



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:15 AM UTC

PDB ID : 3VQ2 / pdb_00003vq2
Title : Crystal structure of mouse TLR4/MD-2/LPS complex
Authors : Ohto, U.; Shimizu, T.
Deposited on : 2012-03-17
Resolution : 2.48 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

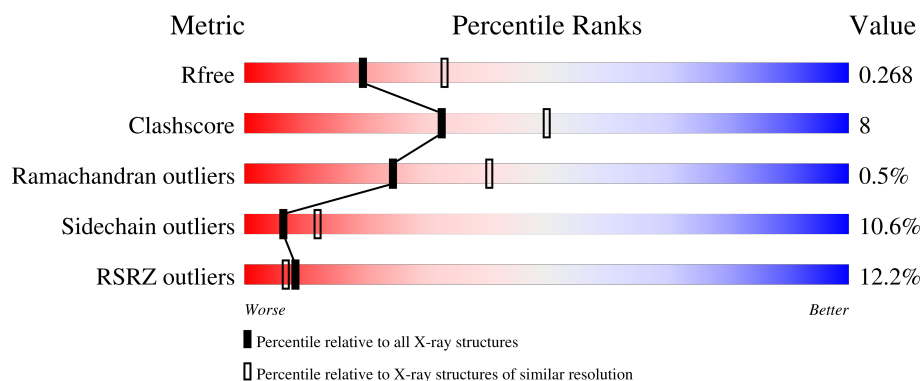
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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.



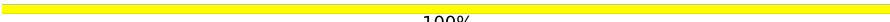
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	606	12% 73% 19% • •
1	B	606	12% 74% 19% • •
2	C	144	5% 65% 25% • • 6%
2	D	144	12% 60% 28% 6% 6%
3	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	F	2	 100%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 11815 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Toll-like receptor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4637	2972	764	875	26			
1	B	581	Total	C	N	O	S	0	0	0
			4637	2972	764	875	26			

- Molecule 2 is a protein called Lymphocyte antigen 96.

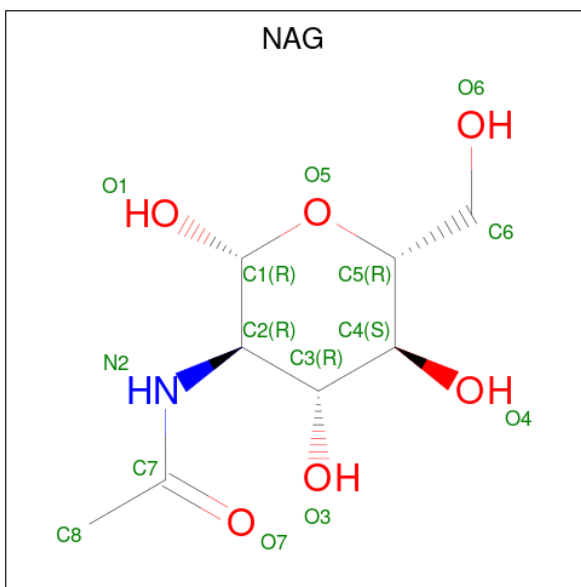
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	135	Total	C	N	O	S	0	0	0
			1092	706	182	197	7			
2	D	135	Total	C	N	O	S	0	0	0
			1092	706	182	197	7			

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



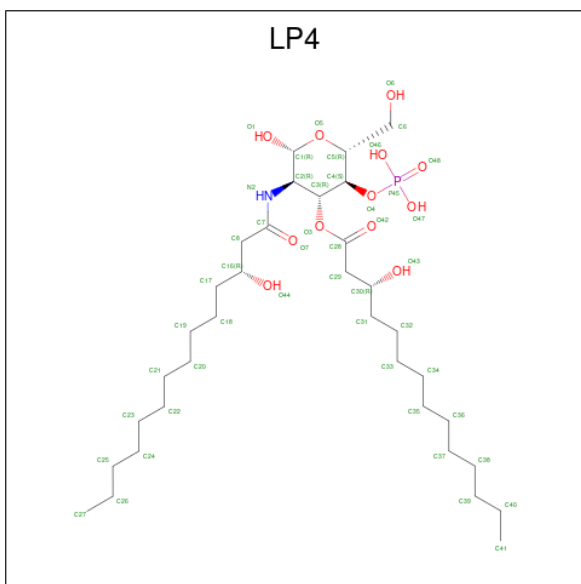
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



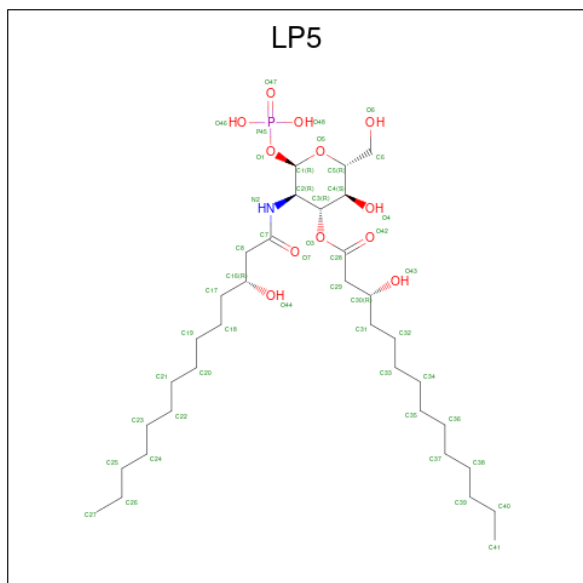
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is 2-deoxy-3-O-[(3R)-3-hydroxytetradecanoyl]-2-[[[(3R)-3-hydroxytetradecanoyl]amino]-4-O-phosphono-beta-D-glucopyranose (CCD ID: LP4) (formula: $C_{34}H_{66}NO_{12}P$).



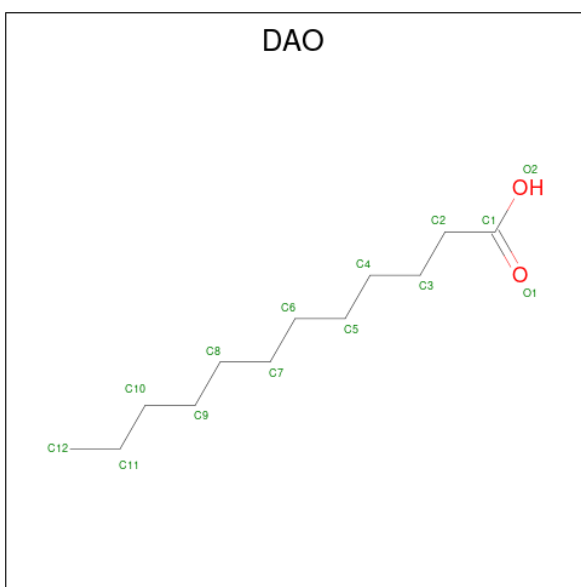
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total 45	C 32	N 1	O 11	P 1	0	0
5	D	1	Total 45	C 32	N 1	O 11	P 1	0	0

- Molecule 6 is (R)-((2R,3S,4R,5R,6R)-3-HYDROXY-2-(HYDROXYMETHYL)-5-((R)-3-HYDROXYTETRADECANAMIDO)-6-(PHOSPHONOOXY)TETRAHYDRO-2H-PYRAN-4-YL) 3-HYDROXYTETRADECANOATE (CCD ID: LP5) (formula: $C_{34}H_{66}NO_{12}P$).



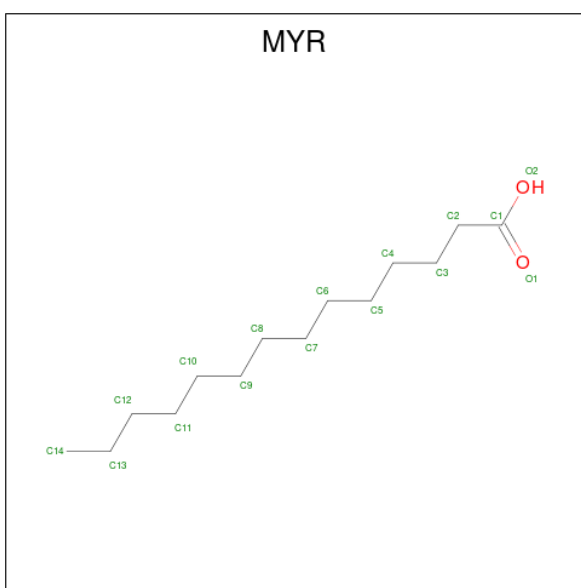
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total 48	C 34	N 1	O 12	P 1	0	0
6	D	1	Total 48	C 34	N 1	O 12	P 1	0	0

- Molecule 7 is LAURIC ACID (CCD ID: DAO) (formula: $C_{12}H_{24}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			13	12	1		
7	D	1	Total	C	O	0	0
			13	12	1		

- Molecule 8 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			15	14	1		
8	D	1	Total	C	O	0	0
			15	14	1		

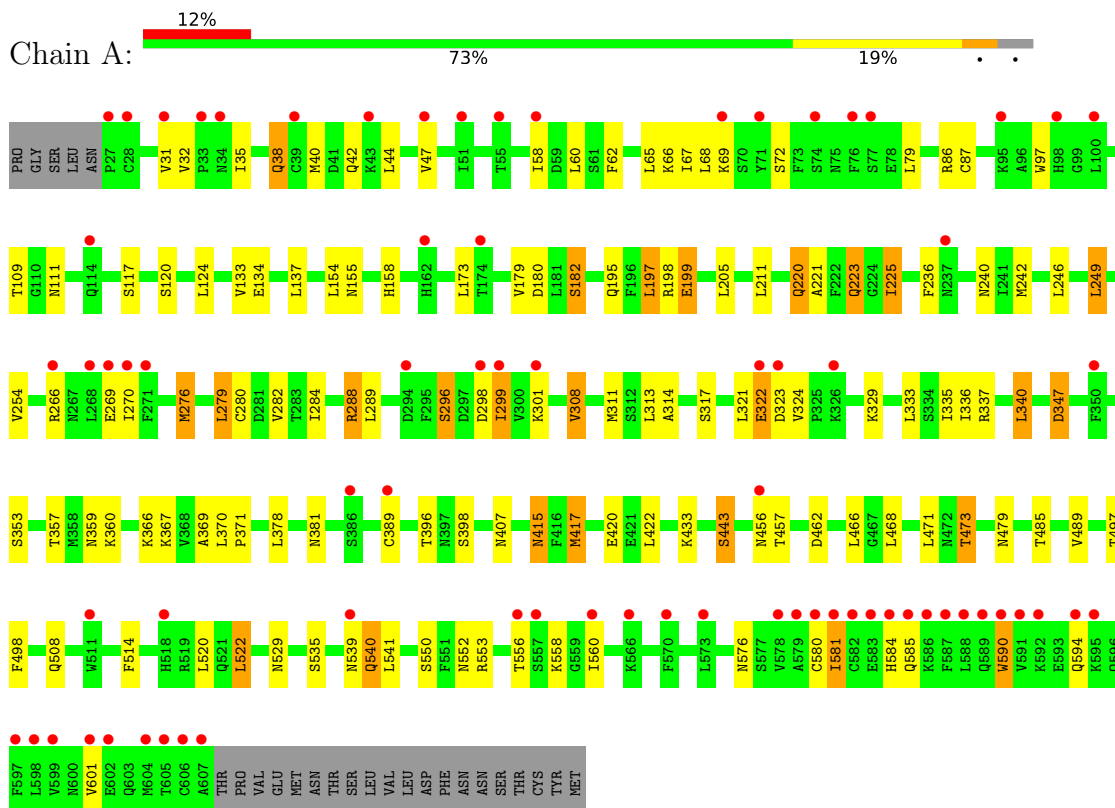
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	8	Total 8	O 8	0	0
9	B	9	Total 9	O 9	0	0

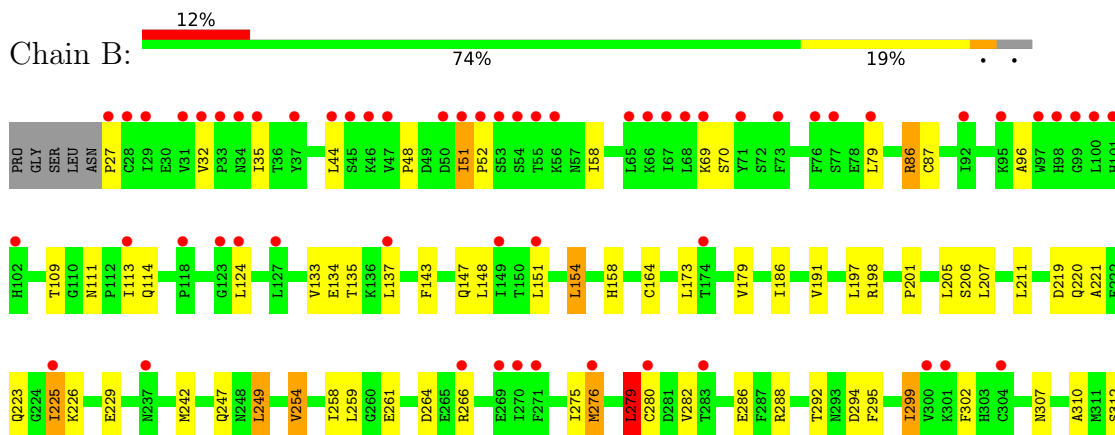
3 Residue-property plots [i](#)

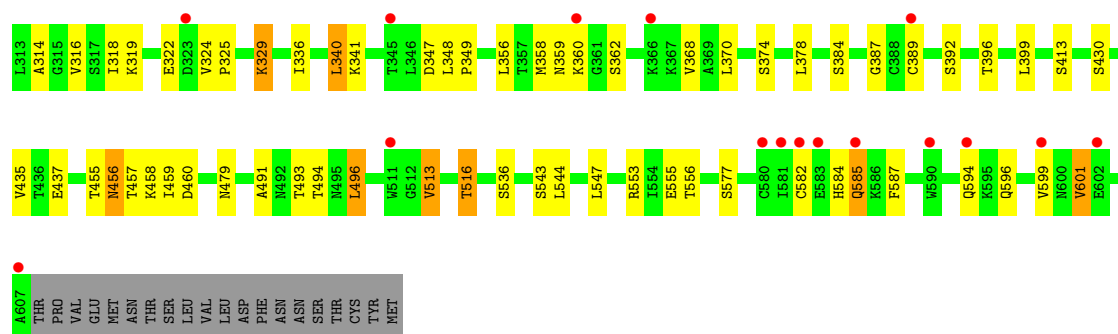
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Toll-like receptor 4

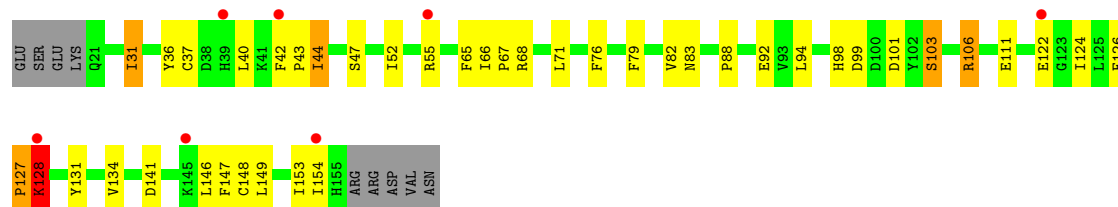


- Molecule 1: Toll-like receptor 4

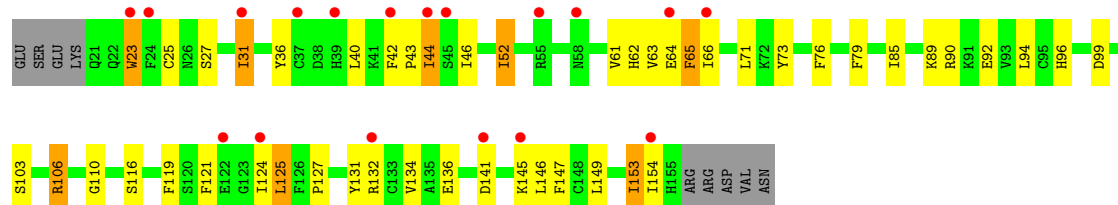




• Molecule 2: Lymphocyte antigen 96



• Molecule 2: Lymphocyte antigen 96



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.81Å 144.32Å 86.94Å 90.00° 95.16° 90.00°	Depositor
Resolution (Å)	86.59 – 2.48 86.59 – 2.48	Depositor EDS
% Data completeness (in resolution range)	98.4 (86.59-2.48) 98.8 (86.59-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.221 , 0.267 0.226 , 0.268	Depositor DCC
R_{free} test set	3775 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11815	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DAO, MYR, NAG, LP5, LP4

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	0.68	0/4735	0.86	1/6414 (0.0%)
1	B	0.67	0/4735	0.84	8/6414 (0.1%)
2	C	0.72	0/1123	0.86	3/1519 (0.2%)
2	D	0.70	0/1123	0.84	2/1519 (0.1%)
All	All	0.68	0/11716	0.85	14/15866 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	ILE	CA-C-N	7.33	129.00	119.84
1	B	51	ILE	C-N-CA	7.33	129.00	119.84
1	A	249	LEU	N-CA-C	-5.96	106.00	113.28
1	B	279	LEU	N-CA-C	5.70	117.50	111.28
2	C	127	PRO	CA-C-N	5.42	131.46	121.70
2	C	127	PRO	C-N-CA	5.42	131.46	121.70
1	B	601	VAL	CB-CA-C	-5.37	104.89	112.14
2	C	128	LYS	N-CA-C	-5.36	95.99	111.00
2	D	65	PHE	N-CA-C	5.28	116.16	108.14
1	B	254	VAL	CB-CA-C	-5.21	103.07	110.83
2	D	52	ILE	N-CA-C	5.17	115.78	107.98
1	B	513	VAL	N-CA-C	5.16	116.50	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	143	PHE	CA-C-N	5.09	126.21	119.84
1	B	143	PHE	C-N-CA	5.09	126.21	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	323	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4637	0	4611	76	0
1	B	4637	0	4613	63	0
2	C	1092	0	1051	29	0
2	D	1092	0	1051	33	0
3	E	28	0	25	1	0
3	F	28	0	25	0	0
4	A	42	0	39	2	0
5	C	45	0	53	0	0
5	D	45	0	53	0	0
6	C	48	0	63	1	0
6	D	48	0	63	2	0
7	C	13	0	23	0	0
7	D	13	0	23	2	0
8	C	15	0	27	0	0
8	D	15	0	27	0	0
9	A	8	0	0	0	0
9	B	9	0	0	0	0
All	All	11815	0	11747	187	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 (187) 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:B:556:THR:HG21	1:B:584:HIS:CG	2.12	0.84
1:A:87:CYS:H	1:A:111:ASN:HD21	1.25	0.84
2:C:44:ILE:HD13	2:C:149:LEU:HD21	1.58	0.83
1:B:295:PHE:CE1	1:B:299:ILE:HG21	2.22	0.74
1:B:387:GLY:HA2	1:B:413:SER:HB3	1.70	0.73
1:A:367:LYS:H	1:A:367:LYS:HD2	1.55	0.71
2:C:127:PRO:HB2	2:C:128:LYS:HB2	1.73	0.70
1:A:529:ASN:HB3	1:A:553:ARG:NH2	2.09	0.68
2:C:127:PRO:CB	2:C:128:LYS:HB2	2.25	0.67
2:D:36:TYR:HE2	2:D:44:ILE:HD12	1.60	0.66
1:B:86:ARG:NH1	2:D:110:GLY:O	2.29	0.66
1:A:417:MET:HE1	2:D:125:LEU:N	2.11	0.65
2:D:127:PRO:HD2	2:D:131:TYR:OH	1.96	0.65
1:B:556:THR:HG22	1:B:587:PHE:CD2	2.31	0.65
1:A:367:LYS:HD2	1:A:367:LYS:N	2.11	0.65
2:C:44:ILE:CD1	2:C:149:LEU:HD21	2.26	0.64
2:D:62:HIS:HD2	2:D:116:SER:OG	1.79	0.64
1:B:286:GLU:HG3	1:B:310:ALA:HB3	1.80	0.63
1:B:86:ARG:HH11	1:B:86:ARG:HB2	1.64	0.63
4:A:804:NAG:H5	3:E:1:NAG:H83	1.79	0.63
2:D:79:PHE:HB2	2:D:134:VAL:HG22	1.81	0.62
6:D:301:LP5:H232	7:D:302:DAO:H81	1.81	0.62
1:B:276:MET:HG3	1:B:279:LEU:HD22	1.82	0.62
2:C:82:VAL:HG22	2:C:131:TYR:CE2	2.35	0.61
1:A:322:GLU:HG2	1:A:322:GLU:O	2.00	0.60
1:A:417:MET:HE1	2:D:125:LEU:H	1.65	0.59
1:B:556:THR:HG21	1:B:584:HIS:HB3	1.83	0.59
1:B:340:LEU:H	1:B:359:ASN:HD21	1.50	0.59
1:A:550:SER:OG	4:A:804:NAG:H82	2.02	0.58
1:B:288:ARG:HG2	1:B:312:SER:HB2	1.84	0.58
1:A:134:GLU:HA	1:A:158:HIS:O	2.03	0.58
1:A:220:GLN:HG3	1:A:223:GLN:HE21	1.68	0.58
1:B:58:ILE:HG22	1:B:79:LEU:HD11	1.84	0.57
1:A:69:LYS:O	1:A:72:SER:OG	2.20	0.57
1:A:195:GLN:HG2	1:A:199:GLU:OE2	2.05	0.57
1:A:552:ASN:HB2	1:A:576:ASN:HD21	1.70	0.57
1:A:553:ARG:HH22	1:B:553:ARG:HH22	1.52	0.57
2:D:76:PHE:HE1	2:D:94:LEU:HD12	1.68	0.57
2:C:131:TYR:HB2	2:C:153:ILE:HB	1.86	0.57
2:D:44:ILE:HD11	2:D:147:PHE:HB2	1.87	0.57
2:C:103:SER:O	2:C:106:ARG:HG3	2.04	0.56
1:A:299:ILE:HG12	1:A:299:ILE:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:PHE:CZ	1:B:299:ILE:CG2	2.88	0.56
1:A:462:ASP:HB2	2:D:85:ILE:HG23	1.87	0.55
1:B:556:THR:HG21	1:B:584:HIS:CB	2.35	0.55
1:B:87:CYS:H	1:B:111:ASN:HD21	1.52	0.55
1:A:66:LYS:C	1:A:67:ILE:HG13	2.31	0.55
2:C:88:PRO:HG3	1:B:460:ASP:HB3	1.87	0.55
1:A:313:LEU:HD12	1:A:335:ILE:HD12	1.87	0.55
1:A:556:THR:HG21	1:A:584:HIS:CB	2.37	0.55
1:A:42:GLN:HB2	1:A:44:LEU:HG	1.89	0.55
1:A:340:LEU:H	1:A:359:ASN:HD21	1.56	0.54
1:B:225:ILE:O	1:B:225:ILE:HG13	2.06	0.54
1:B:276:MET:HB3	1:B:302:PHE:CE2	2.43	0.54
1:A:337:ARG:HH12	2:C:101:ASP:CG	2.16	0.53
1:B:374:SER:HA	1:B:399:LEU:HA	1.90	0.53
1:A:276:MET:HG3	1:A:279:LEU:CD2	2.38	0.53
1:B:206:SER:HB3	1:B:229:GLU:HG2	1.89	0.53
1:A:87:CYS:H	1:A:111:ASN:ND2	2.02	0.53
1:A:333:LEU:HD11	1:A:335:ILE:HD11	1.91	0.53
1:A:236:PHE:CD1	1:A:242:MET:HG3	2.44	0.52
1:B:279:LEU:O	1:B:282:VAL:HG22	2.10	0.52
1:B:201:PRO:HB3	1:B:226:LYS:HE3	1.92	0.52
1:B:387:GLY:HA2	1:B:413:SER:CB	2.39	0.52
1:B:258:ILE:HG13	1:B:288:ARG:HB2	1.92	0.52
1:B:27:PRO:HA	1:B:51:ILE:HD11	1.91	0.51
1:A:514:PHE:HB3	1:A:541:LEU:HD21	1.91	0.51
1:A:456:ASN:ND2	1:B:456:ASN:HD21	2.07	0.51
1:B:319:LYS:HD2	1:B:341:LYS:HE2	1.93	0.51
2:C:31:ILE:HG13	2:C:31:ILE:O	2.10	0.51
2:C:44:ILE:HD11	2:C:147:PHE:HB2	1.92	0.51
1:A:269:GLU:HG2	1:A:270:ILE:H	1.76	0.51
1:B:295:PHE:CZ	1:B:299:ILE:HG21	2.44	0.51
2:D:31:ILE:HG13	2:D:154:ILE:HB	1.93	0.51
2:D:36:TYR:CE2	2:D:44:ILE:HD12	2.45	0.50
1:A:32:VAL:HG12	1:A:35:ILE:HB	1.94	0.49
2:D:42:PHE:HD1	2:D:146:LEU:O	1.94	0.49
1:A:415:ASN:O	1:A:443:SER:OG	2.29	0.49
1:A:381:ASN:H	1:A:407:ASN:ND2	2.10	0.49
1:A:296:SER:O	1:A:299:ILE:HG22	2.12	0.49
1:A:180:ASP:OD1	1:A:182:SER:HB2	2.13	0.49
2:C:76:PHE:HE1	2:C:94:LEU:HD12	1.78	0.49
2:C:127:PRO:O	2:C:131:TYR:OH	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:ARG:NH1	2:D:99:ASP:OD2	2.46	0.49
2:D:103:SER:O	2:D:106:ARG:HG3	2.12	0.49
1:A:539:ASN:O	1:A:540:GLN:HB2	2.13	0.49
1:A:288:ARG:NH1	2:C:99:ASP:OD2	2.46	0.49
2:D:124:ILE:CG2	2:D:125:LEU:N	2.75	0.48
1:A:415:ASN:ND2	1:A:415:ASN:H	2.11	0.48
1:B:87:CYS:H	1:B:111:ASN:ND2	2.11	0.48
1:A:556:THR:HG21	1:A:584:HIS:CG	2.49	0.48
2:D:62:HIS:CD2	2:D:116:SER:OG	2.65	0.48
2:C:126:PHE:HZ	6:C:301:LP5:H321	1.78	0.48
1:B:314:ALA:HA	1:B:336:ILE:O	2.13	0.48
1:A:370:LEU:O	1:A:396:THR:HB	2.14	0.47
1:A:415:ASN:HD21	2:D:125:LEU:H	1.62	0.47
1:B:249:LEU:HB3	1:B:282:VAL:HG11	1.95	0.47
1:A:58:ILE:HG22	1:A:79:LEU:HD11	1.97	0.47
1:A:197:LEU:HD23	1:A:225:ILE:HD12	1.95	0.47
1:B:307:ASN:HA	1:B:329:LYS:HG3	1.97	0.47
2:D:134:VAL:HA	2:D:149:LEU:O	2.14	0.47
1:A:155:ASN:HD22	1:A:155:ASN:C	2.22	0.47
1:A:381:ASN:H	1:A:407:ASN:HD21	1.61	0.47
2:D:23:TRP:CZ2	2:D:25:CYS:HB3	2.50	0.47
1:A:296:SER:O	1:A:299:ILE:CG2	2.63	0.47
2:C:55:ARG:O	2:C:122:GLU:O	2.32	0.47
1:B:111:ASN:O	1:B:135:THR:HA	2.15	0.47
1:A:179:VAL:HG23	1:A:205:LEU:HD11	1.97	0.47
1:A:87:CYS:N	1:A:111:ASN:HD21	2.02	0.46
1:A:347:ASP:HB3	1:A:369:ALA:HB3	1.96	0.46
1:B:44:LEU:HD13	1:B:48:PRO:HG3	1.98	0.46
1:A:301:LYS:O	1:A:301:LYS:HG2	2.13	0.46
1:B:134:GLU:HA	1:B:158:HIS:O	2.14	0.46
1:B:430:SER:O	1:B:455:THR:HA	2.15	0.46
1:A:282:VAL:HG23	1:A:284:ILE:HG13	1.96	0.46
2:C:79:PHE:HB2	2:C:134:VAL:HG22	1.97	0.46
1:B:544:LEU:HD21	1:B:547:LEU:HB2	1.97	0.46
1:A:62:PHE:CZ	2:C:68:ARG:HD3	2.51	0.46
1:A:308:VAL:HG11	1:A:311:MET:HE2	1.97	0.46
1:B:109:THR:HA	1:B:133:VAL:O	2.16	0.46
1:B:370:LEU:O	1:B:396:THR:HB	2.16	0.46
1:A:590:TRP:O	1:A:594:GLN:HB2	2.16	0.45
1:B:491:ALA:O	1:B:516:THR:HG21	2.16	0.45
1:A:473:THR:HG23	1:A:498:PHE:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:92:GLU:OE2	2:C:92:GLU:HA	2.16	0.45
1:A:457:THR:O	1:A:479:ASN:HB3	2.17	0.45
1:A:65:LEU:O	1:A:67:ILE:N	2.41	0.45
2:C:83:ASN:HD21	2:C:128:LYS:HB3	1.81	0.45
1:A:468:LEU:HD13	1:A:471:LEU:HD22	1.99	0.44
2:C:37:CYS:HB2	2:C:148:CYS:HB3	1.86	0.44
6:D:301:LP5:H16	6:D:301:LP5:H191	1.81	0.44
1:B:457:THR:O	1:B:479:ASN:HB3	2.17	0.44
2:C:42:PHE:CD2	2:C:68:ARG:HG3	2.51	0.44
2:D:46:ILE:HG13	2:D:63:VAL:HG22	2.00	0.44
1:A:539:ASN:O	1:A:540:GLN:CB	2.65	0.44
2:D:61:VAL:HG23	2:D:119:PHE:CD2	2.52	0.44
1:B:316:VAL:HG12	1:B:318:ILE:H	1.82	0.44
2:D:73:TYR:CD1	2:D:141:ASP:HB3	2.52	0.44
1:B:242:MET:HG2	1:B:275:ILE:CG2	2.48	0.44
2:C:31:ILE:HD11	2:C:154:ILE:HD12	2.00	0.43
1:B:493:THR:HB	1:B:496:LEU:HD22	1.99	0.43
1:B:86:ARG:HD2	2:D:66:ILE:HG21	2.01	0.43
1:A:86:ARG:HD3	2:C:66:ILE:HG21	2.01	0.43
2:D:124:ILE:HG22	2:D:125:LEU:N	2.33	0.43
1:B:264:ASP:OD1	2:D:103:SER:HB3	2.19	0.43
2:D:90:ARG:NH1	2:D:92:GLU:OE2	2.52	0.43
1:A:417:MET:HB3	1:A:417:MET:HE3	1.71	0.43
2:D:90:ARG:NH1	7:D:302:DAO:H31	2.34	0.43
1:B:179:VAL:HG23	1:B:205:LEU:HD11	2.00	0.42
2:D:42:PHE:HA	2:D:43:PRO:HD3	1.94	0.42
1:A:485:THR:HG22	1:A:508:GLN:HB2	2.01	0.42
1:A:497:THR:HA	1:A:520:LEU:HA	2.02	0.42
1:B:348:LEU:HA	1:B:349:PRO:HD3	1.87	0.42
2:D:131:TYR:HB2	2:D:153:ILE:HB	2.01	0.42
1:A:220:GLN:HG3	1:A:223:GLN:NE2	2.34	0.42
1:A:276:MET:HG3	1:A:279:LEU:HD23	2.01	0.42
1:A:522:LEU:C	1:A:522:LEU:HD13	2.45	0.42
1:A:242:MET:O	1:A:246:LEU:HG	2.19	0.42
2:C:67:PRO:HD2	2:C:111:GLU:O	2.19	0.42
1:B:70:SER:HA	1:B:96:ALA:HA	2.01	0.42
1:B:555:GLU:O	1:B:556:THR:HG23	2.20	0.42
1:B:585:GLN:H	1:B:585:GLN:HG3	1.66	0.42
1:B:164:CYS:O	1:B:164:CYS:SG	2.77	0.42
1:A:38:GLN:HE22	1:A:40:MET:HE3	1.84	0.41
1:A:462:ASP:HA	1:A:489:VAL:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:MET:HE1	2:D:96:HIS:CE1	2.55	0.41
2:C:98:HIS:O	2:C:99:ASP:C	2.62	0.41
2:C:43:PRO:C	2:C:44:ILE:HG13	2.45	0.41
1:A:553:ARG:NH2	1:B:553:ARG:HH22	2.18	0.41
2:C:36:TYR:HE2	2:C:44:ILE:HD12	1.85	0.41
2:C:141:ASP:OD1	2:C:141:ASP:N	2.53	0.41
1:A:109:THR:HA	1:A:133:VAL:O	2.21	0.41
1:B:32:VAL:CG1	1:B:35:ILE:HB	2.51	0.41
1:B:324:VAL:HA	1:B:325:PRO:HD3	1.92	0.41
1:B:198:ARG:NH2	1:B:221:ALA:O	2.54	0.41
1:B:295:PHE:CZ	1:B:299:ILE:HG22	2.56	0.41
2:D:52:ILE:HG23	2:D:121:PHE:HZ	1.85	0.41
1:A:276:MET:HG3	1:A:279:LEU:HD22	2.02	0.41
1:A:370:LEU:HA	1:A:371:PRO:HD2	1.97	0.41
1:B:164:CYS:HB2	1:B:186:ILE:HG21	2.03	0.41
1:B:292:THR:HG22	1:B:294:ASP:O	2.21	0.41
1:A:97:TRP:NE1	1:A:120:SER:O	2.54	0.40
2:D:64:GLU:O	2:D:65:PHE:HB3	2.21	0.40
1:B:151:LEU:HD21	1:B:154:LEU:HD23	2.03	0.40
1:A:198:ARG:NH2	1:A:221:ALA:O	2.55	0.40
1:A:314:ALA:HA	1:A:336:ILE:O	2.20	0.40
1:A:556:THR:HG21	1:A:584:HIS:CD2	2.57	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 X-ray entries followed by that with respect to entries of similar resolution.

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	579/606 (96%)	533 (92%)	43 (7%)	3 (0%)	24	40
1	B	579/606 (96%)	529 (91%)	47 (8%)	3 (0%)	24	40
2	C	133/144 (92%)	127 (96%)	5 (4%)	1 (1%)	16	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	133/144 (92%)	129 (97%)	4 (3%)	0	100	100
All	All	1424/1500 (95%)	1318 (93%)	99 (7%)	7 (0%)	24	40

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	581	ILE
2	C	128	LYS
1	B	52	PRO
1	A	317	SER
1	A	560	ILE
1	B	114	GLN
1	B	362	SER

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 X-ray entries followed by that with respect to entries of similar resolution.

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	540/564 (96%)	480 (89%)	60 (11%)	6	11
1	B	540/564 (96%)	484 (90%)	56 (10%)	7	12
2	C	122/131 (93%)	111 (91%)	11 (9%)	9	17
2	D	122/131 (93%)	109 (89%)	13 (11%)	6	12
All	All	1324/1390 (95%)	1184 (89%)	140 (11%)	6	12

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	VAL
1	A	38	GLN
1	A	47	VAL
1	A	60	LEU
1	A	68	LEU
1	A	117	SER
1	A	124	LEU

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Mol	Chain	Res	Type
1	A	137	LEU
1	A	154	LEU
1	A	173	LEU
1	A	182	SER
1	A	197	LEU
1	A	199	GLU
1	A	211	LEU
1	A	220	GLN
1	A	223	GLN
1	A	225	ILE
1	A	240	ASN
1	A	249	LEU
1	A	254	VAL
1	A	266	ARG
1	A	276	MET
1	A	279	LEU
1	A	280	CYS
1	A	288	ARG
1	A	289	LEU
1	A	296	SER
1	A	298	ASP
1	A	299	ILE
1	A	308	VAL
1	A	321	LEU
1	A	322	GLU
1	A	324	VAL
1	A	329	LYS
1	A	340	LEU
1	A	347	ASP
1	A	353	SER
1	A	357	THR
1	A	360	LYS
1	A	366	LYS
1	A	378	LEU
1	A	389	CYS
1	A	398	SER
1	A	415	ASN
1	A	417	MET
1	A	420	GLU
1	A	422	LEU
1	A	433	LYS
1	A	443	SER

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Mol	Chain	Res	Type
1	A	466	LEU
1	A	473	THR
1	A	522	LEU
1	A	535	SER
1	A	540	GLN
1	A	558	LYS
1	A	580	CYS
1	A	581	ILE
1	A	585	GLN
1	A	590	TRP
1	A	601	VAL
2	C	31	ILE
2	C	40	LEU
2	C	44	ILE
2	C	47	SER
2	C	52	ILE
2	C	65	PHE
2	C	71	LEU
2	C	103	SER
2	C	106	ARG
2	C	124	ILE
2	C	146	LEU
1	B	69	LYS
1	B	86	ARG
1	B	113	ILE
1	B	124	LEU
1	B	137	LEU
1	B	147	GLN
1	B	148	LEU
1	B	154	LEU
1	B	173	LEU
1	B	191	VAL
1	B	197	LEU
1	B	207	LEU
1	B	211	LEU
1	B	219	ASP
1	B	220	GLN
1	B	223	GLN
1	B	225	ILE
1	B	247	GLN
1	B	249	LEU
1	B	254	VAL

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Mol	Chain	Res	Type
1	B	259	LEU
1	B	261	GLU
1	B	266	ARG
1	B	276	MET
1	B	279	LEU
1	B	280	CYS
1	B	299	ILE
1	B	322	GLU
1	B	329	LYS
1	B	340	LEU
1	B	347	ASP
1	B	356	LEU
1	B	360	LYS
1	B	368	VAL
1	B	378	LEU
1	B	384	SER
1	B	389	CYS
1	B	392	SER
1	B	435	VAL
1	B	437	GLU
1	B	456	ASN
1	B	458	LYS
1	B	459	ILE
1	B	494	THR
1	B	496	LEU
1	B	513	VAL
1	B	516	THR
1	B	536	SER
1	B	543	SER
1	B	577	SER
1	B	582	CYS
1	B	585	GLN
1	B	594	GLN
1	B	596	GLN
1	B	599	VAL
1	B	601	VAL
2	D	23	TRP
2	D	27	SER
2	D	31	ILE
2	D	40	LEU
2	D	44	ILE
2	D	71	LEU

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Mol	Chain	Res	Type
2	D	89	LYS
2	D	106	ARG
2	D	125	LEU
2	D	132	ARG
2	D	136	GLU
2	D	145	LYS
2	D	153	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	102	HIS
1	A	111	ASN
1	A	129	ASN
1	A	155	ASN
1	A	223	GLN
1	A	247	GLN
1	A	267	ASN
1	A	327	HIS
1	A	359	ASN
1	A	407	ASN
1	A	415	ASN
1	A	428	GLN
1	A	429	HIS
1	A	456	ASN
1	A	508	GLN
1	A	521	GLN
1	A	537	HIS
1	A	539	ASN
1	A	540	GLN
1	A	562	GLN
1	A	576	ASN
1	A	584	HIS
1	A	594	GLN
2	C	39	HIS
2	C	155	HIS
1	B	42	GLN
1	B	102	HIS
1	B	111	ASN
1	B	129	ASN
1	B	147	GLN

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Mol	Chain	Res	Type
1	B	155	ASN
1	B	162	HIS
1	B	175	ASN
1	B	192	ASN
1	B	200	ASN
1	B	223	GLN
1	B	267	ASN
1	B	339	GLN
1	B	359	ASN
1	B	423	GLN
1	B	484	ASN
1	B	521	GLN
1	B	537	HIS
1	B	584	HIS
1	B	589	GLN
1	B	600	ASN
2	D	21	GLN
2	D	62	HIS
2	D	83	ASN
2	D	96	HIS
2	D	114	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

4 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	E	1	3,1	14,14,15	1.50	1 (7%)	17,19,21	2.11	3 (17%)
3	NAG	E	2	3	14,14,15	0.67	0	17,19,21	1.39	1 (5%)
3	NAG	F	1	3,1	14,14,15	0.54	0	17,19,21	1.38	3 (17%)
3	NAG	F	2	3	14,14,15	0.59	0	17,19,21	1.38	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	NAG	O5-C1	-5.23	1.34	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	O5-C1-C2	-6.99	100.47	111.29
3	E	2	NAG	C4-C3-C2	4.09	117.01	111.02
3	F	2	NAG	C1-O5-C5	3.83	117.32	112.19
3	F	1	NAG	C1-O5-C5	3.66	117.10	112.19
3	E	1	NAG	C2-N2-C7	-2.89	119.02	122.90
3	F	1	NAG	C6-C5-C4	-2.38	107.19	113.02
3	F	1	NAG	O4-C4-C5	-2.19	103.92	109.32
3	F	2	NAG	C2-N2-C7	2.10	125.71	122.90
3	E	1	NAG	C6-C5-C4	-2.06	107.97	113.02

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6

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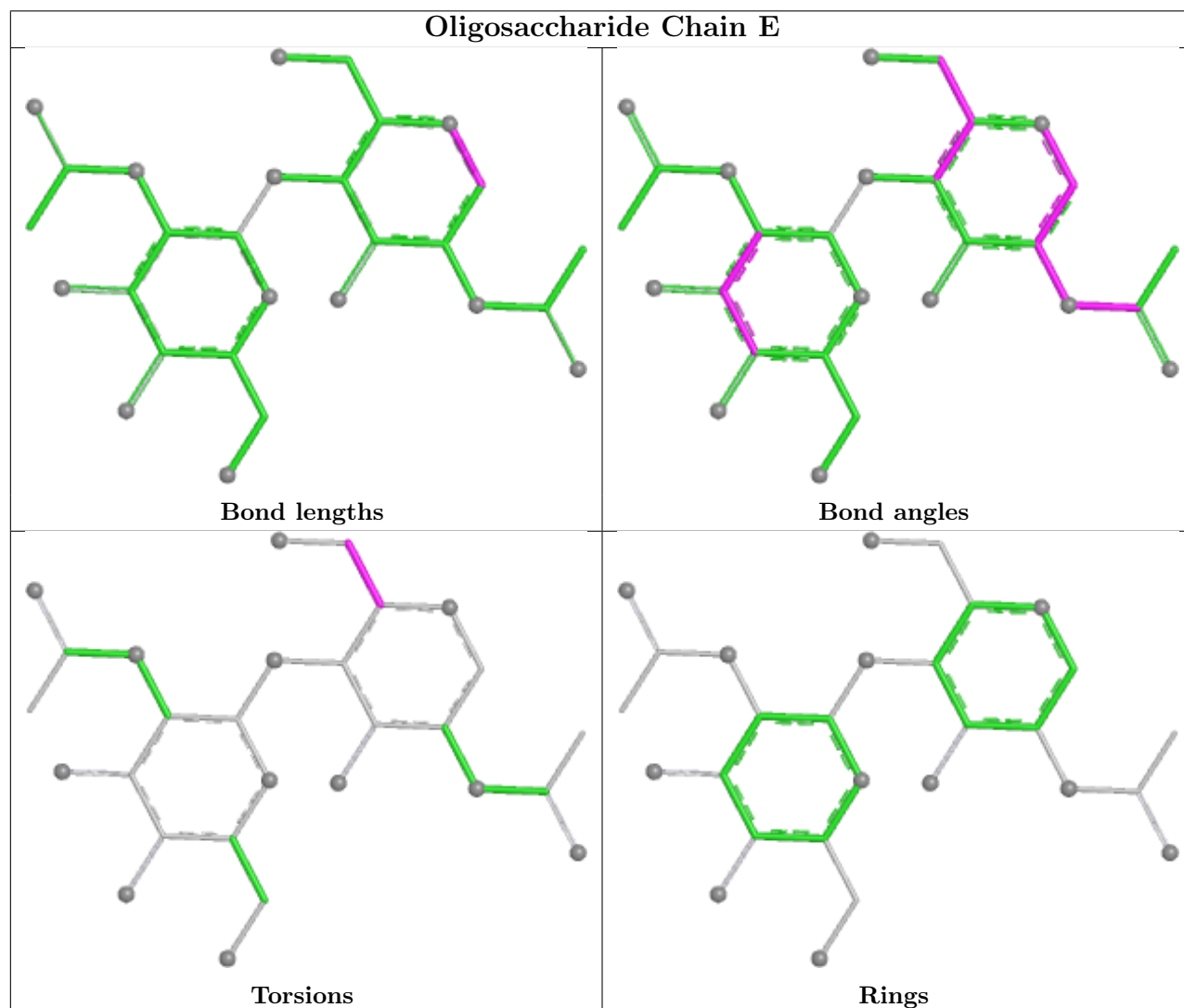
Mol	Chain	Res	Type	Atoms
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	F	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6

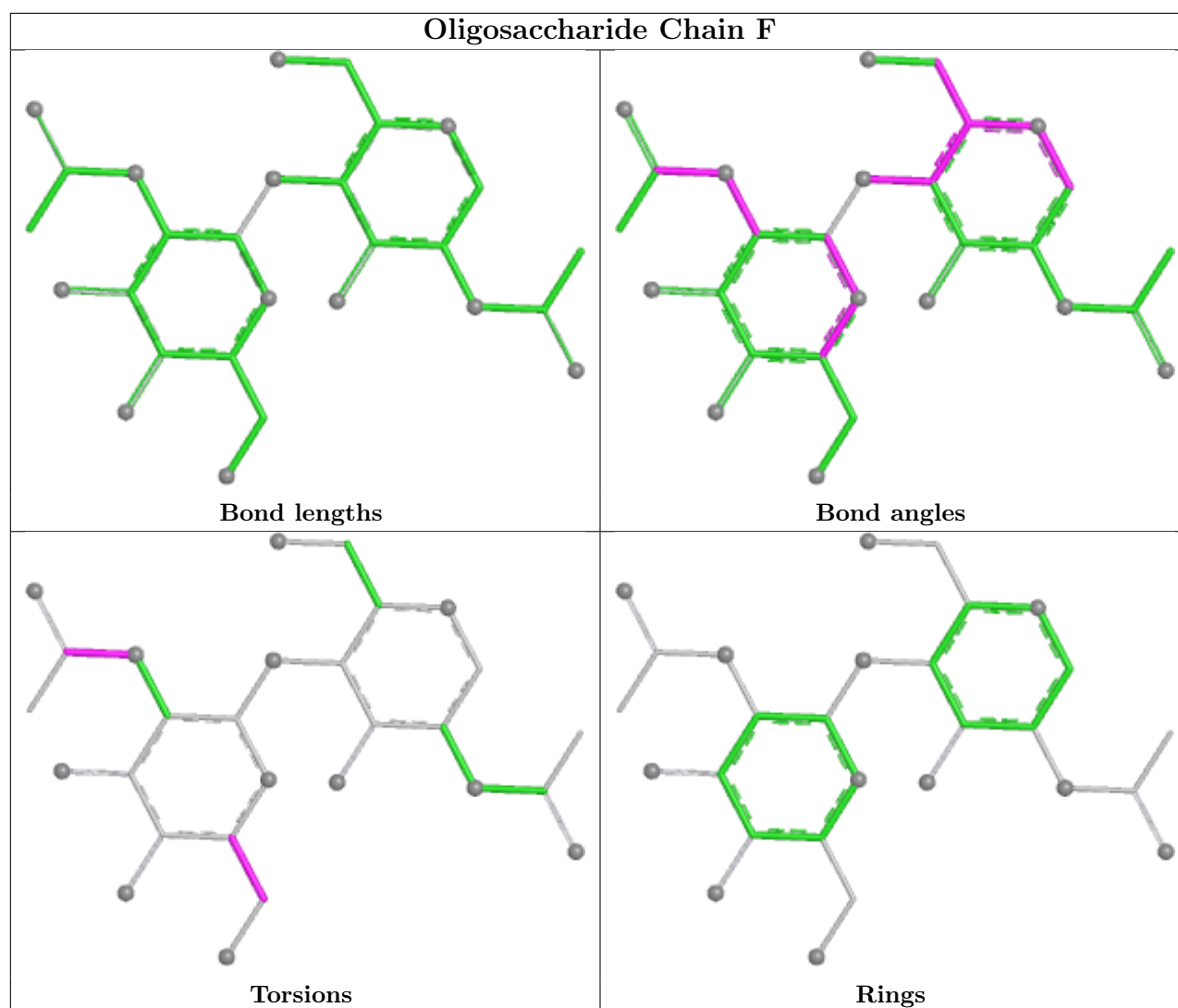
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	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](#)

11 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	NAG	A	804	-	14,14,15	0.52	0	17,19,21	0.83	0
8	MYR	D	303	5	14,14,15	0.89	1 (7%)	13,13,15	0.72	0
4	NAG	A	801	1	14,14,15	0.72	1 (7%)	17,19,21	1.97	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	DAO	D	302	5	12,12,13	0.98	1 (8%)	11,11,13	0.61	0
5	LP4	C	300	7,6,8	45,45,48	0.80	2 (4%)	54,56,60	1.01	2 (3%)
5	LP4	D	300	7,6,8	45,45,48	0.71	0	54,56,60	1.13	4 (7%)
6	LP5	C	301	5	47,48,48	0.93	4 (8%)	58,60,60	1.31	5 (8%)
6	LP5	D	301	5	47,48,48	0.88	1 (2%)	58,60,60	1.10	6 (10%)
4	NAG	A	800	1	14,14,15	1.78	1 (7%)	17,19,21	2.39	4 (23%)
7	DAO	C	302	5	12,12,13	0.96	1 (8%)	11,11,13	0.61	0
8	MYR	C	303	5	14,14,15	0.89	1 (7%)	13,13,15	0.69	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	NAG	A	804	-	-	2/6/23/26	0/1/1/1
8	MYR	D	303	5	-	9/12/12/13	-
4	NAG	A	801	1	-	2/6/23/26	0/1/1/1
7	DAO	D	302	5	-	5/10/10/11	-
5	LP4	C	300	7,6,8	-	12/43/60/65	0/1/1/1
5	LP4	D	300	7,6,8	-	13/43/60/65	0/1/1/1
6	LP5	C	301	5	-	17/44/65/65	0/1/1/1
6	LP5	D	301	5	-	16/44/65/65	0/1/1/1
4	NAG	A	800	1	-	2/6/23/26	0/1/1/1
7	DAO	C	302	5	-	5/10/10/11	-
8	MYR	C	303	5	-	10/12/12/13	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800	NAG	O5-C1	-6.36	1.33	1.43
6	D	301	LP5	P45-O47	3.42	1.61	1.50
7	D	302	DAO	O2-C1	-3.32	1.25	1.42
7	C	302	DAO	O2-C1	-3.24	1.25	1.42
8	D	303	MYR	O2-C1	-3.23	1.25	1.42
8	C	303	MYR	O2-C1	-3.22	1.25	1.42
6	C	301	LP5	P45-O47	3.11	1.60	1.50
6	C	301	LP5	P45-O1	2.57	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	NAG	C1-C2	2.34	1.55	1.52
5	C	300	LP4	C29-C28	2.15	1.54	1.50
5	C	300	LP4	C3-C2	2.12	1.55	1.52
6	C	301	LP5	O3-C3	-2.06	1.41	1.44
6	C	301	LP5	P45-O46	2.04	1.62	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	NAG	C1-O5-C5	-7.98	101.49	112.19
4	A	801	NAG	C1-O5-C5	5.50	119.56	112.19
4	A	801	NAG	C2-N2-C7	-3.53	118.17	122.90
6	C	301	LP5	C8-C7-N2	-3.50	111.47	116.25
5	D	300	LP4	C1-C2-N2	-3.46	104.99	110.43
6	C	301	LP5	C3-O3-C28	3.41	123.13	117.59
4	A	800	NAG	O5-C1-C2	-3.16	106.40	111.29
5	D	300	LP4	C3-O3-C28	-2.90	112.87	117.59
6	C	301	LP5	C1-C2-N2	-2.71	106.36	110.92
4	A	801	NAG	O5-C1-C2	-2.63	107.22	111.29
4	A	800	NAG	C4-C3-C2	-2.61	107.19	111.02
4	A	800	NAG	O5-C5-C6	2.58	112.69	107.66
5	C	300	LP4	O47-P45-O4	-2.58	95.78	105.85
6	D	301	LP5	C3-O3-C28	-2.47	113.57	117.59
6	C	301	LP5	O1-P45-O47	-2.40	100.79	109.33
6	D	301	LP5	C3-C2-N2	-2.39	107.09	110.91
6	C	301	LP5	C17-C16-C8	-2.39	104.85	112.88
4	A	801	NAG	C3-C4-C5	-2.28	106.10	110.23
6	D	301	LP5	C8-C7-N2	-2.27	113.16	116.25
5	D	300	LP4	O5-C5-C6	2.22	111.99	107.66
6	D	301	LP5	O5-C1-O1	-2.22	108.46	111.36
5	C	300	LP4	C1-C2-N2	-2.22	106.94	110.43
5	D	300	LP4	O46-P45-O48	2.19	119.37	110.83
4	A	801	NAG	C1-C2-N2	2.17	113.85	110.43
6	D	301	LP5	O46-P45-O48	2.09	115.64	107.80
6	D	301	LP5	O46-P45-O47	-2.09	102.70	110.83

There are no chirality outliers.

All (93) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	300	LP4	C17-C16-C8-C7
5	C	300	LP4	O44-C16-C8-C7

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Mol	Chain	Res	Type	Atoms
5	C	300	LP4	C8-C16-C17-C18
5	D	300	LP4	C17-C16-C8-C7
5	D	300	LP4	O44-C16-C8-C7
5	D	300	LP4	C8-C16-C17-C18
5	D	300	LP4	O44-C16-C17-C18
6	C	301	LP5	O44-C16-C8-C7
6	C	301	LP5	C17-C16-C8-C7
6	D	301	LP5	N2-C7-C8-C16
6	D	301	LP5	O7-C7-C8-C16
6	D	301	LP5	O44-C16-C8-C7
6	D	301	LP5	C17-C16-C8-C7
4	A	800	NAG	C4-C5-C6-O6
4	A	800	NAG	O5-C5-C6-O6
5	C	300	LP4	O44-C16-C17-C18
4	A	804	NAG	C4-C5-C6-O6
4	A	804	NAG	O5-C5-C6-O6
6	C	301	LP5	O5-C5-C6-O6
7	D	302	DAO	C11-C10-C9-C8
8	C	303	MYR	C4-C5-C6-C7
8	C	303	MYR	C6-C7-C8-C9
5	C	300	LP4	C34-C35-C36-C37
6	C	301	LP5	C18-C19-C20-C21
7	C	302	DAO	C11-C10-C9-C8
6	D	301	LP5	C20-C21-C22-C23
8	C	303	MYR	C9-C10-C11-C12
6	C	301	LP5	C36-C37-C38-C39
8	D	303	MYR	C6-C7-C8-C9
6	D	301	LP5	C23-C24-C25-C26
4	A	801	NAG	C4-C5-C6-O6
5	D	300	LP4	C17-C18-C19-C20
6	D	301	LP5	C37-C38-C39-C40
6	C	301	LP5	C31-C32-C33-C34
6	C	301	LP5	C4-C5-C6-O6
6	C	301	LP5	C17-C18-C19-C20
6	D	301	LP5	C19-C20-C21-C22
7	C	302	DAO	C3-C4-C5-C6
6	C	301	LP5	C23-C24-C25-C26
6	C	301	LP5	C20-C21-C22-C23
6	D	301	LP5	C31-C32-C33-C34
7	C	302	DAO	C5-C6-C7-C8
8	D	303	MYR	C4-C5-C6-C7
8	D	303	MYR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
7	D	302	DAO	O2-C1-C2-C3
8	C	303	MYR	C1-C2-C3-C4
8	D	303	MYR	C1-C2-C3-C4
5	D	300	LP4	C37-C38-C39-C40
6	C	301	LP5	C19-C20-C21-C22
8	C	303	MYR	C2-C3-C4-C5
5	D	300	LP4	C34-C35-C36-C37
7	D	302	DAO	C5-C6-C7-C8
6	C	301	LP5	C37-C38-C39-C40
6	D	301	LP5	C17-C18-C19-C20
7	D	302	DAO	C2-C3-C4-C5
6	D	301	LP5	C18-C19-C20-C21
6	C	301	LP5	C24-C25-C26-C27
6	D	301	LP5	C24-C25-C26-C27
6	D	301	LP5	C38-C39-C40-C41
7	D	302	DAO	C9-C10-C11-C12
5	C	300	LP4	C17-C18-C19-C20
4	A	801	NAG	O5-C5-C6-O6
6	C	301	LP5	O43-C30-C31-C32
8	D	303	MYR	C11-C12-C13-C14
5	D	300	LP4	C16-C17-C18-C19
8	D	303	MYR	C2-C3-C4-C5
8	D	303	MYR	C5-C6-C7-C8
6	D	301	LP5	O5-C5-C6-O6
8	C	303	MYR	C5-C6-C7-C8
5	C	300	LP4	C37-C38-C39-C40
5	C	300	LP4	C19-C20-C21-C22
5	C	300	LP4	C4-O4-P45-O48
6	D	301	LP5	C4-C5-C6-O6
5	D	300	LP4	C29-C28-O3-C3
6	C	301	LP5	C35-C36-C37-C38
8	C	303	MYR	C7-C8-C9-C10
5	C	300	LP4	C16-C17-C18-C19
8	C	303	MYR	C3-C4-C5-C6
5	D	300	LP4	C18-C19-C20-C21
8	D	303	MYR	C3-C4-C5-C6
7	C	302	DAO	C2-C3-C4-C5
8	C	303	MYR	O2-C1-C2-C3
6	C	301	LP5	C30-C31-C32-C33
6	D	301	LP5	C30-C31-C32-C33
6	C	301	LP5	O7-C7-C8-C16
5	C	300	LP4	C36-C37-C38-C39

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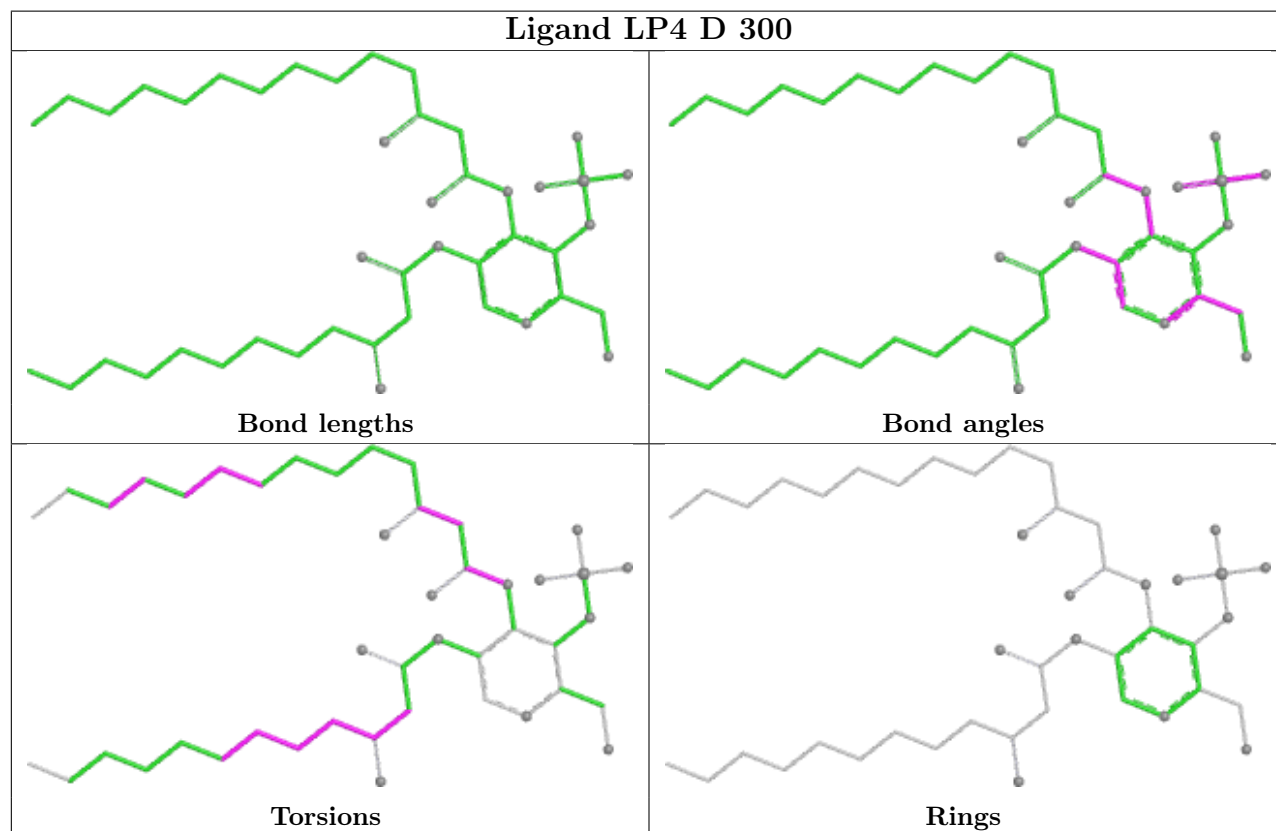
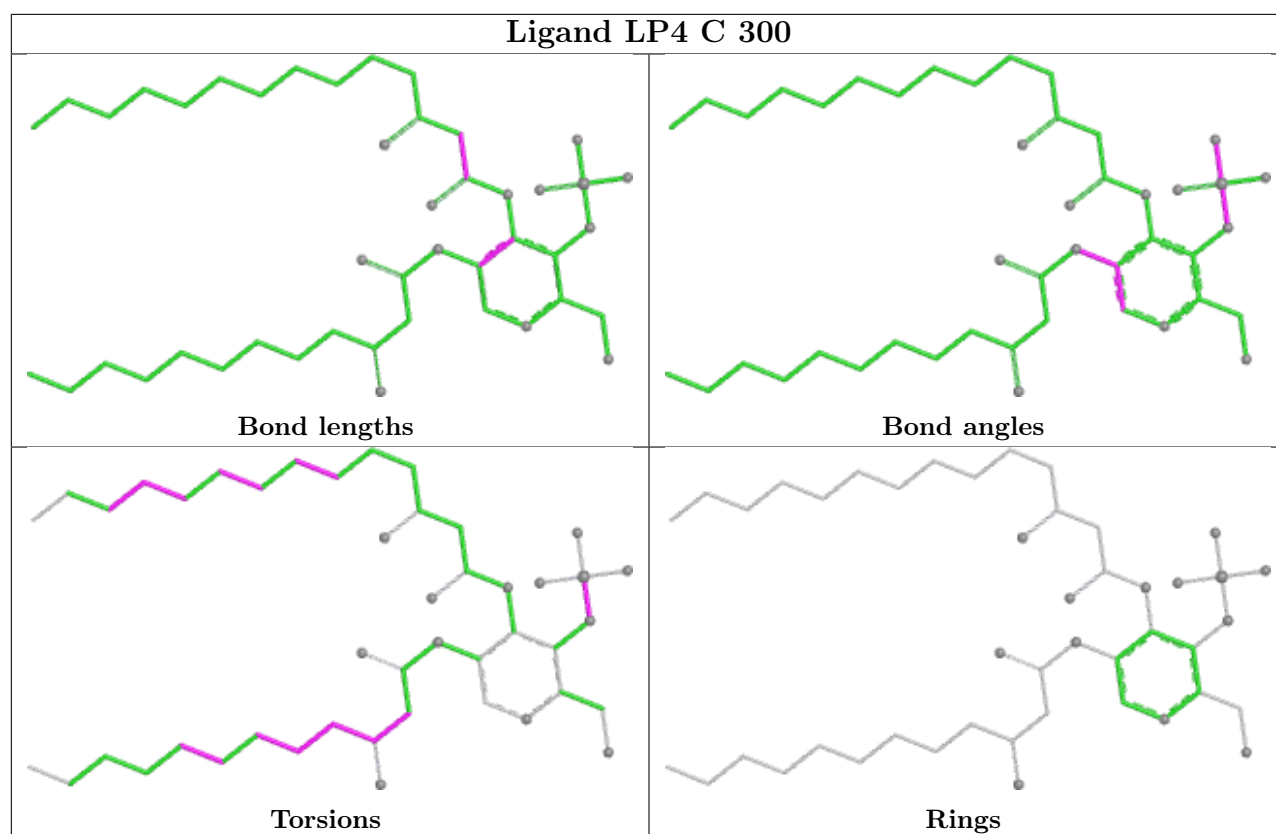
Mol	Chain	Res	Type	Atoms
7	C	302	DAO	O2-C1-C2-C3
5	D	300	LP4	C28-C29-C30-C31
5	D	300	LP4	O42-C28-O3-C3
5	D	300	LP4	C35-C36-C37-C38
8	C	303	MYR	C11-C12-C13-C14
5	C	300	LP4	C32-C33-C34-C35
8	D	303	MYR	O2-C1-C2-C3

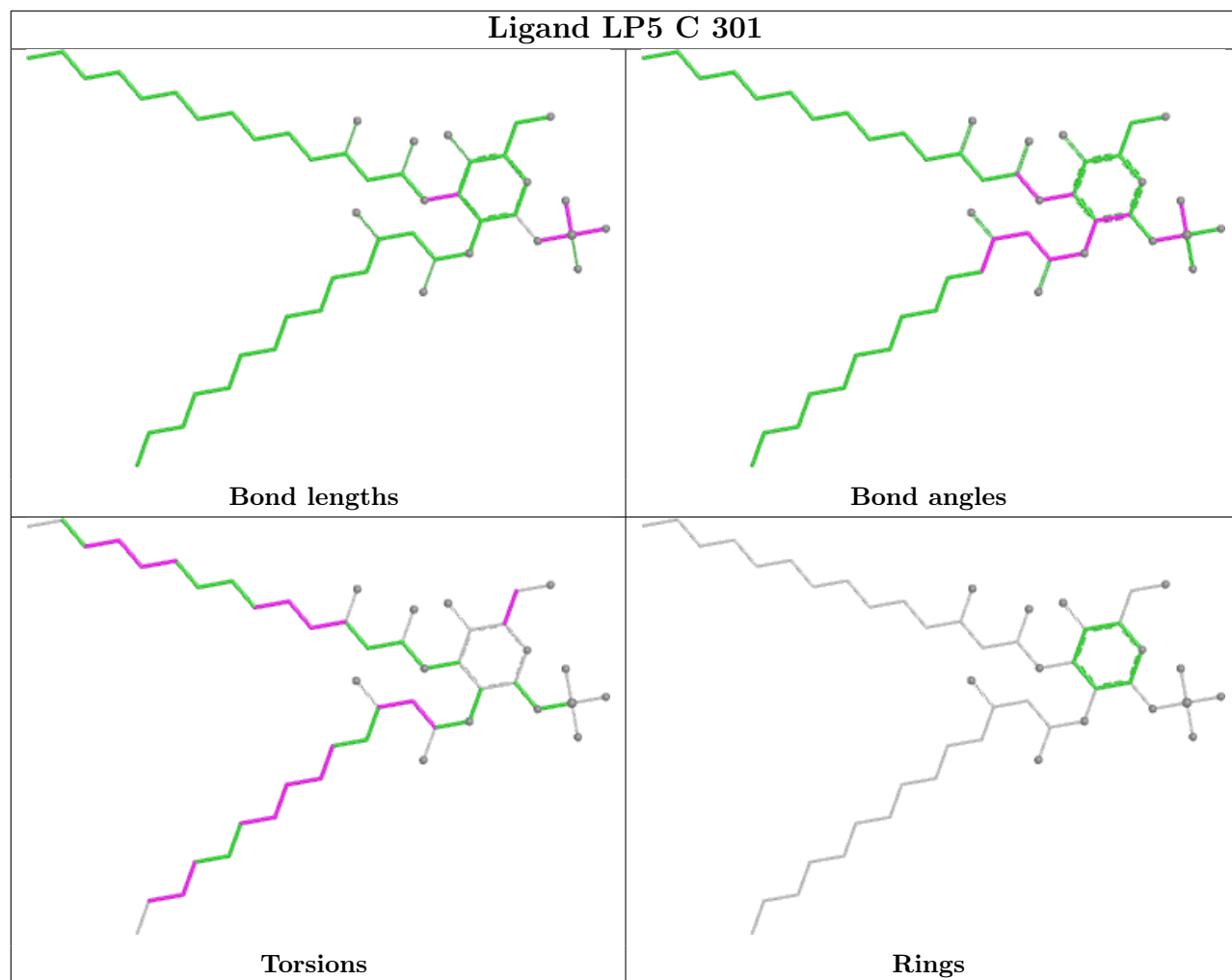
There are no ring outliers.

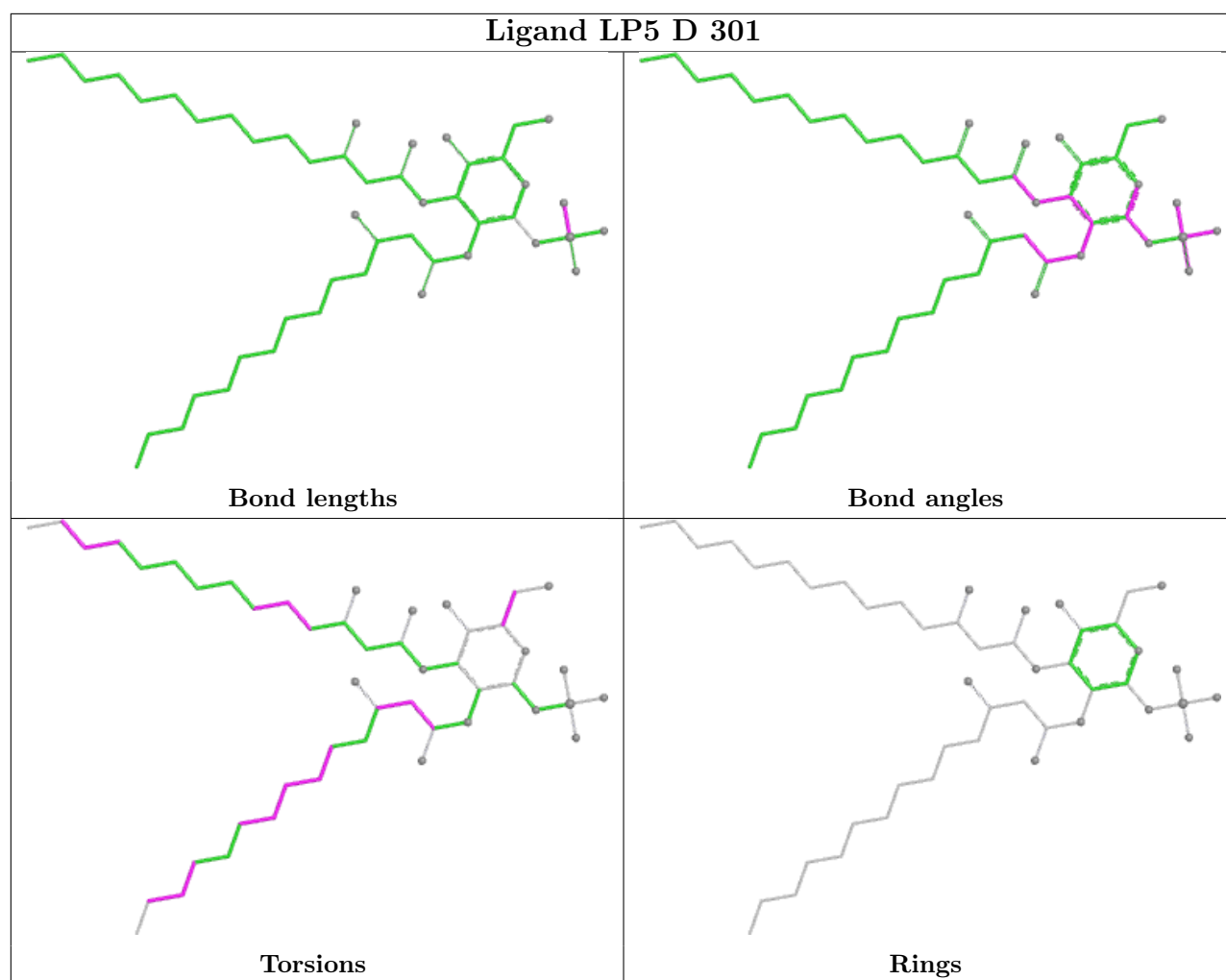
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	804	NAG	2	0
7	D	302	DAO	2	0
6	C	301	LP5	1	0
6	D	301	LP5	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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	581/606 (95%)	0.78	74 (12%) 8 6	42, 65, 119, 169	0
1	B	581/606 (95%)	0.75	75 (12%) 7 6	38, 68, 128, 184	0
2	C	135/144 (93%)	0.60	7 (5%) 33 29	36, 64, 92, 112	2 (1%)
2	D	135/144 (93%)	0.98	18 (13%) 7 5	37, 71, 97, 142	2 (1%)
All	All	1432/1500 (95%)	0.77	174 (12%) 8 7	36, 67, 121, 184	4 (0%)

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	145	LYS	8.5
1	A	579	ALA	7.7
1	A	587	PHE	6.3
1	A	581	ILE	6.2
1	B	27	PRO	5.8
2	C	145	LYS	5.7
1	B	55	THR	5.6
1	B	594	GLN	5.6
1	A	591	VAL	5.5
1	A	590	TRP	5.5
1	A	27	PRO	5.4
1	A	582	CYS	5.3
1	A	556	THR	5.2
1	A	511	TRP	5.2
1	B	67	ILE	5.0
2	D	154	ILE	4.9
1	A	588	LEU	4.9
1	B	31	VAL	4.7
1	B	270	ILE	4.6
1	A	270	ILE	4.5
2	C	154	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	607	ALA	4.4
1	A	580	CYS	4.3
1	A	601	VAL	4.3
1	A	585	GLN	4.1
1	B	51	ILE	4.1
1	B	607	ALA	3.9
1	B	71	TYR	3.9
1	B	37	TYR	3.8
1	A	560	ILE	3.8
1	A	598	LEU	3.8
1	B	582	CYS	3.7
2	C	128	LYS	3.7
1	A	322	GLU	3.6
1	B	97	TRP	3.6
2	D	122	GLU	3.6
1	B	511	TRP	3.6
1	B	99	GLY	3.5
1	B	35	ILE	3.5
1	A	599	VAL	3.5
1	B	52	PRO	3.5
1	A	589	GLN	3.5
1	A	98	HIS	3.4
1	B	50	ASP	3.4
1	B	301	LYS	3.4
1	A	74	SER	3.4
1	B	53	SER	3.4
1	B	581	ILE	3.3
2	D	23	TRP	3.3
1	B	54	SER	3.3
1	B	102	HIS	3.3
1	B	123	GLY	3.3
1	B	585	GLN	3.2
1	A	604	MET	3.2
1	A	557	SER	3.2
1	A	76	PHE	3.2
1	A	299	ILE	3.2
1	A	350	PHE	3.1
1	A	456	ASN	3.1
1	B	599	VAL	3.1
1	B	590	TRP	3.0
2	D	124	ILE	3.0
1	B	76	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	118	PRO	2.9
1	A	69	LYS	2.9
1	A	301	LYS	2.9
1	B	101	HIS	2.9
1	B	66	LYS	2.9
2	D	44	ILE	2.9
1	B	98	HIS	2.9
1	B	300	VAL	2.9
1	B	323	ASP	2.9
2	D	42	PHE	2.9
2	D	45	SER	2.9
1	B	124	LEU	2.9
1	B	345	THR	2.8
1	B	100	LEU	2.8
2	D	31	ILE	2.8
1	A	594	GLN	2.8
1	B	304	CYS	2.8
2	D	64	GLU	2.8
1	B	271	PHE	2.8
1	A	71	TYR	2.8
1	A	578	VAL	2.8
1	B	266	ARG	2.8
1	B	360	LYS	2.8
2	C	39	HIS	2.7
1	B	34	ASN	2.7
1	A	592	LYS	2.7
1	B	32	VAL	2.7
1	B	46	LYS	2.7
1	A	114	GLN	2.7
1	A	584	HIS	2.7
1	A	606	CYS	2.7
1	B	580	CYS	2.7
1	B	73	PHE	2.7
1	A	602	GLU	2.6
1	B	583	GLU	2.6
1	A	586	LYS	2.6
1	A	58	ILE	2.6
1	A	389	CYS	2.6
1	A	605	THR	2.6
1	A	47	VAL	2.6
1	B	174	THR	2.6
1	A	266	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	29	ILE	2.5
1	B	77	SER	2.5
2	D	39	HIS	2.5
2	D	55	ARG	2.5
1	B	237	ASN	2.5
1	A	323	ASP	2.5
2	C	122	GLU	2.4
1	A	268	LEU	2.4
1	A	55	THR	2.4
1	A	566	LYS	2.4
1	A	237	ASN	2.4
1	A	33	PRO	2.4
1	A	595	LYS	2.4
1	B	45	SER	2.3
1	A	518	HIS	2.3
1	B	65	LEU	2.3
1	A	39	CYS	2.3
1	B	602	GLU	2.3
1	A	31	VAL	2.3
2	D	58	ASN	2.3
1	B	33	PRO	2.3
1	B	113	ILE	2.3
1	A	573	LEU	2.3
1	B	68	LEU	2.3
1	B	69	LYS	2.3
2	D	141	ASP	2.3
1	A	43	LYS	2.2
1	A	100	LEU	2.2
1	B	149	ILE	2.2
1	A	271	PHE	2.2
1	A	34	ASN	2.2
1	B	28	CYS	2.2
1	A	77	SER	2.2
1	B	269	GLU	2.2
1	B	389	CYS	2.2
2	D	66	ILE	2.2
1	A	95	LYS	2.2
1	B	56	LYS	2.2
1	B	366	LYS	2.2
1	A	162	HIS	2.2
1	B	276	MET	2.2
1	A	28	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	55	ARG	2.2
2	C	42	PHE	2.2
1	B	47	VAL	2.1
1	B	127	LEU	2.1
1	B	283	THR	2.1
1	B	280	CYS	2.1
1	A	570	PHE	2.1
2	D	37	CYS	2.1
1	A	597	PHE	2.1
1	B	44	LEU	2.1
2	D	132	ARG	2.1
1	A	269	GLU	2.1
1	A	326	LYS	2.1
1	A	174	THR	2.1
1	B	92	ILE	2.1
2	D	24	PHE	2.0
1	A	539	ASN	2.0
1	B	79	LEU	2.0
1	A	583	GLU	2.0
1	A	298	ASP	2.0
1	A	386	SER	2.0
1	B	137	LEU	2.0
1	B	151	LEU	2.0
1	B	95	LYS	2.0
1	A	51	ILE	2.0
1	B	225	ILE	2.0
1	A	294	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	F	2	14/15	0.77	0.18	63,78,94,120	0

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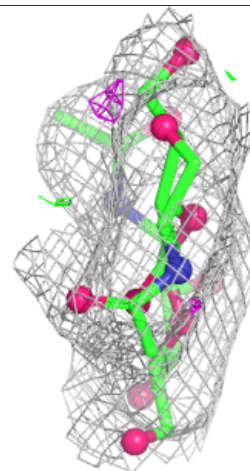
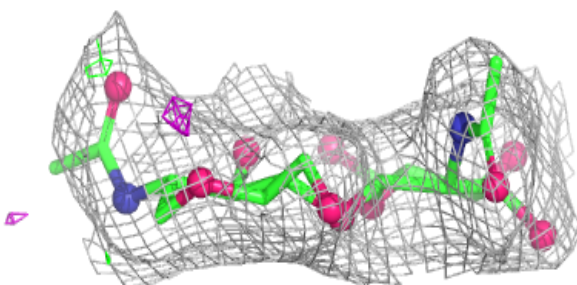
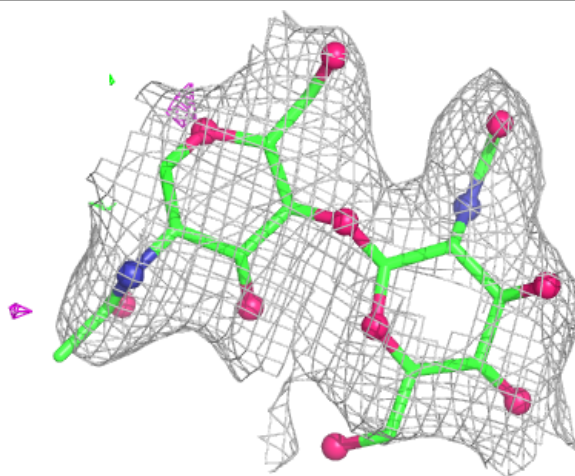
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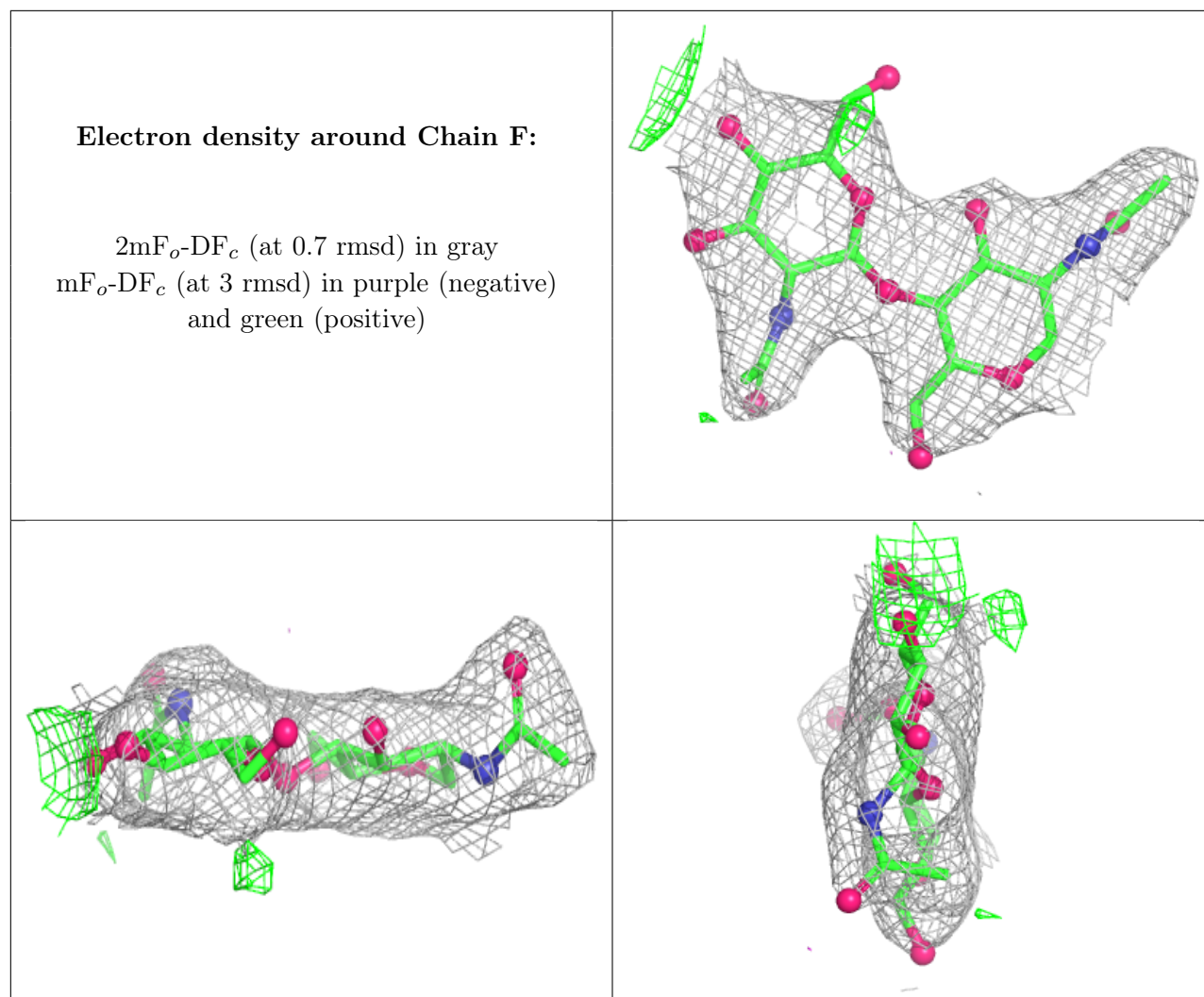
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	E	2	14/15	0.83	0.14	79,94,120,130	0
3	NAG	E	1	14/15	0.92	0.15	65,75,85,96	0
3	NAG	F	1	14/15	0.96	0.10	47,54,70,80	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	801	14/15	0.77	0.19	71,82,105,111	0
4	NAG	A	804	14/15	0.81	0.18	81,105,125,136	0
5	LP4	D	300	45/48	0.90	0.15	60,72,90,96	0
8	MYR	D	303	15/16	0.90	0.24	66,91,101,116	0
5	LP4	C	300	45/48	0.91	0.14	45,64,81,99	0
4	NAG	A	800	14/15	0.93	0.10	59,73,84,85	0
7	DAO	D	302	13/14	0.94	0.17	72,82,97,103	0
8	MYR	C	303	15/16	0.94	0.20	68,79,99,122	0
7	DAO	C	302	13/14	0.94	0.16	68,75,88,90	0

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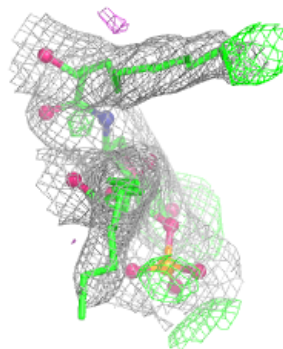
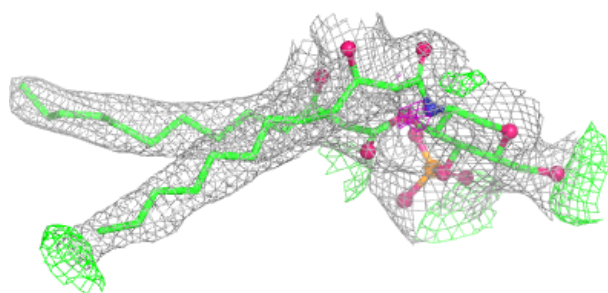
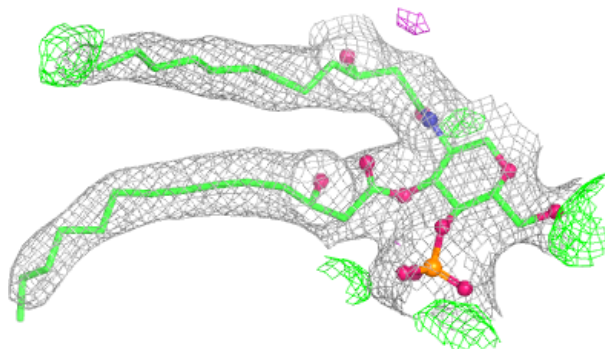
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	LP5	D	301	48/48	0.95	0.13	52,78,102,119	0
6	LP5	C	301	48/48	0.96	0.12	48,68,102,109	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

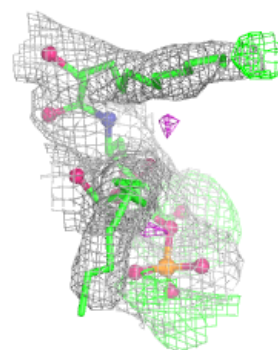
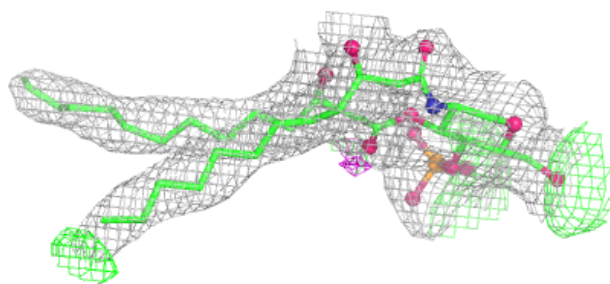
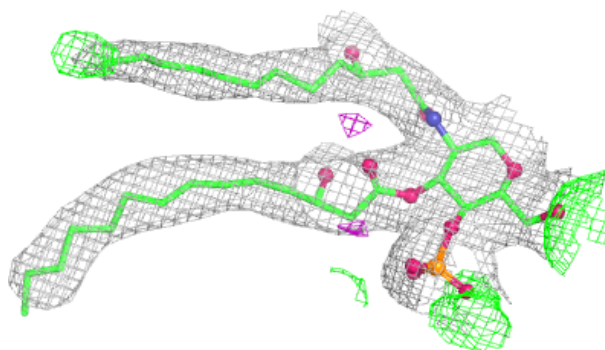
Electron density around LP4 D 300:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

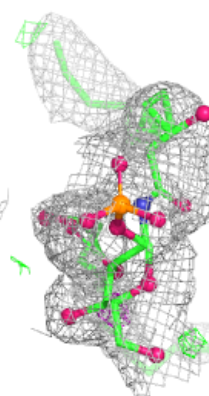
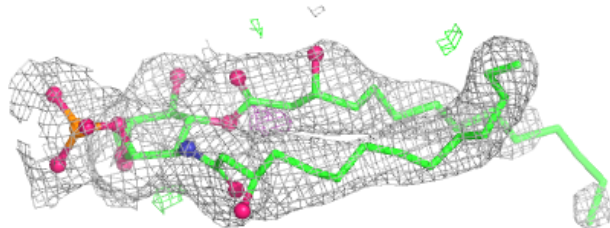
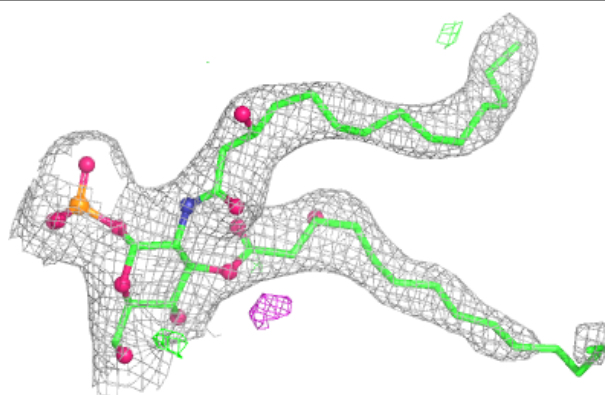


Electron density around LP4 C 300:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

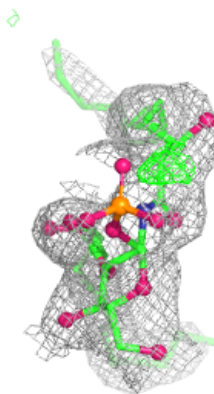
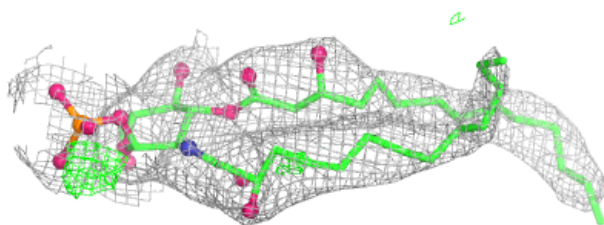
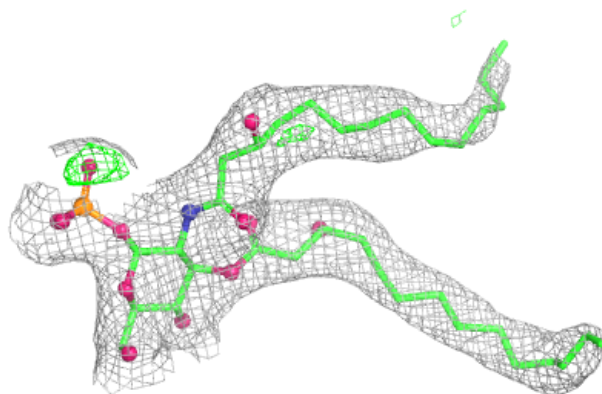
**Electron density around LP5 D 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LP5 C 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.