



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:53 AM UTC

PDB ID : 5JMY / pdb_00005jmy
Title : NEPRILYSIN COMPLEXED WITH LBQ657
Authors : Schiering, N.; Wiesmann, C.
Deposited on : 2016-04-29
Resolution : 2.00 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

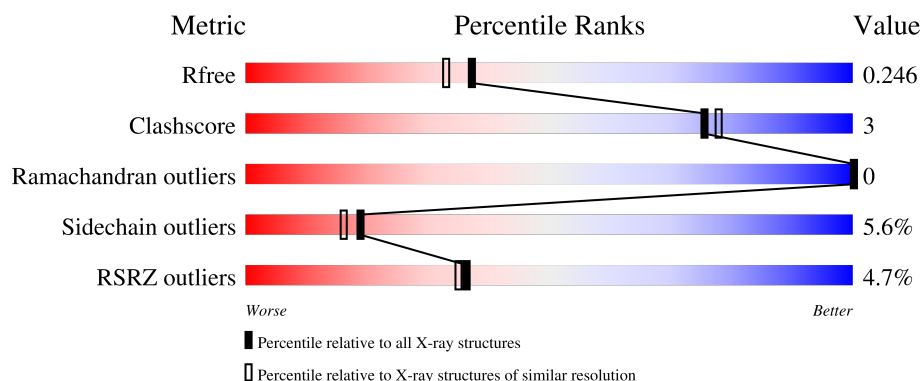
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	698	9% 87% 11%
1	B	698	9% 87% 12%
2	C	2	50% 50%
2	D	2	50% 50%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12295 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 Neprilysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	696	Total	C	N	O	S	0	2	0
			5612	3549	961	1076	26			
1	B	696	Total	C	N	O	S	0	0	0
			5595	3538	957	1074	26			

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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

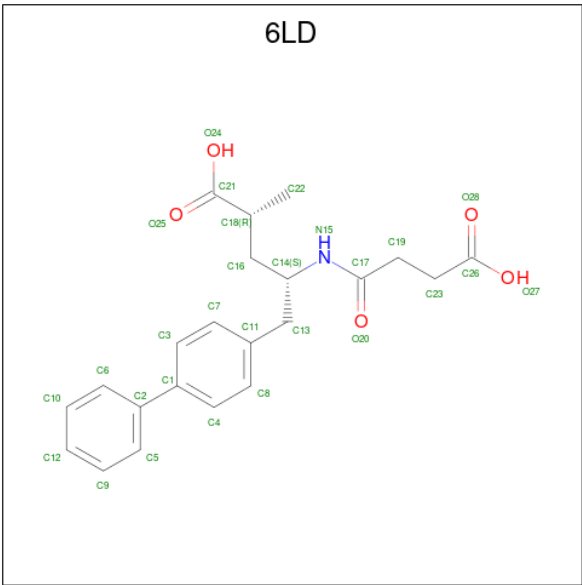


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		

- Molecule 5 is Sacubitrilat (CCD ID: 6LD) (formula: C₂₂H₂₅NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			28	22	1	5		
5	B	1	Total	C	N	O	0	0
			28	22	1	5		

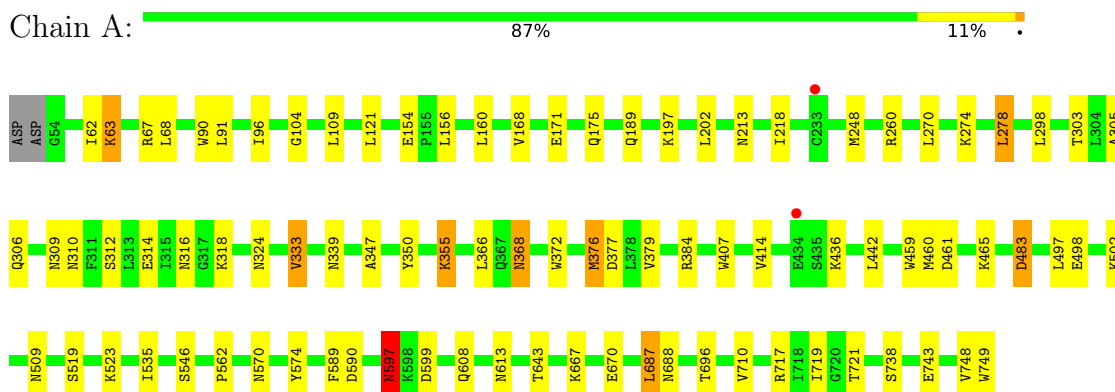
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	514	Total	O	0	0
			514	514		
6	B	376	Total	O	0	0
			376	376		

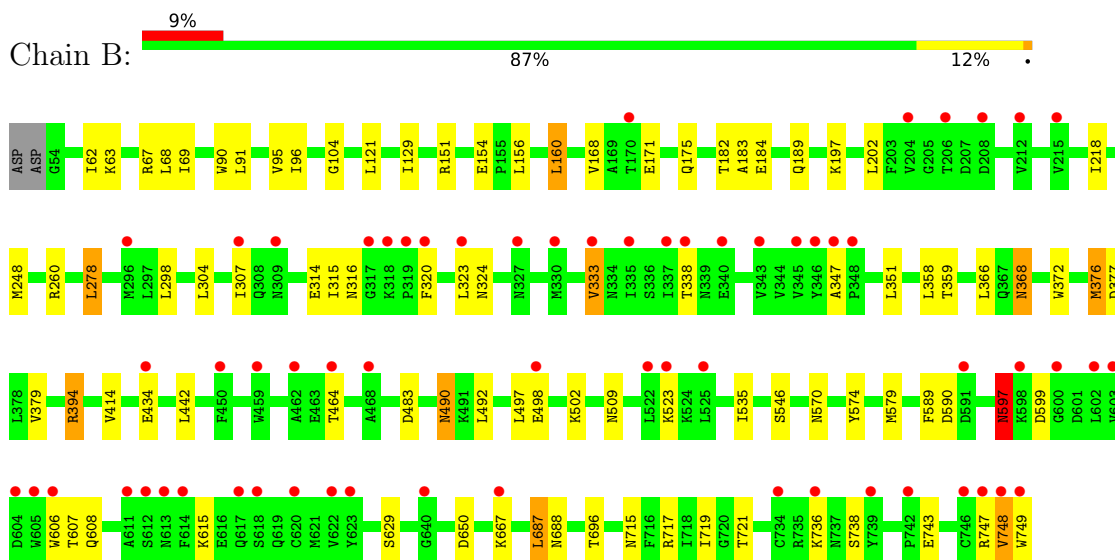
3 Residue-property plots

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 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: Neprilysin



- Molecule 1: Neprilysin



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





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

Chain D:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.74Å 109.14Å 248.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.28 – 2.00 29.28 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.28-2.00) 98.2 (29.28-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.00Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.186 , 0.228 0.201 , 0.246	Depositor DCC
R_{free} test set	4992 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12295	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 6LD, NAG, ZN

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	0.86	0/5731	1.26	17/7752 (0.2%)
1	B	0.83	1/5713 (0.0%)	1.28	10/7727 (0.1%)
All	All	0.85	1/11444 (0.0%)	1.27	27/15479 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	160	LEU	CA-C	5.11	1.57	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	738	SER	N-CA-C	-7.19	101.03	110.53
1	A	738	SER	N-CA-C	-7.04	101.24	110.53
1	A	597	ASN	CA-CB-CG	6.92	119.52	112.60
1	B	597	ASN	CA-CB-CG	6.90	119.50	112.60
1	B	615	LYS	CA-C-N	6.39	129.36	120.29
1	B	615	LYS	C-N-CA	6.39	129.36	120.29
1	A	309	ASN	CA-C-N	6.25	128.65	120.28
1	A	309	ASN	C-N-CA	6.25	128.65	120.28
1	B	316	ASN	CA-CB-CG	5.83	118.43	112.60
1	B	377	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	213	ASN	CA-CB-CG	5.73	118.33	112.60
1	B	590	ASP	CA-CB-CG	5.72	118.32	112.60
1	A	590	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	316	ASN	CA-CB-CG	5.54	118.14	112.60
1	A	461	ASP	CA-C-N	5.48	127.89	120.38
1	A	461	ASP	C-N-CA	5.48	127.89	120.38
1	A	377	ASP	CA-CB-CG	5.39	117.99	112.60
1	B	748	VAL	N-CA-CB	5.29	119.95	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	719	ILE	CB-CG1-CD1	5.26	124.85	113.80
1	B	324	ASN	CA-CB-CG	5.21	117.81	112.60
1	A	310	ASN	N-CA-C	5.13	116.88	111.28
1	A	436	LYS	CA-C-N	5.10	127.53	120.29
1	A	436	LYS	C-N-CA	5.10	127.53	120.29
1	A	324	ASN	CA-CB-CG	5.03	117.63	112.60
1	A	483	ASP	CA-C-N	5.02	127.71	120.38
1	A	483	ASP	C-N-CA	5.02	127.71	120.38
1	B	394	ARG	N-CA-CB	5.00	118.04	110.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5612	0	5460	33	0
1	B	5595	0	5446	37	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
3	A	42	0	39	0	0
3	B	42	0	39	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	28	0	0	0	0
5	B	28	0	0	0	0
6	A	514	0	0	1	0
6	B	376	0	0	1	0
All	All	12295	0	11034	67	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 3.

All (67) 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:202:LEU:HD23	1:A:218:ILE:HD11	1.70	0.72
1:A:460:MET:HE3	1:A:465:LYS:HG2	1.70	0.72
1:B:202:LEU:HD23	1:B:218:ILE:HD11	1.72	0.71
1:A:305:ALA:HB2	1:A:339:ASN:HB3	1.77	0.67
1:B:168:VAL:H	1:B:368:ASN:HD21	1.44	0.65
1:B:183:ALA:HB2	1:B:315:ILE:HG21	1.79	0.64
1:A:168:VAL:H	1:A:368:ASN:HD21	1.43	0.64
1:A:333:VAL:HG11	1:A:523:LYS:HB3	1.79	0.62
1:B:333:VAL:HG11	1:B:523:LYS:HB3	1.79	0.62
1:A:67:ARG:HH22	1:A:688:ASN:HD21	1.47	0.62
1:A:407:TRP:CZ2	1:B:95:VAL:HG11	2.34	0.61
1:B:502:LYS:H	1:B:509:ASN:HD21	1.50	0.59
1:A:502:LYS:H	1:A:509:ASN:HD21	1.52	0.58
1:A:67:ARG:HH22	1:A:688:ASN:ND2	2.03	0.56
1:B:589:PHE:HB3	1:B:749:TRP:CZ2	2.41	0.56
1:A:589:PHE:HB3	1:A:749:TRP:CZ2	2.41	0.56
1:A:96:ILE:HD11	1:A:696:THR:HG23	1.90	0.53
1:B:67:ARG:HH22	1:B:688:ASN:ND2	2.07	0.52
1:B:121:LEU:HD13	1:B:414:VAL:HG21	1.92	0.52
1:B:67:ARG:HH22	1:B:688:ASN:HD21	1.57	0.51
1:A:67:ARG:HH12	1:A:688:ASN:ND2	2.09	0.51
1:B:67:ARG:HH12	1:B:688:ASN:ND2	2.09	0.51
1:A:597:ASN:HD22	1:A:597:ASN:C	2.18	0.50
1:B:597:ASN:C	1:B:597:ASN:HD22	2.18	0.50
1:A:62:ILE:HG13	1:B:62:ILE:HG13	1.94	0.50
1:A:278:LEU:HD11	1:A:366:LEU:HD23	1.94	0.50
1:A:535:ILE:HD13	1:A:546:SER:HB2	1.94	0.50
1:B:67:ARG:HH12	1:B:688:ASN:HD22	1.60	0.50
1:A:597:ASN:ND2	1:A:599:ASP:H	2.10	0.50
1:B:570:ASN:O	1:B:574:TYR:HD1	1.94	0.49
1:B:597:ASN:ND2	1:B:599:ASP:H	2.11	0.49
1:A:372:TRP:CE2	1:A:376:MET:HG3	2.48	0.48
1:B:372:TRP:CE2	1:B:376:MET:HG3	2.48	0.48
1:A:347:ALA:HB1	1:A:350:TYR:HB3	1.95	0.48
1:B:278:LEU:HD11	1:B:366:LEU:HD23	1.93	0.48
1:B:96:ILE:HD11	1:B:696:THR:HG23	1.95	0.48
1:A:121:LEU:HD13	1:A:414[A]:VAL:HG21	1.96	0.48
1:A:570:ASN:O	1:A:574:TYR:HD1	1.96	0.48
1:B:464:THR:HG23	1:B:607:THR:HG23	1.96	0.47
1:A:68:LEU:HD22	1:A:687:LEU:HD13	1.96	0.47
1:A:67:ARG:HH12	1:A:688:ASN:HD22	1.63	0.47
1:B:535:ILE:HD13	1:B:546:SER:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:GLU:HB3	1:B:359:THR:HG22	1.97	0.46
1:A:90:TRP:CZ2	1:A:104:GLY:HA2	2.51	0.45
1:B:315:ILE:HD11	1:B:358:LEU:HD23	1.98	0.45
1:B:715:ASN:O	1:B:719:ILE:HD12	2.16	0.45
1:B:304:LEU:HD13	1:B:323:LEU:HA	1.99	0.45
1:A:459:TRP:HB2	1:A:613:ASN:HB3	1.99	0.45
1:B:68:LEU:HD22	1:B:687:LEU:HD13	2.00	0.44
1:A:303:THR:H	1:A:306:GLN:HE21	1.64	0.44
1:A:270:LEU:HB2	6:A:1264:HOH:O	2.18	0.44
1:B:90:TRP:CZ2	1:B:104:GLY:HA2	2.52	0.43
1:B:579:MET:HE1	1:B:650:ASP:HA	2.01	0.43
1:B:717:ARG:O	1:B:721:THR:HG23	2.19	0.43
1:B:464:THR:HG22	1:B:606:TRP:HA	2.01	0.42
1:B:248:MET:HG2	1:B:372:TRP:CE2	2.54	0.42
1:B:304:LEU:HA	1:B:307:ILE:HD12	2.01	0.42
1:A:248:MET:HG2	1:A:372:TRP:CE2	2.55	0.42
1:B:490:ASN:HB2	6:B:1145:HOH:O	2.19	0.42
1:A:109:LEU:HD11	1:A:562:PRO:HD2	2.02	0.41
1:B:184:GLU:HG3	1:B:320:PHE:CE1	2.56	0.41
1:A:63:LYS:HD2	1:B:69:ILE:CG2	2.50	0.41
1:B:347:ALA:O	1:B:351:LEU:HG	2.20	0.41
1:A:312:SER:O	1:A:355:LYS:HG3	2.20	0.41
1:A:643:THR:HA	1:A:710:VAL:O	2.21	0.41
1:B:129:ILE:HD11	1:B:492:LEU:HD23	2.02	0.40
1:A:717:ARG:O	1:A:721:THR:HG23	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 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	696/698 (100%)	677 (97%)	19 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	694/698 (99%)	672 (97%)	22 (3%)	0	100	100
All	All	1390/1396 (100%)	1349 (97%)	41 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	607/607 (100%)	574 (95%)	33 (5%)	20	17
1	B	605/607 (100%)	570 (94%)	35 (6%)	18	15
All	All	1212/1214 (100%)	1144 (94%)	68 (6%)	19	16

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LYS
1	A	91	LEU
1	A	154	GLU
1	A	156	LEU
1	A	160	LEU
1	A	171	GLU
1	A	175	GLN
1	A	189	GLN
1	A	197	LYS
1	A	260	ARG
1	A	274	LYS
1	A	278	LEU
1	A	298	LEU
1	A	314	GLU
1	A	318	LYS
1	A	333	VAL
1	A	355	LYS
1	A	368	ASN

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Mol	Chain	Res	Type
1	A	376	MET
1	A	379	VAL
1	A	384	ARG
1	A	442	LEU
1	A	483	ASP
1	A	497	LEU
1	A	498	GLU
1	A	519	SER
1	A	597	ASN
1	A	608	GLN
1	A	667	LYS
1	A	670	GLU
1	A	687	LEU
1	A	743	GLU
1	A	748	VAL
1	B	63	LYS
1	B	91	LEU
1	B	151	ARG
1	B	154	GLU
1	B	156	LEU
1	B	160	LEU
1	B	171	GLU
1	B	175	GLN
1	B	182	THR
1	B	189	GLN
1	B	197	LYS
1	B	260	ARG
1	B	278	LEU
1	B	298	LEU
1	B	333	VAL
1	B	338	THR
1	B	368	ASN
1	B	376	MET
1	B	379	VAL
1	B	394	ARG
1	B	434	GLU
1	B	442	LEU
1	B	483	ASP
1	B	490	ASN
1	B	497	LEU
1	B	498	GLU
1	B	597	ASN

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Mol	Chain	Res	Type
1	B	608	GLN
1	B	629	SER
1	B	667	LYS
1	B	687	LEU
1	B	736	LYS
1	B	743	GLU
1	B	747	ARG
1	B	748	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	306	GLN
1	A	368	ASN
1	A	415	ASN
1	A	490	ASN
1	A	494	ASN
1	A	509	ASN
1	A	550	ASN
1	A	597	ASN
1	A	619	GLN
1	A	642	ASN
1	A	662	GLN
1	A	688	ASN
1	B	105	ASN
1	B	213	ASN
1	B	310	ASN
1	B	368	ASN
1	B	415	ASN
1	B	452	GLN
1	B	494	ASN
1	B	509	ASN
1	B	550	ASN
1	B	551	GLN
1	B	597	ASN
1	B	619	GLN
1	B	642	ASN
1	B	662	GLN
1	B	688	ASN

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 ⓘ

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$
2	NAG	C	1	1,2	14,14,15	0.22	0	17,19,21	0.56	0
2	NAG	C	2	2	14,14,15	0.32	0	17,19,21	0.81	1 (5%)
2	NAG	D	1	1,2	14,14,15	0.31	0	17,19,21	0.57	0
2	NAG	D	2	2	14,14,15	0.30	0	17,19,21	0.87	1 (5%)

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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C1-O5-C5	2.98	116.18	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	2.75	115.87	112.19

There are no chirality outliers.

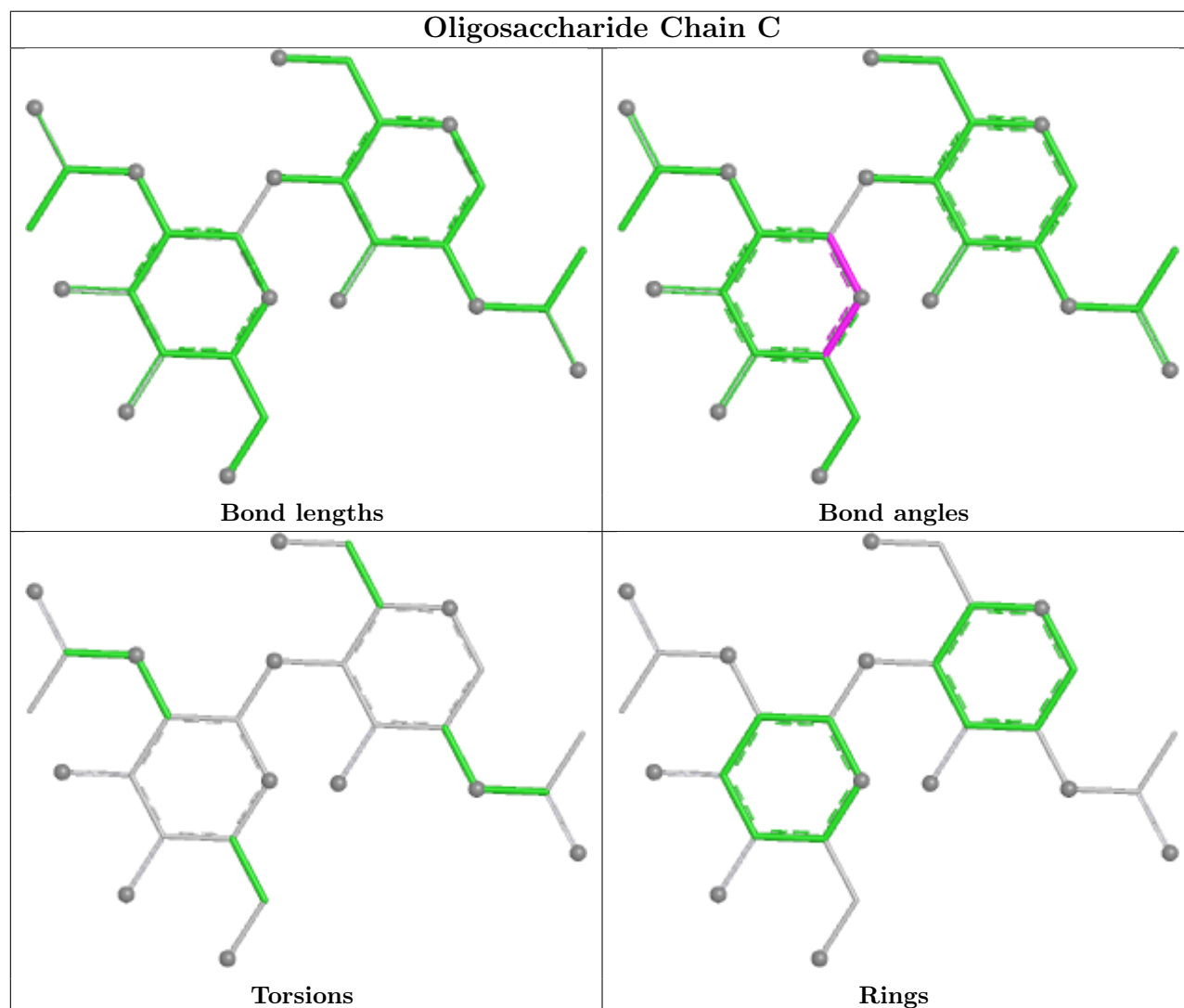
All (2) torsion outliers are listed below:

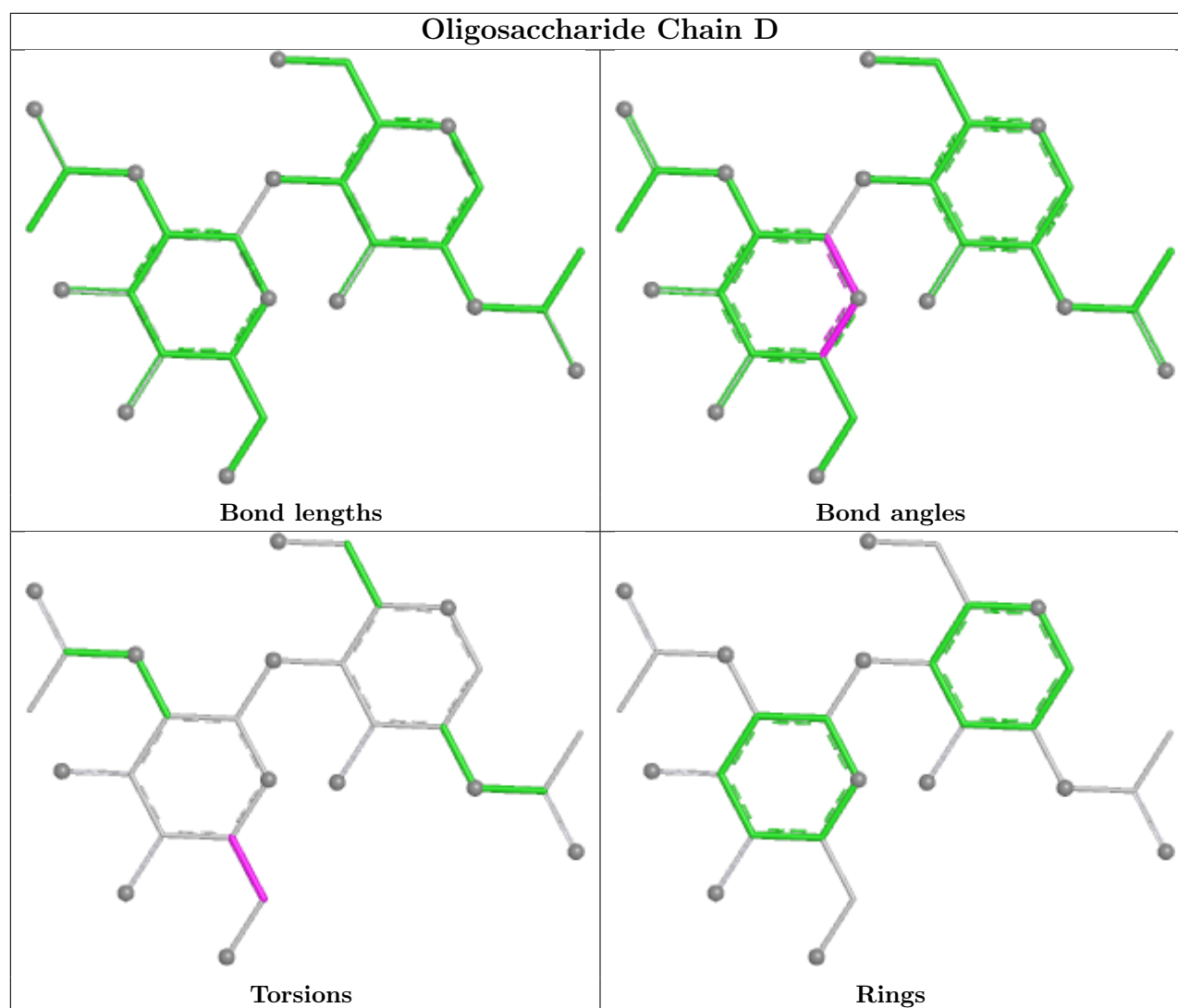
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\# Z > 2$
5	6LD	A	807	4	29,29,29	1.25	1 (3%)	37,38,38	1.13	2 (5%)
3	NAG	B	801	1	14,14,15	0.33	0	17,19,21	0.80	1 (5%)
3	NAG	A	802	1	14,14,15	0.30	0	17,19,21	0.79	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	805	1	14,14,15	0.33	0	17,19,21	0.61	0
5	6LD	B	807	4	29,29,29	1.04	1 (3%)	37,38,38	1.05	3 (8%)
3	NAG	B	805	1	14,14,15	0.36	0	17,19,21	0.50	0
3	NAG	B	802	1	14,14,15	0.31	0	17,19,21	0.74	1 (5%)
3	NAG	A	801	1	14,14,15	0.33	0	17,19,21	0.65	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
5	6LD	A	807	4	-	2/25/25/25	0/2/2/2
3	NAG	B	801	1	-	0/6/23/26	0/1/1/1
3	NAG	A	802	1	-	1/6/23/26	0/1/1/1
3	NAG	A	805	1	-	0/6/23/26	0/1/1/1
5	6LD	B	807	4	-	3/25/25/25	0/2/2/2
3	NAG	B	805	1	-	0/6/23/26	0/1/1/1
3	NAG	B	802	1	-	0/6/23/26	0/1/1/1
3	NAG	A	801	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	807	6LD	C10-C6	2.34	1.42	1.38
5	B	807	6LD	C8-C4	2.07	1.42	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	807	6LD	C11-C13-C14	-3.28	106.49	113.71
5	B	807	6LD	O20-C17-C19	-3.23	116.17	122.02
5	A	807	6LD	C16-C14-N15	-3.04	103.04	110.62
3	A	802	NAG	C1-O5-C5	2.87	116.03	112.19
3	B	801	NAG	C1-O5-C5	2.65	115.74	112.19
3	B	802	NAG	C1-O5-C5	2.62	115.69	112.19
5	B	807	6LD	C11-C13-C14	-2.60	107.99	113.71
5	B	807	6LD	C19-C17-N15	2.35	120.00	115.86

There are no chirality outliers.

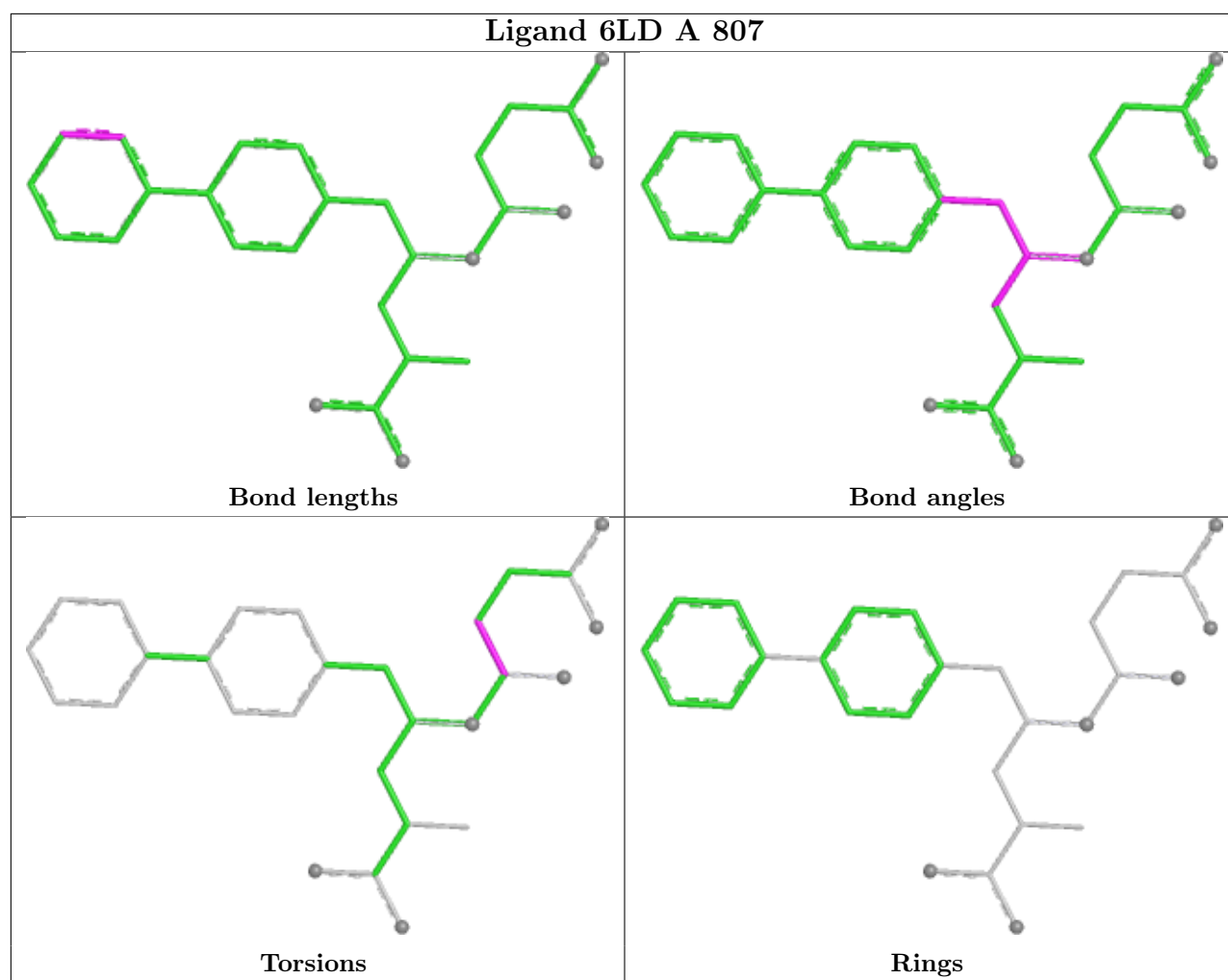
All (6) torsion outliers are listed below:

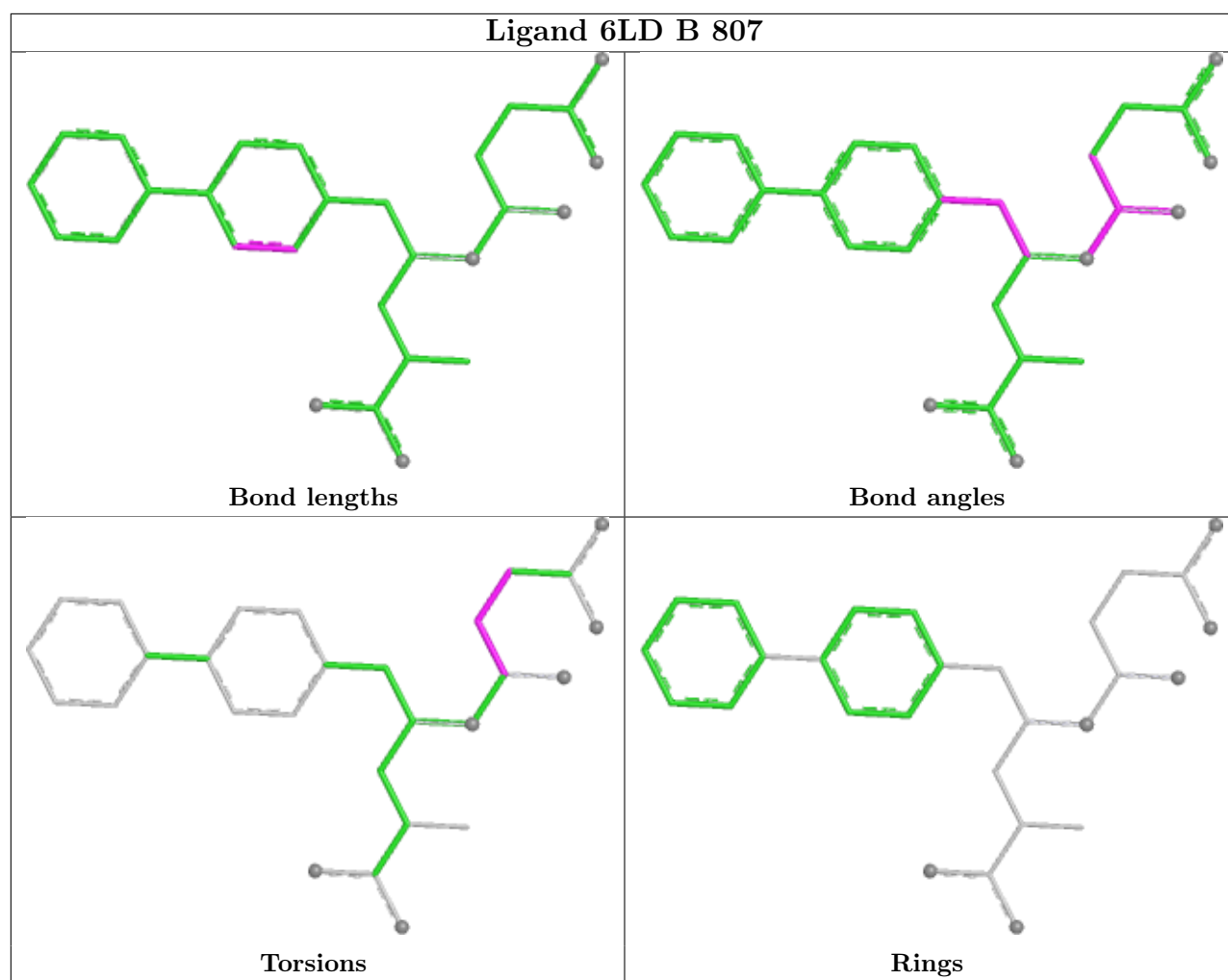
Mol	Chain	Res	Type	Atoms
5	B	807	6LD	N15-C17-C19-C23
5	B	807	6LD	O20-C17-C19-C23
5	A	807	6LD	N15-C17-C19-C23
5	A	807	6LD	O20-C17-C19-C23
3	A	802	NAG	O5-C5-C6-O6
5	B	807	6LD	C17-C19-C23-C26

There are no ring outliers.

No monomer is involved in short contacts.

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	696/698 (99%)	-0.11	2 (0%) 90 89	10, 34, 60, 83	2 (0%)
1	B	696/698 (99%)	0.52	63 (9%) 15 13	22, 45, 73, 88	0
All	All	1392/1396 (99%)	0.20	65 (4%) 36 35	10, 40, 70, 88	2 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	323	LEU	3.8
1	B	600	GLY	3.6
1	B	605	TRP	3.5
1	B	620	CYS	3.4
1	B	525	LEU	3.3
1	B	611	ALA	3.1
1	B	333	VAL	3.0
1	B	320	PHE	2.9
1	B	462	ALA	2.9
1	B	614	PHE	2.8
1	B	622	VAL	2.8
1	B	602	LEU	2.8
1	B	603	VAL	2.8
1	B	739	TYR	2.7
1	B	522	LEU	2.7
1	B	523	LYS	2.7
1	B	338	THR	2.6
1	B	307	ILE	2.6
1	B	317	GLY	2.5
1	B	204	VAL	2.5
1	B	618	SER	2.5
1	B	330	MET	2.5
1	B	337	ILE	2.5
1	B	327	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	319	PRO	2.4
1	B	340	GLU	2.4
1	B	747	ARG	2.4
1	B	170	THR	2.4
1	B	734	CYS	2.4
1	B	623	TYR	2.3
1	A	434	GLU	2.3
1	B	748	VAL	2.3
1	B	749	TRP	2.3
1	B	434	GLU	2.3
1	B	742	PRO	2.3
1	B	604	ASP	2.3
1	B	335	ILE	2.3
1	B	309	ASN	2.3
1	B	746	CYS	2.3
1	B	459	TRP	2.3
1	B	667	LYS	2.2
1	B	617	GLN	2.2
1	B	212	VAL	2.2
1	B	598	LYS	2.2
1	B	347	ALA	2.2
1	B	346	TYR	2.2
1	B	612	SER	2.2
1	B	606	TRP	2.2
1	B	343	VAL	2.1
1	B	591	ASP	2.1
1	B	450	PHE	2.1
1	B	736	LYS	2.1
1	B	464	THR	2.1
1	B	640	GLY	2.1
1	B	345	VAL	2.1
1	B	318	LYS	2.1
1	B	498	GLU	2.1
1	B	208	ASP	2.1
1	B	215	VAL	2.1
1	B	296	MET	2.0
1	A	233	CYS	2.0
1	B	468	ALA	2.0
1	B	613	ASN	2.0
1	B	206	THR	2.0
1	B	348	PRO	2.0

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

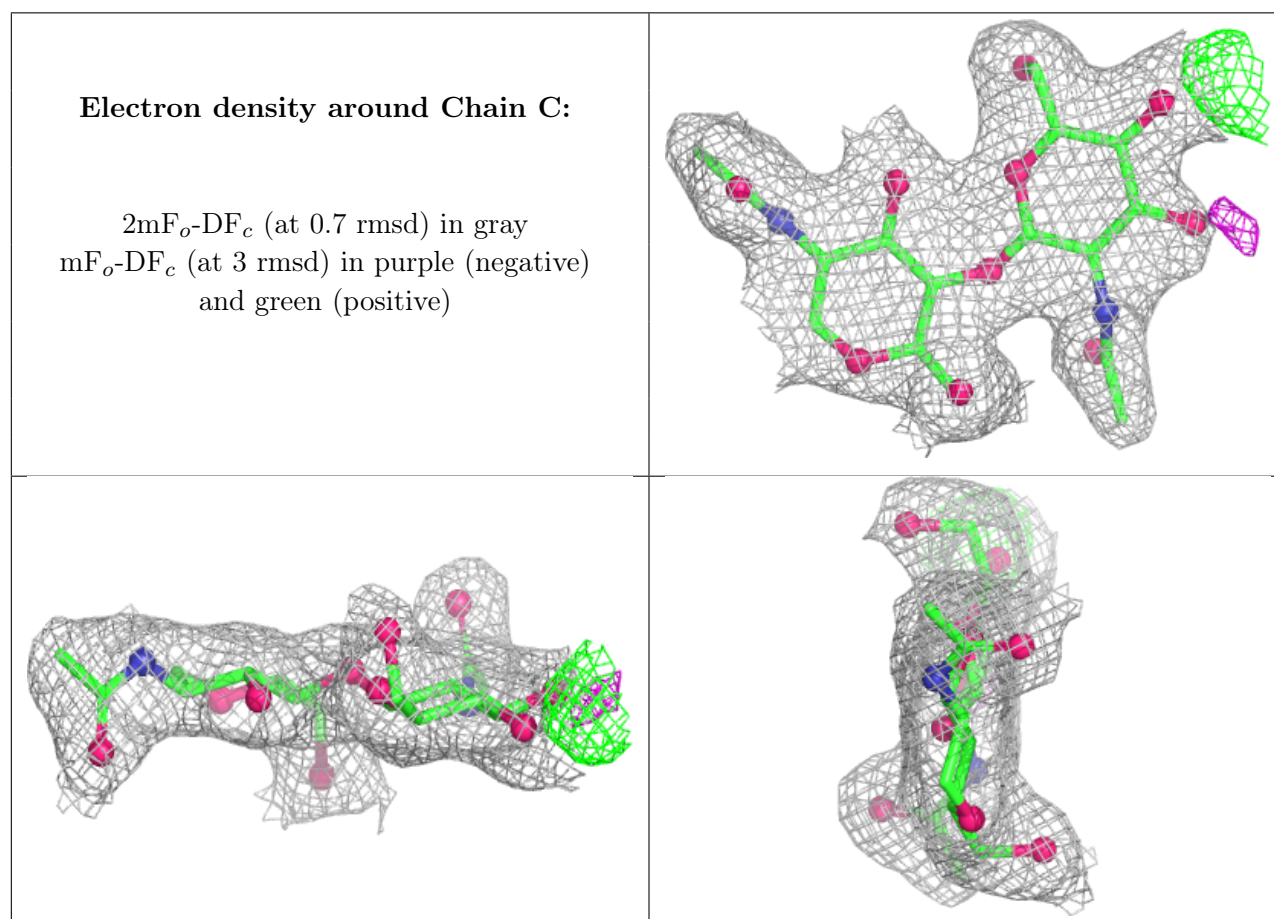
There are no non-standard protein/DNA/RNA residues in this entry.

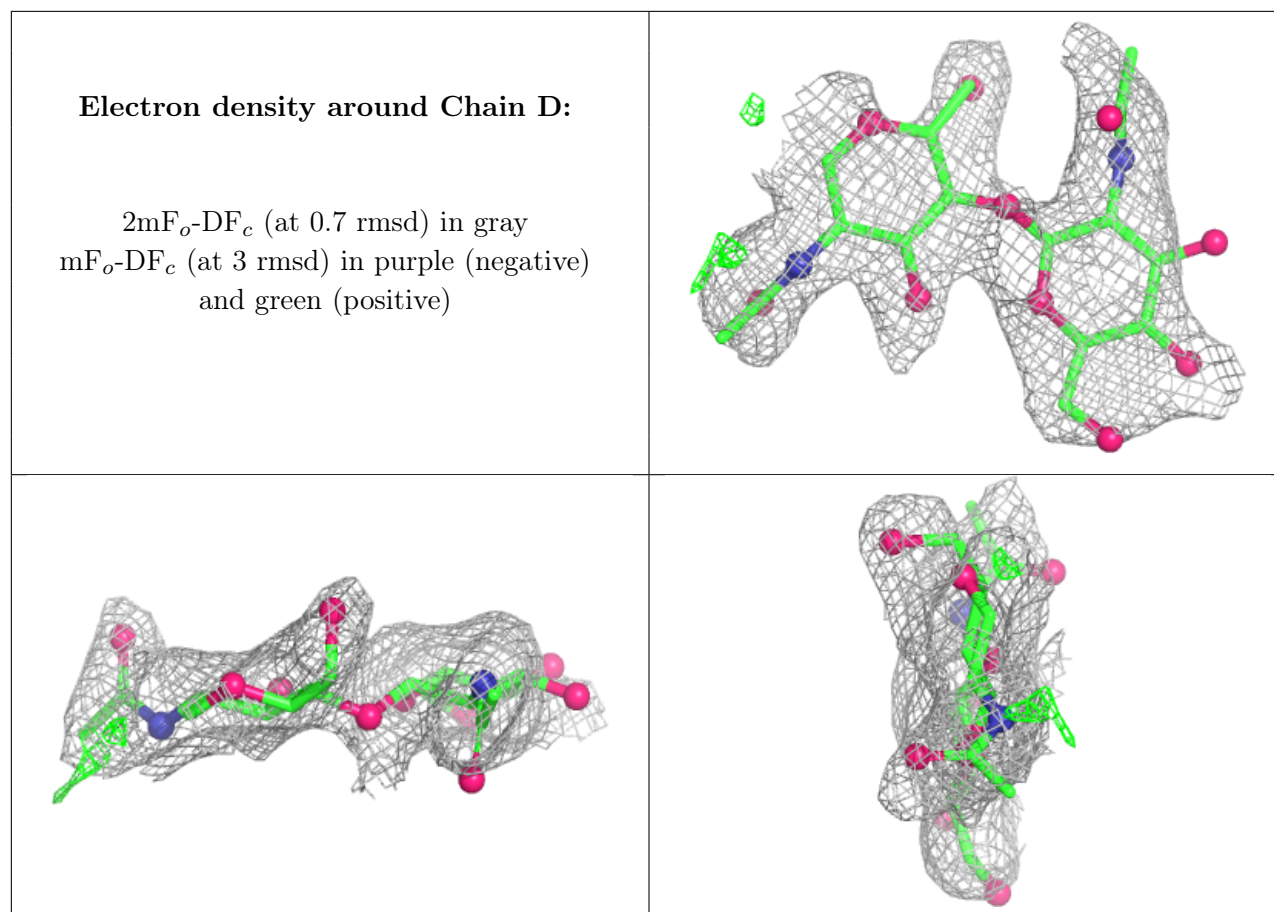
6.3 Carbohydrates [i](#)

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
2	NAG	D	2	14/15	0.70	0.14	95,97,100,103	0
2	NAG	D	1	14/15	0.77	0.16	73,82,87,92	0
2	NAG	C	2	14/15	0.83	0.10	43,48,53,54	0
2	NAG	C	1	14/15	0.95	0.06	27,34,38,41	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.





6.4 Ligands [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.

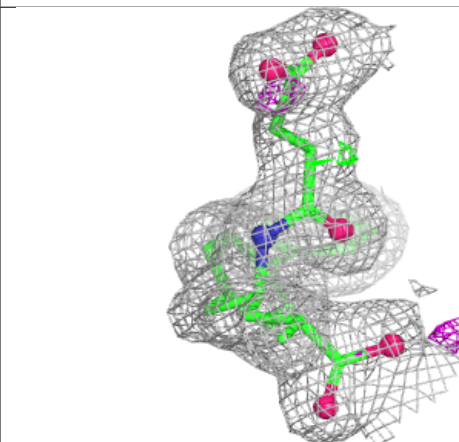
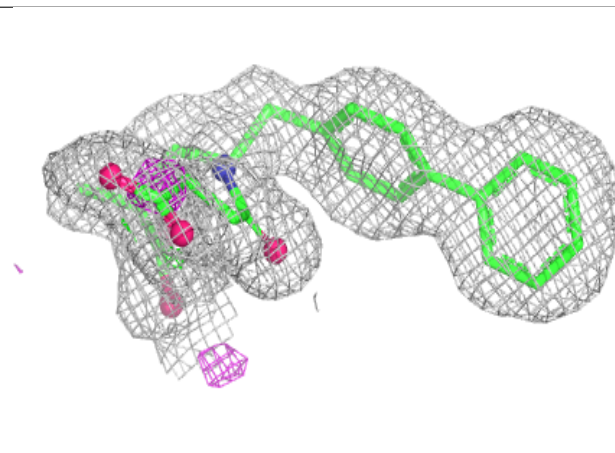
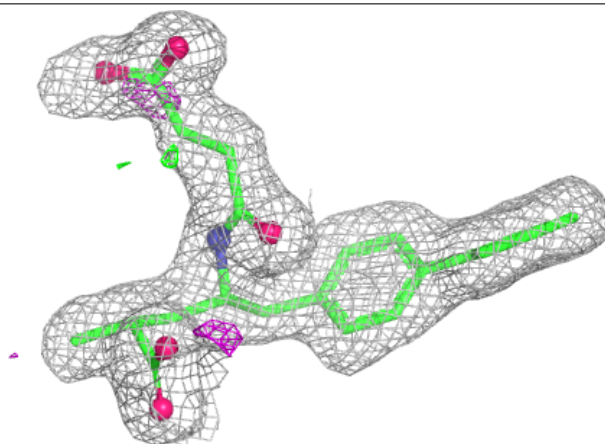
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	A	805	14/15	0.72	0.12	67,73,78,79	0
3	NAG	B	801	14/15	0.72	0.14	64,74,80,83	0
3	NAG	B	805	14/15	0.75	0.13	79,80,81,82	0
3	NAG	A	801	14/15	0.83	0.10	49,55,57,62	0
3	NAG	B	802	14/15	0.85	0.12	62,65,79,79	0
3	NAG	A	802	14/15	0.90	0.10	51,53,60,61	0
5	6LD	A	807	28/28	0.96	0.06	17,22,34,38	0
5	6LD	B	807	28/28	0.96	0.06	18,27,35,39	0
4	ZN	B	806	1/1	0.99	0.02	31,31,31,31	0
4	ZN	A	806	1/1	1.00	0.02	24,24,24,24	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.

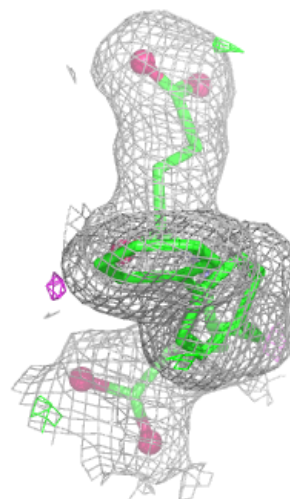
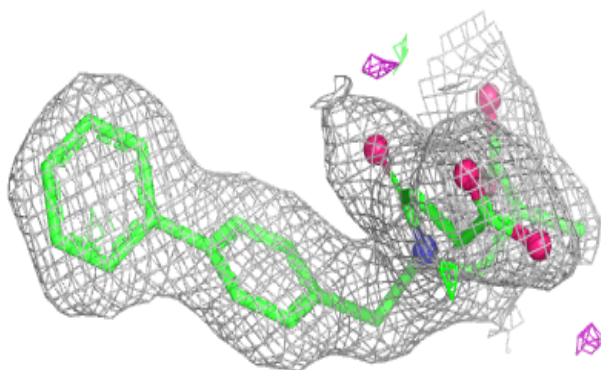
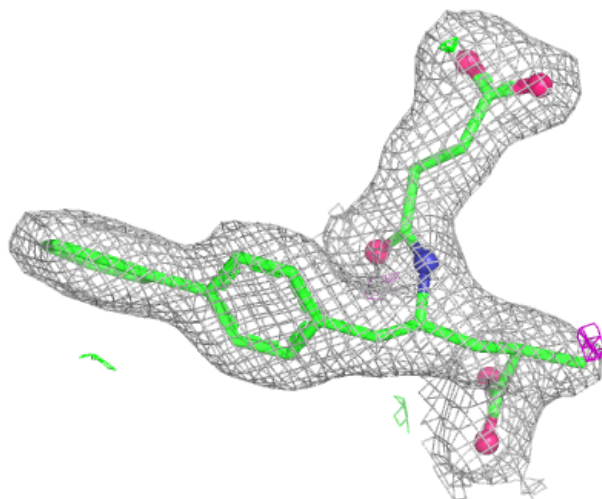
Electron density around 6LD A 807:

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



Electron density around 6LD B 807:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.