WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Nov 29, 2022 – 05:09 AM EST

|		
PDB ID	:	7V07
EMDB ID	:	EMD-26940
Title	:	Band 3-I-TM local refinement from erythrocyte ankyrin-1 complex consensus reconstruction
Authors	:	Vallese, F.; Kim, K.; Yen, L.Y.; Johnston, J.D.; Noble, A.J.; Cali, T.; Clarke, O.B.
Deposited on	:	2022-05-10
Resolution	:	2.80 Å(reported)

1   Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.80 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	Percentile Ranks	Value
Clashscore		8
Ramachandran outliers		0.3%
Sidechain outliers		5.6%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures
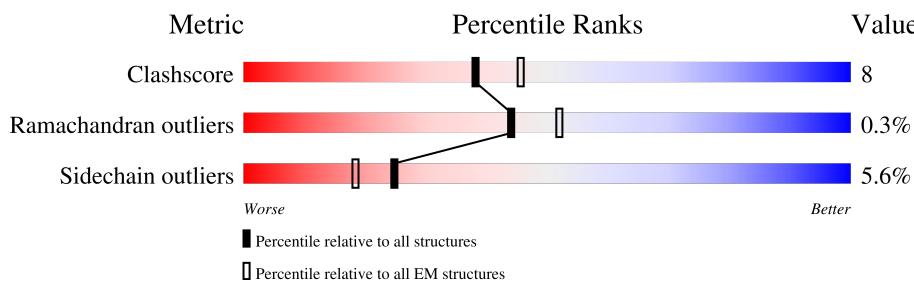
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	B	150	13% 19% 7% 73%
1	D	150	7% 20% 7% 73%
2	C	911	· 43% 13% · 43%
2	E	911	· 47% 9% · 43%
3	A	6	83% 33% 67%
3	F	6	83% 67% 33%
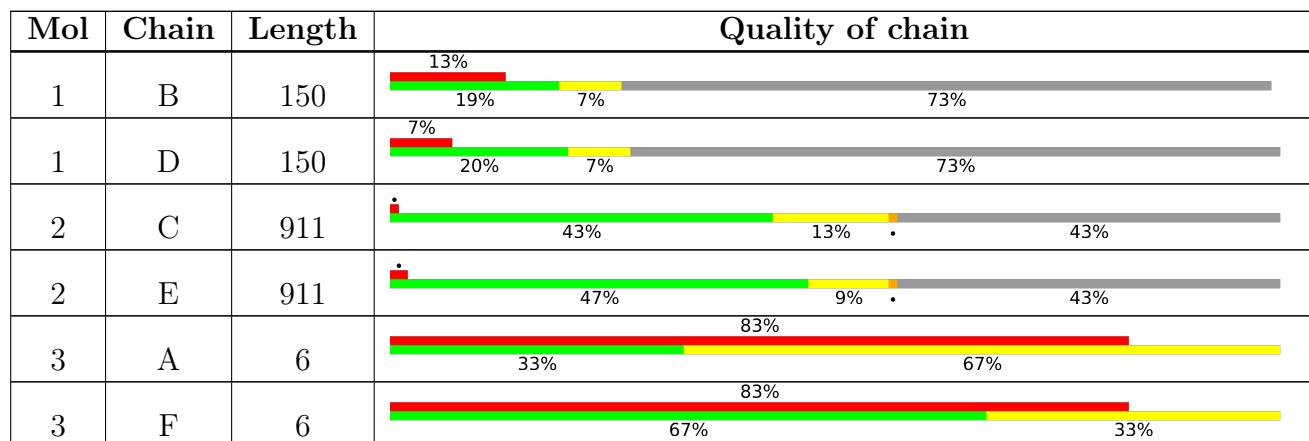
2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 9162 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 Glycophorin-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	40	Total	C	N	O	S	0	0
			302	198	51	52	1		
1	D	40	Total	C	N	O	S	0	0
			302	198	51	52	1		

- Molecule 2 is a protein called Band 3 anion transport protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	517	Total	C	N	O	S	0	0
			4063	2718	651	676	18		
2	E	517	Total	C	N	O	S	0	0
			4063	2718	651	676	18		

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)]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.
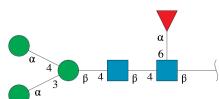
Mol	Chain	Residues	Atoms				AltConf	Trace
3	A	6	Total	C	N	O	0	0
			71	40	2	29		
3	F	6	Total	C	N	O	0	0
			71	40	2	29		

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).
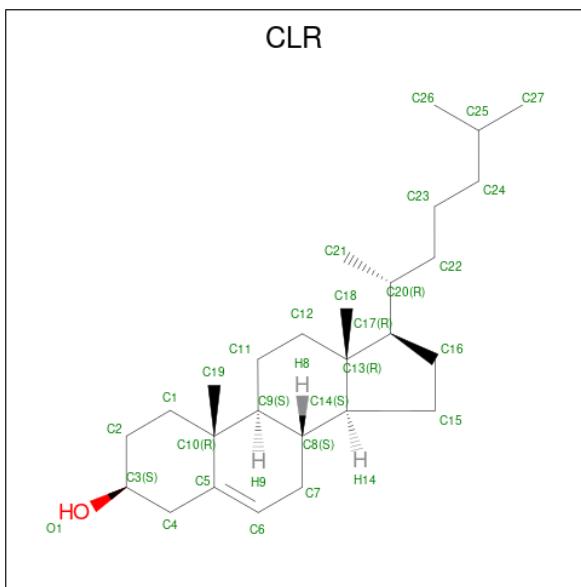
Mol	Chain	Residues	Atoms			AltConf
4	C	1	Total	C	O	0
			56	54	2	
4	C	1	Total	C	O	0
			56	54	2	
4	E	1	Total	C	O	0
			56	54	2	
4	E	1	Total	C	O	0
			56	54	2	

- Molecule 5 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: $C_{32}H_{65}NO_8P$).
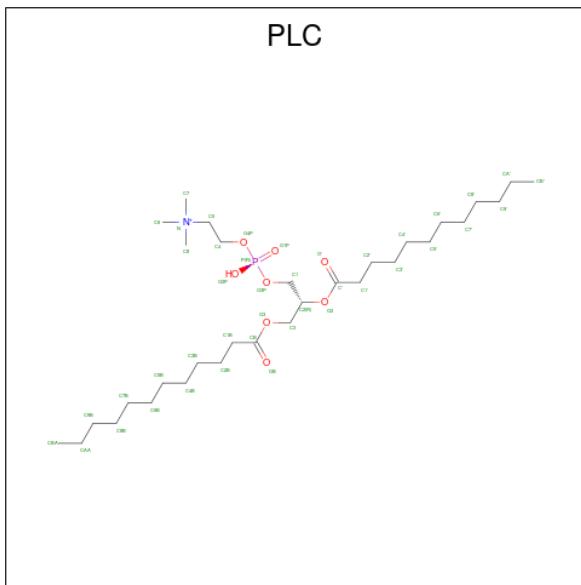
Mol	Chain	Residues	Atoms					AltConf
5	C	1	Total	C	N	O	P	0
			42	32	1	8	1	
5	E	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 6 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5 -diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (three-letter code: PIO) (formula: $C_{25}H_{49}O_{19}P_3$) (labeled as "Ligand of Interest" by depositor).
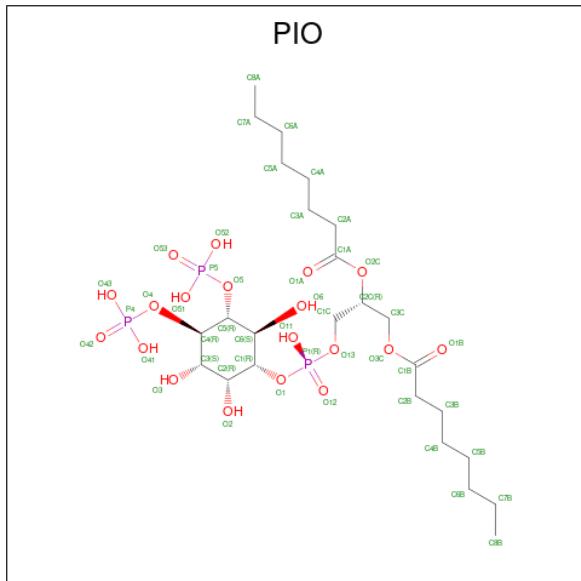

| Mol	Chain	Residues	Atoms				AltConf
6	E	1	Total	C	O	P	0
			94	50	38	6	
6	E	1	Total	C	O	P	0
			94	50	38	6	

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: Glycophorin-A

Chain B:

• Molecule 1: Glycophorin-A

Chain D:

• Molecule 2: Band 3 anion transport protein

Chain C:

SER GLY ASP PRO SER GLN PRO LEU LEU PRO GLN HIS SER SER LEU GLU THR GLN LEU PHE CYS GLU GLN GLY ASP GLY GLY THR GLU GLY HIS SER PRO GLY ILE LEU GLU LYS ILE PRO ASP SER GLU ALA THR LEU LEU VAL LEU VAL GLY ARG ALA ASP PHE LEU GLU GLN PRO

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

ALA GLN SER ARG GLY GLU LEU HIS LEU GLU GLY PHE LEU ASP CYS SER LEU VAL LEU PRO PRO THR ASP ALA PRO SER GLU GLN ALA LEU LEU SER LEU VAL PRO VAL GLN ARG GLU LEU LEU ARG ARG ARG TYR GLN SER SER PRO ALA LYS PRO ASP SER SER PHE TYR LYS

GLY LEU ASP ASN GLY GLY PRO ASP ASP **P371** T375 R384 D385 A400 V405 F411 S418 K430 T431 R432 M435 G436 V437 S438 E439 L440 A456 F464 L469 E473 C479 E480 T481 N482 G483 L484 E485 Y486 I487 R490 V491 W492 F495

V505 E508 F511 R514 S517 Q521 S529 F537 I541 F544 Q545 D546 H547 P548 L549 Q550 K551 T552 Y553 N554 Y555 L558 M559 K562 P563 Q564 G565 P566 L567 L575 T581 L588 R589 K590 F591 K592 S595 Y596 F597 P598 G599 K600 L601 R602 R603

G606 D607 F608 G609 V610 M617 I624 T629 P635 D636 K639 N642 S643 A645 R646 I650 H651 P652 L653 R656 P660 I661 W662 M663 M664 L672 I676 L680 E681 S682 K691 L704 L707 A716 M721 A726 T727 G742 K743

ALA SER THR PRO GLY ALA ALA **A751** Q752 L780 S781 R782 I783 V787 L788 F789 G790 I791 F792 S799 L805 I809 L812 F813 K814 P815 P816 K817 Y818 D821 V825 K826 K829 T830 W831 L844 K851 I864 L873 D890 A891 K892 A893 T894 PHE ASP

GLU GLU GLU GLY ARG ASP GLU TYR ASP GLU VAL ALA MET PRO VAL

• Molecule 2: Band 3 anion transport protein

Chain E:
47%　　　9%　•　　43%

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

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

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

SER GLY ASP PRO SER GLN PRO LEU LEU PRO GLN HIS SER SER LEU GLU THR GLN LEU PHE CYS GLU GLN GLY ASP GLY GLY THR GLU GLY HIS SER PRO SER GLY ILE LEU GLU LYS ILE PRO ASP SER GLU ALA THR LEU VAL LEU VAL GLY ARG ALA ASP PHE LEU GLU GLN PRO

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

ALA GLN SER ARG GLY GLU LEU LEU HIS SER LEU GLU GLY PHE LEU ASP CYS SER LEU VAL LEU PRO PRO THR ASP ALA PRO SER GLU GLN ALA LEU LEU SER LEU VAL PRO VAL GLN ARG GLU LEU LEU ARG ARG ARG TYR GLN SER SER PRO ALA LYS PRO ASP SER SER PHE TYR LYS

GLY LEU ASP ASN GLY GLY PRO ASP ASP **P371** R384 T398 D399 A400 F401 V405 L406 S418 L426 T431 Q434 M435 L440 A456 Q457 F464 E473 E480 Y486 I487 V488 Q489 R490 V491 W492 L499 F511 R518 E522 I523 I528

F537 I541 K542 Q545 P548 L549 Y555 L558 M559 V560 P561 K562 P566 L588 R589 K590 F591 K592 Y596 F597 P598 G599 K600 D607 F608 G609 S613 Q625 T629 S644 A645 R646 G654 L655 R656 P660 I661 W662 M663 M664 F665 A666 L669

L672 I678 F679 L680 E681 S682 S700 L704 L718 F719 G720 M721 P722 S725 A726 V729 H734 G742 K743 ALA SER THR PRO GLY ALA ALA A751 Q752 S762 M776 F792 I803 F806 I809 L812 P815 P816 K817 Y818 H819 P820 D821 V822

P823 Y824 V825 K826 Q840 K851 S856 D889 D890 A891 K892 A893 T894 PHE ASP GLU GLU GLY ARG ASP GLU TYR ASP GLU VAL ALA MET PRO VAL

• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)]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

83%

Chain A:
33%
67%

NAG1 NAG2 BMA3 MAN4 MAN5 FUC6

• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)]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

83%

Chain F:
67%
33%

NAG1 NAG2 BMA3 MAN4 MAN5 FUC6

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	226351	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Patch CTF (cryoSPARC v3) followed by per particle defocus refinement and refinement of higher order aberrations (cryoSPARC v3)	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/Å^2)$	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.436	Depositor
Minimum map value	-2.964	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.162	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	157.7, 157.7, 157.7	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.415, 0.415, 0.415	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	B	0.25	0/307	0.56	0/415
1	D	0.26	0/307	0.57	0/415
2	C	0.32	0/4166	0.54	0/5665
2	E	0.32	0/4166	0.52	0/5665
All	All	0.32	0/8946	0.53	0/12160

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	302	0	309	7	0
1	D	302	0	309	5	0
2	C	4063	0	4262	79	0
2	E	4063	0	4262	52	0
3	A	71	0	61	1	0
3	F	71	0	61	0	0
4	C	56	0	92	3	0
4	E	56	0	92	5	0
5	C	42	0	64	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	42	0	64	6	0
6	E	94	0	88	10	0
All	All	9162	0	9664	150	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 8.

All (150) 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)
2:C:430:LYS:HD2	2:C:473:GLU:HA	1.53	0.90
2:C:831:TRP:HB3	4:C:1002:CLR:H193	1.62	0.82
2:E:431:THR:HG22	2:E:434:GLN:HB2	1.60	0.81
2:E:545:GLN:HB3	5:E:1003:PLC:H51	1.68	0.76
2:E:522:GLU:HG2	2:E:803:ILE:HG23	1.67	0.75
5:C:1003:PLC:H2A1	5:C:1003:PLC:H5'2	1.69	0.73
2:E:537:PHE:HE1	5:E:1003:PLC:H9A2	1.54	0.72
2:C:831:TRP:HB3	4:C:1002:CLR:H111	1.72	0.70
2:E:600:LYS:H	2:E:600:LYS:HE2	1.57	0.70
2:C:544:PHE:HB3	5:C:1003:PLC:H2	1.74	0.69
2:C:562:LYS:HE2	2:C:563:PRO:HD2	1.75	0.67
2:C:430:LYS:HG2	2:C:473:GLU:HG2	1.77	0.66
2:C:537:PHE:HE1	5:C:1003:PLC:H9A1	1.60	0.66
2:C:598:PRO:HD2	2:C:601:LEU:HD23	1.78	0.66
2:C:487:ILE:HG23	2:C:650:ILE:HG21	1.78	0.65
6:E:1005:PIO:H7A	6:E:1005:PIO:H7BA	1.78	0.65
2:C:636:ASP:OD2	2:C:639:LYS:NZ	2.30	0.65
2:E:431:THR:CG2	2:E:434:GLN:HB2	2.27	0.65
2:C:529:SER:HG	2:C:799:SER:HG	1.44	0.65
2:C:559:MET:SD	2:C:567:LEU:HD11	2.37	0.65
2:C:813:PHE:HA	6:E:1005:PIO:H6A	1.79	0.64
2:C:644:SER:O	2:C:656:ARG:NH2	2.31	0.64
2:E:499:LEU:HD13	4:E:1001:CLR:H273	1.79	0.64
2:E:803:ILE:HG22	2:E:806:PHE:H	1.62	0.63
1:D:103:VAL:O	1:D:107:ILE:HD12	2.00	0.62
6:E:1004:PIO:H6AA	6:E:1004:PIO:H7BA	1.81	0.61
2:E:734:HIS:NE2	2:E:762:SER:OG	2.33	0.61
2:C:550:GLN:HG3	2:C:553:TYR:CZ	2.36	0.61
5:E:1003:PLC:H2A2	5:E:1003:PLC:H5'2	1.84	0.60
2:C:716:ALA:HB1	2:C:721:MET:HB2	1.84	0.59
1:B:89:GLU:OE2	2:C:651:HIS:ND1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:521:GLN:OE1	2:C:691:LYS:NZ	2.36	0.59
2:C:400:ALA:HA	2:C:405:VAL:HG21	1.84	0.58
2:E:431:THR:O	2:E:434:GLN:HG3	2.04	0.57
2:E:457:GLN:HE21	2:E:700:SER:HB3	1.68	0.57
2:C:672:LEU:O	2:C:676:ILE:HD12	2.04	0.57
2:E:435:MET:HE3	2:E:722:PRO:HG3	1.88	0.56
2:E:549:LEU:HD12	5:E:1003:PLC:H2'2	1.88	0.55
2:C:805:LEU:HD21	2:C:844:LEU:HD11	1.86	0.55
2:C:479:CYS:HB3	2:C:484:LEU:O	2.06	0.55
2:E:825:VAL:HG12	2:E:826:LYS:HD3	1.88	0.55
2:E:663:MET:HA	2:E:666:ALA:HB3	1.88	0.55
1:D:87:PHE:HB3	1:D:91:GLU:HB3	1.90	0.54
2:C:375:THR:HG21	2:C:384:ARG:HE	1.72	0.54
2:C:439:GLU:HG2	2:C:646:ARG:HH12	1.73	0.54
2:C:595:SER:O	2:E:815:PRO:HD2	2.08	0.54
2:C:642:ASN:OD1	3:A:1:NAG:N2	2.40	0.53
2:C:680:LEU:HD21	2:C:864:ILE:HD11	1.90	0.53
2:E:491:VAL:HG22	2:E:718:LEU:HA	1.89	0.53
2:E:678:ILE:HG12	2:E:725:SER:HB2	1.91	0.53
2:E:598:PRO:HD3	6:E:1005:PIO:H5A	1.91	0.53
2:C:559:MET:HE1	2:C:563:PRO:HG3	1.90	0.53
2:C:780:LEU:HA	2:C:783:ILE:HD12	1.91	0.53
2:C:558:LEU:HD12	2:C:564:GLN:HG3	1.92	0.52
2:C:817:LYS:HD2	2:C:818:TYR:CE2	2.45	0.52
2:E:400:ALA:HA	2:E:405:VAL:HG21	1.92	0.52
2:C:469:LEU:O	2:C:473:GLU:HG3	2.09	0.52
2:E:817:LYS:HD2	6:E:1004:PIO:H5	1.91	0.52
2:C:682:SER:HA	2:C:726:ALA:HB3	1.92	0.51
2:C:440:LEU:HD11	2:C:464:PHE:HB2	1.93	0.51
4:E:1002:CLR:H161	6:E:1004:PIO:H3C	1.92	0.50
2:C:545:GLN:HB3	5:C:1003:PLC:H51	1.93	0.50
2:C:505:VAL:HG21	2:C:707:LEU:HB2	1.93	0.50
2:C:651:HIS:HD2	2:C:653:LEU:H	1.58	0.50
1:D:90:PRO:HA	1:D:93:THR:HG22	1.93	0.49
2:C:486:TYR:CZ	2:C:490:ARG:HD2	2.47	0.49
2:C:550:GLN:HG3	2:C:553:TYR:CE2	2.47	0.49
2:E:541:ILE:O	2:E:545:GLN:HG3	2.12	0.49
2:E:592:LYS:NZ	2:E:607:ASP:OD1	2.45	0.49
2:C:487:ILE:HG23	2:C:650:ILE:CG2	2.43	0.49
2:E:809:ILE:HA	2:E:812:LEU:HD12	1.95	0.49
2:C:547:HIS:ND1	2:C:567:LEU:HB2	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:1005:PIO:H6AA	6:E:1005:PIO:H5B	1.96	0.48
2:C:592:LYS:HG3	2:C:606:GLY:HA3	1.94	0.48
2:C:430:LYS:HD2	2:C:473:GLU:CA	2.36	0.47
2:C:581:THR:HG23	2:C:790:GLY:HA3	1.96	0.47
2:E:492:TRP:CE2	2:E:664:MET:HG2	2.50	0.47
2:E:669:LEU:HD12	2:E:669:LEU:H	1.79	0.47
2:E:817:LYS:HE3	2:E:817:LYS:HB2	1.38	0.47
2:C:485:GLU:H	2:C:485:GLU:HG3	1.53	0.47
2:C:438:SER:OG	2:C:439:GLU:OE2	2.32	0.46
2:C:548:PRO:HD2	2:C:566:PRO:HB3	1.98	0.46
2:E:486:TYR:CZ	2:E:490:ARG:HD2	2.50	0.46
2:E:596:TYR:O	2:E:597:PHE:HB2	2.16	0.46
2:C:588:LEU:HD13	2:C:609:GLY:HA2	1.98	0.45
2:C:624:ILE:HD11	5:E:1003:PLC:H4'2	1.98	0.45
2:E:398:THR:HA	2:E:401:PHE:CD1	2.51	0.45
2:C:375:THR:OG1	2:C:508:GLU:OE2	2.25	0.45
2:C:418:SER:HB2	2:C:792:PHE:HZ	1.82	0.45
2:E:523:ILE:HD11	2:E:840:GLN:HG2	1.99	0.45
4:C:1001:CLR:H162	4:C:1001:CLR:H221	1.51	0.45
4:E:1001:CLR:H221	4:E:1001:CLR:H162	1.54	0.45
2:C:581:THR:HG21	2:C:787:VAL:HA	1.98	0.44
2:E:682:SER:HA	2:E:726:ALA:HB3	1.99	0.44
2:E:456:ALA:HB2	2:E:704:LEU:HD23	1.98	0.44
2:C:558:LEU:H	2:C:558:LEU:HG	1.47	0.44
2:C:430:LYS:HE2	2:C:430:LYS:HB2	1.58	0.44
1:B:92:ILE:HG12	2:C:653:LEU:HG	2.00	0.44
2:C:541:ILE:O	2:C:545:GLN:HG3	2.18	0.44
2:E:426:LEU:HD23	2:E:426:LEU:HA	1.71	0.44
2:E:488:VAL:HG21	2:E:654:GLY:HA2	2.00	0.44
2:C:581:THR:HB	2:C:617:MET:HG3	1.99	0.44
2:C:825:VAL:HG12	2:C:826:LYS:HE2	2.00	0.43
2:C:599:GLY:N	6:E:1004:PIO:O3	2.52	0.43
2:C:484:LEU:CD2	2:C:663:MET:HG3	2.48	0.43
2:E:418:SER:HB2	2:E:792:PHE:HZ	1.82	0.43
2:C:411:PHE:CD1	2:C:610:VAL:HG11	2.54	0.43
6:E:1004:PIO:H8AB	6:E:1004:PIO:H5AA	1.69	0.43
2:C:660:PRO:HB2	2:C:662:TRP:CD1	2.54	0.43
2:E:528:ILE:HG22	2:E:729:VAL:HG23	2.01	0.43
1:B:99:VAL:O	1:B:103:VAL:HG12	2.19	0.43
1:D:79:GLU:OE2	2:E:656:ARG:NH1	2.51	0.43
2:C:562:LYS:HE2	2:C:562:LYS:HB2	1.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:600:LYS:HG3	2:C:601:LEU:N	2.33	0.42
2:C:873:LEU:HD23	2:C:873:LEU:HA	1.89	0.42
2:E:680:LEU:HD23	2:E:680:LEU:HA	1.80	0.42
1:B:110:ILE:O	1:B:114:ILE:HG12	2.18	0.42
2:E:548:PRO:HD2	2:E:566:PRO:HB3	2.00	0.42
2:C:809:ILE:O	2:C:812:LEU:HB2	2.19	0.42
2:E:440:LEU:HD11	2:E:464:PHE:HB2	2.00	0.42
2:E:588:LEU:HD13	2:E:609:GLY:HA2	2.02	0.42
1:B:114:ILE:HG22	1:B:115:ARG:H	1.83	0.42
2:C:551:LYS:H	2:C:551:LYS:HG2	1.64	0.42
1:B:90:PRO:HA	1:B:93:THR:HG22	2.01	0.41
2:E:537:PHE:O	2:E:541:ILE:HD12	2.20	0.41
2:C:815:PRO:HA	2:C:816:PRO:HD3	1.94	0.41
2:C:590:LYS:HE3	2:C:590:LYS:HB3	1.66	0.41
2:E:660:PRO:HB2	2:E:662:TRP:CD1	2.55	0.41
2:C:418:SER:OG	2:C:788:LEU:HD13	2.21	0.41
2:C:437:VAL:HB	2:C:635:PRO:HG3	2.02	0.41
2:C:541:ILE:HD13	2:C:541:ILE:N	2.35	0.41
2:C:562:LYS:CE	2:C:563:PRO:HD2	2.47	0.41
2:C:492:TRP:CE2	2:C:664:MET:HG2	2.55	0.41
2:C:596:TYR:O	2:C:597:PHE:HB2	2.21	0.41
2:E:541:ILE:HG23	5:E:1003:PLC:OB	2.21	0.41
2:E:646:ARG:NH1	2:E:720:GLY:O	2.50	0.41
4:E:1002:CLR:H211	4:E:1002:CLR:H263	2.02	0.41
1:B:81:VAL:O	2:C:656:ARG:NH1	2.50	0.41
2:C:456:ALA:HB2	2:C:704:LEU:HD23	2.03	0.41
2:E:518:ARG:O	2:E:522:GLU:HB2	2.21	0.41
2:E:625:GLN:O	2:E:625:GLN:HG2	2.20	0.41
4:E:1001:CLR:H213	4:E:1001:CLR:H232	1.97	0.41
2:E:542:LYS:HA	2:E:542:LYS:HD2	1.83	0.41
2:E:823:PRO:HB3	2:E:893:ALA:HA	2.02	0.40
2:C:548:PRO:HG2	2:C:550:GLN:NE2	2.36	0.40
2:C:575:LEU:HD11	5:C:1003:PLC:H8A1	2.03	0.40
1:D:110:ILE:O	1:D:114:ILE:HG12	2.22	0.40
2:E:600:LYS:H	2:E:600:LYS:CE	2.31	0.40
2:E:398:THR:HA	2:E:401:PHE:CE1	2.56	0.40
6:E:1005:PIO:H8BA	6:E:1005:PIO:H5BA	1.93	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	B	38/150 (25%)	36 (95%)	2 (5%)	0	100	100
1	D	38/150 (25%)	38 (100%)	0	0	100	100
2	C	513/911 (56%)	502 (98%)	10 (2%)	1 (0%)	47	78
2	E	513/911 (56%)	503 (98%)	8 (2%)	2 (0%)	34	66
All	All	1102/2122 (52%)	1079 (98%)	20 (2%)	3 (0%)	44	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	597	PHE
2	C	597	PHE
2	E	819	HIS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	31/136 (23%)	30 (97%)	1 (3%)	39	73
1	D	31/136 (23%)	30 (97%)	1 (3%)	39	73
2	C	444/786 (56%)	417 (94%)	27 (6%)	18	48
2	E	444/786 (56%)	420 (95%)	24 (5%)	22	53
All	All	950/1844 (52%)	897 (94%)	53 (6%)	25	51

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	100	MET
1	D	86	HIS
2	C	384	ARG
2	C	385	ASP
2	C	430	LYS
2	C	432	ARG
2	C	435	MET
2	C	480	GLU
2	C	481	THR
2	C	482	ASN
2	C	495	PHE
2	C	511	PHE
2	C	514	ARG
2	C	517	SER
2	C	529	SER
2	C	541	ILE
2	C	550	GLN
2	C	558	LEU
2	C	562	LYS
2	C	602	ARG
2	C	603	ARG
2	C	629	THR
2	C	643	SER
2	C	646	ARG
2	C	727	THR
2	C	782	ARG
2	C	821	ASP
2	C	829	LYS
2	C	851	LYS
2	E	384	ARG
2	E	406	LEU
2	E	426	LEU
2	E	435	MET
2	E	473	GLU
2	E	480	GLU
2	E	511	PHE
2	E	590	LYS
2	E	600	LYS
2	E	613	SER
2	E	625	GLN
2	E	629	THR
2	E	644	SER
2	E	646	ARG

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Mol	Chain	Res	Type
2	E	656	ARG
2	E	669	LEU
2	E	672	LEU
2	E	681	GLU
2	E	752	GLN
2	E	762	SER
2	E	776	MET
2	E	817	LYS
2	E	851	LYS
2	E	856	SER

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

Mol	Chain	Res	Type
2	C	550	GLN
2	C	564	GLN
2	E	457	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 ⓘ

12 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	A	1	2,3	14,14,15	0.39	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	NAG	A	2	3	14,14,15	0.18	0	17,19,21	0.35	0
3	BMA	A	3	3	11,11,12	1.24	1 (9%)	15,15,17	1.26	2 (13%)
3	MAN	A	4	3	11,11,12	1.36	1 (9%)	15,15,17	2.10	4 (26%)
3	MAN	A	5	3	11,11,12	0.25	0	15,15,17	0.44	0
3	FUC	A	6	3	10,10,11	0.70	0	14,14,16	1.03	3 (21%)
3	NAG	F	1	2,3	14,14,15	0.26	0	17,19,21	0.38	0
3	NAG	F	2	3	14,14,15	0.18	0	17,19,21	0.35	0
3	BMA	F	3	3	11,11,12	1.42	2 (18%)	15,15,17	1.32	3 (20%)
3	MAN	F	4	3	11,11,12	0.99	1 (9%)	15,15,17	1.48	2 (13%)
3	MAN	F	5	3	11,11,12	0.23	0	15,15,17	0.39	0
3	FUC	F	6	3	10,10,11	0.72	0	14,14,16	0.87	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	A	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	A	2	3	-	0/6/23/26	0/1/1/1
3	BMA	A	3	3	-	2/2/19/22	0/1/1/1
3	MAN	A	4	3	-	1/2/19/22	0/1/1/1
3	MAN	A	5	3	-	0/2/19/22	1/1/1/1
3	FUC	A	6	3	-	-	0/1/1/1
3	NAG	F	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	1/2/19/22	1/1/1/1
3	MAN	F	5	3	-	0/2/19/22	0/1/1/1
3	FUC	F	6	3	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4	MAN	C1-C2	3.67	1.60	1.52
3	A	3	BMA	C1-C2	2.95	1.58	1.52
3	F	3	BMA	C1-C2	2.41	1.57	1.52
3	F	4	MAN	C1-C2	2.27	1.57	1.52
3	F	3	BMA	C4-C5	2.22	1.57	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	4	MAN	C1-O5-C5	5.79	120.03	112.19
3	F	4	MAN	C1-O5-C5	4.62	118.45	112.19
3	A	4	MAN	O5-C1-C2	3.35	115.94	110.77
3	A	4	MAN	C1-C2-C3	3.15	113.53	109.67
3	A	3	BMA	O2-C2-C3	-3.08	103.96	110.14
3	F	3	BMA	O2-C2-C3	-2.77	104.59	110.14
3	A	4	MAN	O2-C2-C3	-2.22	105.69	110.14
3	F	3	BMA	O5-C1-C2	-2.17	107.42	110.77
3	F	4	MAN	O2-C2-C3	-2.16	105.82	110.14
3	F	3	BMA	C2-C3-C4	-2.07	107.31	110.89
3	A	6	FUC	C1-O5-C5	2.07	117.46	112.78
3	A	3	BMA	O2-C2-C1	2.03	113.31	109.15
3	A	6	FUC	O5-C5-C4	2.03	113.16	109.52
3	A	6	FUC	O2-C2-C1	2.01	113.25	109.15

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	NAG	O5-C5-C6-O6
3	A	3	BMA	C4-C5-C6-O6
3	A	1	NAG	C4-C5-C6-O6
3	A	3	BMA	O5-C5-C6-O6
3	A	4	MAN	O5-C5-C6-O6
3	F	4	MAN	O5-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5	MAN	C1-C2-C3-C4-C5-O5
3	F	4	MAN	C1-C2-C3-C4-C5-O5

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	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.

Oligosaccharide Chain A

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings
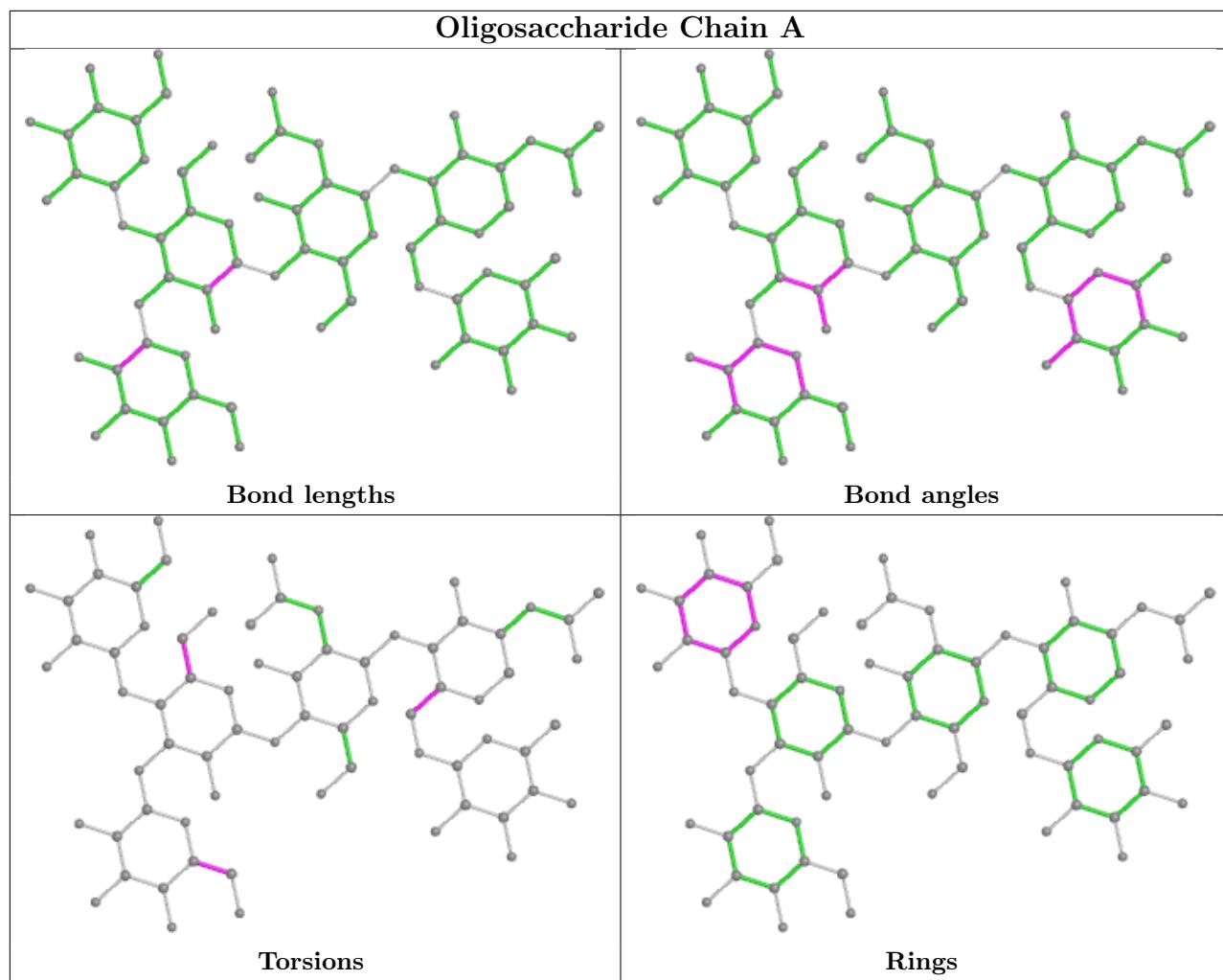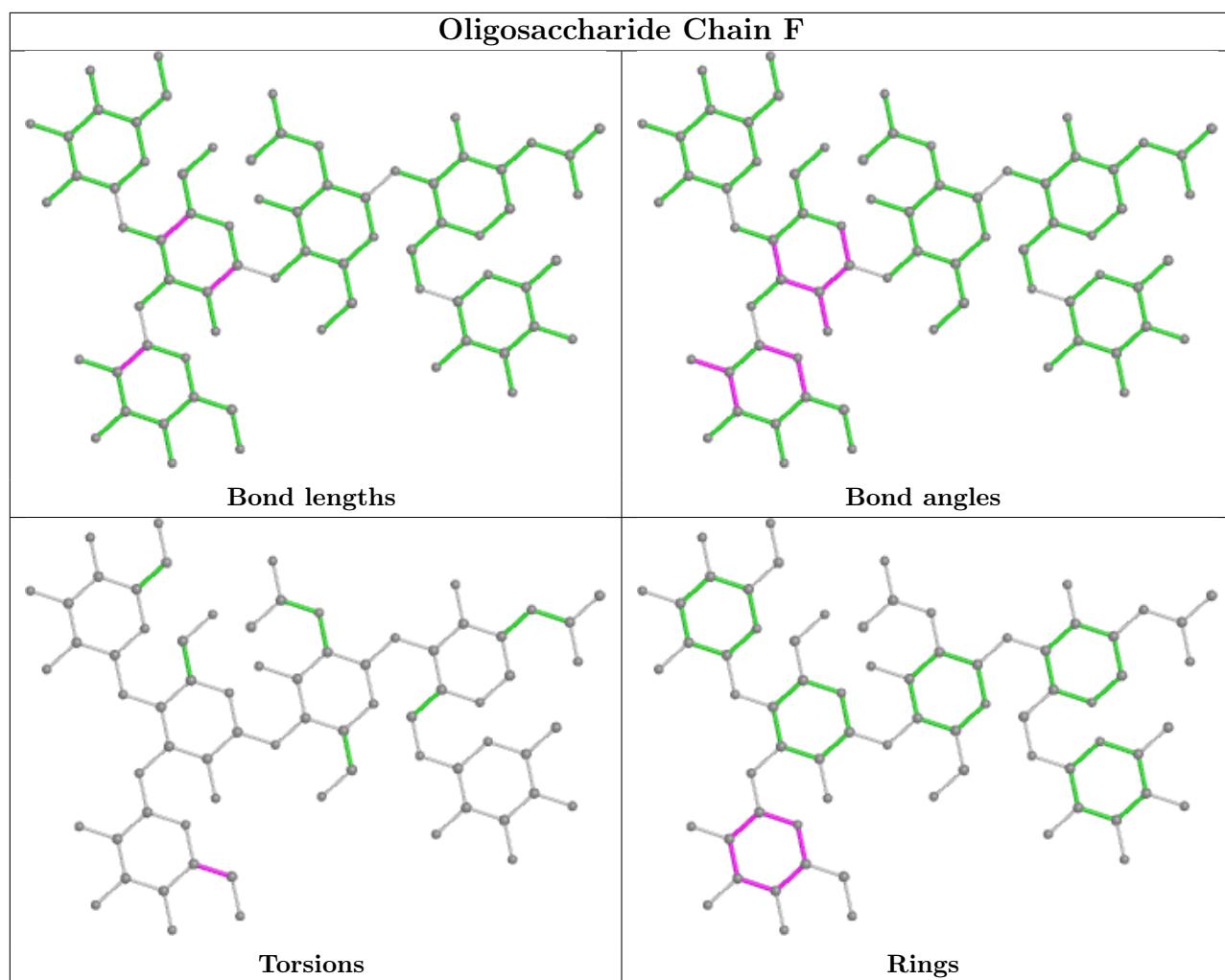
5.6 Ligand geometry ⓘ

8 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	$\#|Z| > 2$
4	CLR	E	1002	-	31,31,31	0.29	0	48,48,48	0.35	0
6	PIO	E	1005	-	47,47,47	0.44	0	61,65,65	0.51	0
5	PLC	C	1003	-	41,41,41	0.31	0	47,49,49	0.31	0
4	CLR	C	1001	-	31,31,31	0.37	0	48,48,48	0.66	0
6	PIO	E	1004	-	47,47,47	0.46	0	61,65,65	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	CLR	E	1001	-	31,31,31	0.39	0	48,48,48	0.55	0
4	CLR	C	1002	-	31,31,31	0.31	0	48,48,48	0.43	0
5	PLC	E	1003	-	41,41,41	0.33	0	47,49,49	0.37	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
4	CLR	E	1002	-	-	8/10/68/68	0/4/4/4
6	PIO	E	1005	-	-	23/44/68/68	0/1/1/1
5	PLC	C	1003	-	-	22/45/45/45	-
4	CLR	C	1001	-	-	8/10/68/68	0/4/4/4
6	PIO	E	1004	-	-	25/44/68/68	0/1/1/1
4	CLR	E	1001	-	-	8/10/68/68	0/4/4/4
4	CLR	C	1002	-	-	9/10/68/68	0/4/4/4
5	PLC	E	1003	-	-	21/45/45/45	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (124) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1003	PLC	O3P-C1-C2-O2
5	E	1003	PLC	O4P-C4-C5-N
5	E	1003	PLC	C1'-C'-O2-C2
5	E	1003	PLC	C4-O4P-P-O3P
6	E	1004	PIO	C1C-O13-P1-O11
6	E	1004	PIO	C2A-C1A-O2C-C2C
6	E	1005	PIO	C1C-O13-P1-O11
6	E	1005	PIO	C2A-C1A-O2C-C2C
6	E	1005	PIO	O2C-C2C-C3C-O3C
6	E	1004	PIO	C2B-C1B-O3C-C3C
6	E	1004	PIO	O1B-C1B-O3C-C3C
5	E	1003	PLC	O'-C'-O2-C2
4	C	1002	CLR	C21-C20-C22-C23
4	E	1001	CLR	C21-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
4	E	1002	CLR	C21-C20-C22-C23
4	C	1001	CLR	C16-C17-C20-C21
4	E	1001	CLR	C16-C17-C20-C21
4	C	1001	CLR	C13-C17-C20-C21
6	E	1004	PIO	O1A-C1A-O2C-C2C
6	E	1005	PIO	O1A-C1A-O2C-C2C
4	C	1001	CLR	C21-C20-C22-C23
5	E	1003	PLC	C4-C5-N-C8
4	E	1001	CLR	C13-C17-C20-C21
4	C	1001	CLR	C16-C17-C20-C22
6	E	1005	PIO	C2B-C1B-O3C-C3C
4	C	1001	CLR	C13-C17-C20-C22
4	C	1002	CLR	C13-C17-C20-C22
4	E	1001	CLR	C13-C17-C20-C22
4	C	1001	CLR	C17-C20-C22-C23
4	E	1001	CLR	C17-C20-C22-C23
4	E	1002	CLR	C17-C20-C22-C23
4	C	1001	CLR	C20-C22-C23-C24
4	E	1001	CLR	C20-C22-C23-C24
4	C	1001	CLR	C22-C23-C24-C25
4	E	1002	CLR	C20-C22-C23-C24
4	E	1001	CLR	C16-C17-C20-C22
5	E	1003	PLC	C'-C1'-C2'-C3'
5	E	1003	PLC	CB-C1B-C2B-C3B
6	E	1004	PIO	C1B-C2B-C3B-C4B
6	E	1005	PIO	O1B-C1B-O3C-C3C
4	E	1002	CLR	C13-C17-C20-C22
4	C	1002	CLR	C20-C22-C23-C24
4	E	1001	CLR	C22-C23-C24-C25
5	C	1003	PLC	C4-O4P-P-O3P
6	E	1005	PIO	C1C-O13-P1-O1
4	C	1002	CLR	C13-C17-C20-C21
5	E	1003	PLC	C4-C5-N-C6
6	E	1005	PIO	C1C-C2C-O2C-C1A
6	E	1004	PIO	C4B-C5B-C6B-C7B
6	E	1005	PIO	C1B-C2B-C3B-C4B
4	C	1002	CLR	C17-C20-C22-C23
4	C	1002	CLR	C16-C17-C20-C21
5	E	1003	PLC	C4'-C5'-C6'-C7'
5	E	1003	PLC	C1B-C2B-C3B-C4B
6	E	1005	PIO	C4B-C5B-C6B-C7B
5	E	1003	PLC	C4-C5-N-C7

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Mol	Chain	Res	Type	Atoms
5	C	1003	PLC	C5B-C6B-C7B-C8B
5	C	1003	PLC	C6B-C7B-C8B-C9B
6	E	1004	PIO	C2A-C3A-C4A-C5A
4	C	1002	CLR	C23-C24-C25-C26
4	C	1002	CLR	C23-C24-C25-C27
5	C	1003	PLC	C4'-C5'-C6'-C7'
6	E	1004	PIO	C2B-C3B-C4B-C5B
5	C	1003	PLC	C7'-C8'-C9'-CA'
5	E	1003	PLC	C2B-C3B-C4B-C5B
5	E	1003	PLC	C7B-C8B-C9B-CAA
4	C	1002	CLR	C16-C17-C20-C22
6	E	1004	PIO	C5A-C6A-C7A-C8A
6	E	1005	PIO	C3A-C4A-C5A-C6A
4	E	1002	CLR	C16-C17-C20-C21
4	E	1002	CLR	C13-C17-C20-C21
5	C	1003	PLC	C1'-C'-O2-C2
5	C	1003	PLC	C5'-C6'-C7'-C8'
6	E	1005	PIO	C2B-C3B-C4B-C5B
6	E	1004	PIO	C1C-O13-P1-O1
4	E	1002	CLR	C16-C17-C20-C22
5	C	1003	PLC	O'-C'-O2-C2
4	E	1002	CLR	C22-C23-C24-C25
5	C	1003	PLC	C1B-CB-O3-C3
6	E	1004	PIO	C5B-C6B-C7B-C8B
5	E	1003	PLC	C8B-C9B-CAA-CBA
6	E	1004	PIO	C3A-C4A-C5A-C6A
6	E	1005	PIO	C5B-C6B-C7B-C8B
5	C	1003	PLC	OB-CB-O3-C3
5	C	1003	PLC	O3P-C1-C2-C3
5	E	1003	PLC	C6B-C7B-C8B-C9B
5	E	1003	PLC	C1-C2-C3-O3
6	E	1004	PIO	O2C-C2C-C3C-O3C
6	E	1005	PIO	C4A-C5A-C6A-C7A
6	E	1004	PIO	C5-O5-P5-O53
6	E	1005	PIO	C2A-C3A-C4A-C5A
5	E	1003	PLC	C3'-C4'-C5'-C6'
6	E	1005	PIO	C1C-C2C-C3C-O3C
5	E	1003	PLC	O2-C2-C3-O3
5	C	1003	PLC	C4B-C5B-C6B-C7B
5	C	1003	PLC	C4-O4P-P-O2P
5	E	1003	PLC	C4-O4P-P-O2P
6	E	1004	PIO	C1C-O13-P1-O12

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Mol	Chain	Res	Type	Atoms
6	E	1004	PIO	O13-C1C-C2C-C3C
5	E	1003	PLC	C2-C1-O3P-P
6	E	1004	PIO	C1C-C2C-O2C-C1A
5	C	1003	PLC	C1B-C2B-C3B-C4B
6	E	1004	PIO	C4A-C5A-C6A-C7A
5	C	1003	PLC	C'-C1'-C2'-C3'
6	E	1004	PIO	C1C-C2C-C3C-O3C
5	C	1003	PLC	C8'-C9'-CA'-CB'
6	E	1005	PIO	C1-O1-P1-O11
5	E	1003	PLC	C1'-C2'-C3'-C4'
5	C	1003	PLC	C3'-C4'-C5'-C6'
6	E	1004	PIO	C4-O4-P4-O42
6	E	1005	PIO	C5-O5-P5-O53
6	E	1005	PIO	O2C-C1A-C2A-C3A
6	E	1004	PIO	C4-O4-P4-O43
6	E	1004	PIO	C5-O5-P5-O52
6	E	1005	PIO	C5-O5-P5-O52
6	E	1004	PIO	O2C-C1A-C2A-C3A
6	E	1005	PIO	C1-O1-P1-O13
5	C	1003	PLC	C2B-C1B-CB-O3
6	E	1005	PIO	C2C-C1C-O13-P1
6	E	1005	PIO	O1A-C1A-C2A-C3A
6	E	1004	PIO	O1A-C1A-C2A-C3A
5	C	1003	PLC	C8B-C9B-CAA-CBA
5	C	1003	PLC	O2-C'-C1'-C2'
5	C	1003	PLC	C2B-C1B-CB-OB

There are no ring outliers.

8 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1002	CLR	2	0
6	E	1005	PIO	5	0
5	C	1003	PLC	5	0
4	C	1001	CLR	1	0
6	E	1004	PIO	5	0
4	E	1001	CLR	3	0
4	C	1002	CLR	2	0
5	E	1003	PLC	6	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand CLR E 1002

Ligand PIO E 1005

Ligand PLC C 1003

Bond lengths

Bond angles

Torsions

Rings

Ligand CLR C 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand PIO E 1004

Bond lengths

Bond angles

Torsions

Rings

Ligand CLR E 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand CLR C 1002

Bond lengths

Bond angles

Torsions

Rings

Ligand PLC E 1003

Bond lengths

Bond angles

Torsions

Rings
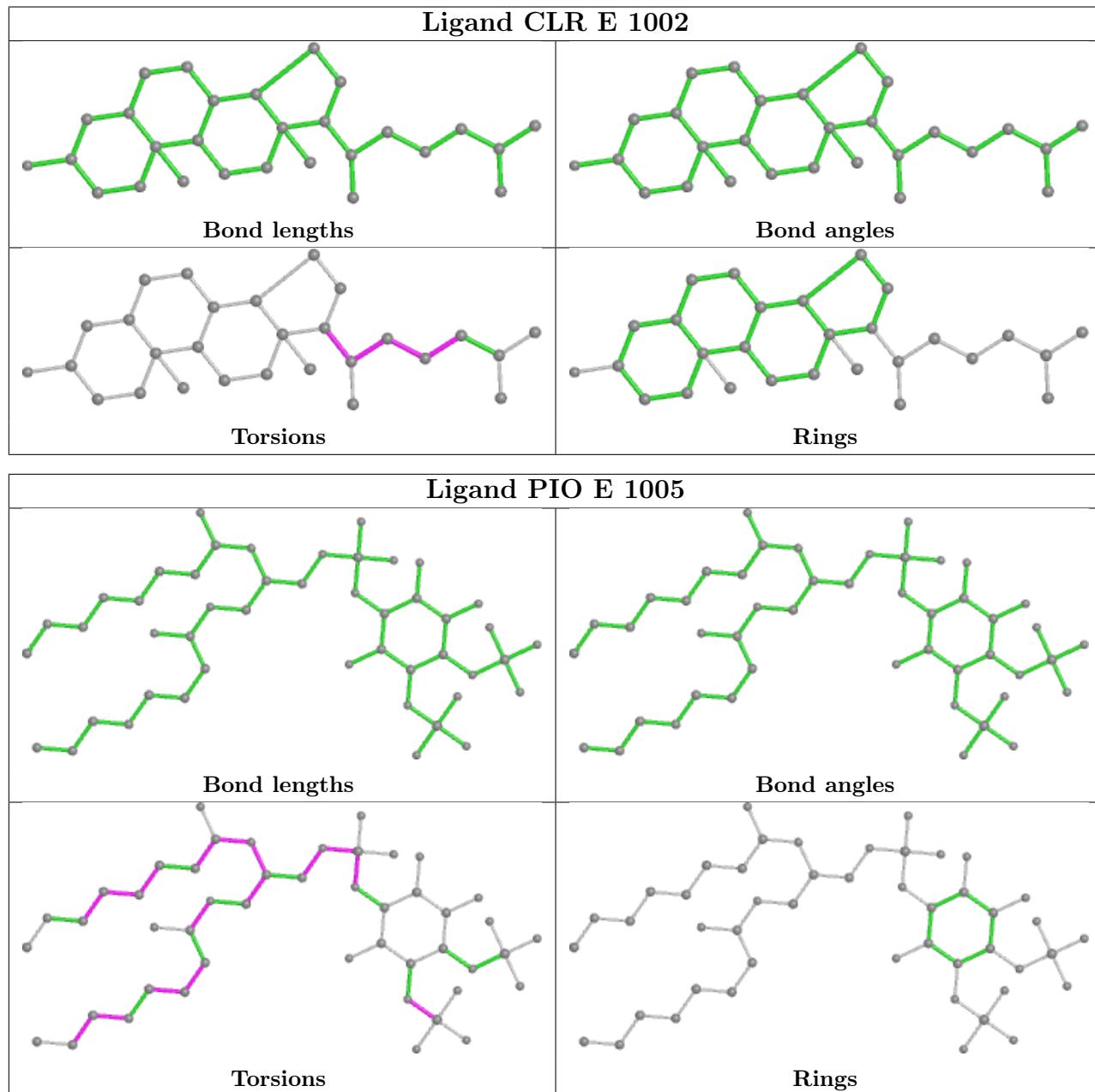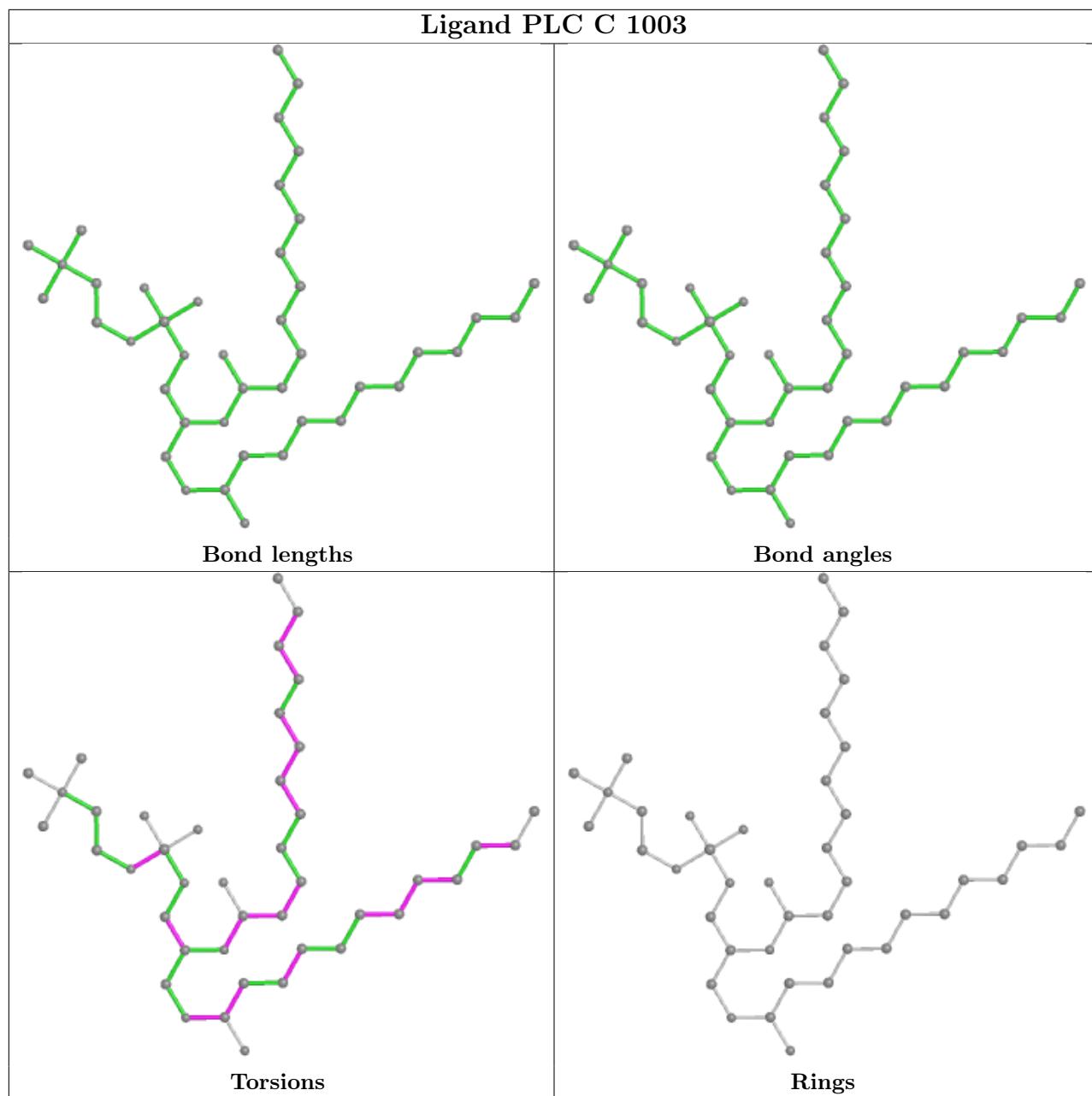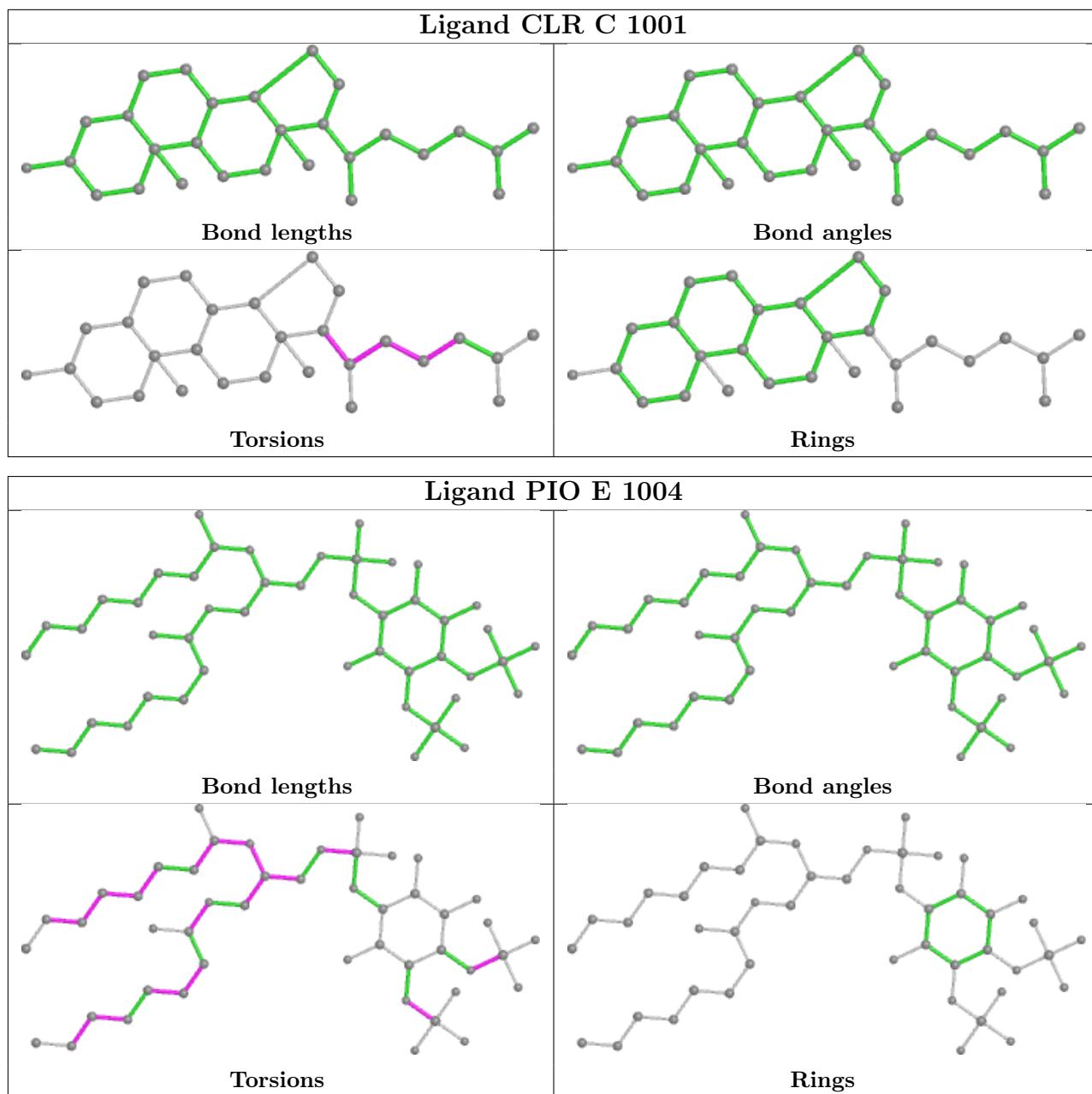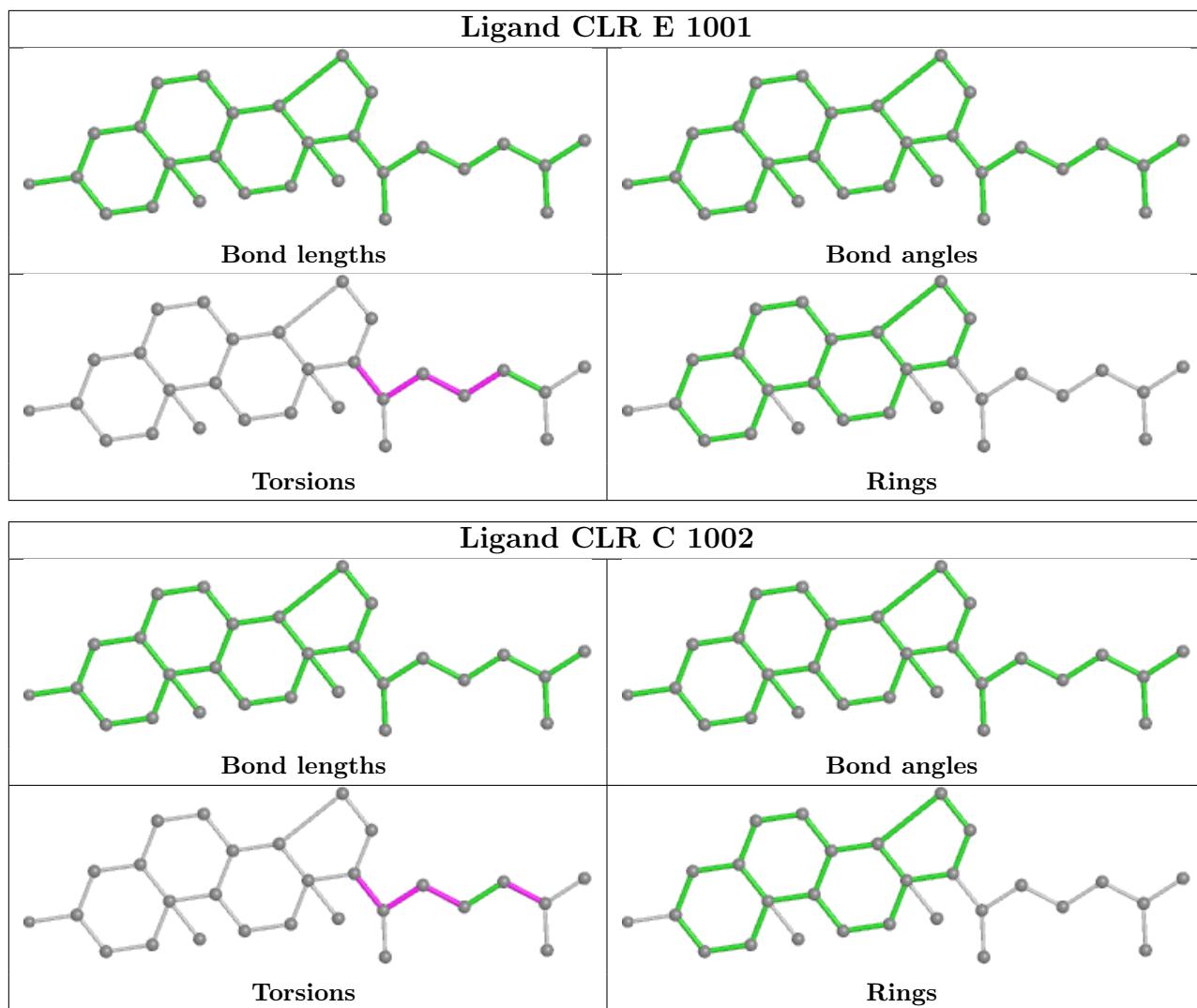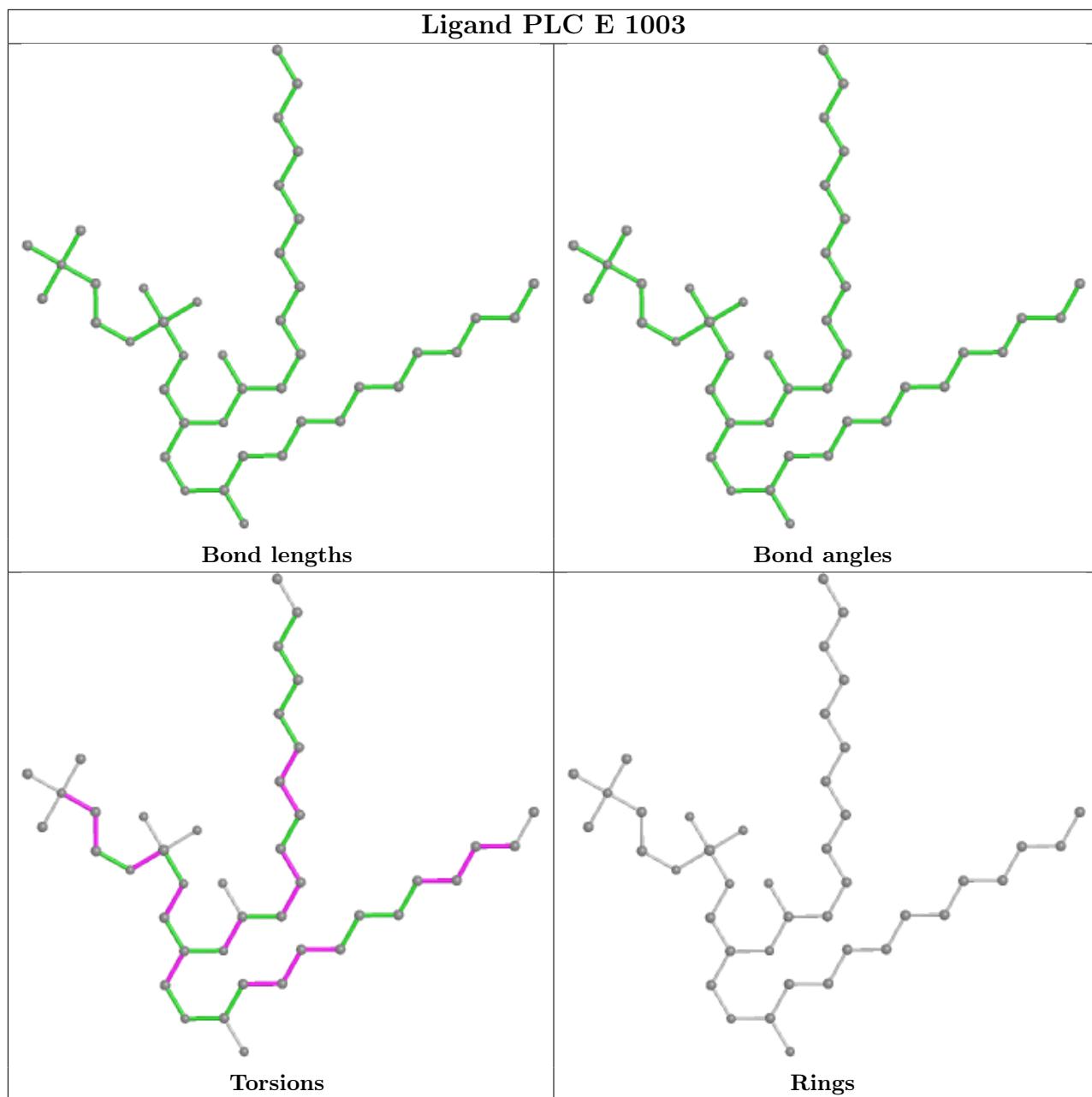
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6　Map visualisation　ⓘ

This section contains visualisations of the EMDB entry EMD-26940. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1　Orthogonal projections　ⓘ
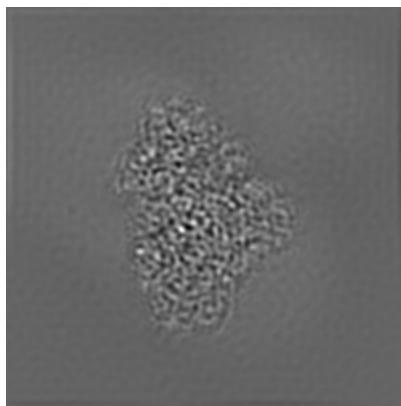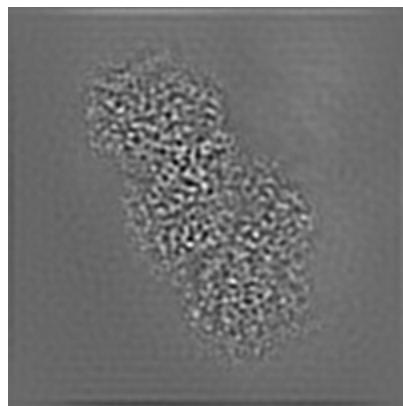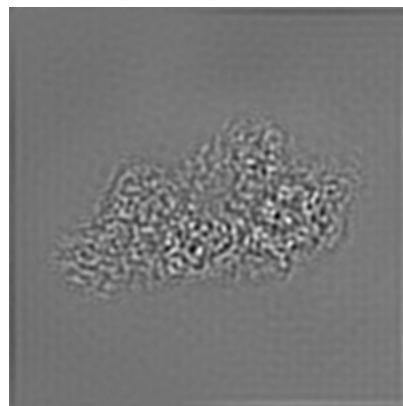
6.1.1　Primary map

X　　　　　　　　Y　　　　　　　　Z

6.1.2　Raw map

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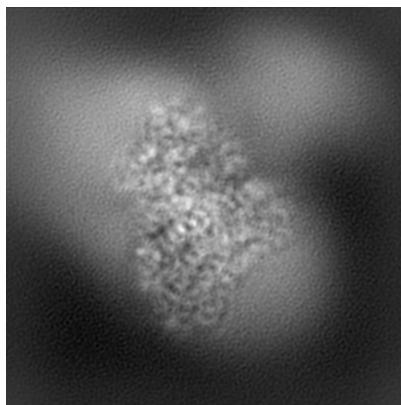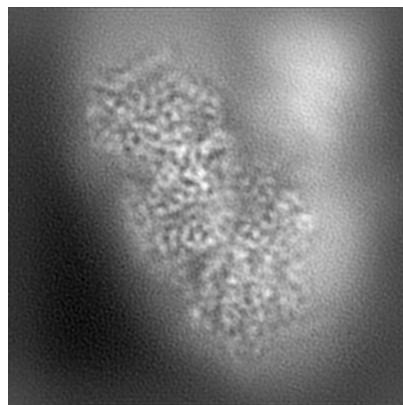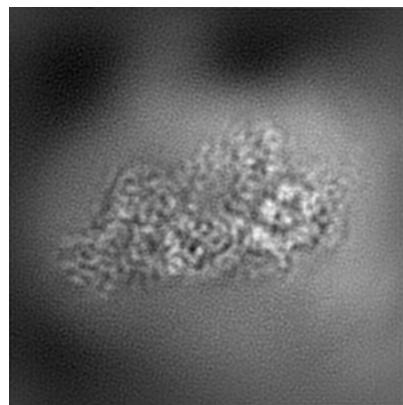
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
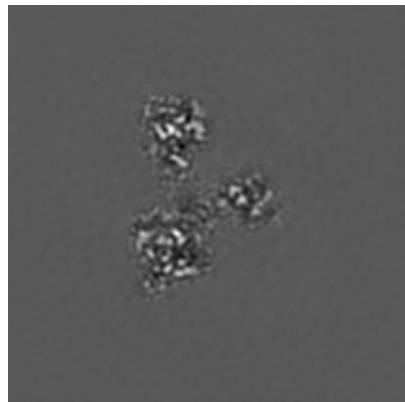
6.2.1 Primary map
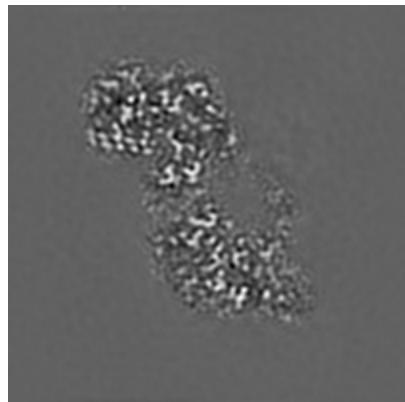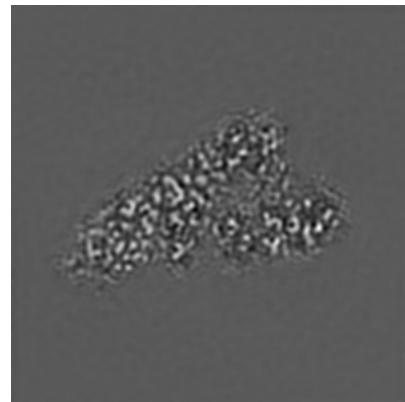
X Index: 190	Y Index: 190	Z Index: 190

6.2.2 Raw map
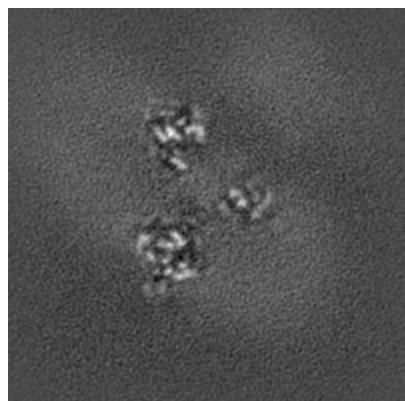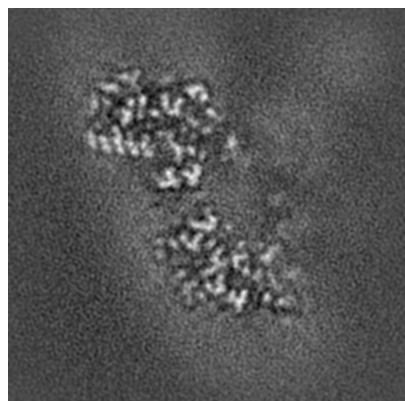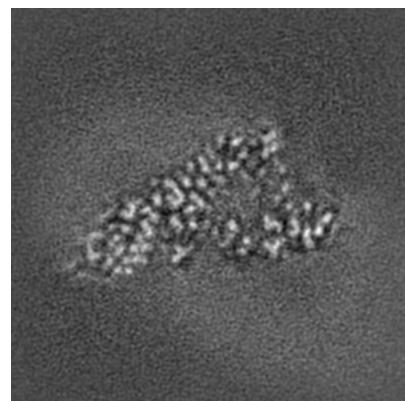
X Index: 190	Y Index: 190	Z Index: 190

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

6.3   Largest variance slices   ⓘ
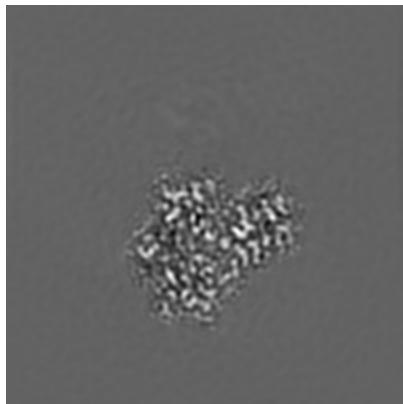
6.3.1   Primary map
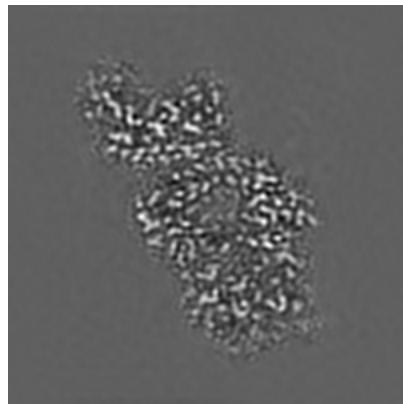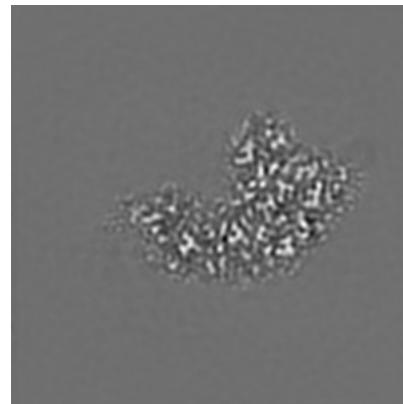
| X Index: 247 | Y Index: 162 | Z Index: 160 |

6.3.2   Raw map
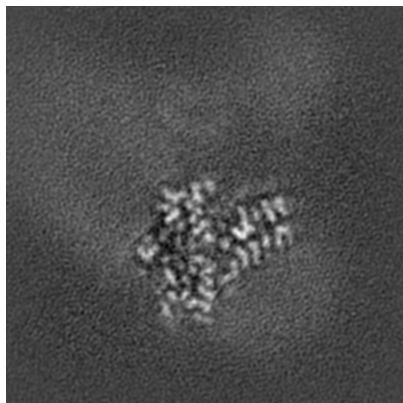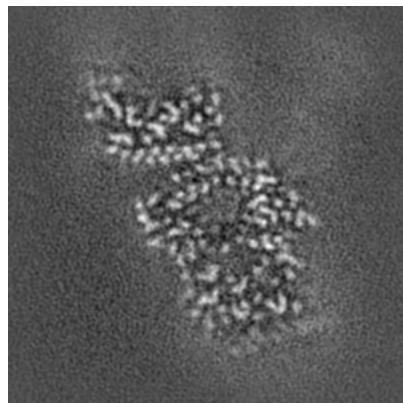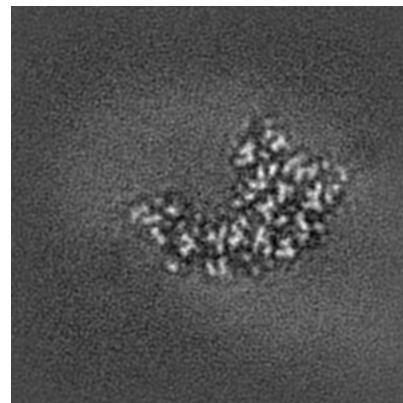
| X Index: 247 | Y Index: 162 | Z Index: 161 |

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

X Y Z
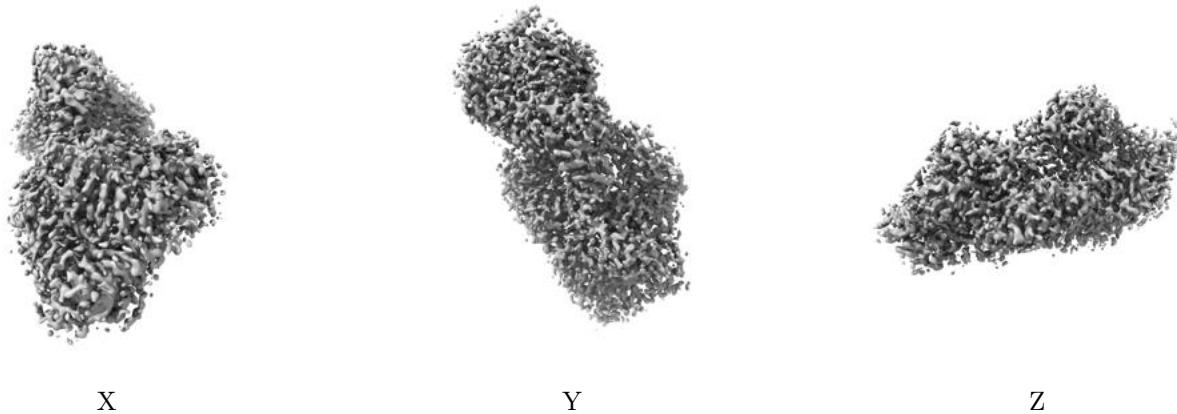
The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

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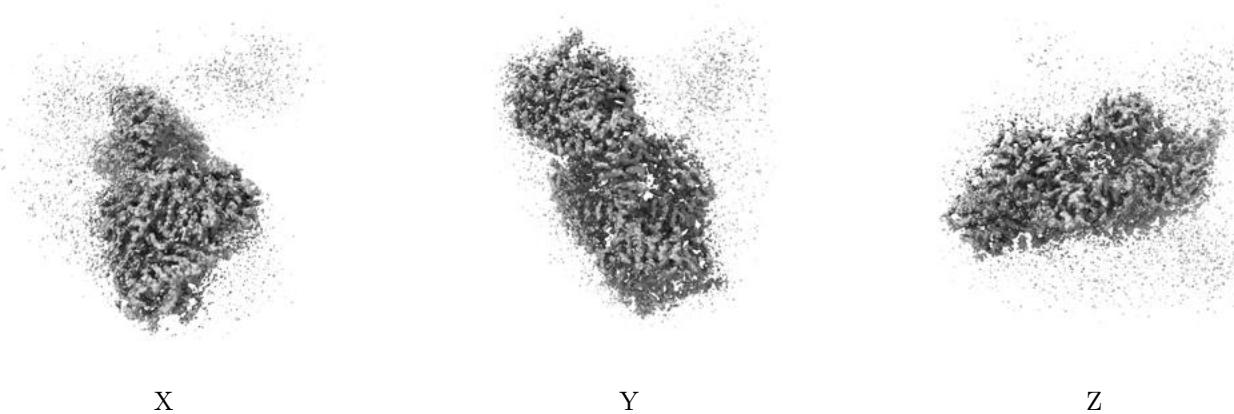
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

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

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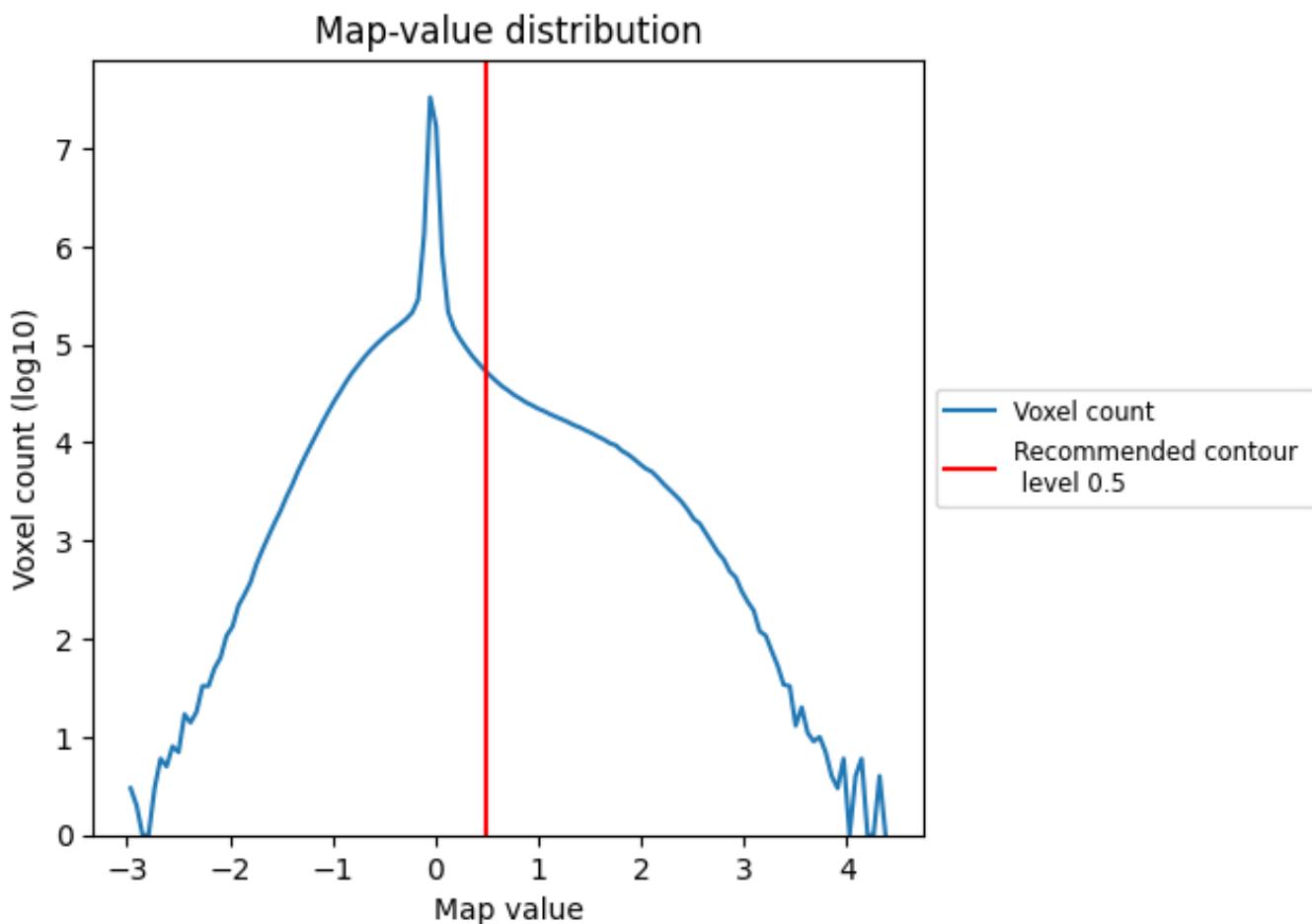
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
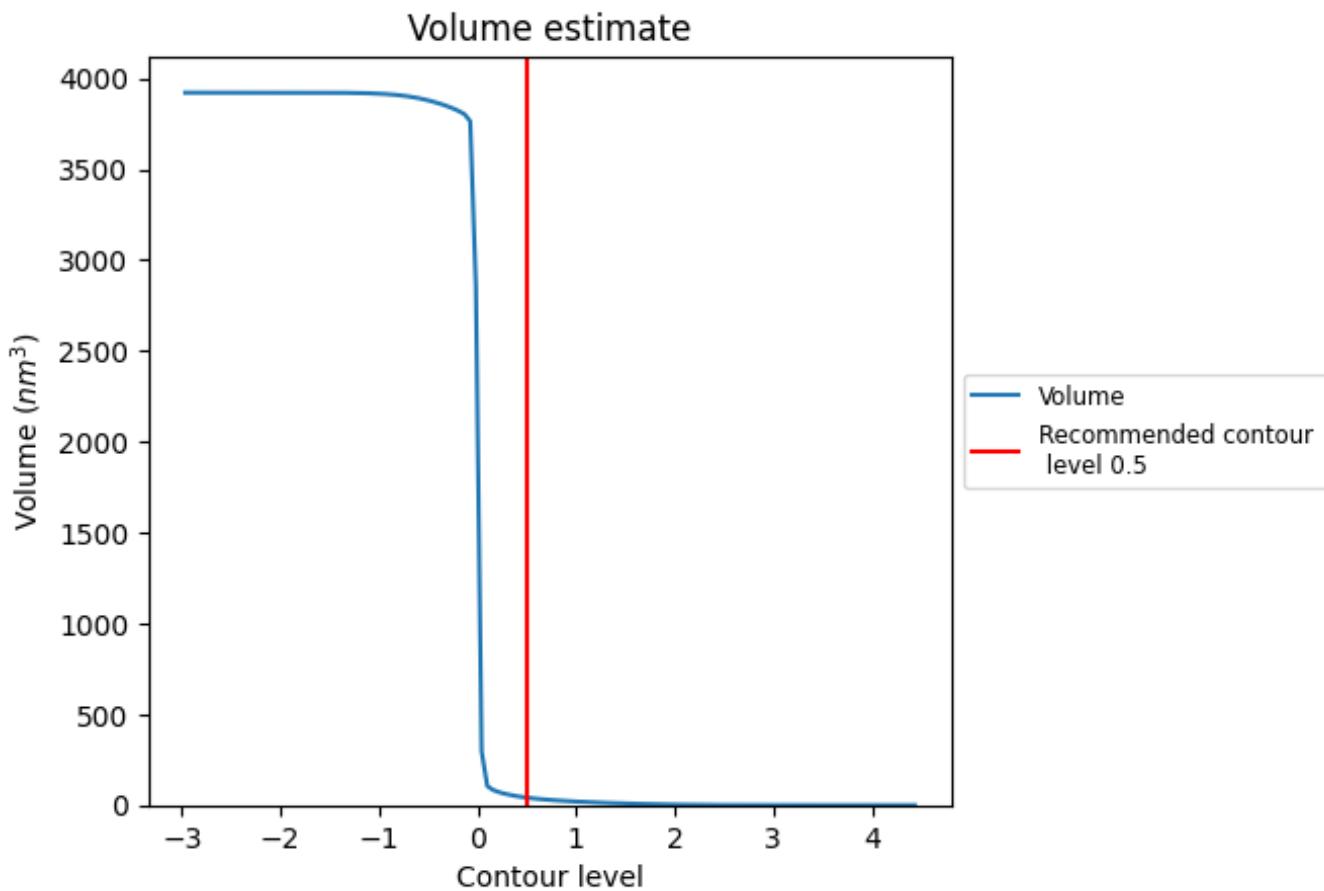
The volume at the recommended contour level is 41 nm^3; this corresponds to an approximate mass of 37 kDa.

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 ⓘ
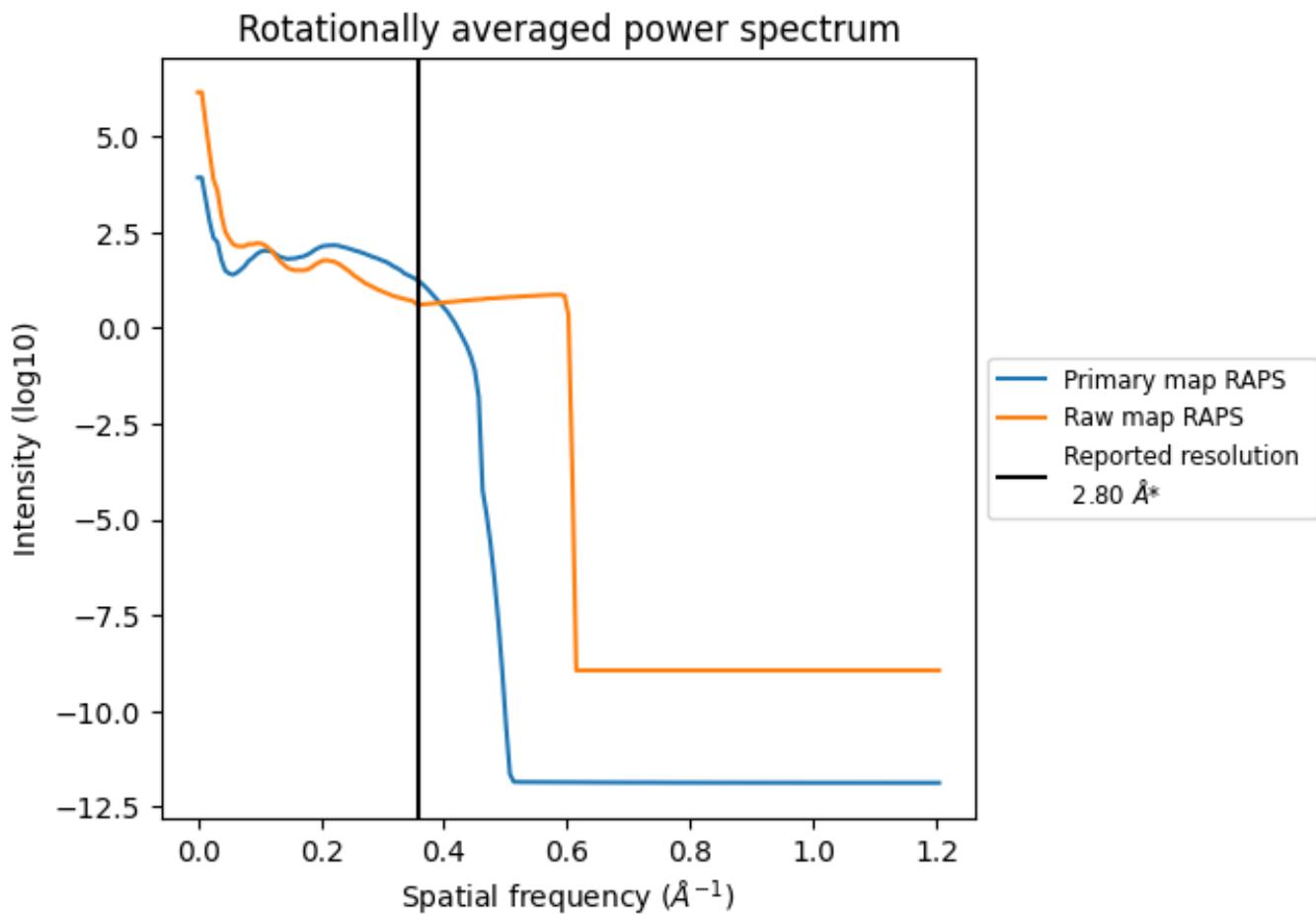
*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ
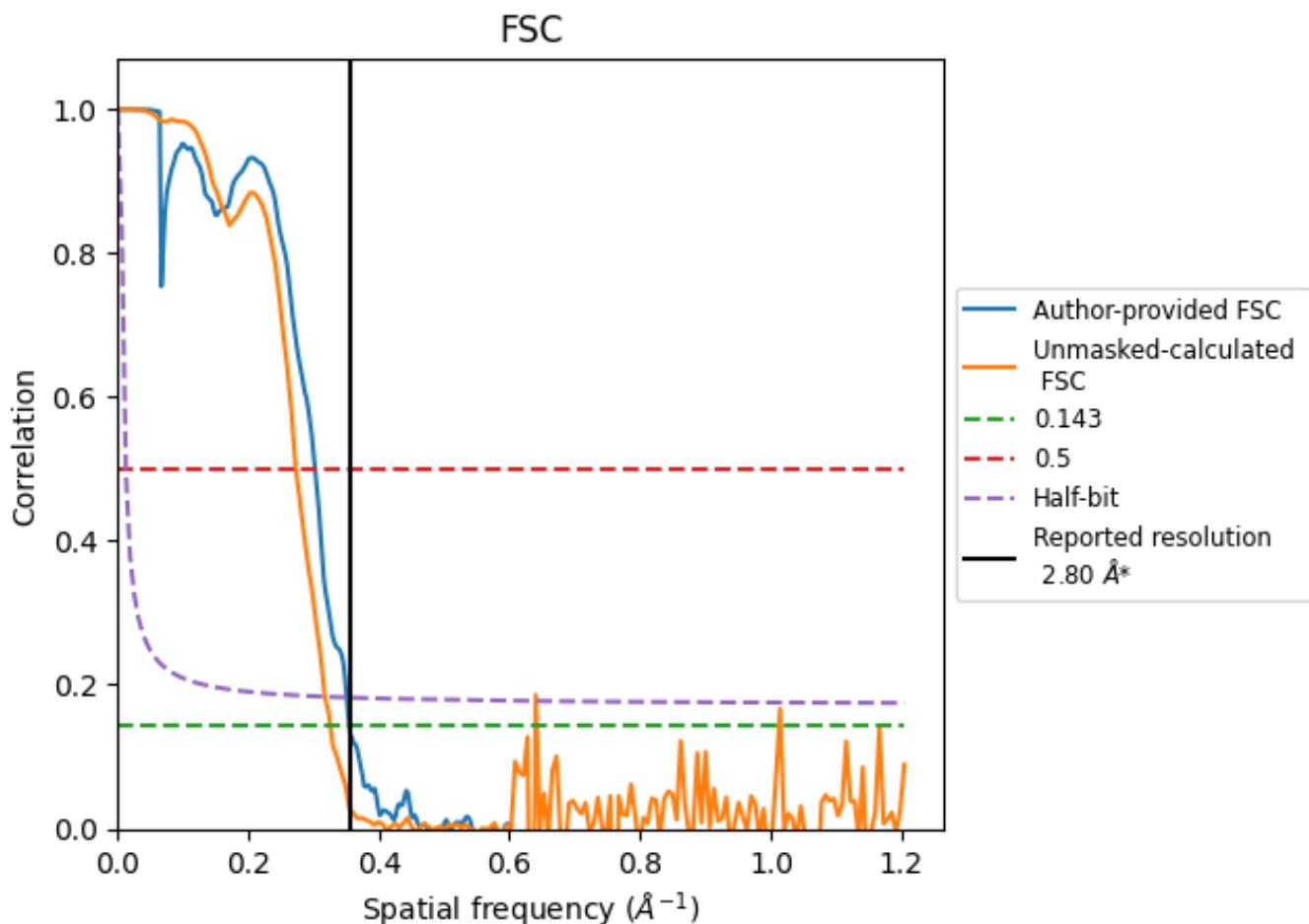
*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8.2   Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.82	3.31	2.85
Unmasked-calculated*	3.07	3.67	3.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-26940 and PDB model 7V07. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay ⓘ

| X | Y | Z |
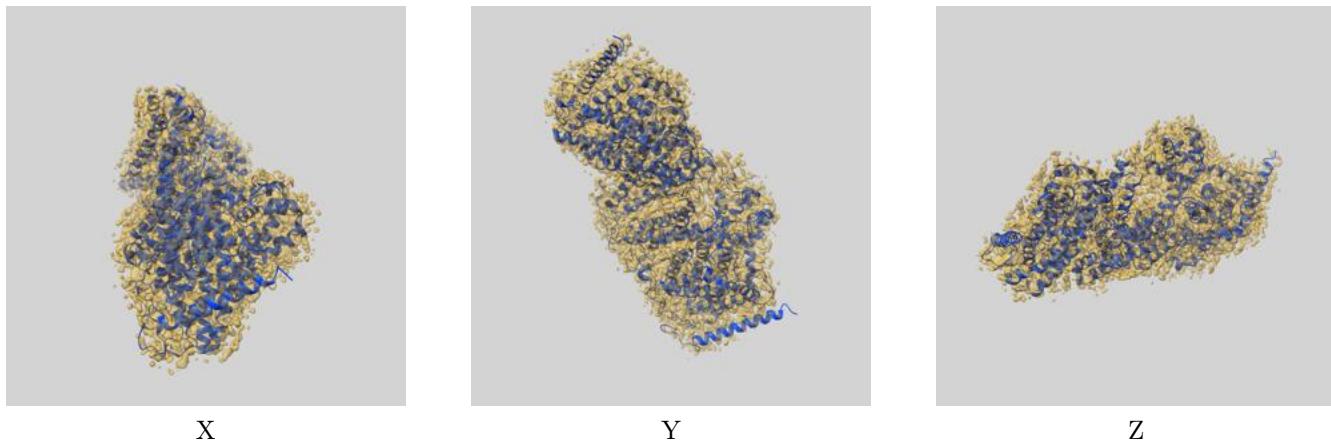
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Q-score mapped to coordinate model ⓘ

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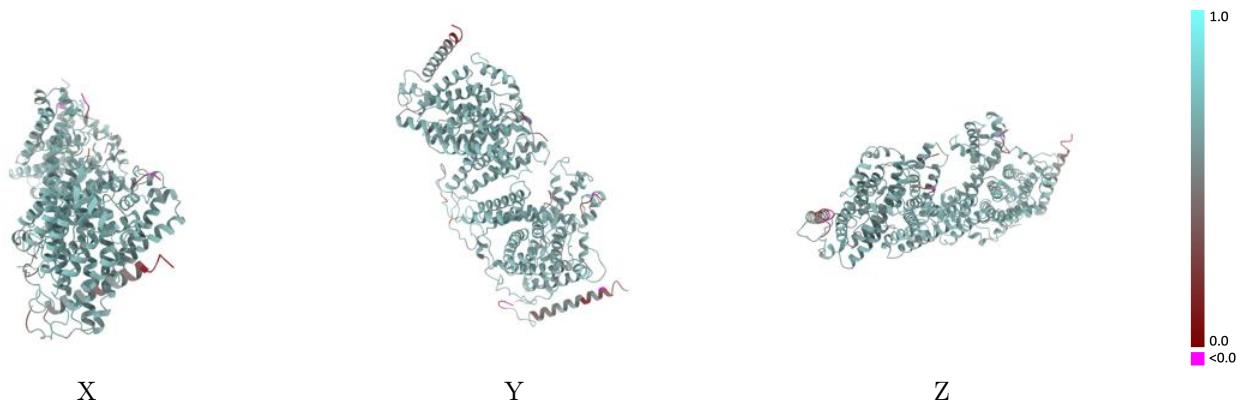
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3　Atom inclusion mapped to coordinate model ⓘ

X　　　　　　　　　　　　　Y　　　　　　　　　　　　　Z
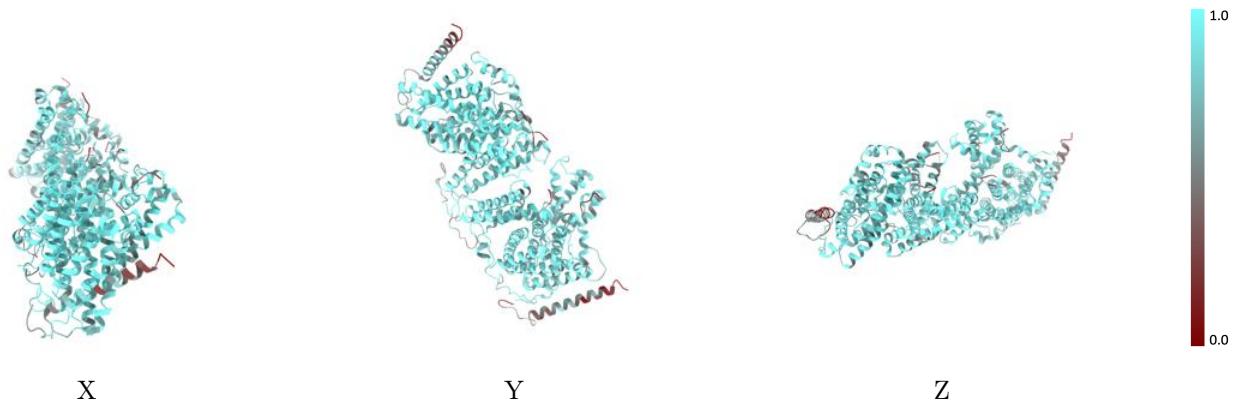
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4   Atom inclusion ⓘ
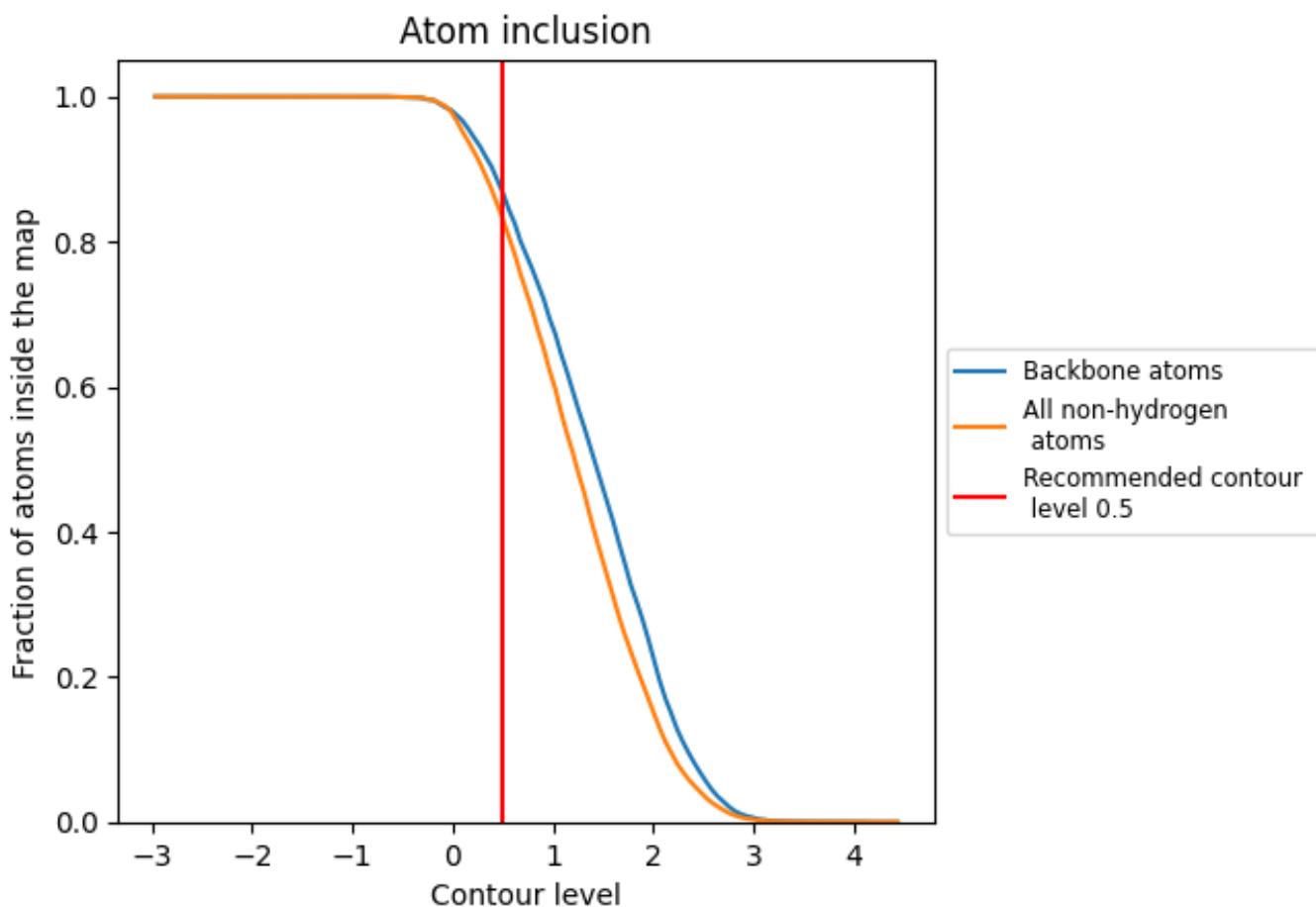
At the recommended contour level, 87% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8317	0.6040
A	0.1690	0.2750
B	0.3939	0.4050
C	0.8605	0.6200
D	0.5455	0.4490
E	0.8763	0.6250
F	0.2254	0.2590

1.0

0.0
<0.0