



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 03:19 AM UTC

PDB ID : 8ESV / pdb_00008esv
EMDB ID : EMD-28580
Title : Structure of human ADAM10-Tspan15 complex bound to 11G2 vFab
Authors : Lipper, C.H.; Blacklow, S.C.
Deposited on : 2022-10-14
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

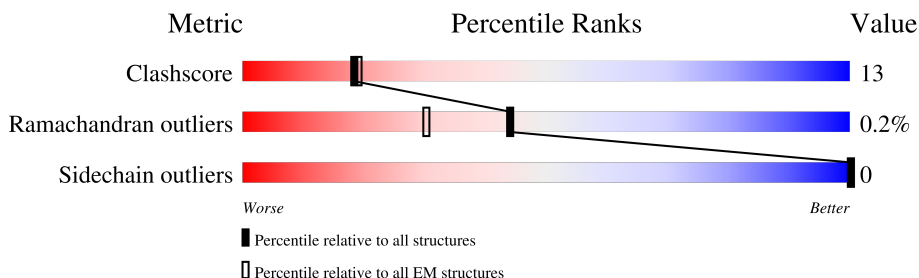
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	543	56% 26% 18%
2	B	306	65% 18% 17%
3	H	225	44% 10% 46%
4	L	221	35% 15% 50%
5	C	4	100%
6	D	3	67% 33%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7222 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 Disintegrin and metalloproteinase domain-containing protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	446	Total	C	N	O	S	0	0
			3306	2036	591	641	38		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	206	ASP	-	expression tag	UNP O14672
A	207	TYR	-	expression tag	UNP O14672
A	208	LYS	-	expression tag	UNP O14672
A	209	ASP	-	expression tag	UNP O14672
A	210	ASP	-	expression tag	UNP O14672
A	211	ASP	-	expression tag	UNP O14672
A	212	ASP	-	expression tag	UNP O14672
A	213	LYS	-	expression tag	UNP O14672

- Molecule 2 is a protein called Tetraspanin-15.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	255	Total	C	N	O	S	0	0
			2006	1320	317	353	16		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	MET	-	initiating methionine	UNP O95858
B	-10	HIS	-	expression tag	UNP O95858
B	-9	HIS	-	expression tag	UNP O95858
B	-8	HIS	-	expression tag	UNP O95858
B	-7	HIS	-	expression tag	UNP O95858
B	-6	HIS	-	expression tag	UNP O95858
B	-5	HIS	-	expression tag	UNP O95858
B	-4	ASP	-	expression tag	UNP O95858

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	ASP	-	expression tag	UNP O95858
B	-2	ASP	-	expression tag	UNP O95858
B	-1	ASP	-	expression tag	UNP O95858
B	0	LYS	-	expression tag	UNP O95858

- Molecule 3 is a protein called 11G2 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	121	Total	C	N	O	S	0	0
			909	572	155	179	3		

- Molecule 4 is a protein called 11G2 Fab Light Chain.

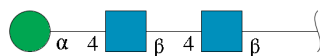
Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	111	Total	C	N	O	S	0	0
			794	497	132	160	5		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
5	C	4	Total	C	N	O	0	0
			50	28	2	20		

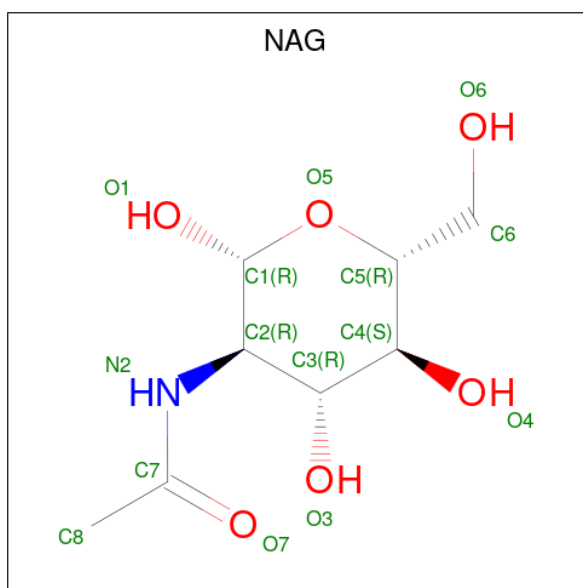
- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

$C_8H_{15}NO_6$).



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

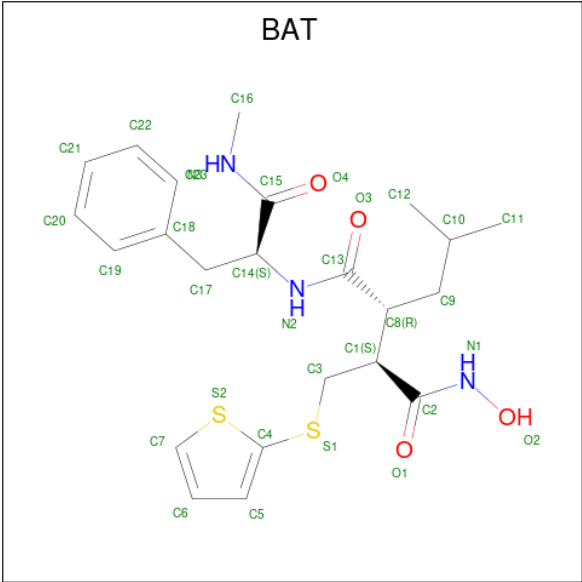
- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	Ca	0
			1	1	

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

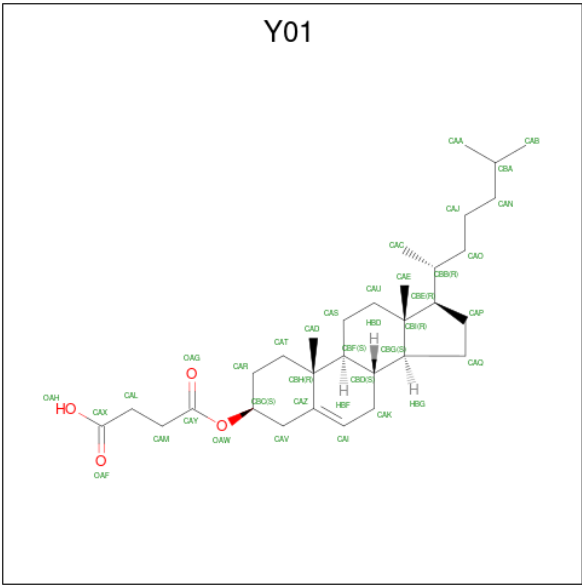
Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total	Zn	0
			1	1	

- Molecule 10 is 4-(N-HYDROXYAMINO)-2R-ISOBUTYL-2S-(2-THIENYLTHIOMETHYL)SUCCINYL-L-PHENYLALANINE-N-METHYLAMIDE (CCD ID: BAT) (formula: $C_{23}H_{31}N_3O_4S_2$).

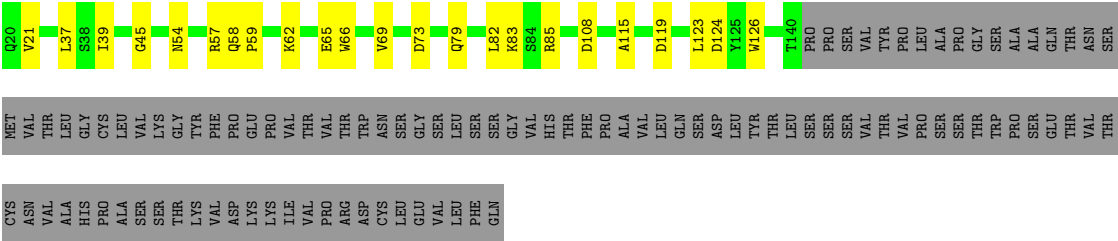


Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	S	0
			32	23	3	4	2	

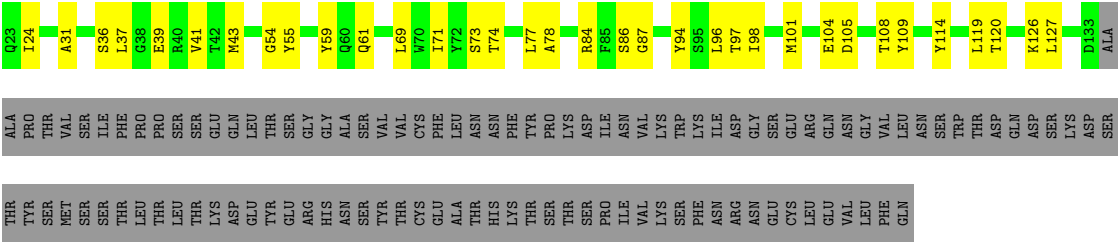
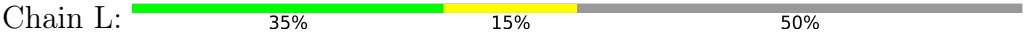
- Molecule 11 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$).



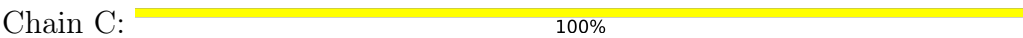
Mol	Chain	Residues	Atoms			AltConf
11	B	1	Total	C	O	0
			35	31	4	
11	B	1	Total	C	O	0
			35	31	4	



• Molecule 4: 11G2 Fab Light Chain



• Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 6: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	178031	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.99	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	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: ZN, MAN, CA, BAT, NAG, Y01

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	0.13	0/3373	0.38	0/4564
2	B	0.12	0/2049	0.32	0/2785
3	H	0.09	0/928	0.26	0/1264
4	L	0.12	0/812	0.31	0/1107
All	All	0.12	0/7162	0.34	0/9720

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 [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	3306	0	3029	107	0
2	B	2006	0	2010	44	0
3	H	909	0	872	19	0
4	L	794	0	737	24	0
5	C	50	0	43	4	0
6	D	39	0	34	0	0
7	A	14	0	13	1	0
8	A	1	0	0	0	0
9	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	32	0	30	4	0
11	B	70	0	98	3	0
All	All	7222	0	6866	184	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 13.

All (184) 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:656:ARG:NH2	2:B:48:GLU:HG2	1.92	0.84
3:H:66:TRP:O	3:H:79:GLN:OE1	2.07	0.72
2:B:186:CYS:HA	2:B:214:ILE:HA	1.70	0.72
1:A:288:ASN:HB2	5:C:1:NAG:H61	1.73	0.70
1:A:549:LYS:HD2	1:A:553:THR:HG21	1.76	0.67
1:A:580:CYS:H	1:A:598:CYS:HA	1.61	0.66
1:A:536:CYS:O	1:A:537:ASN:ND2	2.30	0.65
2:B:220:THR:O	2:B:224:ILE:HG12	1.97	0.64
1:A:387:HIS:HE2	1:A:393:HIS:CD2	2.07	0.62
2:B:116:PHE:HB3	2:B:119:GLN:OE1	1.99	0.62
1:A:279:THR:HG22	1:A:281:ALA:H	1.64	0.62
1:A:503:CYS:SG	1:A:504:SER:N	2.73	0.62
2:B:153:LYS:NZ	2:B:215:TYR:OH	2.31	0.61
1:A:320:ASP:O	1:A:366:GLN:NE2	2.34	0.61
2:B:204:ASP:OD1	2:B:205:LYS:NZ	2.32	0.61
1:A:593:LEU:HG	1:A:632:CYS:HB3	1.83	0.60
2:B:211:GLN:HG2	2:B:216:VAL:HG21	1.82	0.60
1:A:310:ASP:O	1:A:346:LYS:NZ	2.32	0.60
1:A:380:THR:O	1:A:384:GLU:HG2	2.02	0.59
2:B:213:VAL:HG13	2:B:214:ILE:HG23	1.84	0.59
2:B:204:ASP:OD1	2:B:205:LYS:N	2.36	0.59
1:A:656:ARG:HH22	2:B:48:GLU:CG	2.16	0.59
1:A:615:TRP:CD1	1:A:618:HIS:HD1	2.21	0.58
1:A:258:GLN:HE21	1:A:269:SER:HB2	1.68	0.58
1:A:606:THR:HG21	1:A:614:GLN:HG3	1.85	0.58
1:A:557:ARG:O	1:A:558:HIS:ND1	2.35	0.58
1:A:572:CYS:HB3	1:A:577:LEU:HG	1.85	0.58
1:A:391:SER:HB3	1:A:440:ILE:HG13	1.86	0.58
1:A:656:ARG:NH2	2:B:48:GLU:CG	2.68	0.57
1:A:592:GLU:HA	1:A:595:HIS:CE1	2.40	0.56
2:B:132:ILE:HA	2:B:135:TYR:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:37:LEU:HD21	3:H:39:ILE:HD11	1.88	0.56
1:A:374:PRO:HD2	1:A:375:LYS:H	1.70	0.56
1:A:552:PHE:HB3	1:A:574:LYS:HA	1.87	0.56
1:A:579:GLU:HA	1:A:598:CYS:HB3	1.88	0.55
1:A:299:LYS:O	1:A:303:LEU:HD12	2.06	0.55
1:A:493:ARG:NH2	4:L:114:TYR:O	2.32	0.55
1:A:239:ARG:NH2	1:A:478:GLN:OE1	2.39	0.55
1:A:564:ASN:HD21	7:A:801:NAG:H5	1.72	0.55
1:A:226:ILE:HG21	1:A:246:ILE:HD12	1.88	0.54
1:A:389:PHE:HB3	1:A:440:ILE:HG12	1.89	0.54
1:A:599:MET:HG3	1:A:604:PRO:HA	1.90	0.54
1:A:273:LYS:HB3	1:A:312:TYR:CE1	2.43	0.54
1:A:276:ARG:HA	1:A:478:GLN:HE22	1.73	0.54
3:H:85:ARG:NH2	3:H:108:ASP:OD2	2.41	0.53
1:A:262:PHE:O	1:A:264:GLY:N	2.41	0.53
1:A:514:GLN:OE1	1:A:514:GLN:N	2.39	0.53
2:B:120:THR:HB	11:B:301:Y01:HAQ2	1.91	0.53
1:A:276:ARG:NH2	5:C:1:NAG:H5	2.24	0.53
4:L:36:SER:N	4:L:39:GLU:OE1	2.42	0.53
5:C:1:NAG:H62	5:C:2:NAG:N2	2.24	0.53
1:A:363:ILE:HD11	1:A:380:THR:HG23	1.91	0.52
2:B:159:ASP:N	2:B:159:ASP:OD1	2.40	0.52
1:A:273:LYS:HB3	1:A:312:TYR:HE1	1.75	0.52
3:H:66:TRP:CD2	4:L:119:LEU:HB3	2.44	0.52
1:A:562:CYS:HA	1:A:567:CYS:HA	1.92	0.51
2:B:108:ILE:HA	2:B:111:VAL:HG22	1.91	0.51
3:H:57:ARG:NE	3:H:65:GLU:OE1	2.42	0.51
4:L:84:ARG:NH2	4:L:104:GLU:OE2	2.44	0.51
2:B:208:PHE:HA	2:B:211:GLN:HG3	1.92	0.51
3:H:21:VAL:HG22	3:H:45:GLY:HA3	1.92	0.51
1:A:351:SER:OG	1:A:352:ASP:N	2.44	0.51
2:B:150:LYS:HZ1	2:B:184:THR:HG22	1.76	0.51
4:L:43:MET:HE2	4:L:109:TYR:HB2	1.93	0.51
1:A:615:TRP:HD1	1:A:618:HIS:HD1	1.57	0.50
1:A:341:GLY:N	1:A:345:GLU:OE2	2.44	0.50
1:A:375:LYS:HA	1:A:378:HIS:NE2	2.26	0.50
1:A:490:PRO:HB2	3:H:119:ASP:HA	1.93	0.50
1:A:261:ASP:HB3	1:A:266:ARG:HH11	1.76	0.50
1:A:225:TYR:HB2	1:A:312:TYR:CD1	2.47	0.50
2:B:161:ARG:HH21	2:B:207:ARG:HG3	1.76	0.49
4:L:71:ILE:HG12	4:L:77:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:LEU:HD22	1:A:615:TRP:HE1	1.77	0.49
3:H:58:GLN:OE1	4:L:61:GLN:NE2	2.38	0.49
1:A:415:TYR:CD2	1:A:433:SER:HB2	2.47	0.49
2:B:104:ILE:O	2:B:108:ILE:HG12	2.12	0.49
2:B:202:THR:HG21	2:B:214:ILE:HD13	1.93	0.49
1:A:288:ASN:O	1:A:291:ARG:NH1	2.36	0.49
1:A:580:CYS:N	1:A:598:CYS:HA	2.28	0.49
2:B:176:PRO:HG2	2:B:177:LEU:HD12	1.94	0.49
1:A:592:GLU:HA	1:A:595:HIS:HE1	1.78	0.48
1:A:260:THR:HG21	1:A:432:PHE:HB2	1.95	0.48
1:A:384:GLU:OE2	10:A:804:BAT:O2	2.32	0.48
2:B:169:HIS:ND1	2:B:180:GLY:O	2.46	0.48
3:H:123:LEU:O	3:H:126:TRP:NE1	2.45	0.48
1:A:265:ILE:HG22	1:A:267:ASN:H	1.78	0.48
1:A:328:LEU:HD21	1:A:372:VAL:HG21	1.96	0.48
1:A:512:THR:HG23	1:A:518:LYS:HG2	1.95	0.48
2:B:259:VAL:O	2:B:263:ILE:HG12	2.13	0.48
1:A:401:PRO:HD2	1:A:414:ASN:HA	1.94	0.48
1:A:297:VAL:HG23	1:A:362:ILE:HD11	1.95	0.48
2:B:202:THR:HG23	2:B:210:VAL:HG11	1.96	0.48
1:A:262:PHE:HA	1:A:437:ILE:HG23	1.96	0.48
4:L:69:LEU:HD23	4:L:78:ALA:HB2	1.95	0.47
1:A:276:ARG:HH21	5:C:1:NAG:H5	1.79	0.47
1:A:573:GLU:HA	1:A:577:LEU:H	1.78	0.47
1:A:610:THR:HG21	1:A:624:ILE:H	1.80	0.47
1:A:651:ASP:O	1:A:655:ALA:HB3	2.15	0.47
3:H:57:ARG:HH12	3:H:108:ASP:HA	1.79	0.47
3:H:73:ASP:OD1	3:H:73:ASP:N	2.39	0.47
1:A:639:CYS:HA	1:A:645:CYS:HB3	1.97	0.46
1:A:387:HIS:NE2	1:A:393:HIS:CD2	2.79	0.46
2:B:100:GLY:O	2:B:104:ILE:HG22	2.15	0.46
1:A:375:LYS:HD3	2:B:207:ARG:NH1	2.30	0.46
1:A:327:VAL:HA	10:A:804:BAT:H14	1.98	0.46
1:A:577:LEU:HD12	1:A:598:CYS:HB2	1.96	0.46
4:L:74:THR:HG21	4:L:94:TYR:CD2	2.51	0.46
1:A:233:PHE:O	1:A:237:GLY:N	2.48	0.46
2:B:146:ASP:HB3	2:B:184:THR:HG21	1.97	0.46
1:A:485:PHE:HB3	1:A:489:GLN:HG3	1.99	0.46
1:A:327:VAL:HG12	10:A:804:BAT:H23	1.98	0.45
2:B:58:ALA:O	2:B:130:ARG:NE	2.46	0.45
2:B:250:LEU:O	2:B:254:LEU:HG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:57:ARG:HH21	3:H:82:LEU:HD21	1.81	0.45
2:B:85:LEU:O	2:B:86:ARG:HB3	2.15	0.45
2:B:107:LEU:O	2:B:111:VAL:HG13	2.17	0.45
1:A:577:LEU:HB2	1:A:599:MET:O	2.17	0.45
2:B:116:PHE:O	2:B:120:THR:HG22	2.16	0.45
1:A:394:ASP:HB3	1:A:400:THR:HG22	1.98	0.45
2:B:77:SER:O	2:B:81:VAL:HG23	2.17	0.45
1:A:284:LYS:HE2	1:A:284:LYS:HB2	1.77	0.45
3:H:54:ASN:HA	3:H:69:VAL:HG23	1.98	0.45
2:B:83:ALA:HB1	2:B:92:LEU:HG	1.99	0.45
3:H:66:TRP:CD1	4:L:119:LEU:HD22	2.52	0.45
4:L:24:ILE:O	4:L:120:THR:HG21	2.18	0.44
1:A:332:TRP:H	1:A:388:ASN:HD21	1.65	0.44
3:H:62:LYS:HE3	3:H:62:LYS:HB3	1.84	0.44
4:L:59:TYR:CD1	4:L:69:LEU:HA	2.53	0.44
4:L:59:TYR:HD1	4:L:69:LEU:HA	1.82	0.44
1:A:252:ALA:HB2	2:B:208:PHE:CE2	2.53	0.44
1:A:505:PRO:HD3	1:A:515:CYS:SG	2.57	0.44
4:L:41:VAL:HG13	4:L:98:ILE:HD12	1.99	0.44
4:L:108:THR:HG22	4:L:126:LYS:HA	1.98	0.44
1:A:470:GLU:HA	1:A:470:GLU:OE1	2.18	0.44
1:A:580:CYS:HB2	1:A:597:CYS:C	2.43	0.44
1:A:492:GLY:O	4:L:55:TYR:OH	2.36	0.43
4:L:31:ALA:O	4:L:126:LYS:N	2.50	0.43
1:A:220:ASN:OD1	1:A:220:ASN:C	2.61	0.43
1:A:389:PHE:HD2	1:A:440:ILE:HG23	1.83	0.43
1:A:482:GLU:O	1:A:501:LYS:NZ	2.51	0.43
1:A:603:ASP:O	1:A:605:SER:N	2.47	0.43
1:A:220:ASN:HB2	1:A:267:ASN:O	2.18	0.43
1:A:229:ASP:OD1	1:A:229:ASP:C	2.62	0.43
2:B:129:ARG:O	2:B:132:ILE:HG12	2.18	0.43
1:A:331:ALA:HB2	1:A:384:GLU:HB3	2.01	0.43
1:A:654:LEU:HB2	2:B:140:ASP:OD1	2.19	0.43
1:A:631:PRO:HA	1:A:638:TYR:HA	2.00	0.42
2:B:169:HIS:HA	2:B:177:LEU:O	2.19	0.42
11:B:302:Y01:HAO2	11:B:302:Y01:HAP1	1.39	0.42
1:A:285:ASP:OD1	1:A:287:THR:HG22	2.20	0.42
1:A:332:TRP:CD2	1:A:358:LEU:HD13	2.55	0.42
1:A:279:THR:O	1:A:282:ASP:HB3	2.20	0.42
2:B:75:MET:HE3	2:B:75:MET:HB3	1.94	0.42
4:L:54:GLY:HA2	4:L:73:SER:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:CYS:O	1:A:626:LEU:HB2	2.19	0.42
1:A:599:MET:HG2	1:A:600:LYS:O	2.19	0.42
2:B:98:ILE:HG12	11:B:302:Y01:HAB1	2.02	0.42
2:B:85:LEU:HD12	2:B:86:ARG:H	1.85	0.41
4:L:59:TYR:CE1	4:L:69:LEU:HD12	2.55	0.41
1:A:514:GLN:H	1:A:514:GLN:CD	2.25	0.41
1:A:614:GLN:HB3	1:A:615:TRP:CE3	2.55	0.41
4:L:105:ASP:O	4:L:127:LEU:HD22	2.21	0.41
1:A:235:TYR:CD1	1:A:235:TYR:C	2.98	0.41
3:H:54:ASN:N	3:H:115:ALA:O	2.42	0.41
4:L:86:SER:OG	4:L:97:THR:OG1	2.35	0.41
1:A:273:LYS:HD2	1:A:312:TYR:CZ	2.56	0.41
1:A:575:TYR:CD2	1:A:618:HIS:HB3	2.55	0.41
2:B:188:ARG:HD3	2:B:194:VAL:HG22	2.03	0.41
2:B:183:TYR:HA	2:B:198:CYS:SG	2.61	0.41
4:L:87:GLY:HA2	4:L:96:LEU:HA	2.03	0.41
1:A:224:LEU:HD23	1:A:314:LEU:HB2	2.02	0.41
1:A:229:ASP:OD1	1:A:231:LEU:N	2.53	0.41
1:A:458:PRO:HA	1:A:466:GLU:OE1	2.21	0.41
2:B:158:GLU:HG3	2:B:159:ASP:OD1	2.21	0.41
1:A:383:HIS:CG	10:A:804:BAT:H123	2.56	0.41
4:L:37:LEU:HA	4:L:101:MET:HE3	2.03	0.41
3:H:124:ASP:OD1	3:H:124:ASP:N	2.52	0.40
4:L:114:TYR:CD2	4:L:119:LEU:HD12	2.56	0.40
1:A:272:VAL:HG21	1:A:275:ILE:HG12	2.03	0.40
1:A:301:LEU:HD13	1:A:362:ILE:HG23	2.04	0.40
1:A:315:ALA:O	1:A:360:THR:HA	2.22	0.40
1:A:326:GLY:HA3	1:A:368:TYR:CZ	2.56	0.40
3:H:59:PRO:HB2	3:H:62:LYS:HB2	2.04	0.40
3:H:79:GLN:O	3:H:83:LYS:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	442/543 (81%)	394 (89%)	46 (10%)	2 (0%)	24	55
2	B	253/306 (83%)	244 (96%)	9 (4%)	0	100	100
3	H	119/225 (53%)	116 (98%)	3 (2%)	0	100	100
4	L	109/221 (49%)	105 (96%)	4 (4%)	0	100	100
All	All	923/1295 (71%)	859 (93%)	62 (7%)	2 (0%)	44	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	SER
1	A	537	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	352/473 (74%)	352 (100%)	0	100	100
2	B	215/267 (80%)	215 (100%)	0	100	100
3	H	97/196 (50%)	97 (100%)	0	100	100
4	L	83/194 (43%)	83 (100%)	0	100	100
All	All	747/1130 (66%)	747 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	GLN
1	A	258	GLN
1	A	307	GLN
1	A	429	ASN

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Mol	Chain	Res	Type
1	A	449	ASN
1	A	489	GLN
1	A	537	ASN
1	A	564	ASN
1	A	595	HIS
2	B	143	ASN
2	B	211	GLN
4	L	57	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	$\# Z > 2$
5	NAG	C	1	5,1	14,14,15	0.43	0	17,19,21	0.54	0
5	NAG	C	2	5	14,14,15	0.22	0	17,19,21	0.47	0
5	MAN	C	3	5	11,11,12	0.96	0	15,15,17	1.18	2 (13%)
5	MAN	C	4	5	11,11,12	0.80	1 (9%)	15,15,17	1.35	2 (13%)
6	NAG	D	1	1,6	14,14,15	0.34	0	17,19,21	0.44	0
6	NAG	D	2	6	14,14,15	0.22	0	17,19,21	0.46	0
6	MAN	D	3	6	11,11,12	0.66	0	15,15,17	1.02	2 (13%)

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
5	NAG	C	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	2/6/23/26	0/1/1/1
5	MAN	C	3	5	-	1/2/19/22	1/1/1/1
5	MAN	C	4	5	-	1/2/19/22	0/1/1/1
6	NAG	D	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	D	2	6	-	0/6/23/26	0/1/1/1
6	MAN	D	3	6	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	4	MAN	C1-C2	2.05	1.57	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	4	MAN	C1-O5-C5	3.65	117.08	112.19
5	C	3	MAN	C1-O5-C5	2.91	116.08	112.19
6	D	3	MAN	C1-O5-C5	2.42	115.42	112.19
5	C	3	MAN	O3-C3-C2	2.33	114.82	110.05
5	C	4	MAN	O2-C2-C3	-2.25	105.48	110.15
6	D	3	MAN	O2-C2-C3	-2.19	105.62	110.15

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

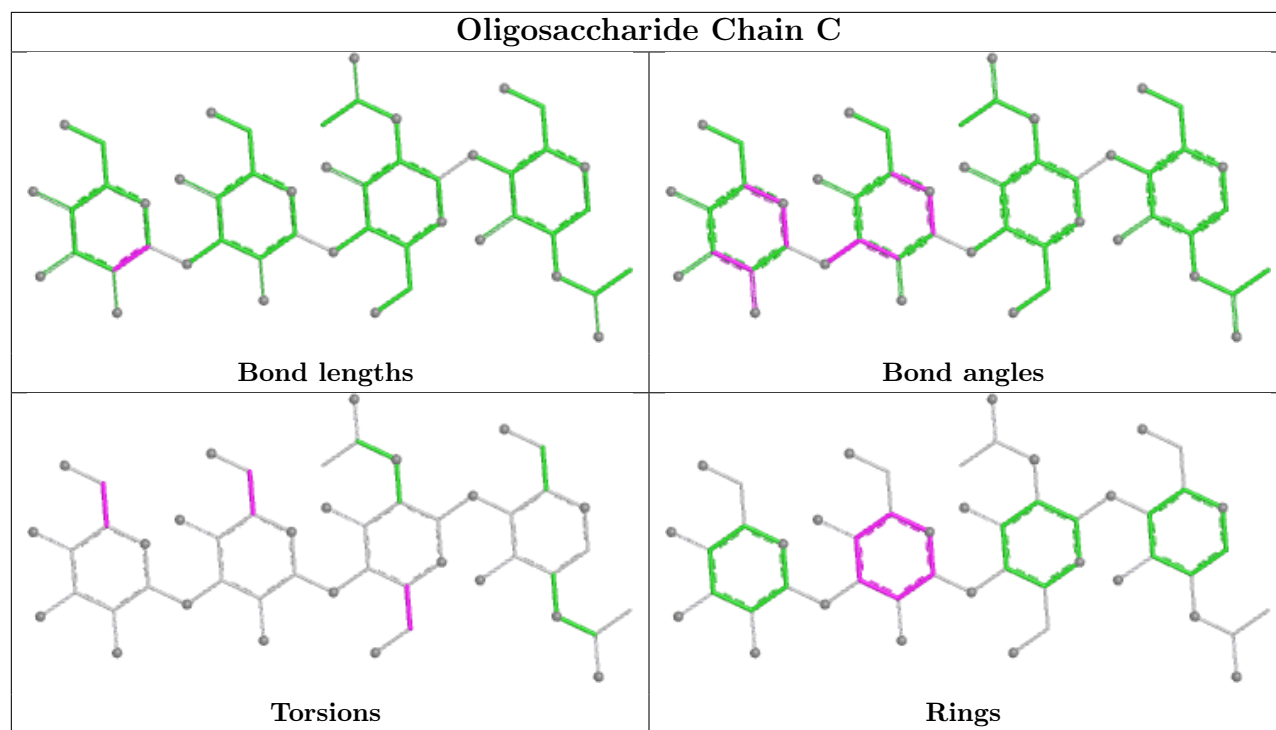
All (1) ring outliers are listed below:

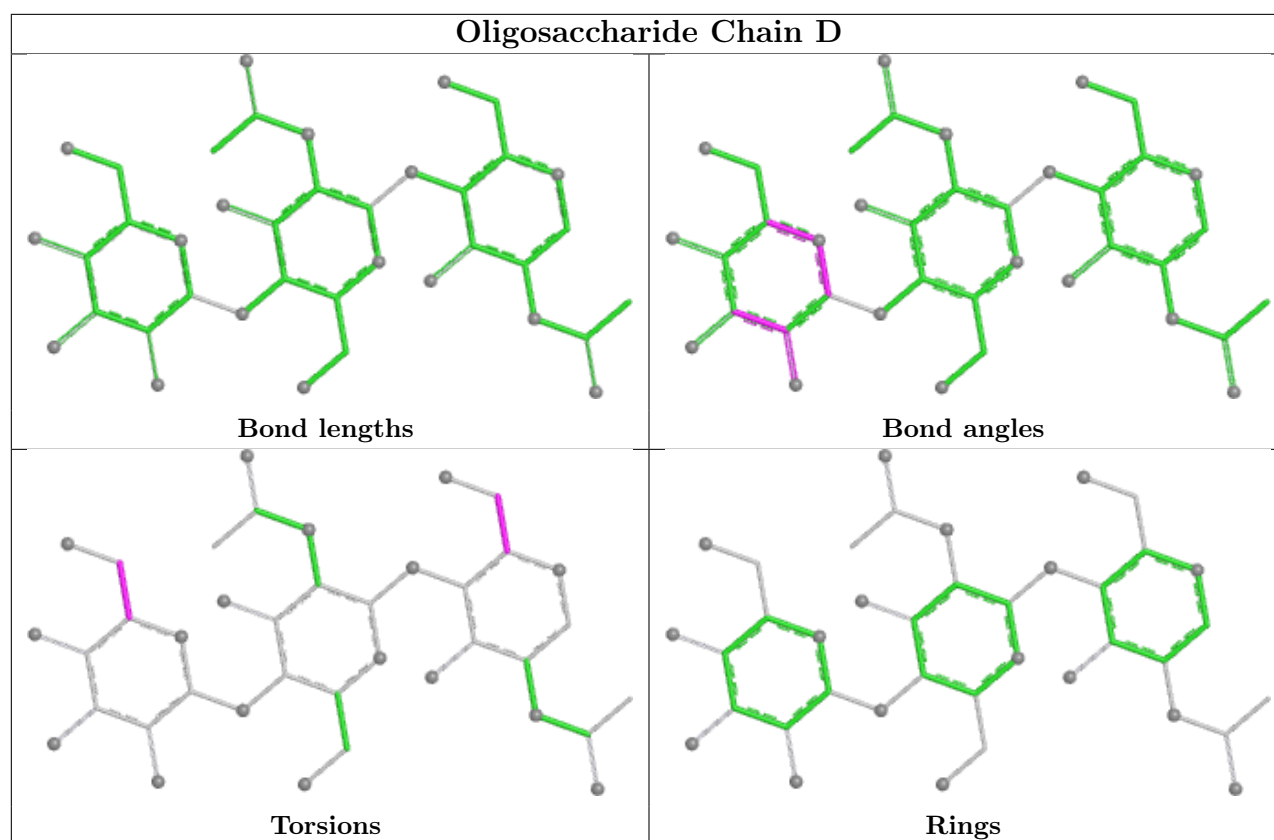
Mol	Chain	Res	Type	Atoms
5	C	3	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	2	NAG	1	0
5	C	1	NAG	4	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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
7	NAG	A	801	1	14,14,15	0.32	0	17,19,21	0.41	0
11	Y01	B	301	-	38,38,38	0.58	0	57,57,57	0.66	0
10	BAT	A	804	9	32,33,33	2.42	10 (31%)	38,43,43	1.68	8 (21%)
11	Y01	B	302	-	38,38,38	0.57	0	57,57,57	0.63	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
7	NAG	A	801	1	-	2/6/23/26	0/1/1/1
11	Y01	B	301	-	-	4/19/77/77	0/4/4/4
10	BAT	A	804	9	-	3/37/37/37	0/2/2/2
11	Y01	B	302	-	-	9/19/77/77	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	804	BAT	C15-N3	8.65	1.45	1.33
10	A	804	BAT	C13-N2	5.30	1.45	1.34
10	A	804	BAT	C4-S2	-4.00	1.55	1.72
10	A	804	BAT	C6-C5	3.60	1.60	1.42
10	A	804	BAT	C4-S1	3.54	1.82	1.75
10	A	804	BAT	C7-S2	-3.18	1.56	1.70
10	A	804	BAT	C6-C7	3.08	1.45	1.34
10	A	804	BAT	O3-C13	-2.47	1.18	1.23
10	A	804	BAT	O1-C2	-2.37	1.18	1.23
10	A	804	BAT	O4-C15	-2.35	1.18	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	804	BAT	C7-S2-C4	5.31	107.61	94.11
10	A	804	BAT	C1-C2-N1	3.30	120.06	115.99
10	A	804	BAT	C8-C13-N2	3.27	119.98	116.01
10	A	804	BAT	C3-S1-C4	3.25	110.02	102.72
10	A	804	BAT	C8-C9-C10	-3.12	110.82	115.82
10	A	804	BAT	C14-C15-N3	2.31	120.48	116.99
10	A	804	BAT	O4-C15-N3	-2.10	119.64	123.13
10	A	804	BAT	C6-C7-S2	-2.09	107.91	113.02

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	B	302	Y01	CAC-CBB-CBE-CAP
11	B	302	Y01	CAC-CBB-CBE-CBI
11	B	302	Y01	CAJ-CAO-CBB-CAC
11	B	302	Y01	CAO-CBB-CBE-CAP
11	B	302	Y01	CAO-CBB-CBE-CBI
11	B	302	Y01	CAJ-CAO-CBB-CBE

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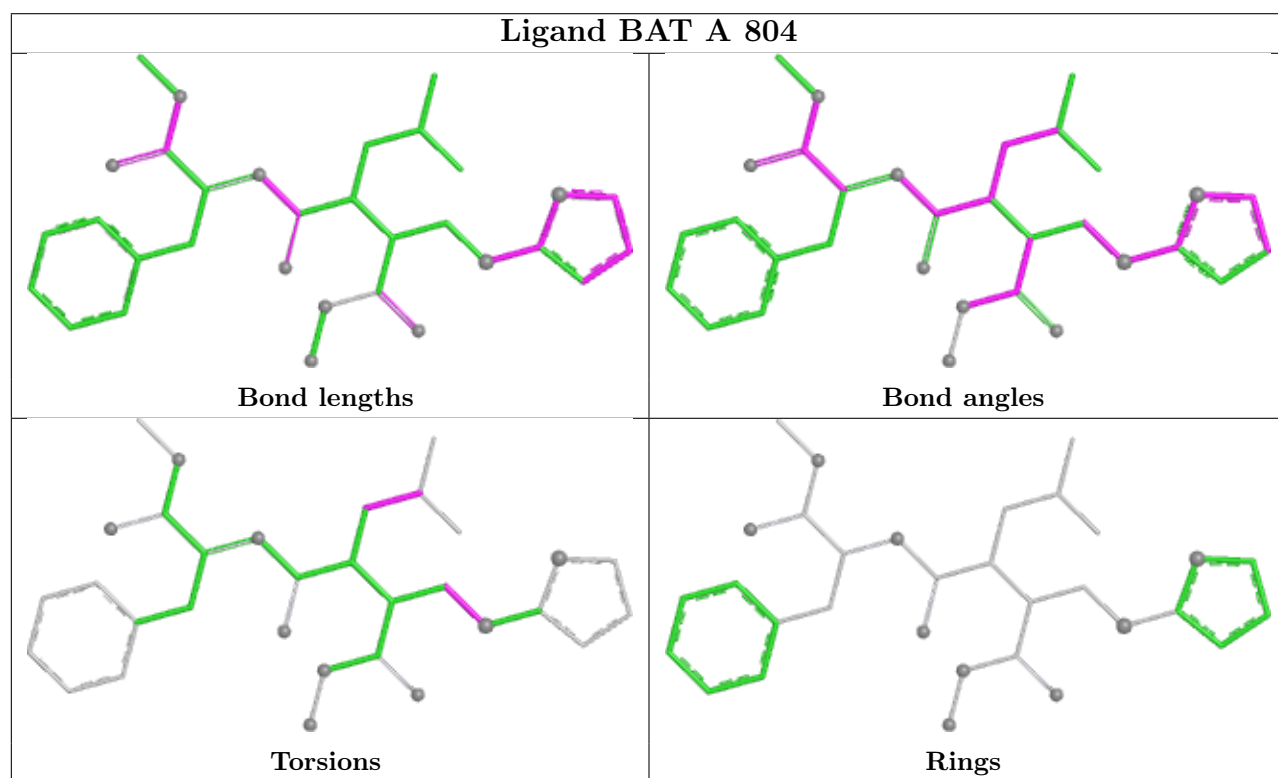
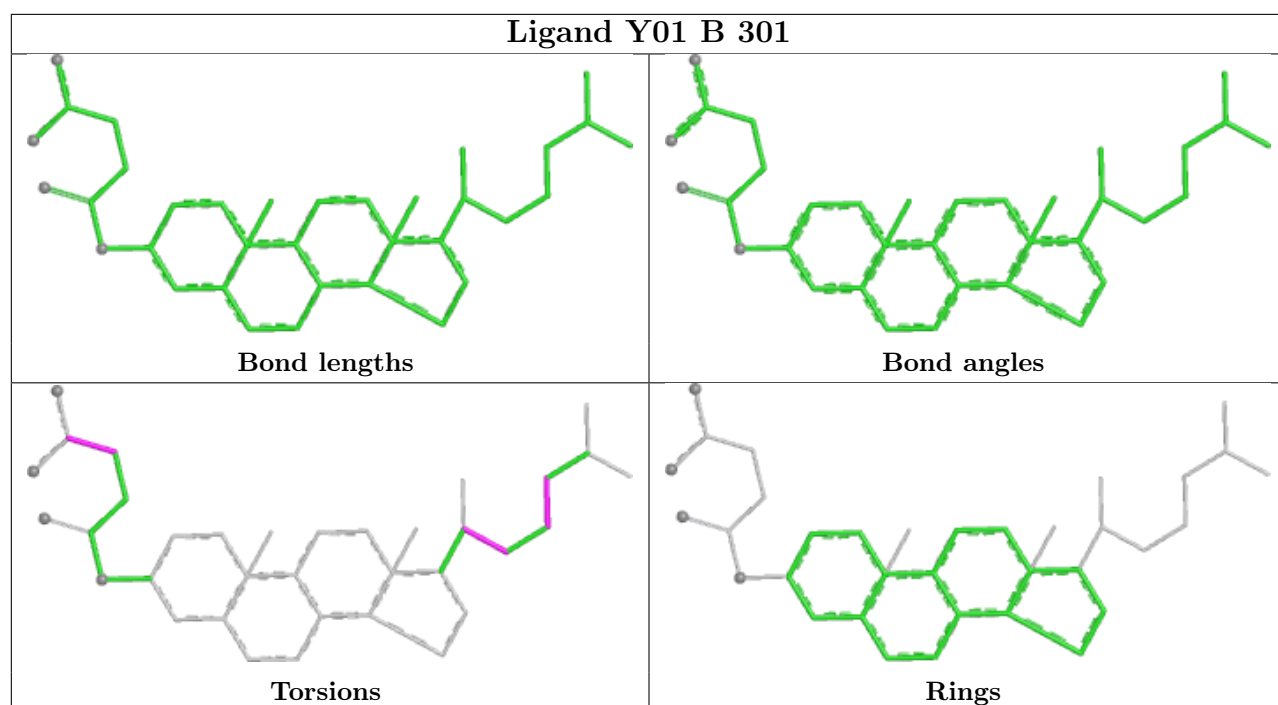
Mol	Chain	Res	Type	Atoms
11	B	301	Y01	CAJ-CAO-CBB-CAC
11	B	301	Y01	CAO-CAJ-CAN-CBA
11	B	302	Y01	CAN-CAJ-CAO-CBB
10	A	804	BAT	C11-C10-C9-C8
7	A	801	NAG	C4-C5-C6-O6
10	A	804	BAT	C1-C3-S1-C4
11	B	301	Y01	CAM-CAL-CAX-OAF
11	B	302	Y01	CAM-CAL-CAX-OAH
11	B	301	Y01	CAM-CAL-CAX-OAH
11	B	302	Y01	CAM-CAL-CAX-OAF
7	A	801	NAG	O5-C5-C6-O6
10	A	804	BAT	C12-C10-C9-C8

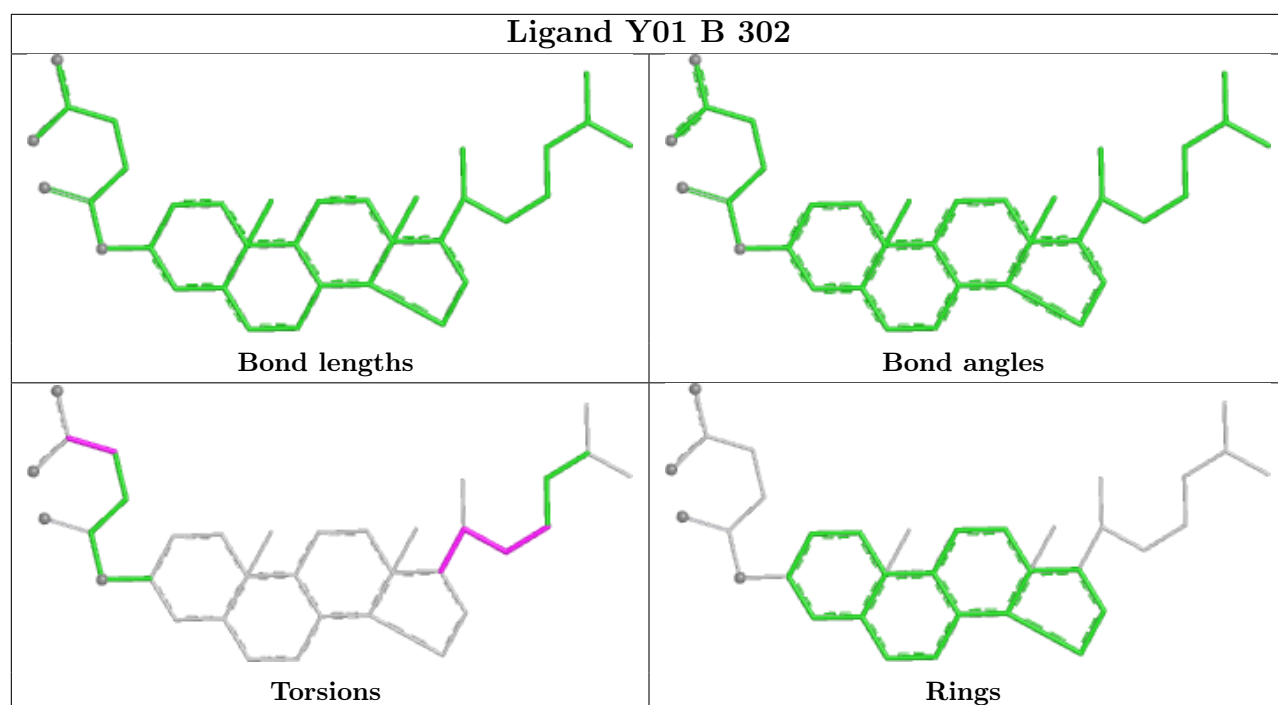
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	801	NAG	1	0
11	B	301	Y01	1	0
10	A	804	BAT	4	0
11	B	302	Y01	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-28580. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 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 ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit

This section was not generated.