



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:38 PM UTC

PDB ID : 1N7D / pdb_00001n7d
Title : Extracellular domain of the LDL receptor
Authors : Rudenko, G.; Henry, L.; Henderson, K.; Ichtchenko, K.; Brown, M.S.; Goldstein, J.L.; Deisenhofer, J.
Deposited on : 2002-11-13
Resolution : 3.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

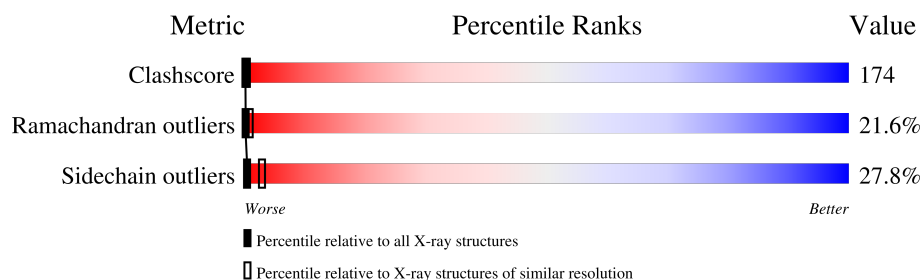
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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))
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	699	
2	B	5	
3	C	4	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	1	-	-	X	-
3	NAG	C	1	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	KEG	A	6003	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4956 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.

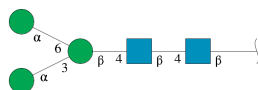
- Molecule 1 is a protein called Low-density lipoprotein receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	639	4702	2874	800	966	62	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	494	GLN	ASN	engineered mutation	UNP P01130
A	636	GLN	ASN	engineered mutation	UNP P01130

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	5	61	34	2	25	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

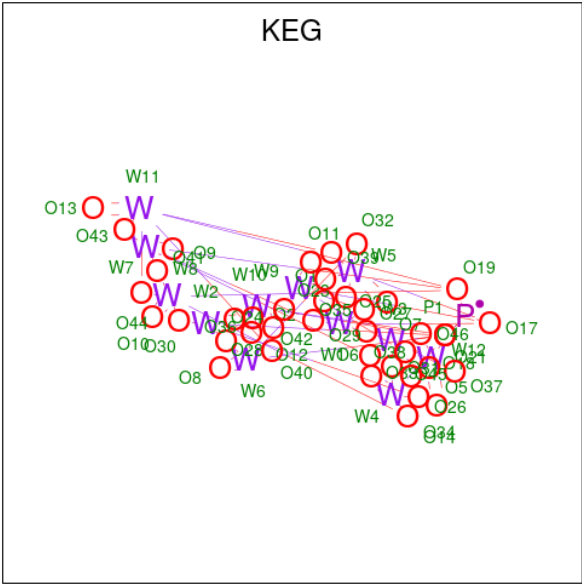


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	Ca	0	0
			8	8		

- Molecule 5 is 12-TUNGSTOPHOSPHATE (CCD ID: KEG) (formula: O₄₀PW₁₂).



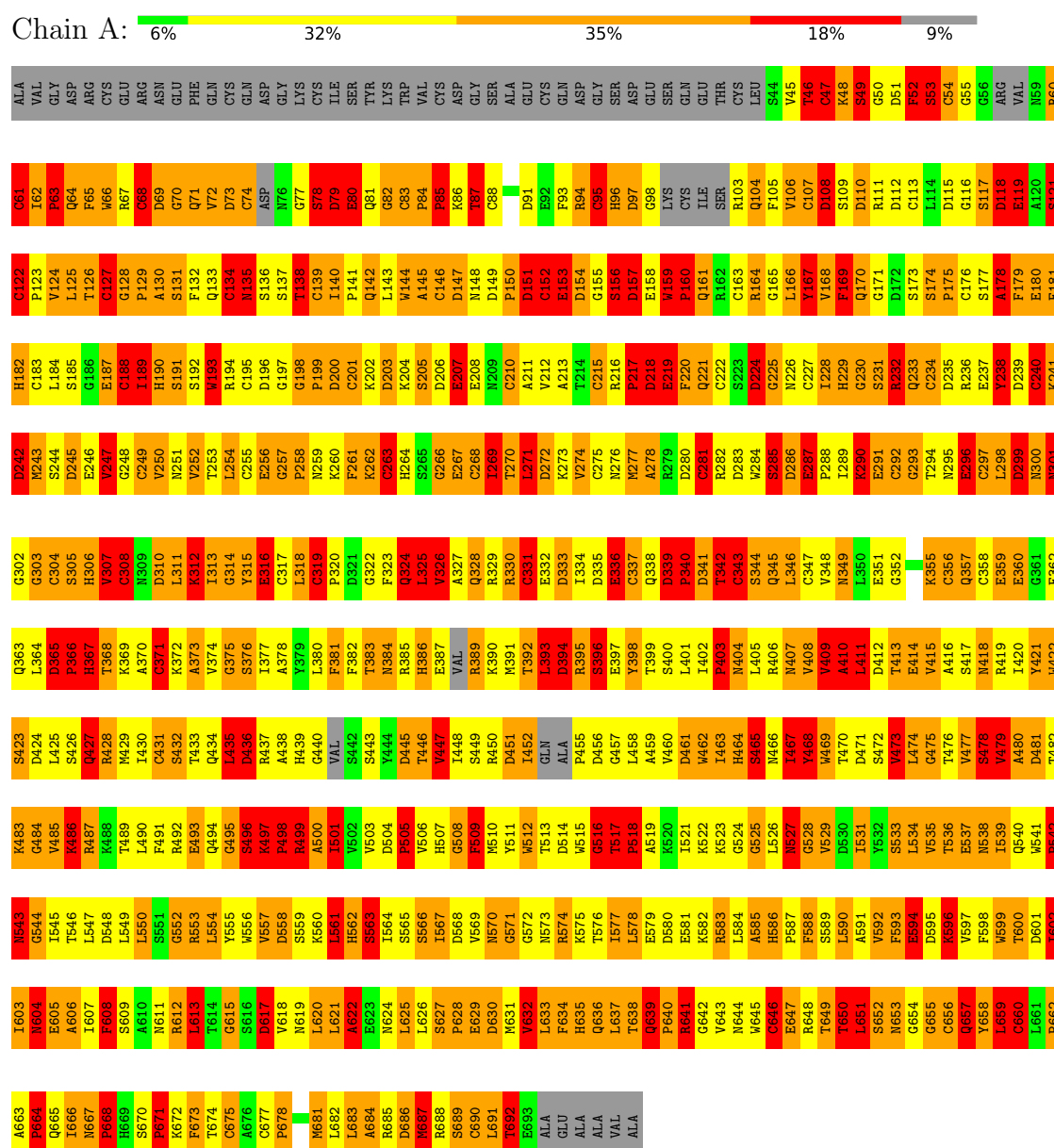
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	O	P	W	0	0
			53	40	1	12		
5	A	1	Total	O	P	W	0	0
			53	40	1	12		
5	A	1	Total	O	P	W	0	0
			29	21	1	7		

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. 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. 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.

Note EDS was not executed.

- Molecule 1: Low-density lipoprotein receptor



- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  20% 80%

MAG1	MAG2	BM13	MAN4	MAN5
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- Molecule 3: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  25% 75%

MAG1	MAG2	BM13	MAN4
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.29Å 185.29Å 85.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.30 – 3.70	Depositor
% Data completeness (in resolution range)	87.8 (45.30-3.70)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.381 , 0.382	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4956	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

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: BMA, KEG, MAN, CA, NAG

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	1.27	39/4796 (0.8%)	2.66	398/6528 (6.1%)

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	2

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	ILE	CA-C	9.75	1.64	1.52
1	A	140	ILE	CA-C	9.22	1.62	1.52
1	A	190	HIS	N-CA	8.19	1.56	1.45
1	A	54	CYS	N-CA	8.18	1.53	1.46
1	A	54	CYS	CA-C	7.49	1.57	1.53

The worst 5 of 398 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	PHE	N-CA-C	-20.73	82.65	111.87
1	A	473	VAL	N-CA-C	-19.62	79.47	108.71
1	A	341	ASP	N-CA-C	-18.42	84.72	112.54
1	A	649	THR	N-CA-C	-18.37	82.95	108.86
1	A	201	CYS	N-CA-C	-17.36	86.02	110.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	TYR	Sidechain
1	A	468	TYR	Sidechain

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	4702	0	4113	1574	4
2	B	61	0	50	25	0
3	C	50	0	43	31	0
4	A	8	0	0	0	0
5	A	135	0	0	19	12
All	All	4956	0	4206	1591	16

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 174.

The worst 5 of 1591 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:586:HIS:CB	1:A:602:ILE:HG21	1.37	1.55
1:A:251:ASN:CA	3:C:1:NAG:H82	1.11	1.54
1:A:586:HIS:HB2	1:A:602:ILE:CG2	1.39	1.51
1:A:251:ASN:HB3	3:C:1:NAG:C8	1.41	1.48
1:A:251:ASN:HB3	3:C:1:NAG:C7	1.43	1.47

The worst 5 of 16 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:6003:KEG:P1	5:A:6003:KEG:O17[4_556]	1.52	0.68
5:A:6003:KEG:P1	5:A:6003:KEG:O18[4_556]	1.52	0.68
5:A:6003:KEG:W1	5:A:6003:KEG:O1[4_556]	1.62	0.58
5:A:6003:KEG:W2	5:A:6003:KEG:O2[4_556]	1.63	0.57
5:A:6003:KEG:O18	5:A:6003:KEG:O18[4_556]	1.70	0.50

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	625/699 (89%)	334 (53%)	156 (25%)	135 (22%)	0 1

5 of 135 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	THR
1	A	47	CYS
1	A	49	SER
1	A	63	PRO
1	A	64	GLN

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	508/614 (83%)	367 (72%)	141 (28%)	0 3

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	577	ILE
1	A	608	PHE
1	A	657	GLN
1	A	242	ASP
1	A	238	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	345	GLN
1	A	407	ASN
1	A	543	ASN
1	A	507	HIS
1	A	538	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 ⓘ

9 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	B	1	1,2	14,14,15	0.78	0	17,19,21	0.69	0
2	NAG	B	2	2	14,14,15	0.88	1 (7%)	17,19,21	0.57	0
2	BMA	B	3	2	11,11,12	0.76	0	15,15,17	0.37	0
2	MAN	B	4	2	11,11,12	14.21	1 (9%)	15,15,17	4.97	2 (13%)
2	MAN	B	5	2	11,11,12	0.90	1 (9%)	15,15,17	0.66	0
3	NAG	C	1	1,3	14,14,15	0.78	0	17,19,21	0.68	0
3	NAG	C	2	3	14,14,15	0.87	1 (7%)	17,19,21	0.56	0
3	BMA	C	3	3	11,11,12	0.76	0	15,15,17	0.37	0
3	MAN	C	4	3	11,11,12	0.89	1 (9%)	15,15,17	0.67	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
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
2	MAN	B	5	2	-	2/2/19/22	0/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	MAN	O6-C6	47.09	3.40	1.42
2	B	5	MAN	C2-C3	2.32	1.56	1.52
2	B	2	NAG	C1-C2	2.30	1.55	1.52
3	C	4	MAN	C2-C3	2.29	1.56	1.52
3	C	2	NAG	C1-C2	2.27	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	MAN	O6-C6-C5	19.01	176.06	111.33
2	B	4	MAN	C1-O5-C5	2.18	115.11	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	5	MAN	C4-C5-C6-O6
3	C	4	MAN	C4-C5-C6-O6
2	B	5	MAN	O5-C5-C6-O6
3	C	4	MAN	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 56 short contacts:

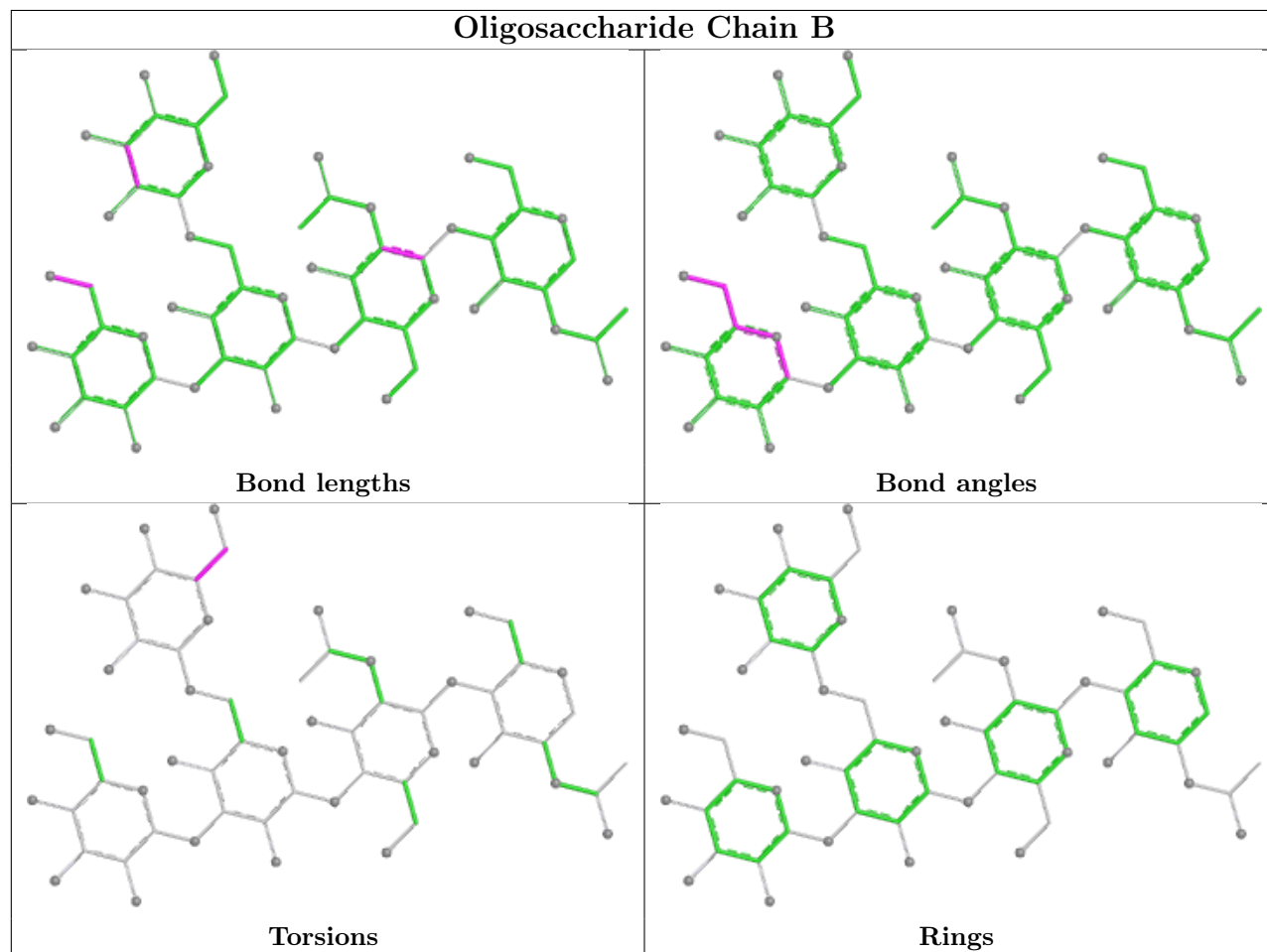
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	31	0

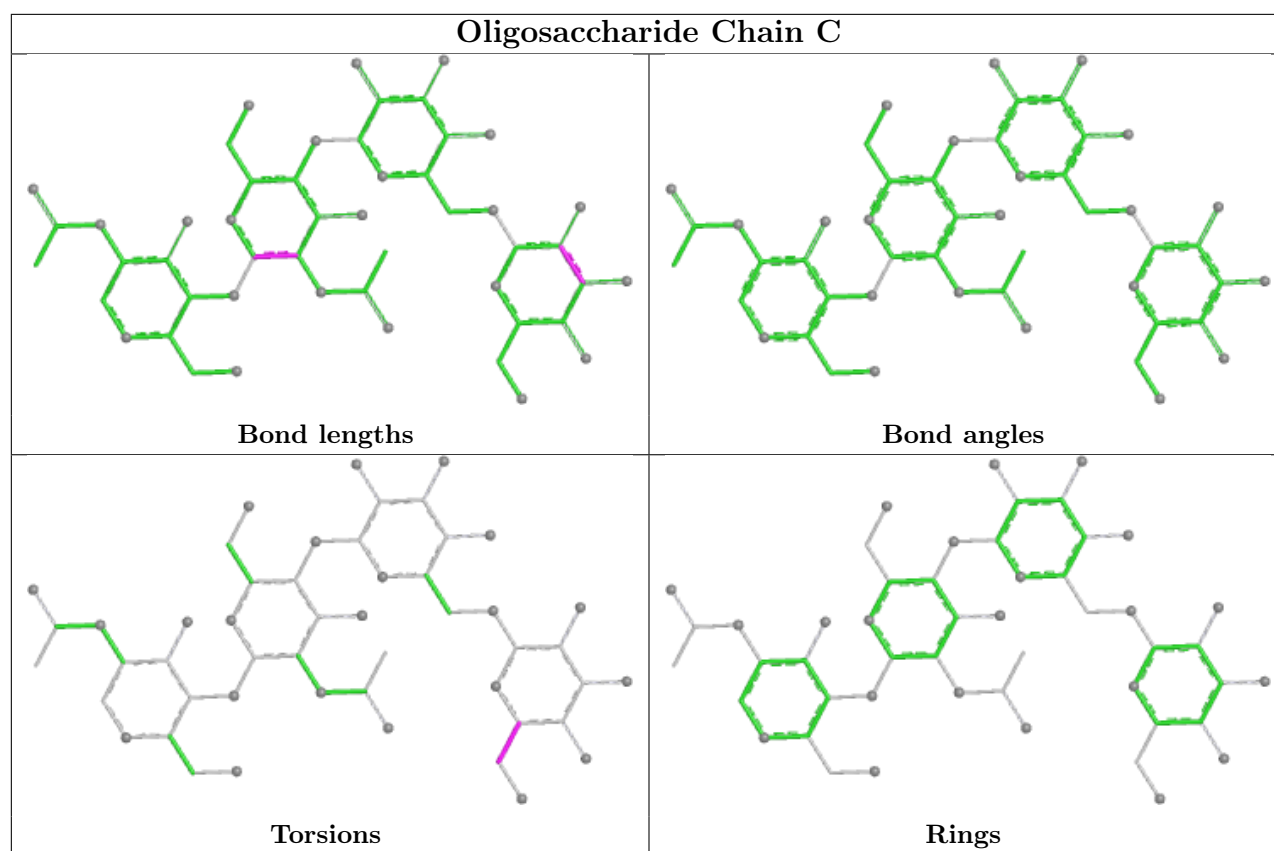
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	25	0

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 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 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	KEG	A	6001	-	76,76,76	3.13	42 (55%)	6,234,234	1.38	2 (33%)
5	KEG	A	6002	-	76,76,76	2.61	32 (42%)	6,234,234	2.76	3 (50%)
5	KEG	A	6003	-	21,37,76	1.27	5 (23%)	0,95,234	-	-

The worst 5 of 79 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	6001	KEG	P1-O18	-7.87	1.27	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	6001	KEG	W2-O28	-7.50	1.55	1.93
5	A	6001	KEG	W1-O29	-7.18	1.60	1.91
5	A	6001	KEG	W3-O33	-7.05	1.61	1.91
5	A	6001	KEG	W6-O36	-7.01	1.58	1.93

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	6002	KEG	O18-P1-O17	-4.86	99.61	108.92
5	A	6002	KEG	O19-P1-O18	3.89	116.37	108.92
5	A	6002	KEG	O19-P1-O17	2.33	113.38	108.92
5	A	6001	KEG	O19-P1-O18	-2.19	104.72	108.92
5	A	6001	KEG	O21-P1-O18	2.09	112.92	108.92

There are no chirality outliers.

There are no torsion outliers.

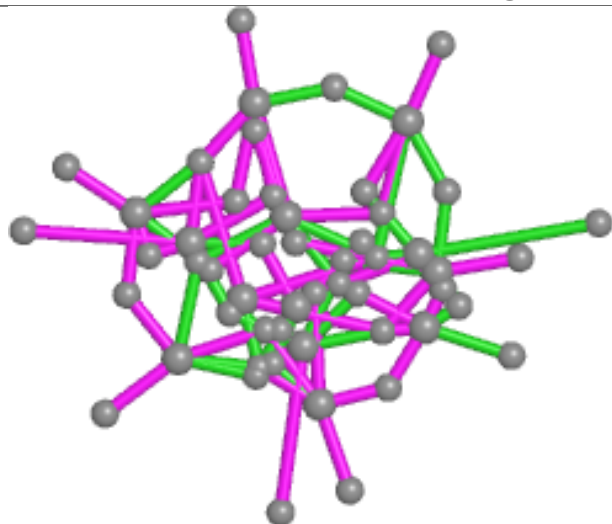
There are no ring outliers.

3 monomers are involved in 31 short contacts:

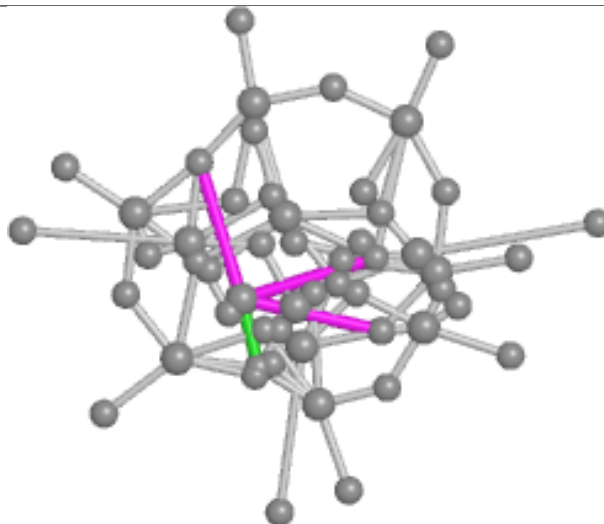
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	6001	KEG	6	0
5	A	6002	KEG	7	0
5	A	6003	KEG	6	12

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.

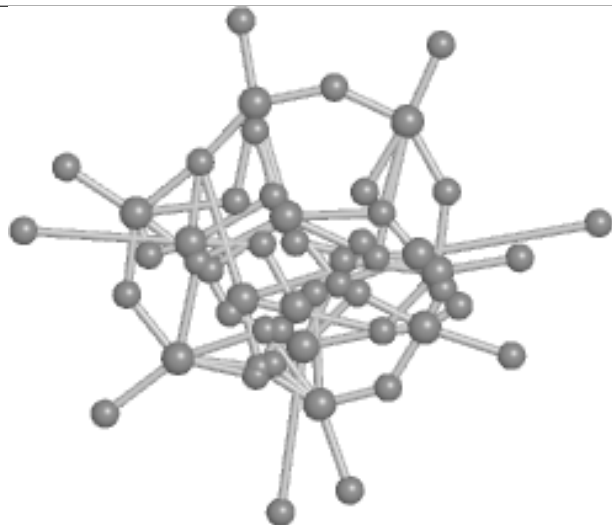
Ligand KEG A 6001



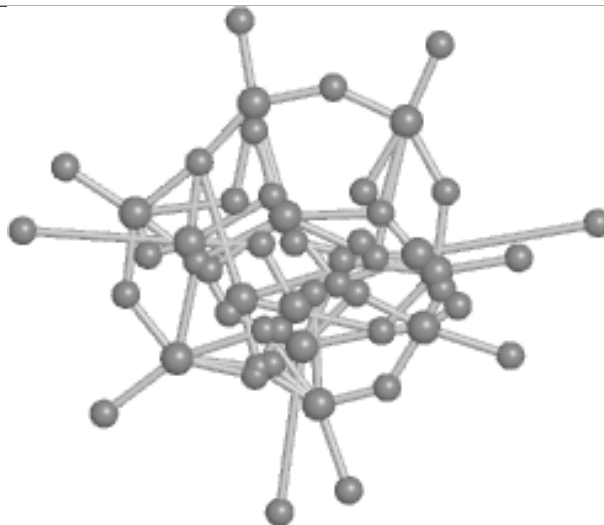
Bond lengths



Bond angles

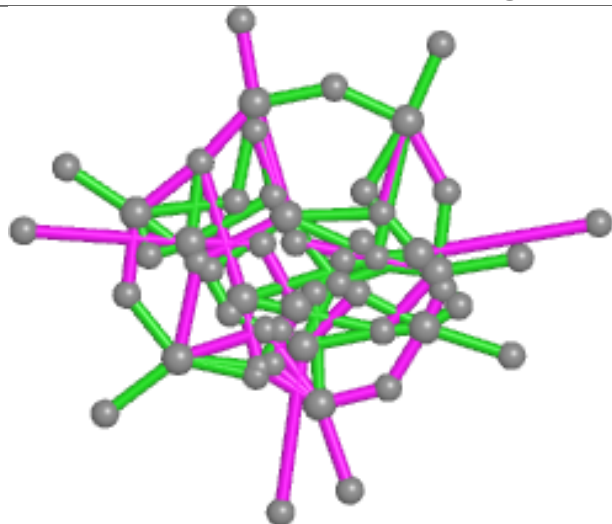


Torsions

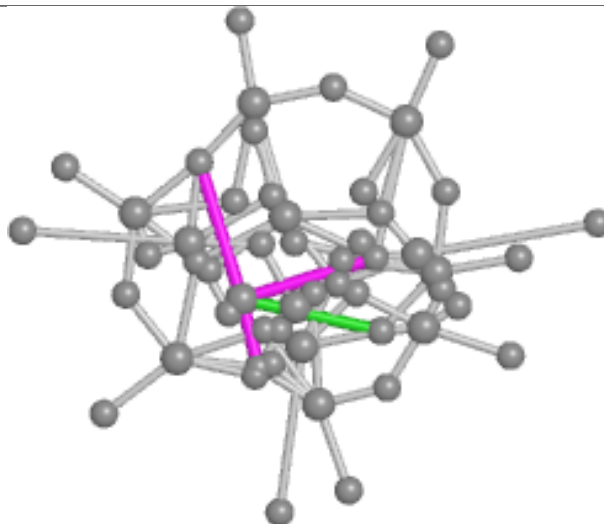


Rings

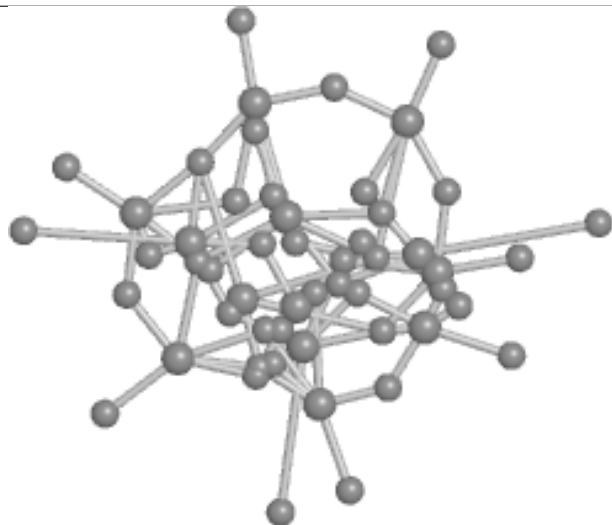
Ligand KEG A 6002



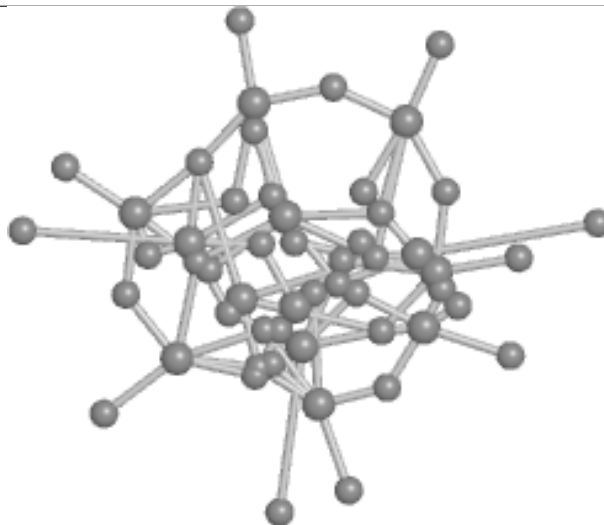
Bond lengths



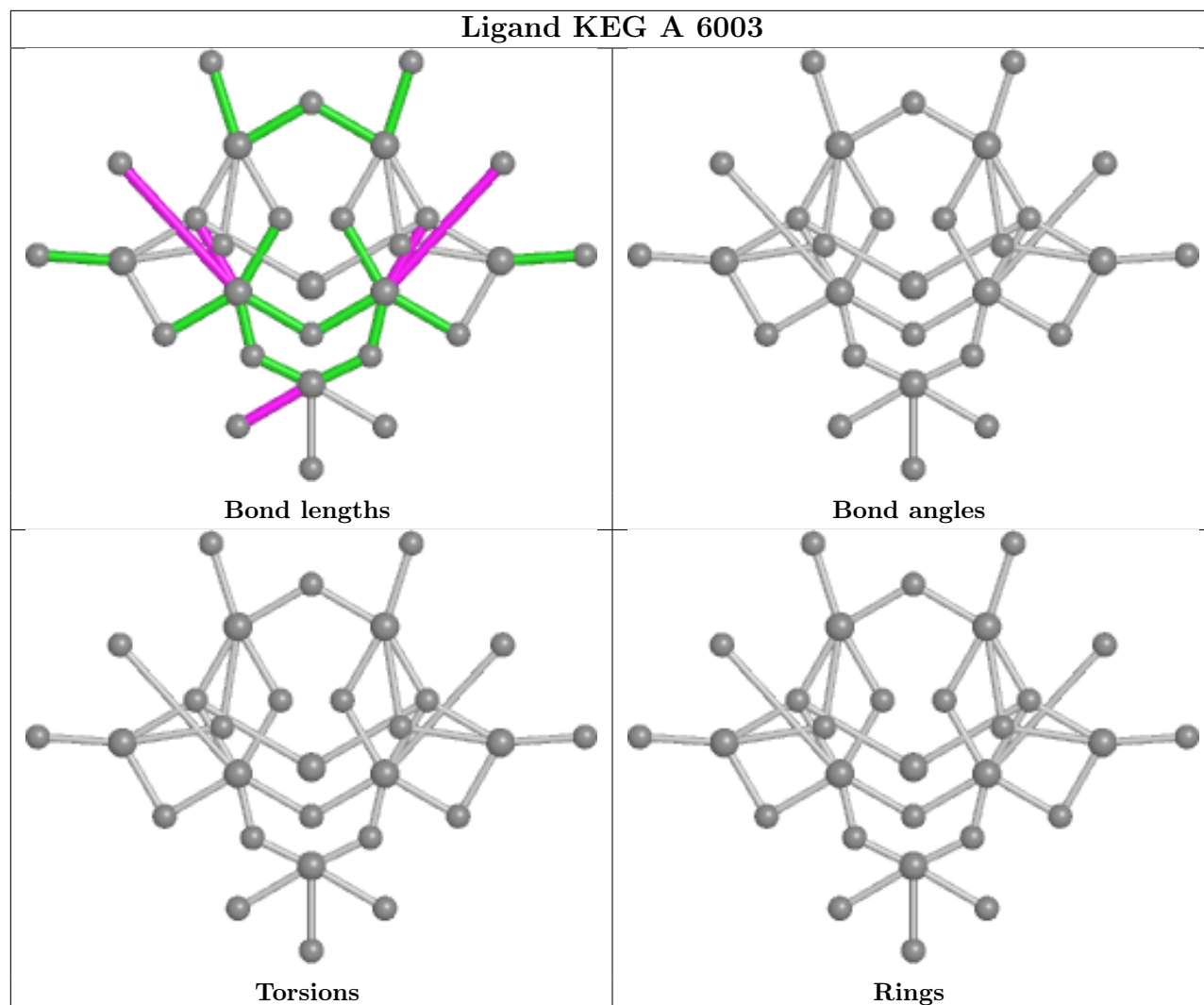
Bond angles



Torsions



Rings



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.