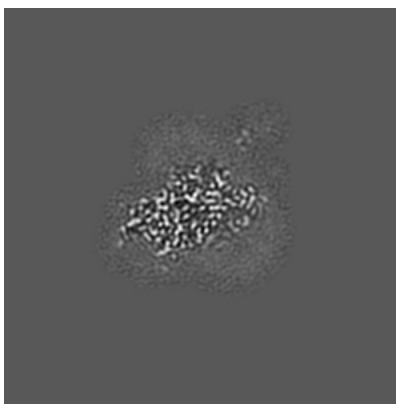
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

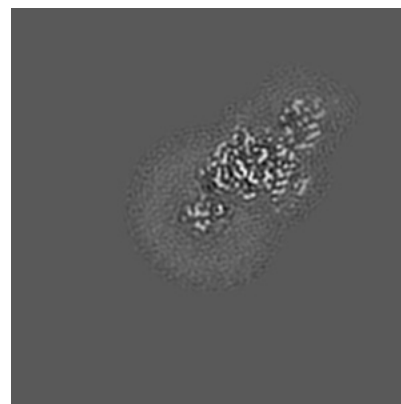
6.3.1 Primary map



X Index: 140



Y Index: 138

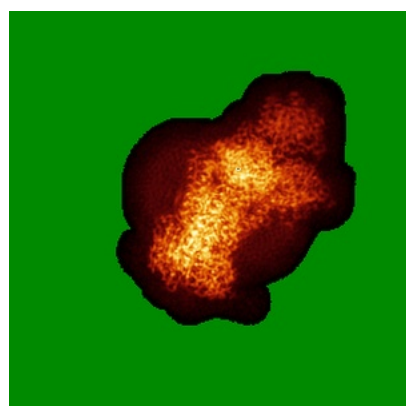


Z Index: 163

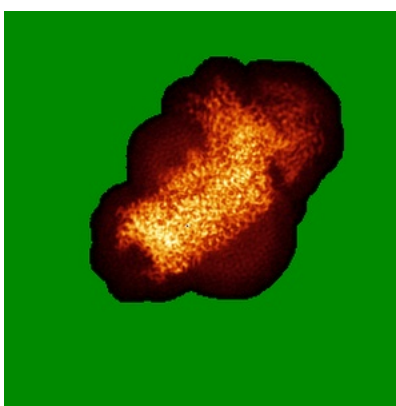
The images above show the largest variance slices of the map in three orthogonal directions.

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

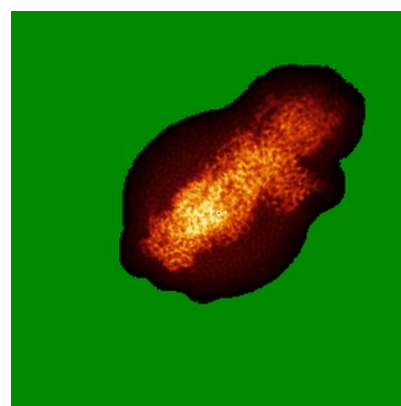
6.4.1 Primary map



X



Y

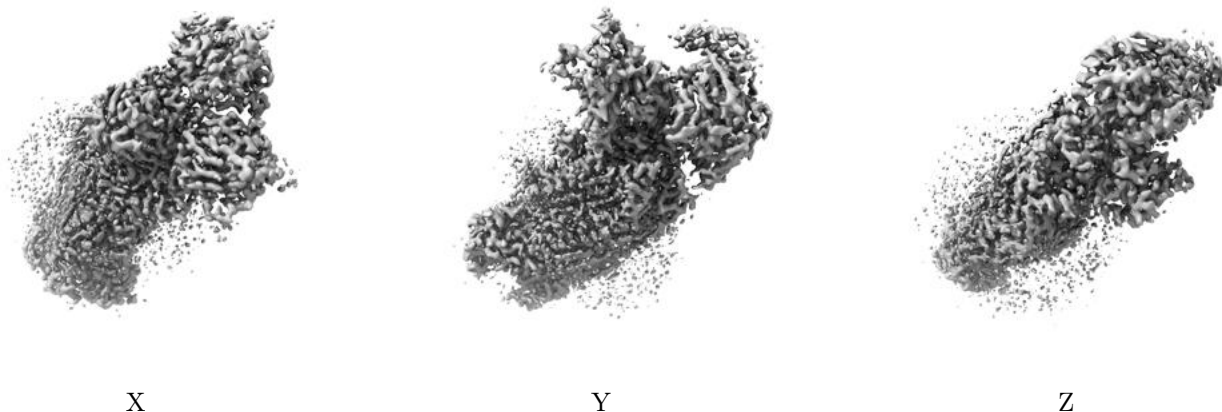


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

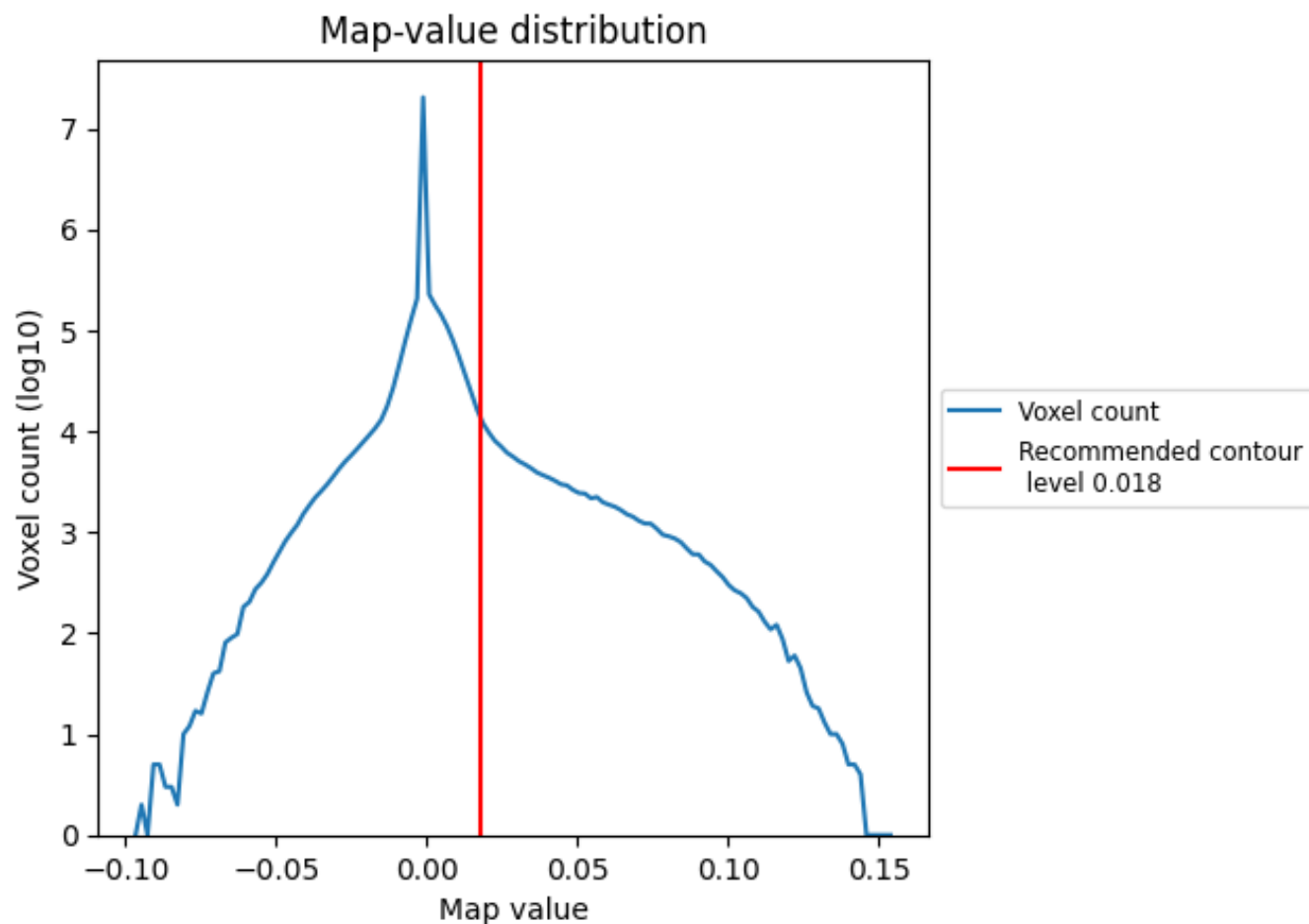
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

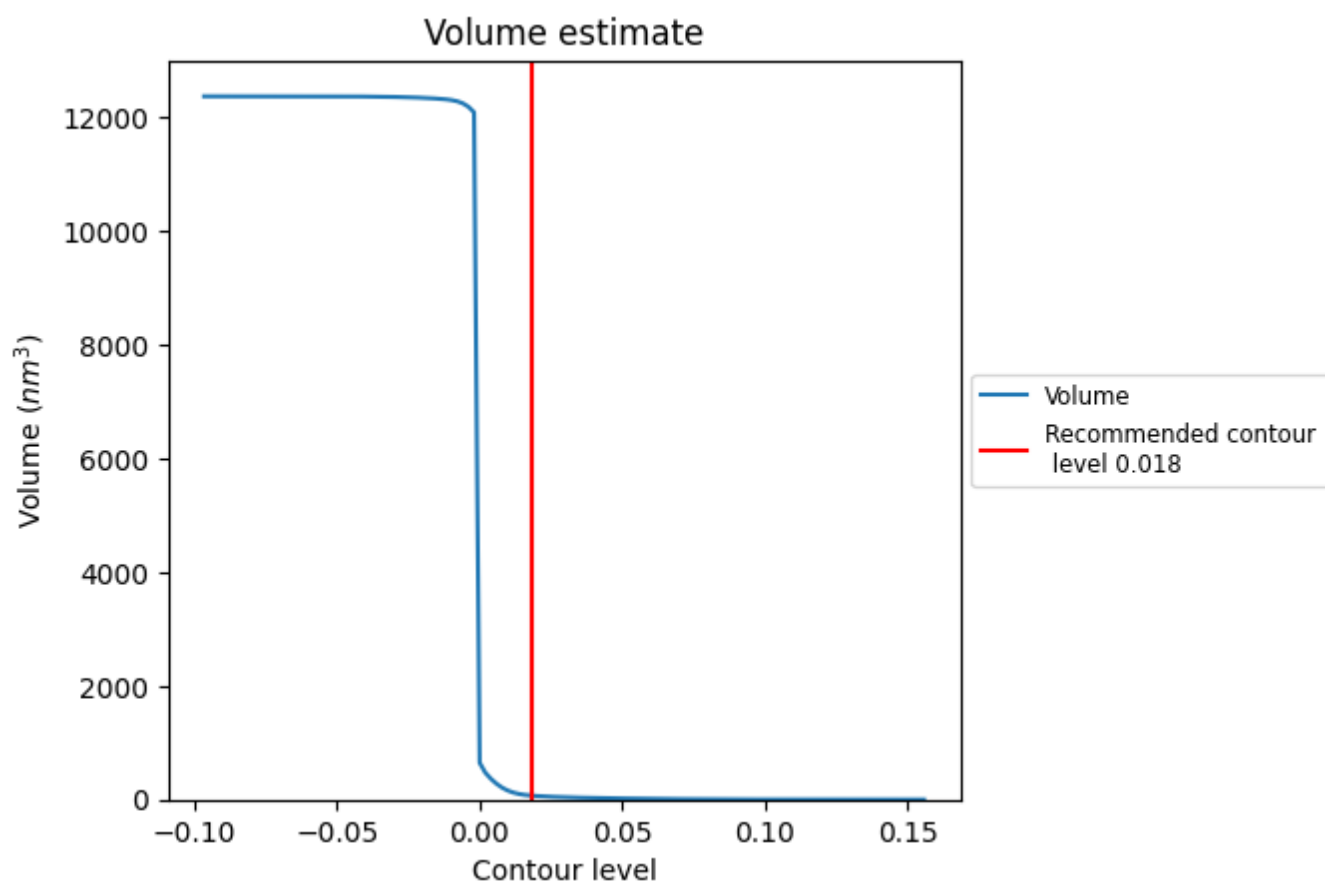
This section contains the results of statistical analysis of the map.

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.

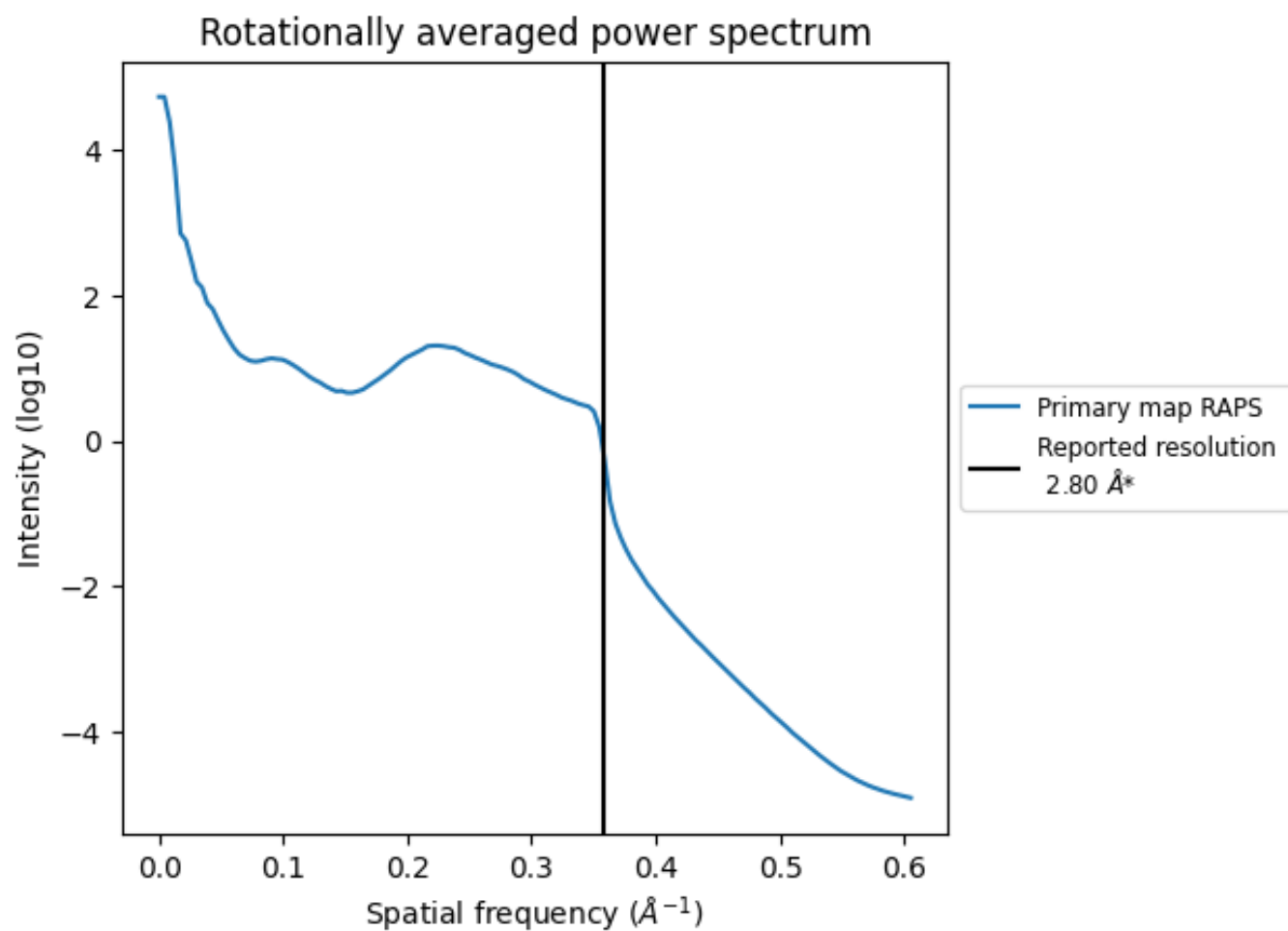
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 70 nm³; this corresponds to an approximate mass of 63 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 0.357 Å⁻¹

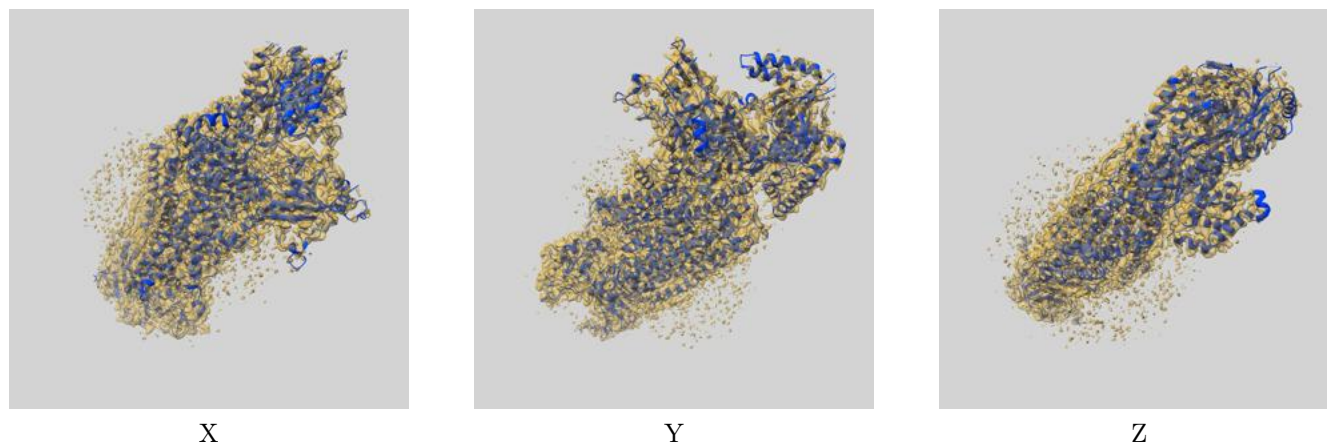
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

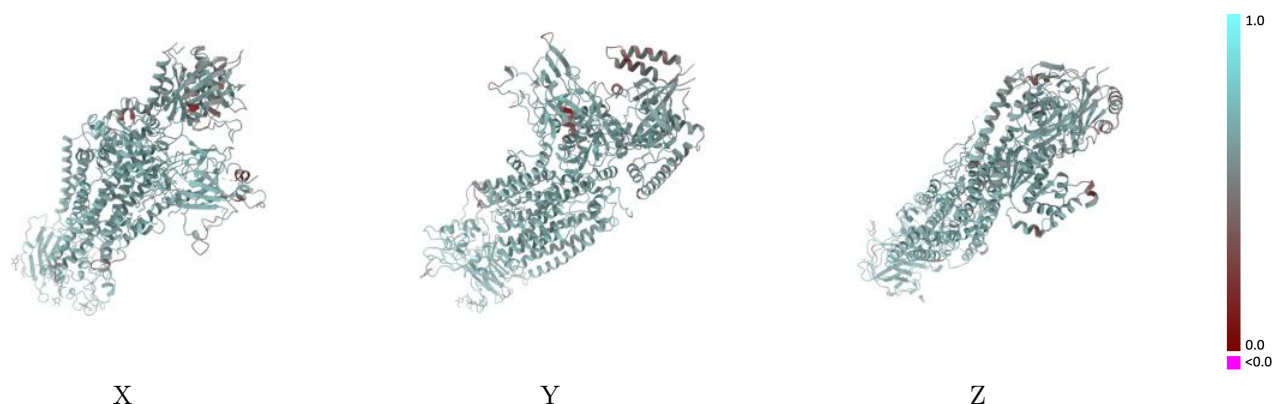
This section contains information regarding the fit between EMDB map EMD-23075 and PDB model 7KYC. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



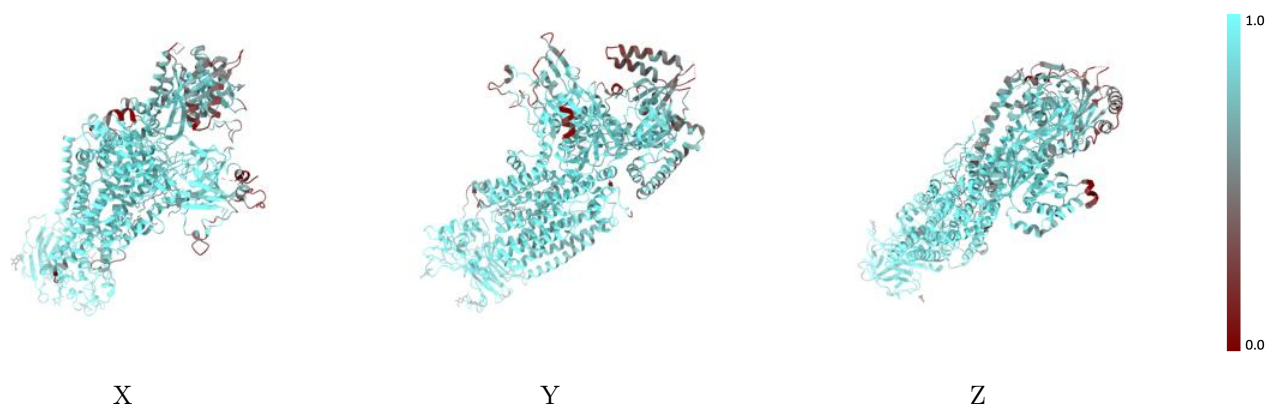
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



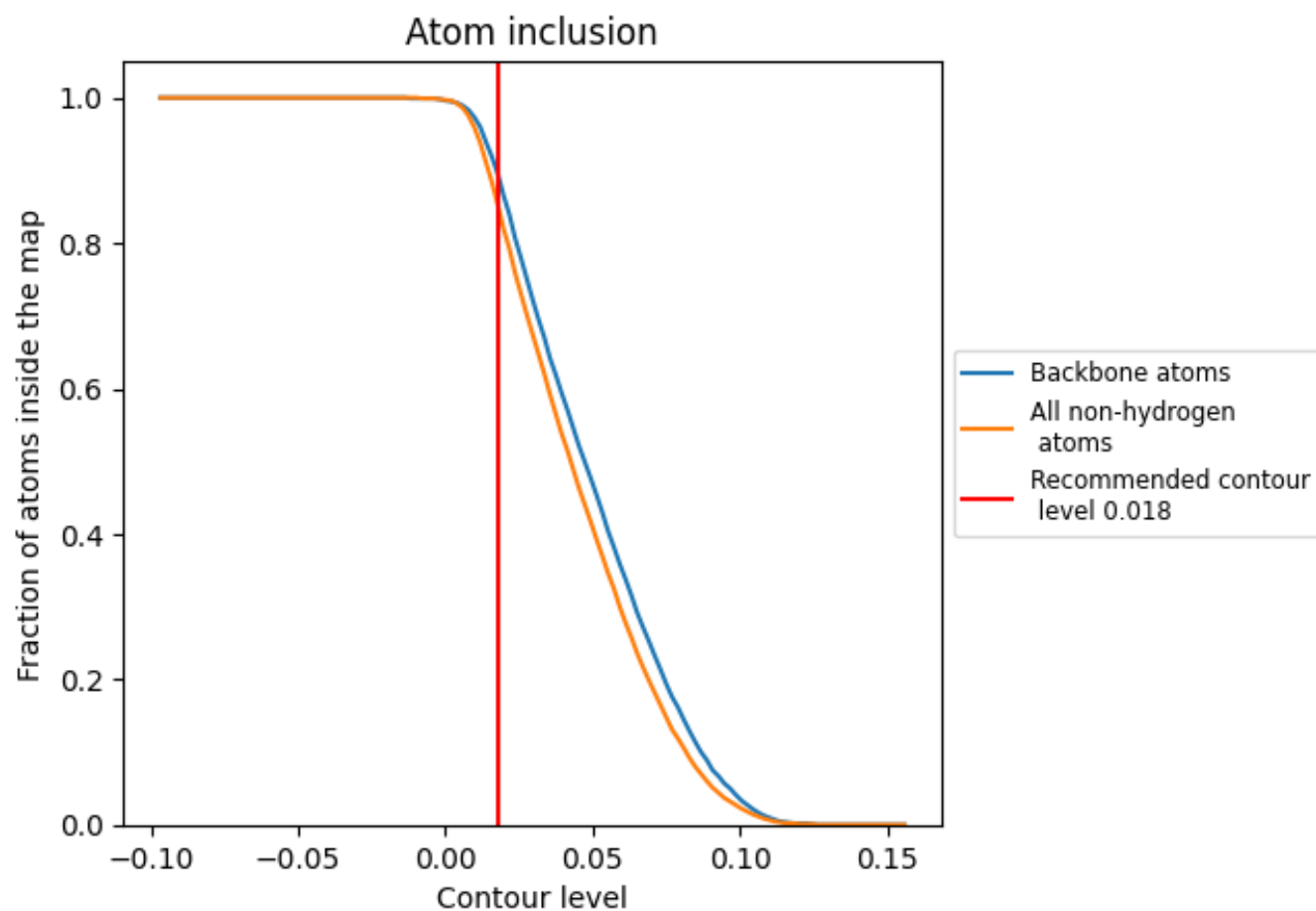
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8500	0.6130
A	0.8300	0.6070
B	0.9150	0.6310
C	0.9490	0.6290
D	0.7860	0.5850
E	0.7500	0.5570

