



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:22 PM UTC

PDB ID : 9HL2 / pdb_00009hl2
Title : Structure of A56/K2 (vaccinia virus)
Authors : Vernuccio, R.; Meola, A.; Guardado-Calvo, P.
Deposited on : 2024-12-04
Resolution : 2.80 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

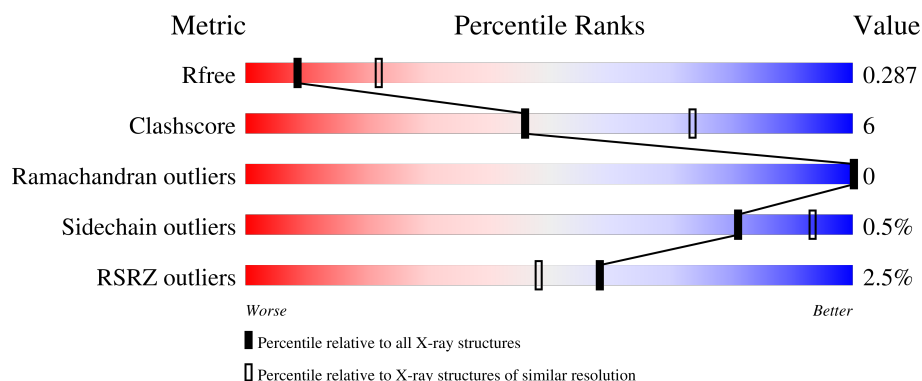
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	413	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>14%</div> <div>13%</div> </div> </div>
2	B	139	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>13%</div> <div>18%</div> </div> </div>
3	C	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
4	D	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3926 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 Superinfection exclusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	360	2913	1873	481	542	17	0	1	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	109	SER	CYS	conflict	UNP P18384
A	370	GLY	-	expression tag	UNP P18384
A	371	SER	-	expression tag	UNP P18384
A	372	GLY	-	expression tag	UNP P18384
A	373	LEU	-	expression tag	UNP P18384
A	374	VAL	-	expression tag	UNP P18384
A	375	PRO	-	expression tag	UNP P18384
A	376	ARG	-	expression tag	UNP P18384
A	377	GLY	-	expression tag	UNP P18384
A	378	SER	-	expression tag	UNP P18384
A	379	GLY	-	expression tag	UNP P18384
A	380	SER	-	expression tag	UNP P18384
A	381	ALA	-	expression tag	UNP P18384
A	382	GLY	-	expression tag	UNP P18384
A	383	TRP	-	expression tag	UNP P18384
A	384	SER	-	expression tag	UNP P18384
A	385	HIS	-	expression tag	UNP P18384
A	386	PRO	-	expression tag	UNP P18384
A	387	GLN	-	expression tag	UNP P18384
A	388	PHE	-	expression tag	UNP P18384
A	389	GLU	-	expression tag	UNP P18384
A	390	LYS	-	expression tag	UNP P18384
A	391	GLY	-	expression tag	UNP P18384
A	392	GLY	-	expression tag	UNP P18384
A	393	GLY	-	expression tag	UNP P18384
A	394	SER	-	expression tag	UNP P18384
A	395	GLY	-	expression tag	UNP P18384

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Chain	Residue	Modelled	Actual	Comment	Reference
A	396	GLY	-	expression tag	UNP P18384
A	397	GLY	-	expression tag	UNP P18384
A	398	SER	-	expression tag	UNP P18384
A	399	GLY	-	expression tag	UNP P18384
A	400	GLY	-	expression tag	UNP P18384
A	401	GLY	-	expression tag	UNP P18384
A	402	SER	-	expression tag	UNP P18384
A	403	TRP	-	expression tag	UNP P18384
A	404	SER	-	expression tag	UNP P18384
A	405	HIS	-	expression tag	UNP P18384
A	406	PRO	-	expression tag	UNP P18384
A	407	GLN	-	expression tag	UNP P18384
A	408	PHE	-	expression tag	UNP P18384
A	409	GLU	-	expression tag	UNP P18384
A	410	LYS	-	expression tag	UNP P18384
A	411	GLY	-	expression tag	UNP P18384
A	412	THR	-	expression tag	UNP P18384
A	413	GLY	-	expression tag	UNP P18384
A	414	GLY	-	expression tag	UNP P18384
A	415	LEU	-	expression tag	UNP P18384
A	416	ASN	-	expression tag	UNP P18384
A	417	ASP	-	expression tag	UNP P18384
A	418	ILE	-	expression tag	UNP P18384
A	419	PHE	-	expression tag	UNP P18384
A	420	GLU	-	expression tag	UNP P18384
A	421	ALA	-	expression tag	UNP P18384
A	422	GLN	-	expression tag	UNP P18384
A	423	LYS	-	expression tag	UNP P18384
A	424	ILE	-	expression tag	UNP P18384
A	425	GLU	-	expression tag	UNP P18384
A	426	TRP	-	expression tag	UNP P18384
A	427	HIS	-	expression tag	UNP P18384
A	428	GLU	-	expression tag	UNP P18384

- Molecule 2 is a protein called Protein OPG185.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	114	Total	C	N	O	S	0	0	0
			905	571	138	192	4			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	15	ARG	-	expression tag	UNP Q01218
B	16	SER	-	expression tag	UNP Q01218
B	134	GLY	-	expression tag	UNP Q01218
B	135	SER	-	expression tag	UNP Q01218
B	136	GLY	-	expression tag	UNP Q01218
B	137	LEU	-	expression tag	UNP Q01218
B	138	VAL	-	expression tag	UNP Q01218
B	139	PRO	-	expression tag	UNP Q01218
B	140	ARG	-	expression tag	UNP Q01218
B	141	GLY	-	expression tag	UNP Q01218
B	142	SER	-	expression tag	UNP Q01218
B	143	GLY	-	expression tag	UNP Q01218
B	144	SER	-	expression tag	UNP Q01218
B	145	GLY	-	expression tag	UNP Q01218
B	146	HIS	-	expression tag	UNP Q01218
B	147	HIS	-	expression tag	UNP Q01218
B	148	HIS	-	expression tag	UNP Q01218
B	149	HIS	-	expression tag	UNP Q01218
B	150	HIS	-	expression tag	UNP Q01218
B	151	HIS	-	expression tag	UNP Q01218
B	152	HIS	-	expression tag	UNP Q01218
B	153	HIS	-	expression tag	UNP Q01218

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



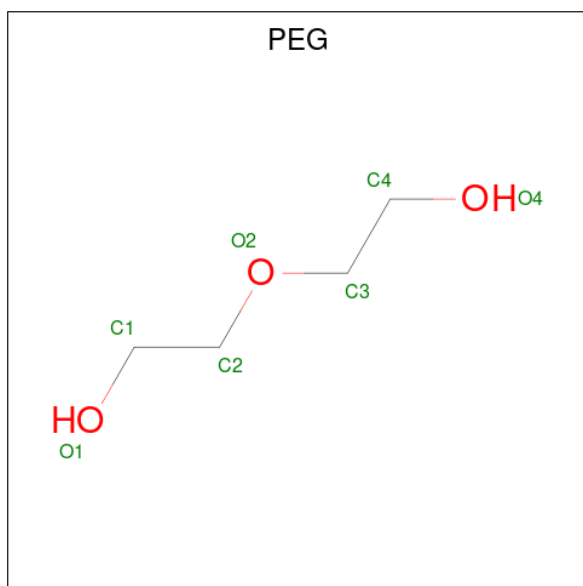
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 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
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).

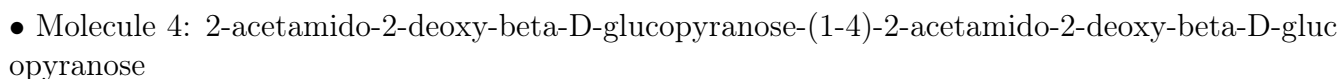
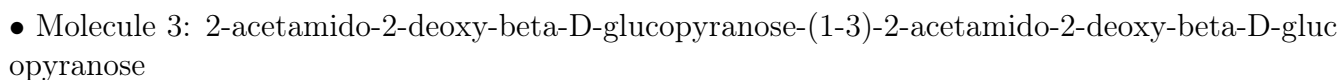


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	20	Total	O	0	0
			20	20		
6	B	4	Total	O	0	0
			4	4		

- Molecule 1: Superinfection exclusion protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	74.37Å 74.37Å 216.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.70 – 2.80 37.70 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (37.70-2.80) 99.8 (37.70-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.233 , 0.287 0.233 , 0.287	Depositor DCC
R_{free} test set	778 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	64.7	Xtriage
Anisotropy	0.632	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3926	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: PEG, 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	0.09	0/2981	0.25	0/4032
2	B	0.10	0/923	0.30	0/1260
All	All	0.09	0/3904	0.26	0/5292

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2913	0	2892	36	0
2	B	905	0	861	11	0
3	C	28	0	25	1	0
4	D	28	0	25	0	0
5	A	21	0	30	0	0
5	B	7	0	10	1	0
6	A	20	0	0	0	0
6	B	4	0	0	0	0
All	All	3926	0	3843	45	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 6.

All (45) 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:26:ILE:HG22	1:A:30:LYS:HE2	1.81	0.63
2:B:30:ALA:HB2	2:B:93:LEU:HD11	1.83	0.61
1:A:198:MET:HE3	1:A:266:LYS:HD2	1.84	0.59
1:A:34:ASP:OD2	1:A:276:ARG:NH2	2.26	0.59
1:A:94:THR:HG21	1:A:224:TYR:HB3	1.85	0.58
1:A:94:THR:HG22	1:A:171:GLY:HA2	1.85	0.58
1:A:99:THR:OG1	1:A:166:THR:OG1	2.19	0.57
1:A:267:LEU:HD12	1:A:268:PRO:HD2	1.85	0.57
1:A:151:ASP:H	1:A:154:MET:HE2	1.70	0.56
1:A:181:LYS:HE2	1:A:199:MET:HG2	1.90	0.54
1:A:128:PHE:HA	1:A:132:ALA:HB2	1.89	0.54
1:A:289:MET:HG3	1:A:297:PHE:HZ	1.73	0.53
1:A:54:PRO:HB3	1:A:300:MET:HE3	1.91	0.52
1:A:281:ILE:HD11	1:A:285:MET:HE3	1.92	0.52
1:A:38:VAL:HG21	1:A:272:ILE:HB	1.93	0.51
1:A:79:THR:HG23	2:B:60:ALA:HB1	1.92	0.51
1:A:332:VAL:HG22	1:A:333:ALA:H	1.75	0.51
1:A:168:TYR:HD1	1:A:326:GLU:HG2	1.76	0.51
1:A:347:PRO:HG2	1:A:365:LYS:HD3	1.95	0.49
1:A:66:THR:HG21	1:A:285:MET:HB3	1.95	0.48
1:A:354:HIS:CE1	1:A:356:ILE:HB	2.49	0.48
1:A:163:ILE:HB	1:A:331:MET:HE3	1.97	0.47
1:A:348:PHE:HD1	1:A:368:SER:HB2	1.81	0.46
2:B:50:LYS:HB3	2:B:54:SER:HB3	1.97	0.46
2:B:43:VAL:HG22	2:B:107:MET:HG2	1.96	0.46
1:A:75:GLY:HA3	2:B:108:THR:HG21	1.98	0.46
1:A:28:ALA:HA	1:A:281:ILE:HG12	1.96	0.46
1:A:235:ILE:HG12	1:A:373:LEU:HB2	1.98	0.45
1:A:76:PRO:O	1:A:79:THR:HB	2.15	0.45
1:A:290:PHE:HA	1:A:307:ILE:O	2.17	0.45
1:A:94:THR:HG22	1:A:172:ILE:H	1.81	0.45
2:B:51:GLU:HB3	2:B:100:THR:HB	1.98	0.44
2:B:36:ARG:HD3	2:B:84:LEU:HA	2.00	0.44
1:A:243:THR:O	1:A:246:ILE:HG22	2.18	0.43
1:A:84:GLY:HA2	1:A:357:THR:HG21	2.00	0.43
1:A:217:TYR:CD1	1:A:236:GLY:HA3	2.53	0.43
1:A:356:ILE:HG13	3:C:1:NAG:H61	2.01	0.43
2:B:78:ASP:OD2	2:B:89:THR:OG1	2.30	0.43
2:B:45:MET:HE2	5:B:201:PEG:H22	2.00	0.43
1:A:181:LYS:HE3	1:A:181:LYS:HB3	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ILE:HD11	1:A:366:VAL:HG22	2.01	0.42
2:B:50:LYS:HG3	2:B:52:PRO:HD2	2.01	0.42
2:B:61:LYS:HA	2:B:61:LYS:HD3	1.86	0.42
1:A:307:ILE:HD13	1:A:331:MET:HB3	2.02	0.41
1:A:47:SER:HB3	1:A:331:MET:HE2	2.03	0.41

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	359/413 (87%)	349 (97%)	10 (3%)	0	100	100
2	B	112/139 (81%)	105 (94%)	7 (6%)	0	100	100
All	All	471/552 (85%)	454 (96%)	17 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	323/358 (90%)	322 (100%)	1 (0%)	86	95
2	B	105/125 (84%)	104 (99%)	1 (1%)	68	88
All	All	428/483 (89%)	426 (100%)	2 (0%)	81	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	THR
2	B	49	TYR

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

Mol	Chain	Res	Type
1	A	36	ASN
1	A	117	GLN
2	B	53	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	$\# Z > 2$
3	NAG	C	1	1,3	14,14,15	0.66	0	17,19,21	2.15	4 (23%)
3	NAG	C	2	3	14,14,15	0.74	0	17,19,21	2.11	6 (35%)
4	NAG	D	1	2,4	14,14,15	0.69	0	17,19,21	0.84	0
4	NAG	D	2	4	14,14,15	0.68	0	17,19,21	1.30	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
3	NAG	C	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
4	NAG	D	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C1-O5-C5	6.91	121.45	112.19
3	C	2	NAG	C4-C3-C2	4.67	117.86	111.02
3	C	2	NAG	C2-N2-C7	3.68	127.83	122.90
4	D	2	NAG	C2-N2-C7	3.62	127.75	122.90
3	C	2	NAG	C1-O5-C5	-3.54	107.44	112.19
3	C	2	NAG	C3-C4-C5	3.29	116.20	110.23
3	C	1	NAG	C3-C4-C5	2.91	115.51	110.23
3	C	2	NAG	O5-C1-C2	-2.86	106.86	111.29
3	C	1	NAG	O5-C1-C2	2.68	115.43	111.29
3	C	1	NAG	C2-N2-C7	2.24	125.91	122.90
3	C	2	NAG	O4-C4-C3	-2.17	105.27	110.38

There are no chirality outliers.

All (9) torsion outliers are listed below:

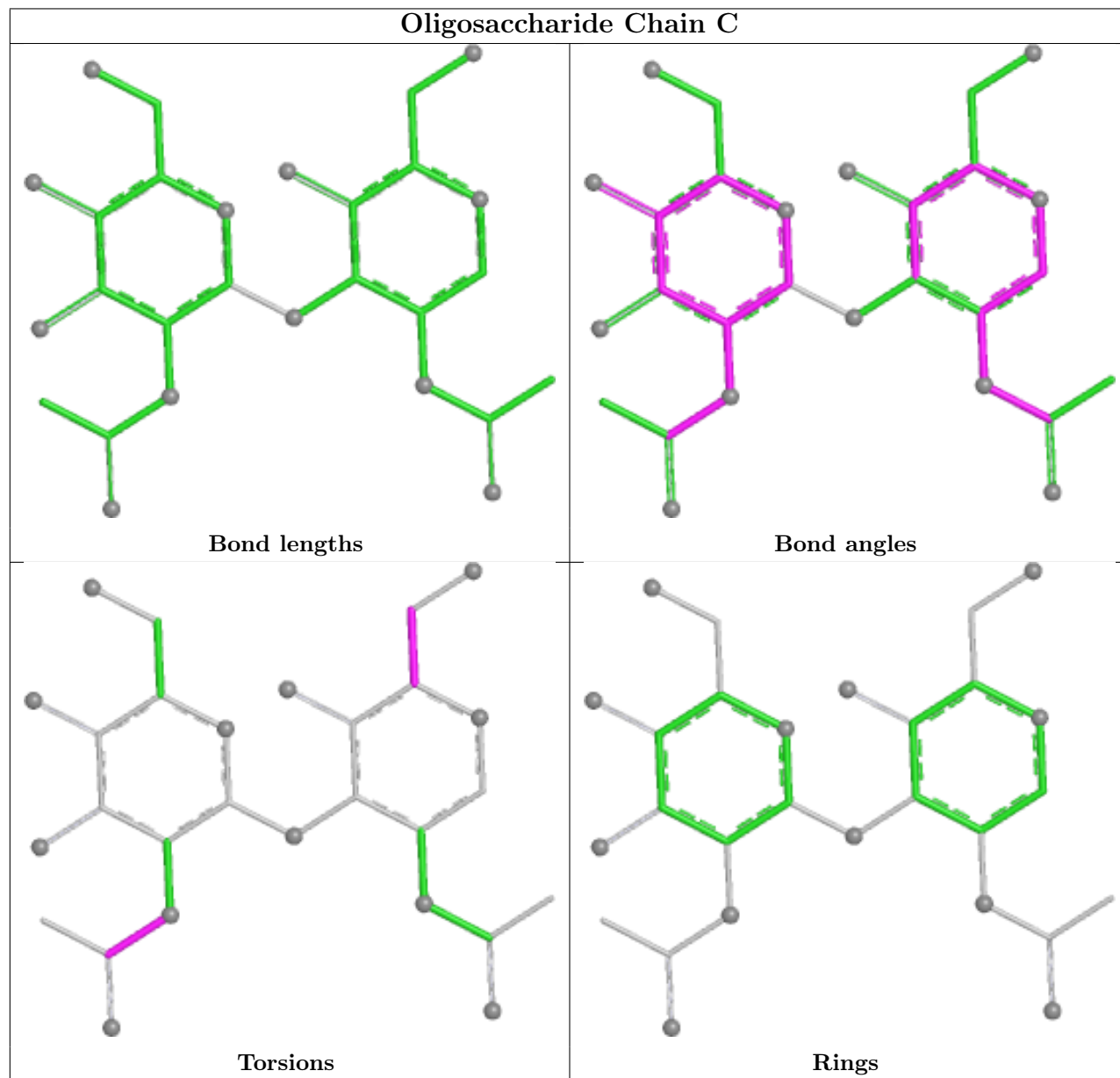
Mol	Chain	Res	Type	Atoms
4	D	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	D	2	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
4	D	2	NAG	C3-C2-N2-C7
4	D	2	NAG	C1-C2-N2-C7

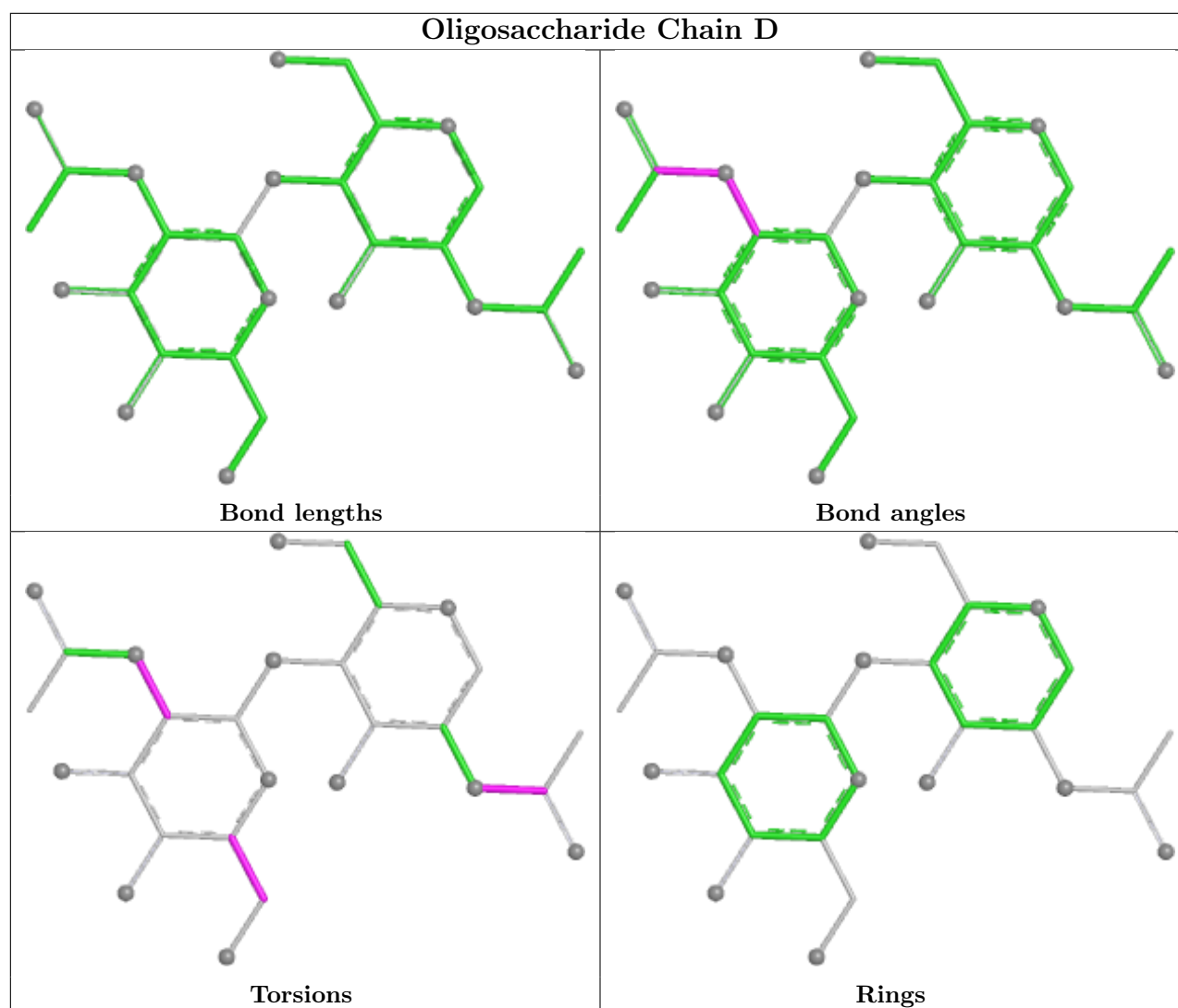
There are no ring outliers.

1 monomer is involved in 1 short contact:

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

4 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	$\# Z > 2$
5	PEG	A	501	-	6,6,6	0.25	0	5,5,5	0.27	0
5	PEG	A	502	-	6,6,6	0.25	0	5,5,5	0.26	0
5	PEG	B	201	-	6,6,6	0.26	0	5,5,5	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PEG	A	503	-	6,6,6	0.25	0	5,5,5	0.26	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	PEG	A	501	-	-	2/4/4/4	-
5	PEG	A	502	-	-	0/4/4/4	-
5	PEG	B	201	-	-	0/4/4/4	-
5	PEG	A	503	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	503	PEG	O2-C3-C4-O4
5	A	501	PEG	O2-C3-C4-O4
5	A	501	PEG	C1-C2-O2-C3
5	A	503	PEG	C4-C3-O2-C2
5	A	503	PEG	C1-C2-O2-C3

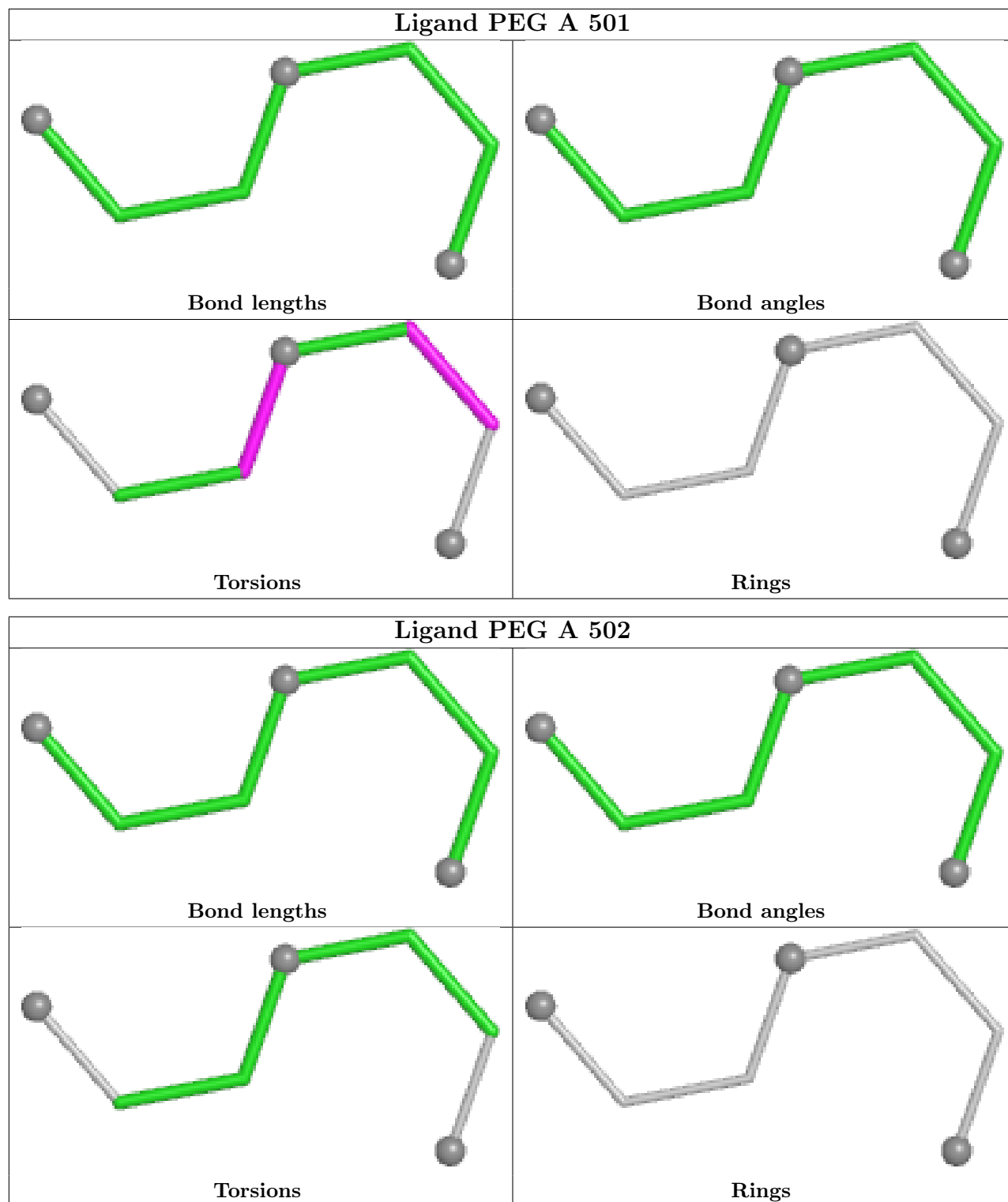
There are no ring outliers.

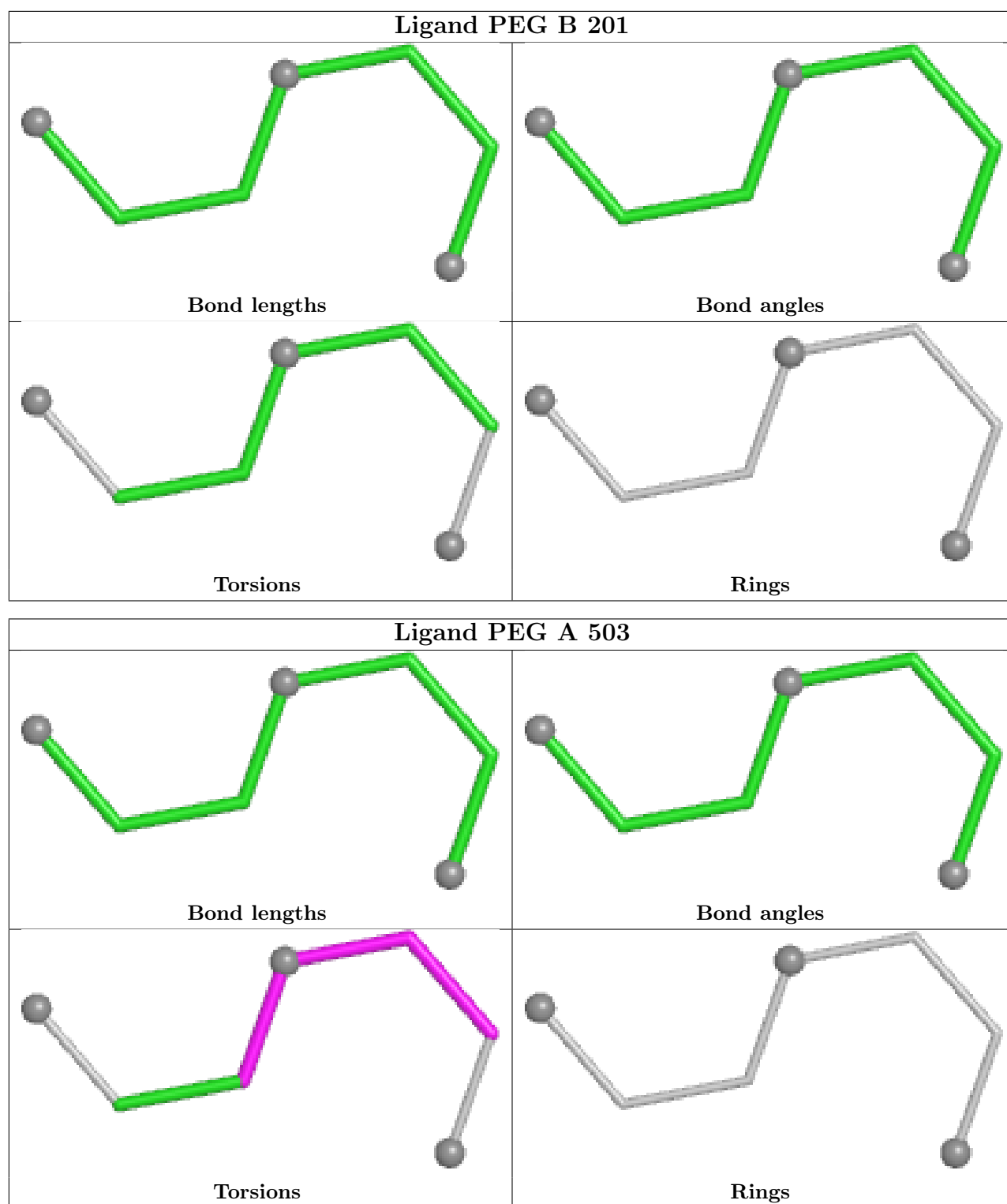
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	201	PEG	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 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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	360/413 (87%)	0.20	8 (2%)	62 52	40, 78, 120, 166	1 (0%)
2	B	114/139 (82%)	0.41	4 (3%)	47 38	70, 86, 147, 221	0
All	All	474/552 (85%)	0.25	12 (2%)	58 48	40, 80, 123, 221	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	51	GLU	3.9
1	A	256[A]	PHE	3.4
2	B	18	PRO	2.9
2	B	54	SER	2.4
1	A	254	TRP	2.3
1	A	187	PHE	2.3
1	A	186	SER	2.3
1	A	193	THR	2.3
1	A	375	PRO	2.2
1	A	244	ASP	2.2
2	B	62	SER	2.1
1	A	151	ASP	2.0

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

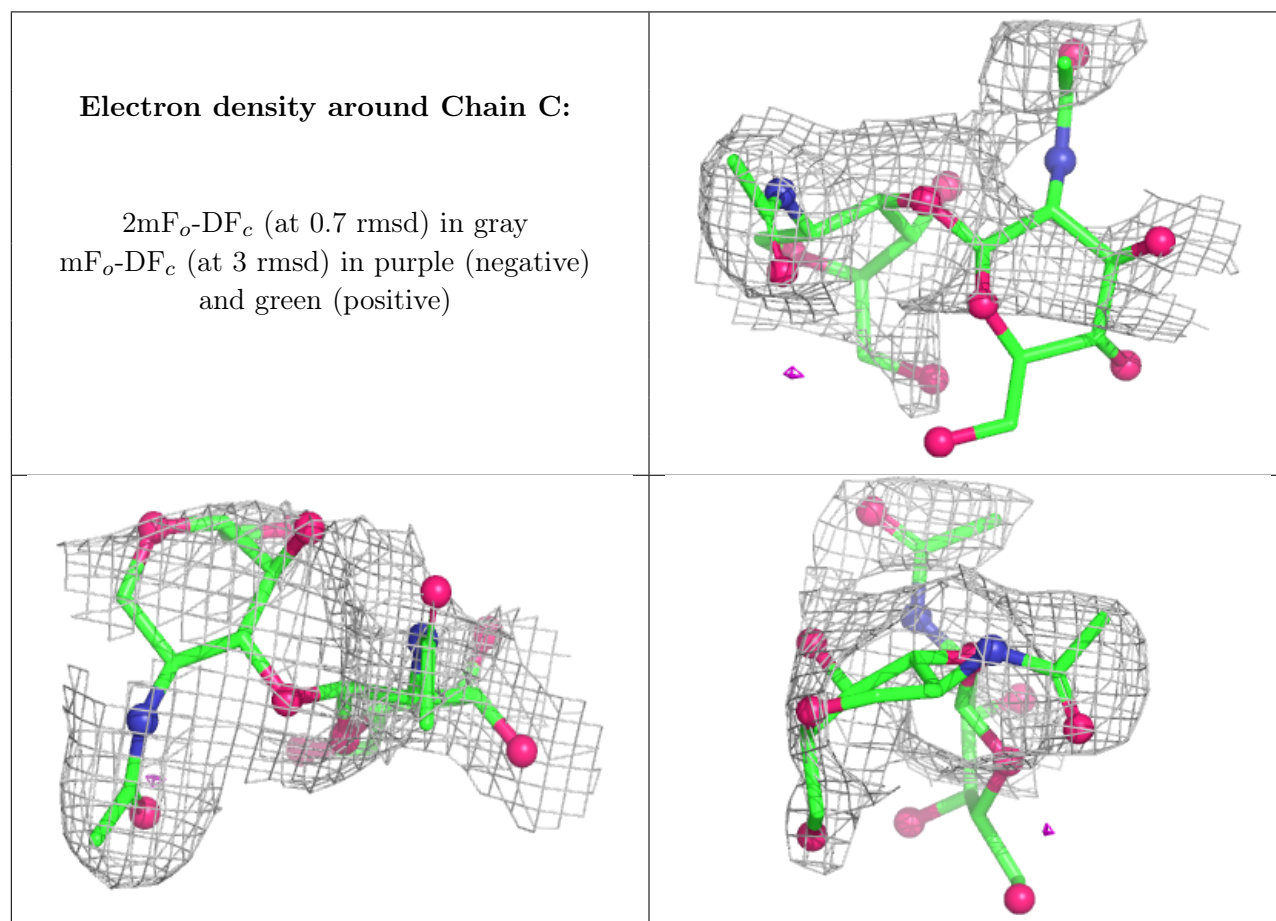
There are no non-standard protein/DNA/RNA residues in this entry.

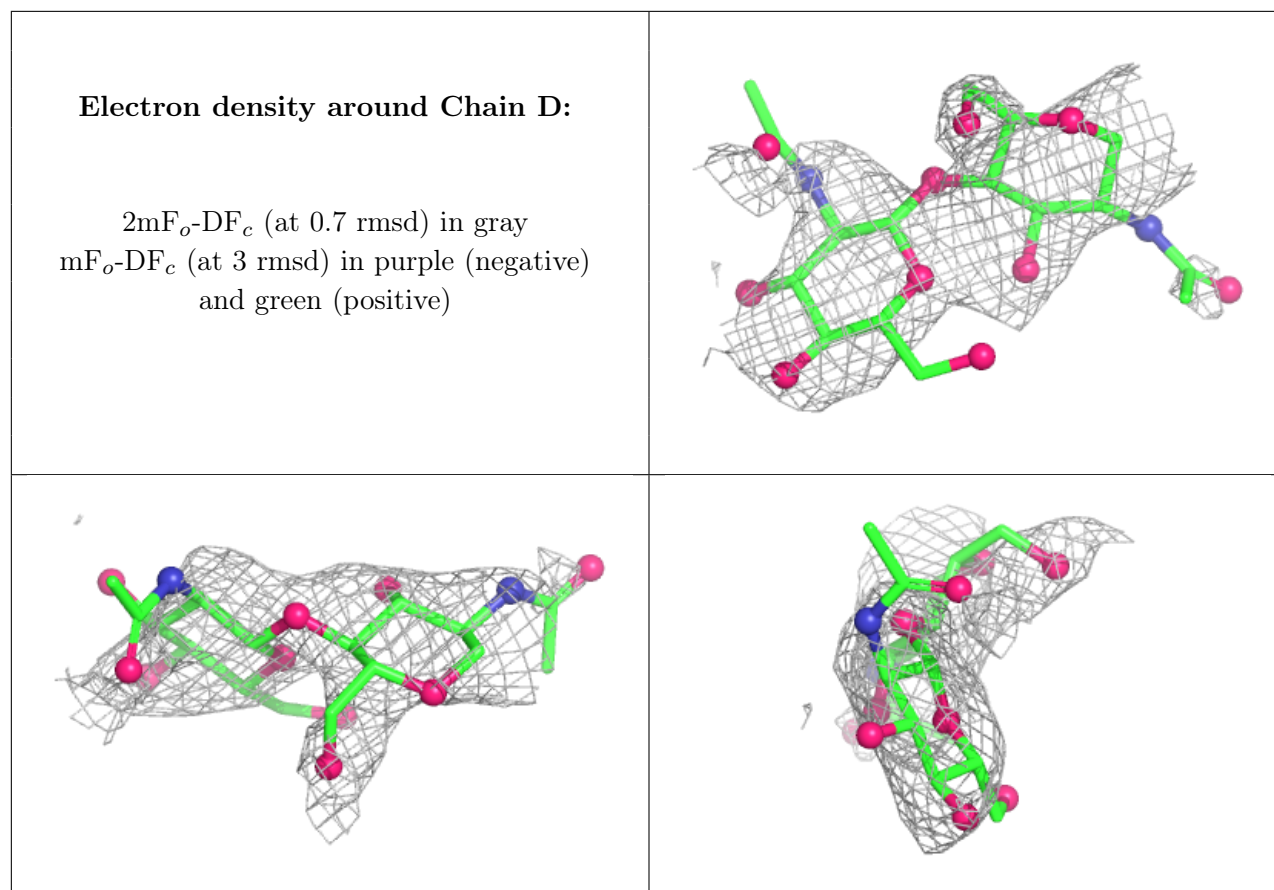
6.3 Carbohydrates [i](#)

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(\AA^2)	Q<0.9
4	NAG	D	2	14/15	0.43	0.15	119,147,156,157	0
3	NAG	C	2	14/15	0.44	0.16	97,138,157,168	0
4	NAG	D	1	14/15	0.56	0.13	107,137,147,151	0
3	NAG	C	1	14/15	0.70	0.12	77,114,130,138	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](#)

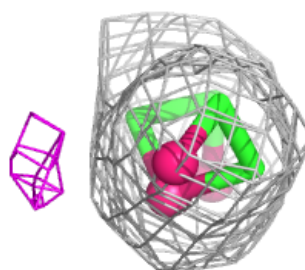
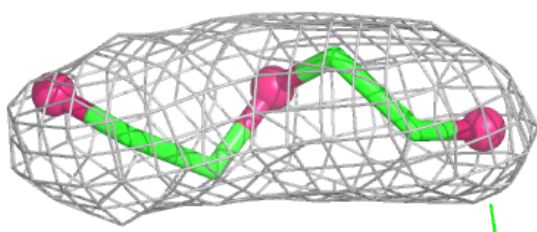
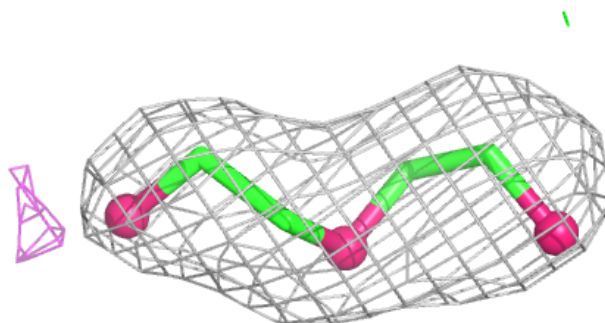
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	PEG	A	502	7/7	0.79	0.14	83,84,98,101	0
5	PEG	A	501	7/7	0.82	0.13	64,68,92,107	0
5	PEG	A	503	7/7	0.83	0.17	82,94,99,103	0
5	PEG	B	201	7/7	0.93	0.20	71,77,84,88	0

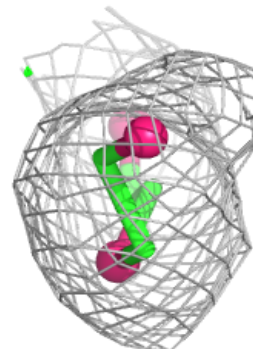
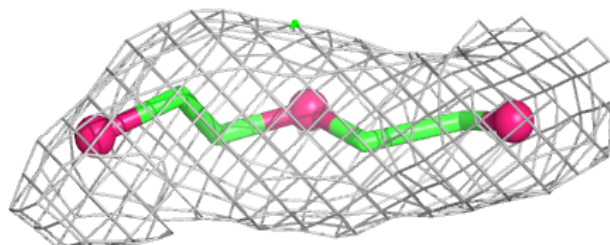
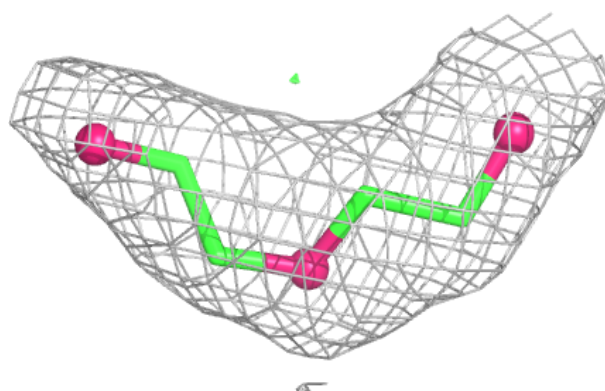
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PEG A 502:

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

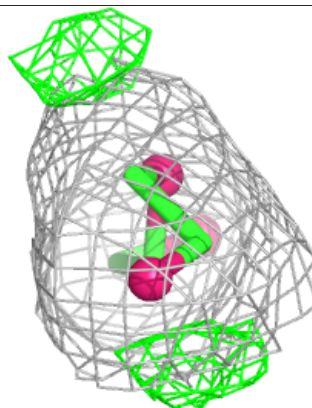
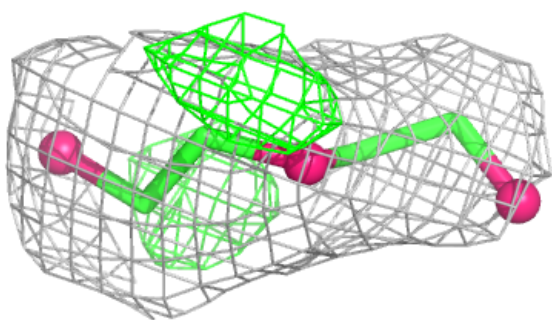
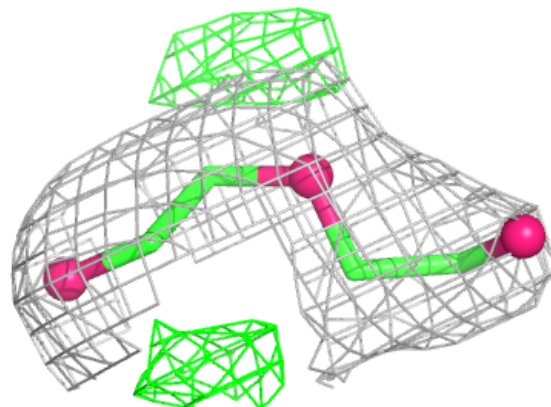
**Electron density around PEG A 501:**

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

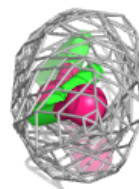
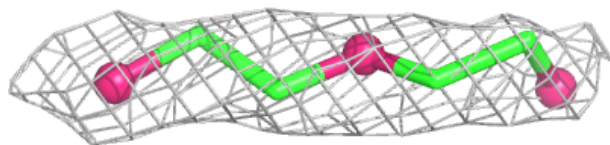
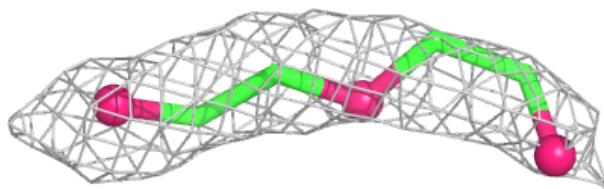


Electron density around PEG A 503:

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

**Electron density around PEG B 201:**

$2mF_o-DF_c$ (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.