



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 04:34 AM BST

PDB ID : 2I36
Title : Crystal structure of trigonal crystal form of ground-state rhodopsin
Authors : Stenkamp, R.E.; Le Trong, I.; Lodowski, D.T.; Salom, D.; Palczewski, K.
Deposited on : 2006-08-17
Resolution : 4.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

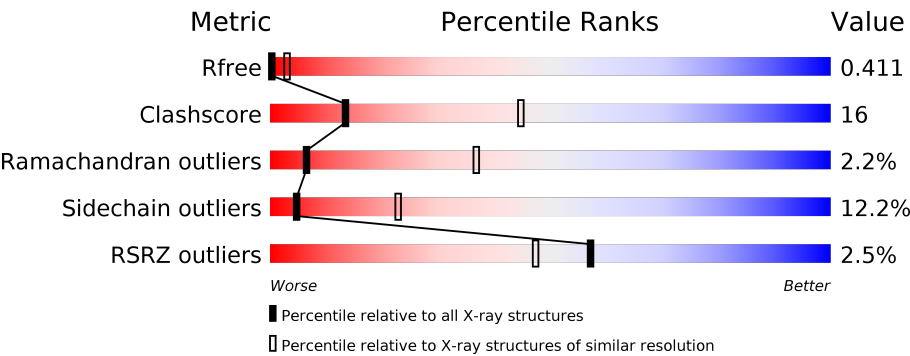
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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.




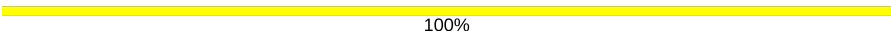

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)

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 on 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	349	
1	B	349	
1	C	349	
2	D	3	
2	F	3	
2	H	3	

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Mol	Chain	Length	Quality of chain
3	E	2	 50%50%
3	G	2	 100%
3	I	2	 50%50%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7883 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 Rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2595	1727	400	442	26			
1	B	315	Total	C	N	O	S	0	0	0
			2502	1667	384	427	24			
1	C	323	Total	C	N	O	S	0	0	0
			2568	1712	394	437	25			

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



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

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



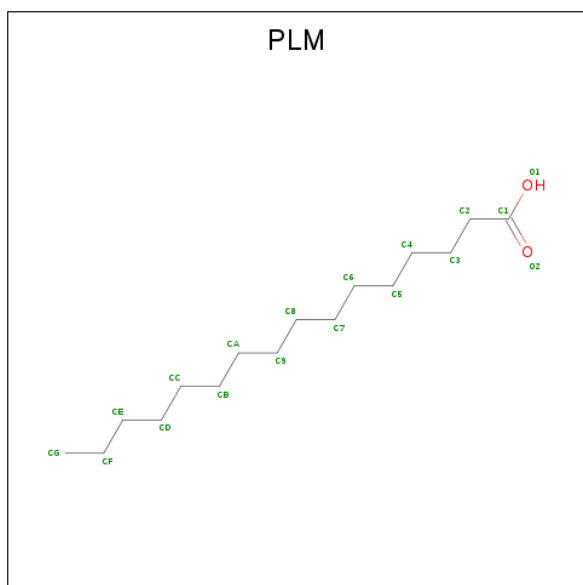
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

- Molecule 4 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).

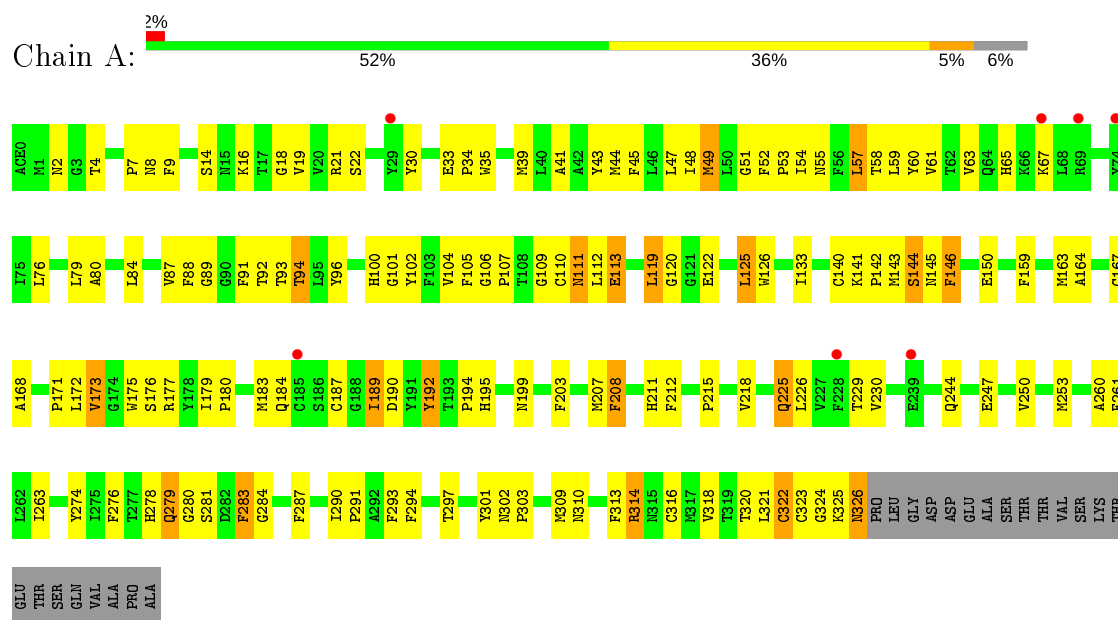


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			17	16	1		

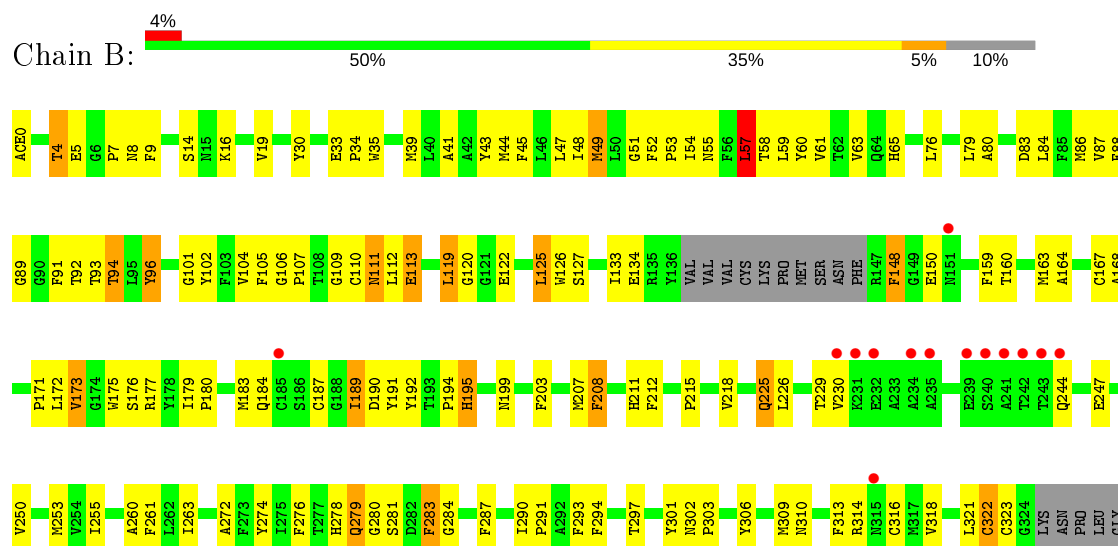
3 Residue-property plots

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: Rhodopsin

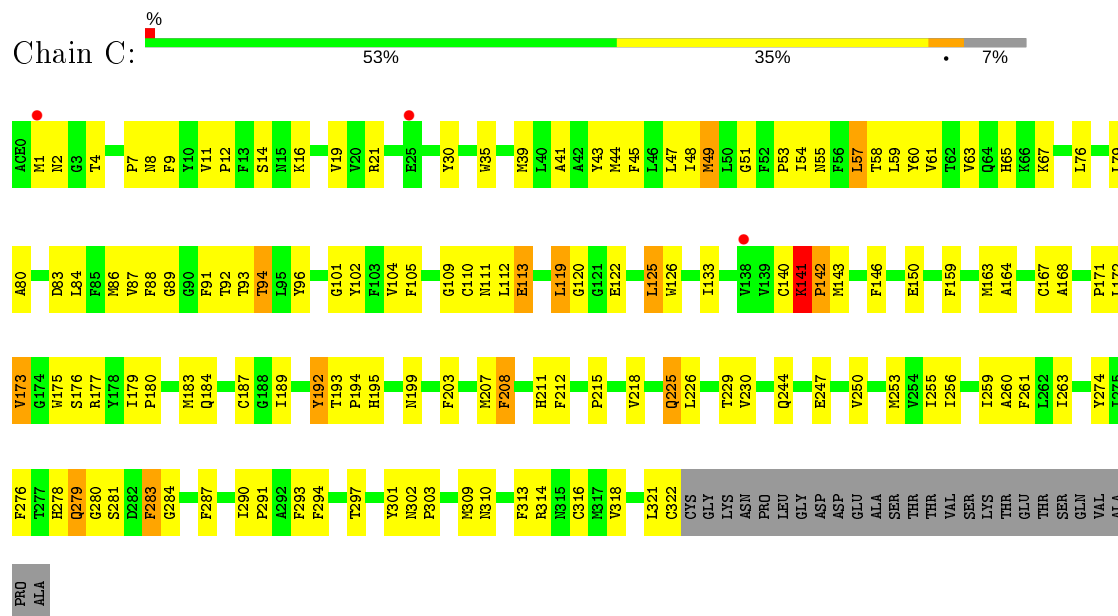


• Molecule 1: Rhodopsin

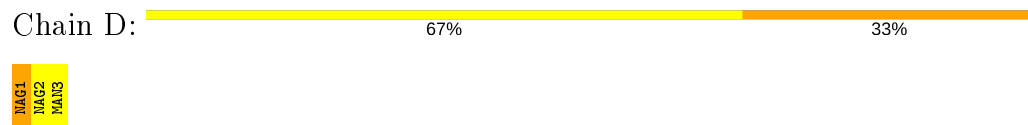


ASP
ASP
GLU
ALA
SER
THR
THR
VAL
SER
LYS
THR
GLU
THR
SER
GLU
VAL
VAL
PRO
PRO
ALA

• Molecule 1: Rhodopsin



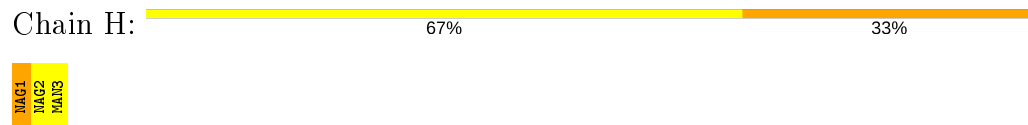
• Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



• Molecule 2: alpha-D-mannopyranose-(1-4)-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





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

Chain G:  100%



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

Chain I:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	159.87Å 159.87Å 142.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 4.10 29.83 – 4.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-4.10) 99.8 (29.83-4.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 4.11Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.382 , 0.412 0.384 , 0.411	Depositor DCC
R_{free} test set	832 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	200.1	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.14 , -6.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.069 for -h,-k,l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	7883	wwPDB-VP
Average B, all atoms (Å ²)	185.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% 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: PLM, NAG, ACE, MAN

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	0.50	0/2675	0.59	0/3645
1	B	0.54	2/2579 (0.1%)	0.60	3/3514 (0.1%)
1	C	0.60	1/2648 (0.0%)	0.58	0/3610
All	All	0.55	3/7902 (0.0%)	0.59	3/10769 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	141	LYS	CE-NZ	17.19	1.92	1.49
1	B	148	PHE	CG-CD2	7.43	1.50	1.38
1	B	148	PHE	CE1-CZ	5.81	1.48	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	PHE	CB-CG-CD1	-5.52	116.94	120.80
1	B	322	CYS	CA-C-N	-5.35	105.43	117.20
1	B	57	LEU	CA-CB-CG	5.14	127.13	115.30

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	2595	0	2569	87	0
1	B	2502	0	2469	85	0
1	C	2568	0	2543	85	0
2	D	39	0	34	1	0
2	F	39	0	34	5	0
2	H	39	0	34	2	0
3	E	28	0	25	1	0
3	G	28	0	25	0	0
3	I	28	0	25	1	0
4	A	17	0	31	0	0
All	All	7883	0	7789	252	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 16.

All (252) 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:C:141:LYS:NZ	1:C:141:LYS:CE	1.92	1.29
1:A:179:ILE:HG13	1:A:180:PRO:HD2	1.54	0.88
2:F:1:NAG:H2	2:H:1:NAG:H83	1.60	0.84
1:C:179:ILE:HG13	1:C:180:PRO:HD2	1.63	0.81
1:B:179:ILE:HG13	1:B:180:PRO:HD2	1.65	0.78
1:A:119:LEU:HD23	1:A:168:ALA:HB3	1.66	0.76
1:C:41:ALA:HA	1:C:44:MET:HB2	1.70	0.72
1:C:119:LEU:HD23	1:C:168:ALA:HB3	1.71	0.72
1:A:41:ALA:HA	1:A:44:MET:HB2	1.71	0.72
1:A:143:MET:HG2	1:A:144:SER:H	1.53	0.72
1:B:41:ALA:HA	1:B:44:MET:HB2	1.70	0.72
1:B:119:LEU:HD23	1:B:168:ALA:HB3	1.71	0.71
1:A:325:LYS:HG2	1:A:326:ASN:N	2.07	0.70
1:A:119:LEU:HD23	1:A:168:ALA:CB	2.22	0.69
1:C:253:MET:SD	1:C:310:ASN:HB2	2.33	0.69
1:C:119:LEU:HD23	1:C:168:ALA:CB	2.23	0.68
1:B:119:LEU:HD23	1:B:168:ALA:CB	2.23	0.68
1:B:180:PRO:HB2	1:B:184:GLN:OE1	1.95	0.67
1:B:253:MET:SD	1:B:310:ASN:HB2	2.36	0.66
1:A:253:MET:SD	1:A:310:ASN:HB2	2.36	0.66
1:B:102:TYR:CZ	1:B:104:VAL:HG12	2.31	0.65
1:B:0:ACE:H1	1:C:193:THR:HA	1.80	0.64
1:C:278:HIS:HB3	1:C:281:SER:HB2	1.79	0.64
1:C:180:PRO:HB2	1:C:184:GLN:OE1	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:PHE:HD1	1:B:283:PHE:H	1.47	0.62
1:B:278:HIS:HB3	1:B:281:SER:HB2	1.80	0.62
1:A:51:GLY:O	1:A:55:ASN:HB2	1.99	0.62
1:A:180:PRO:HB2	1:A:184:GLN:OE1	2.00	0.62
1:A:278:HIS:HB3	1:A:281:SER:HB2	1.82	0.61
1:B:274:TYR:O	1:B:278:HIS:ND1	2.31	0.61
1:A:283:PHE:HD1	1:A:283:PHE:H	1.49	0.61
1:C:278:HIS:O	1:C:280:GLY:N	2.31	0.61
1:B:302:ASN:HB2	1:B:303:PRO:HD3	1.83	0.60
1:C:283:PHE:H	1:C:283:PHE:HD1	1.48	0.60
1:A:250:VAL:HG22	1:A:310:ASN:ND2	2.18	0.59
1:B:278:HIS:O	1:B:280:GLY:N	2.31	0.59
1:C:140:CYS:HB3	1:C:229:THR:HG21	1.83	0.59
1:A:274:TYR:O	1:A:278:HIS:ND1	2.32	0.59
1:B:318:VAL:HA	1:B:321:LEU:HD12	1.85	0.58
1:A:100:HIS:NE2	1:B:96:TYR:OH	2.36	0.58
1:C:302:ASN:HB2	1:C:303:PRO:HD3	1.85	0.57
1:C:51:GLY:O	1:C:55:ASN:HB2	2.04	0.57
1:B:283:PHE:O	1:B:287:PHE:HB2	2.04	0.57
1:A:276:PHE:O	1:A:279:GLN:NE2	2.37	0.57
1:A:302:ASN:HB2	1:A:303:PRO:HD3	1.86	0.56
1:A:53:PRO:O	1:A:57:LEU:HD22	2.06	0.56
1:B:7:PRO:HD2	1:B:9:PHE:CE1	2.41	0.56
1:A:260:ALA:HA	1:A:263:ILE:HD12	1.86	0.56
1:C:102:TYR:CZ	1:C:104:VAL:HG12	2.41	0.56
1:C:93:THR:HB	1:C:113:GLU:HB2	1.89	0.55
1:C:318:VAL:HA	1:C:321:LEU:HD12	1.89	0.55
1:A:325:LYS:HG2	1:A:326:ASN:H	1.72	0.54
1:B:0:ACE:H3	1:C:192:TYR:O	2.07	0.54
1:A:283:PHE:O	1:A:287:PHE:HB2	2.07	0.54
1:B:51:GLY:O	1:B:55:ASN:HB2	2.06	0.54
1:C:283:PHE:O	1:C:287:PHE:HB2	2.07	0.54
1:C:122:GLU:OE2	1:C:211:HIS:HB3	2.08	0.54
1:A:60:TYR:HA	1:A:63:VAL:HG12	1.89	0.54
1:B:122:GLU:OE1	1:B:164:ALA:HA	2.08	0.54
1:C:60:TYR:HA	1:C:63:VAL:HG12	1.89	0.54
1:C:2:ASN:OD1	3:I:1:NAG:O5	2.21	0.53
1:C:45:PHE:O	1:C:49:MET:HB3	2.07	0.53
1:A:290:ILE:N	1:A:291:PRO:HD2	2.24	0.53
1:B:93:THR:HB	1:B:113:GLU:HB2	1.89	0.53
1:B:48:ILE:HG12	1:B:91:PHE:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:ILE:N	1:C:291:PRO:HD2	2.24	0.53
1:A:318:VAL:HA	1:A:321:LEU:HD12	1.91	0.53
1:B:290:ILE:N	1:B:291:PRO:HD2	2.24	0.53
1:C:226:LEU:O	1:C:230:VAL:HG23	2.08	0.53
1:C:260:ALA:HB1	1:C:301:TYR:CE1	2.43	0.52
1:C:225:GLN:O	1:C:225:GLN:NE2	2.42	0.52
1:C:14:SER:C	1:C:16:LYS:H	2.13	0.52
1:A:278:HIS:O	1:A:280:GLY:N	2.32	0.52
1:B:260:ALA:HA	1:B:263:ILE:HD12	1.92	0.52
1:A:7:PRO:HD2	1:A:9:PHE:CE1	2.46	0.51
1:C:260:ALA:HA	1:C:263:ILE:HD12	1.92	0.51
1:B:276:PHE:O	1:B:279:GLN:NE2	2.42	0.51
1:B:60:TYR:HA	1:B:63:VAL:HG12	1.91	0.51
1:C:48:ILE:HG12	1:C:91:PHE:HB3	1.92	0.51
1:B:244:GLN:HA	1:B:247:GLU:HB2	1.93	0.51
1:C:250:VAL:HG22	1:C:310:ASN:ND2	2.24	0.51
1:B:5:GLU:HB2	1:C:1:MET:HB2	1.93	0.51
1:B:126:TRP:CH2	1:B:215:PRO:HG3	2.46	0.51
1:C:141:LYS:NZ	1:C:141:LYS:CD	2.70	0.51
2:F:1:NAG:H82	2:H:1:NAG:H2	1.93	0.51
1:B:47:LEU:HD21	1:B:297:THR:HG22	1.93	0.51
1:A:244:GLN:HA	1:A:247:GLU:HB2	1.92	0.50
1:A:43:TYR:HE2	1:A:293:PHE:HB3	1.77	0.50
1:C:76:LEU:HD23	1:C:79:LEU:HD23	1.93	0.50
1:B:171:PRO:HD3	1:B:203:PHE:CZ	2.46	0.50
1:C:43:TYR:HE2	1:C:293:PHE:HB3	1.77	0.50
1:A:122:GLU:OE2	1:A:211:HIS:HB3	2.12	0.50
1:B:14:SER:C	1:B:16:LYS:H	2.14	0.50
1:A:226:LEU:O	1:A:230:VAL:HG23	2.12	0.50
1:C:55:ASN:OD1	1:C:80:ALA:HA	2.12	0.50
1:B:171:PRO:HA	1:B:176:SER:HB3	1.94	0.49
1:C:21:ARG:NH1	2:F:2:NAG:H62	2.27	0.49
1:B:226:LEU:O	1:B:230:VAL:HG23	2.10	0.49
1:C:253:MET:HG3	1:C:309:MET:HB2	1.93	0.49
1:B:45:PHE:O	1:B:49:MET:HB3	2.12	0.49
1:A:171:PRO:HA	1:A:176:SER:HB3	1.94	0.49
1:B:4:THR:HG21	2:F:1:NAG:H81	1.95	0.49
1:C:142:PRO:HD2	1:C:143:MET:H	1.77	0.49
1:A:125:LEU:HB2	1:A:261:PHE:CZ	2.48	0.49
1:C:54:ILE:HG22	1:C:303:PRO:HB2	1.94	0.49
1:A:180:PRO:HA	1:A:187:CYS:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:THR:HB	1:A:113:GLU:HB2	1.95	0.49
1:A:253:MET:HG3	1:A:309:MET:HB2	1.95	0.49
1:B:43:TYR:HE2	1:B:293:PHE:HB3	1.77	0.49
1:C:119:LEU:HD22	1:C:164:ALA:HB1	1.94	0.49
1:C:53:PRO:O	1:C:57:LEU:HD22	2.12	0.49
1:B:76:LEU:HD23	1:B:79:LEU:HD23	1.94	0.49
1:C:126:TRP:CH2	1:C:215:PRO:HG3	2.48	0.49
1:C:276:PHE:O	1:C:279:GLN:NE2	2.46	0.49
1:B:134:GLU:HA	1:B:148:PHE:HE2	1.77	0.48
1:C:48:ILE:CG2	1:C:87:VAL:HG13	2.43	0.48
1:C:180:PRO:HA	1:C:187:CYS:HA	1.95	0.48
1:C:244:GLN:HA	1:C:247:GLU:HB2	1.94	0.48
1:B:218:VAL:O	1:B:218:VAL:HG12	2.14	0.48
1:A:14:SER:C	1:A:16:LYS:H	2.16	0.48
1:A:179:ILE:HG13	1:A:180:PRO:CD	2.34	0.48
1:A:48:ILE:CG2	1:A:87:VAL:HG13	2.44	0.48
1:B:180:PRO:HA	1:B:187:CYS:HA	1.96	0.48
1:C:7:PRO:HD2	1:C:9:PHE:CE1	2.48	0.48
1:A:76:LEU:HD23	1:A:79:LEU:HD23	1.95	0.48
1:C:140:CYS:SG	1:C:226:LEU:HD11	2.54	0.48
1:A:140:CYS:SG	1:A:229:THR:HG21	2.53	0.47
1:A:45:PHE:O	1:A:49:MET:HB3	2.14	0.47
1:B:105:PHE:HB2	1:B:109:GLY:HA3	1.96	0.47
1:A:100:HIS:CE1	1:B:96:TYR:OH	2.68	0.47
1:A:283:PHE:N	1:A:283:PHE:CD1	2.82	0.47
1:B:253:MET:HG3	1:B:309:MET:HB2	1.96	0.47
1:A:126:TRP:CH2	1:A:215:PRO:HG3	2.49	0.47
1:B:283:PHE:N	1:B:283:PHE:CD1	2.83	0.47
1:C:229:THR:HG22	1:C:229:THR:O	2.14	0.47
1:C:283:PHE:N	1:C:283:PHE:CD1	2.83	0.47
1:A:54:ILE:HG22	1:A:303:PRO:HB2	1.96	0.47
1:A:48:ILE:HG12	1:A:91:PHE:HB3	1.96	0.47
1:A:218:VAL:HG12	1:A:218:VAL:O	2.14	0.47
1:C:256:ILE:HA	1:C:259:ILE:HD12	1.96	0.47
1:C:125:LEU:HB2	1:C:261:PHE:CZ	2.50	0.47
1:A:322:CYS:SG	1:A:325:LYS:HD3	2.54	0.47
1:A:2:ASN:OD1	3:E:1:NAG:O5	2.33	0.47
1:B:65:HIS:CD2	1:B:316:CYS:HB3	2.50	0.46
1:C:218:VAL:O	1:C:218:VAL:HG12	2.15	0.46
1:B:229:THR:O	1:B:229:THR:HG22	2.15	0.46
1:A:229:THR:O	1:A:229:THR:HG22	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:TYR:O	1:C:278:HIS:ND1	2.36	0.46
2:F:1:NAG:O6	2:F:2:NAG:H83	2.15	0.46
1:A:250:VAL:HG22	1:A:310:ASN:HD21	1.79	0.46
1:A:65:HIS:CD2	1:A:316:CYS:HB3	2.51	0.46
1:B:122:GLU:OE2	1:B:211:HIS:HB3	2.15	0.46
1:A:102:TYR:CZ	1:A:104:VAL:HG12	2.51	0.46
1:B:194:PRO:O	1:B:195:HIS:C	2.54	0.46
1:A:175:TRP:CE3	1:A:203:PHE:HD1	2.34	0.46
1:A:19:VAL:HG13	1:A:30:TYR:HB2	1.98	0.46
1:A:35:TRP:O	1:A:39:MET:HB2	2.16	0.46
1:A:119:LEU:HD22	1:A:164:ALA:HB1	1.98	0.46
1:C:105:PHE:HB2	1:C:109:GLY:HA3	1.98	0.46
1:A:225:GLN:NE2	1:A:225:GLN:O	2.49	0.45
1:B:54:ILE:HG22	1:B:303:PRO:HB2	1.98	0.45
1:C:171:PRO:HA	1:C:176:SER:HB3	1.99	0.45
1:A:18:GLY:O	2:D:1:NAG:H61	2.17	0.45
1:B:119:LEU:HD22	1:B:164:ALA:HB1	1.98	0.45
1:C:122:GLU:OE1	1:C:164:ALA:HA	2.16	0.45
1:B:225:GLN:O	1:B:225:GLN:NE2	2.49	0.45
1:B:0:ACE:CH3	1:C:192:TYR:O	2.65	0.45
1:B:260:ALA:HB1	1:B:301:TYR:CE1	2.52	0.45
1:B:55:ASN:OD1	1:B:80:ALA:HA	2.16	0.45
1:A:126:TRP:NE1	1:A:163:MET:HB3	2.31	0.45
1:A:91:PHE:HA	1:A:94:THR:CG2	2.47	0.45
1:A:47:LEU:HD21	1:A:297:THR:HG22	1.99	0.45
1:B:48:ILE:CG2	1:B:87:VAL:HG13	2.47	0.45
1:B:33:GLU:HA	1:B:34:PRO:HD3	1.84	0.45
1:B:35:TRP:O	1:B:39:MET:HB2	2.17	0.45
1:A:55:ASN:OD1	1:A:80:ALA:HA	2.17	0.45
1:A:122:GLU:OE1	1:A:164:ALA:HA	2.17	0.45
1:B:53:PRO:O	1:B:57:LEU:HD22	2.17	0.45
1:A:58:THR:HA	1:A:61:VAL:HG12	1.98	0.44
1:C:175:TRP:CE3	1:C:203:PHE:HD1	2.35	0.44
1:B:255:ILE:O	1:B:255:ILE:HG22	2.18	0.44
1:A:171:PRO:HD3	1:A:203:PHE:CZ	2.52	0.44
1:B:250:VAL:HG22	1:B:310:ASN:ND2	2.32	0.44
1:B:91:PHE:HA	1:B:94:THR:CG2	2.47	0.44
1:C:172:LEU:HD23	1:C:173:VAL:HG13	2.00	0.44
1:C:179:ILE:HG13	1:C:180:PRO:CD	2.42	0.44
1:B:106:GLY:HA3	1:B:107:PRO:HD3	1.87	0.44
1:C:35:TRP:O	1:C:39:MET:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:PHE:HB2	1:A:109:GLY:HA3	2.00	0.44
1:B:125:LEU:HB2	1:B:261:PHE:CZ	2.52	0.44
1:B:303:PRO:HA	1:B:306:TYR:HB3	2.00	0.44
1:C:126:TRP:NE1	1:C:163:MET:HB3	2.32	0.44
1:A:260:ALA:HB1	1:A:301:TYR:CE1	2.53	0.43
1:C:83:ASP:O	1:C:86:MET:HB2	2.18	0.43
1:B:107:PRO:O	1:B:111:ASN:ND2	2.51	0.43
1:B:91:PHE:HA	1:B:94:THR:HG22	2.00	0.43
1:C:253:MET:HG3	1:C:309:MET:CB	2.47	0.43
1:C:91:PHE:HA	1:C:94:THR:CG2	2.48	0.43
1:C:47:LEU:HD21	1:C:297:THR:HG22	1.99	0.43
1:A:314:ARG:NH1	1:B:323:CYS:SG	2.91	0.43
1:C:65:HIS:CD2	1:C:316:CYS:HB3	2.53	0.43
1:B:83:ASP:O	1:B:86:MET:HB2	2.19	0.43
1:A:107:PRO:O	1:A:111:ASN:ND2	2.51	0.43
1:C:11:VAL:HA	1:C:12:PRO:HD3	1.81	0.43
1:C:65:HIS:CE1	1:C:316:CYS:HG	2.36	0.43
1:B:172:LEU:HD23	1:B:173:VAL:HG13	2.01	0.43
1:B:48:ILE:H	1:B:48:ILE:HG13	1.50	0.43
1:C:171:PRO:HD3	1:C:203:PHE:CZ	2.54	0.43
1:A:21:ARG:HB3	1:A:22:SER:H	1.75	0.42
1:A:48:ILE:HG13	1:A:48:ILE:H	1.50	0.42
1:B:175:TRP:CE3	1:B:203:PHE:HD1	2.36	0.42
1:B:306:TYR:O	1:B:310:ASN:HB3	2.19	0.42
1:C:110:CYS:C	1:C:112:LEU:H	2.23	0.42
1:B:19:VAL:HG13	1:B:30:TYR:HB2	2.00	0.42
1:A:100:HIS:CE1	1:B:96:TYR:HH	2.38	0.42
1:B:101:GLY:O	1:B:102:TYR:HB3	2.18	0.42
1:C:58:THR:HA	1:C:61:VAL:HG12	2.00	0.42
1:B:191:TYR:CE1	1:B:272:ALA:HB1	2.54	0.42
1:C:101:GLY:O	1:C:102:TYR:HB3	2.20	0.42
1:A:126:TRP:CD1	1:A:163:MET:HB3	2.55	0.42
1:A:208:PHE:O	1:A:212:PHE:HB3	2.19	0.42
1:A:33:GLU:HA	1:A:34:PRO:HD3	1.86	0.42
1:A:91:PHE:HA	1:A:94:THR:HG22	2.01	0.42
1:B:208:PHE:O	1:B:212:PHE:HB3	2.19	0.42
1:C:65:HIS:C	1:C:67:LYS:H	2.23	0.42
1:B:189:ILE:HD13	1:B:190:ASP:N	2.35	0.42
1:C:250:VAL:HG22	1:C:310:ASN:HD21	1.85	0.42
1:C:255:ILE:O	1:C:255:ILE:HG22	2.20	0.42
1:A:189:ILE:HD13	1:A:190:ASP:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LEU:HD23	1:A:173:VAL:HG13	2.02	0.42
1:A:192:TYR:N	1:A:192:TYR:CD1	2.88	0.42
1:A:65:HIS:C	1:A:67:LYS:H	2.22	0.42
1:C:194:PRO:O	1:C:195:HIS:C	2.59	0.41
1:B:110:CYS:C	1:B:112:LEU:H	2.23	0.41
1:B:126:TRP:NE1	1:B:163:MET:HB3	2.36	0.41
1:A:106:GLY:HA3	1:A:107:PRO:HD3	1.87	0.41
1:B:58:THR:HA	1:B:61:VAL:HG12	2.02	0.41
1:B:127:SER:OG	1:B:160:THR:HG21	2.20	0.41
1:C:208:PHE:O	1:C:212:PHE:HB3	2.20	0.41
1:B:52:PHE:HB3	1:B:53:PRO:HD3	2.02	0.41
1:C:19:VAL:HG13	1:C:30:TYR:HB2	2.02	0.41
1:B:253:MET:HG3	1:B:309:MET:CB	2.50	0.41
1:C:142:PRO:CD	1:C:143:MET:H	2.33	0.41
1:C:140:CYS:SG	1:C:226:LEU:HG	2.61	0.41
1:A:101:GLY:O	1:A:102:TYR:HB3	2.20	0.41
1:A:110:CYS:C	1:A:112:LEU:H	2.25	0.41
1:A:52:PHE:HB3	1:A:53:PRO:HD3	2.03	0.41
1:C:48:ILE:HG13	1:C:48:ILE:H	1.52	0.41
1:A:142:PRO:HD2	1:A:146:PHE:CD1	2.56	0.40
1:C:91:PHE:HA	1:C:94:THR:HG22	2.03	0.40
1:A:194:PRO:O	1:A:195:HIS:C	2.59	0.40
1:A:125:LEU:HB2	1:A:261:PHE:HZ	1.87	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	325/349 (93%)	270 (83%)	47 (14%)	8 (2%)	5	34
1	B	311/349 (89%)	265 (85%)	40 (13%)	6 (2%)	8	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	321/349 (92%)	270 (84%)	44 (14%)	7 (2%)	6	37
All	All	957/1047 (91%)	805 (84%)	131 (14%)	21 (2%)	6	37

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	GLN
1	B	279	GLN
1	C	279	GLN
1	A	111	ASN
1	A	144	SER
1	A	284	GLY
1	A	324	GLY
1	B	111	ASN
1	B	284	GLY
1	C	111	ASN
1	C	284	GLY
1	C	142	PRO
1	A	89	GLY
1	A	120	GLY
1	B	89	GLY
1	B	120	GLY
1	C	89	GLY
1	C	120	GLY
1	C	141	LYS
1	B	195	HIS
1	A	141	LYS

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	278/296 (94%)	242 (87%)	36 (13%)	4	21
1	B	266/296 (90%)	235 (88%)	31 (12%)	5	24
1	C	275/296 (93%)	242 (88%)	33 (12%)	5	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	819/888 (92%)	719 (88%)	100 (12%)	5 23

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	8	ASN
1	A	49	MET
1	A	57	LEU
1	A	59	LEU
1	A	84	LEU
1	A	88	PHE
1	A	92	THR
1	A	94	THR
1	A	96	TYR
1	A	113	GLU
1	A	119	LEU
1	A	125	LEU
1	A	133	ILE
1	A	145	ASN
1	A	146	PHE
1	A	150	GLU
1	A	159	PHE
1	A	167	CYS
1	A	173	VAL
1	A	177	ARG
1	A	183	MET
1	A	189	ILE
1	A	192	TYR
1	A	199	ASN
1	A	207	MET
1	A	208	PHE
1	A	225	GLN
1	A	283	PHE
1	A	294	PHE
1	A	313	PHE
1	A	314	ARG
1	A	320	THR
1	A	322	CYS
1	A	323	CYS
1	A	326	ASN
1	B	4	THR

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Mol	Chain	Res	Type
1	B	8	ASN
1	B	49	MET
1	B	57	LEU
1	B	59	LEU
1	B	84	LEU
1	B	88	PHE
1	B	92	THR
1	B	94	THR
1	B	96	TYR
1	B	113	GLU
1	B	119	LEU
1	B	125	LEU
1	B	133	ILE
1	B	150	GLU
1	B	159	PHE
1	B	167	CYS
1	B	173	VAL
1	B	177	ARG
1	B	183	MET
1	B	189	ILE
1	B	192	TYR
1	B	199	ASN
1	B	207	MET
1	B	208	PHE
1	B	225	GLN
1	B	283	PHE
1	B	294	PHE
1	B	313	PHE
1	B	314	ARG
1	B	322	CYS
1	C	4	THR
1	C	8	ASN
1	C	49	MET
1	C	57	LEU
1	C	59	LEU
1	C	84	LEU
1	C	88	PHE
1	C	92	THR
1	C	94	THR
1	C	96	TYR
1	C	113	GLU
1	C	119	LEU

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Mol	Chain	Res	Type
1	C	125	LEU
1	C	133	ILE
1	C	141	LYS
1	C	146	PHE
1	C	150	GLU
1	C	159	PHE
1	C	167	CYS
1	C	173	VAL
1	C	177	ARG
1	C	183	MET
1	C	189	ILE
1	C	192	TYR
1	C	199	ASN
1	C	207	MET
1	C	208	PHE
1	C	225	GLN
1	C	283	PHE
1	C	294	PHE
1	C	313	PHE
1	C	314	ARG
1	C	322	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	199	ASN
1	A	211	HIS
1	A	225	GLN
1	A	310	ASN
1	B	73	ASN
1	B	199	ASN
1	B	211	HIS
1	B	225	GLN
1	C	8	ASN
1	C	73	ASN
1	C	199	ASN
1	C	211	HIS

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 ⓘ

15 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	D	1	1,2	14,14,15	0.78	0	17,19,21	1.77	4 (23%)
2	NAG	D	2	2	14,14,15	0.85	0	17,19,21	1.36	1 (5%)
2	MAN	D	3	2	11,11,12	0.43	0	15,15,17	1.37	2 (13%)
3	NAG	E	1	1,3	14,14,15	0.63	0	17,19,21	1.64	2 (11%)
3	NAG	E	2	3	14,14,15	0.81	1 (7%)	17,19,21	1.59	2 (11%)
2	NAG	F	1	1,2	14,14,15	0.61	0	17,19,21	1.34	3 (17%)
2	NAG	F	2	2	14,14,15	0.50	0	17,19,21	1.33	2 (11%)
2	MAN	F	3	2	11,11,12	0.59	0	15,15,17	2.06	3 (20%)
3	NAG	G	1	1,3	14,14,15	0.61	0	17,19,21	1.64	2 (11%)
3	NAG	G	2	3	14,14,15	0.68	1 (7%)	17,19,21	1.92	1 (5%)
2	NAG	H	1	1,2	14,14,15	0.75	0	17,19,21	1.56	2 (11%)
2	NAG	H	2	2	14,14,15	0.52	0	17,19,21	1.65	1 (5%)
2	MAN	H	3	2	11,11,12	0.49	0	15,15,17	1.87	5 (33%)
3	NAG	I	1	1,3	14,14,15	0.64	0	17,19,21	2.04	4 (23%)
3	NAG	I	2	3	14,14,15	0.65	0	17,19,21	1.64	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
2	NAG	D	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	MAN	D	3	2	-	1/2/19/22	1/1/1/1
3	NAG	E	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	6/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	MAN	F	3	2	-	1/2/19/22	1/1/1/1
3	NAG	G	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	MAN	H	3	2	-	1/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	NAG	C1-C2	2.17	1.55	1.52
3	G	2	NAG	C1-C2	2.02	1.55	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2	NAG	C1-O5-C5	7.10	121.81	112.19
2	F	3	MAN	C1-O5-C5	6.29	120.72	112.19
3	I	2	NAG	C1-O5-C5	5.81	120.06	112.19
2	H	2	NAG	C1-O5-C5	5.73	119.95	112.19
3	I	1	NAG	C1-O5-C5	5.13	119.14	112.19
2	H	1	NAG	C4-C3-C2	4.98	118.31	111.02
3	E	1	NAG	C4-C3-C2	4.81	118.06	111.02
3	E	2	NAG	C1-O5-C5	4.70	118.55	112.19
3	I	1	NAG	C4-C3-C2	4.41	117.48	111.02
2	H	3	MAN	C1-O5-C5	4.00	117.61	112.19
2	F	2	NAG	C1-O5-C5	4.00	117.61	112.19
2	D	1	NAG	C4-C3-C2	3.98	116.85	111.02
2	D	2	NAG	C4-C3-C2	3.86	116.67	111.02
3	G	1	NAG	C1-O5-C5	3.83	117.38	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	MAN	C1-O5-C5	3.80	117.34	112.19
3	G	1	NAG	C4-C3-C2	3.71	116.45	111.02
2	H	3	MAN	C1-C2-C3	3.51	113.98	109.67
2	D	1	NAG	C2-N2-C7	3.28	127.57	122.90
2	F	1	NAG	C4-C3-C2	3.23	115.75	111.02
3	E	2	NAG	O5-C5-C6	3.21	112.23	107.20
3	E	1	NAG	O5-C5-C6	2.90	111.75	107.20
2	F	1	NAG	C1-O5-C5	2.88	116.09	112.19
2	H	3	MAN	C2-C3-C4	2.73	115.62	110.89
3	I	2	NAG	O5-C5-C6	2.69	111.41	107.20
2	D	3	MAN	O5-C5-C6	2.67	111.39	107.20
2	F	3	MAN	C3-C4-C5	2.57	114.83	110.24
2	D	1	NAG	O5-C1-C2	2.55	115.31	111.29
2	H	1	NAG	C2-N2-C7	2.53	126.51	122.90
2	F	3	MAN	C1-C2-C3	2.41	112.63	109.67
2	F	2	NAG	C2-N2-C7	2.38	126.29	122.90
3	I	1	NAG	O4-C4-C3	2.27	115.61	110.35
2	F	1	NAG	C2-N2-C7	2.23	126.07	122.90
2	H	3	MAN	C6-C5-C4	-2.20	107.84	113.00
2	D	1	NAG	O5-C5-C6	2.19	110.64	107.20
2	H	3	MAN	O5-C5-C6	2.16	110.58	107.20
3	I	1	NAG	O3-C3-C4	-2.09	105.51	110.35

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	F	1	NAG	O7-C7-N2-C2
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	I	2	NAG	C4-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C8-C7-N2-C2
2	F	1	NAG	C1-C2-N2-C7
2	D	2	NAG	O5-C5-C6-O6
2	F	3	MAN	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
3	I	1	NAG	O7-C7-N2-C2
2	D	3	MAN	O5-C5-C6-O6
2	H	3	MAN	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
2	F	1	NAG	C3-C2-N2-C7
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
3	I	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C3-C2-N2-C7

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	3	MAN	C1-C2-C3-C4-C5-O5
2	D	3	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 8 short contacts:

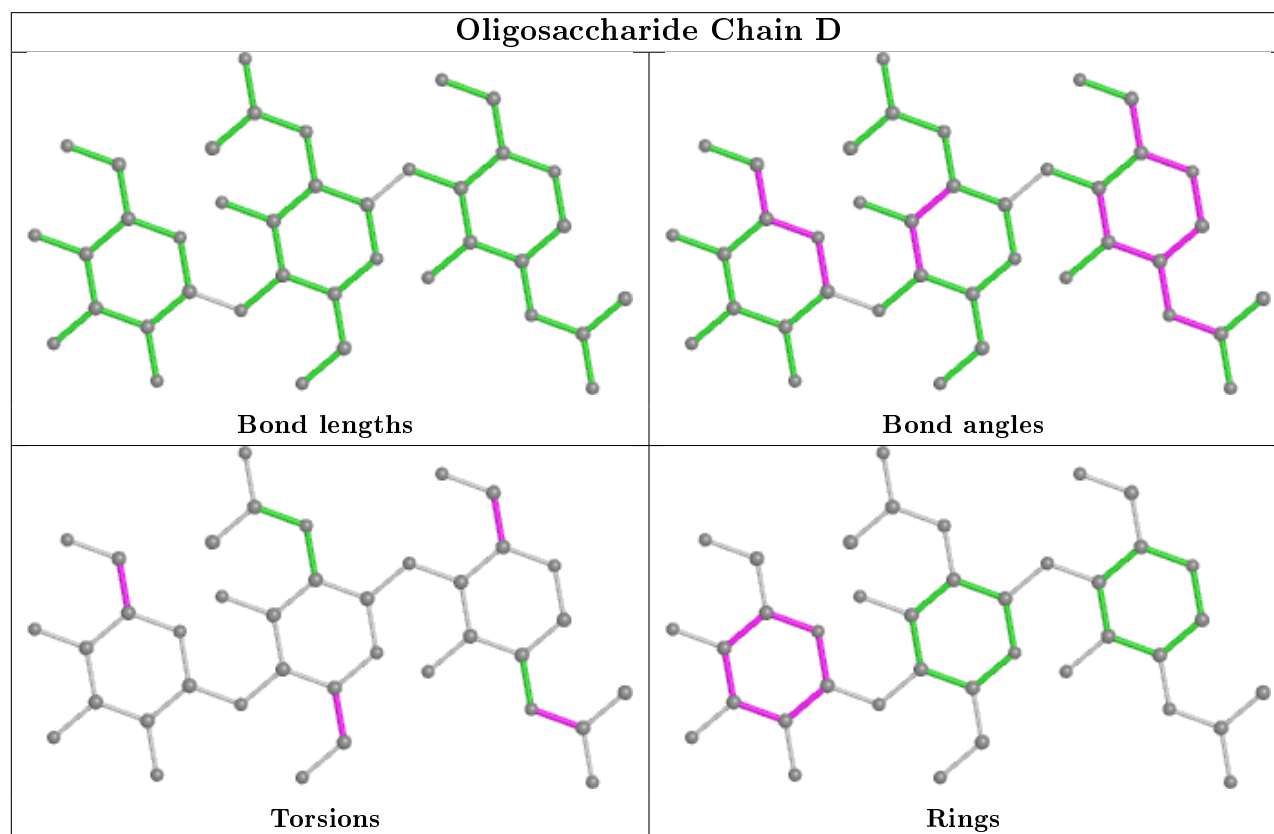
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	NAG	2	0
3	I	1	NAG	1	0
2	F	2	NAG	2	0

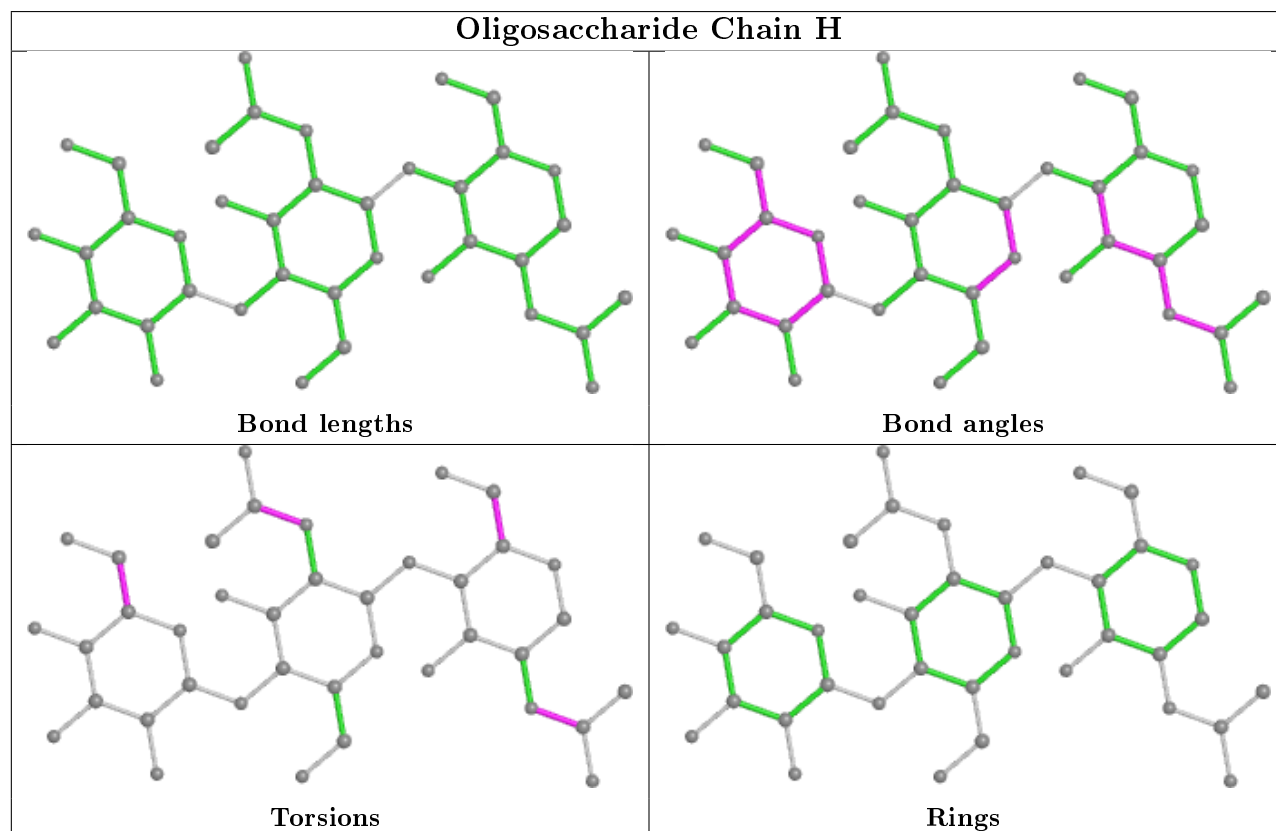
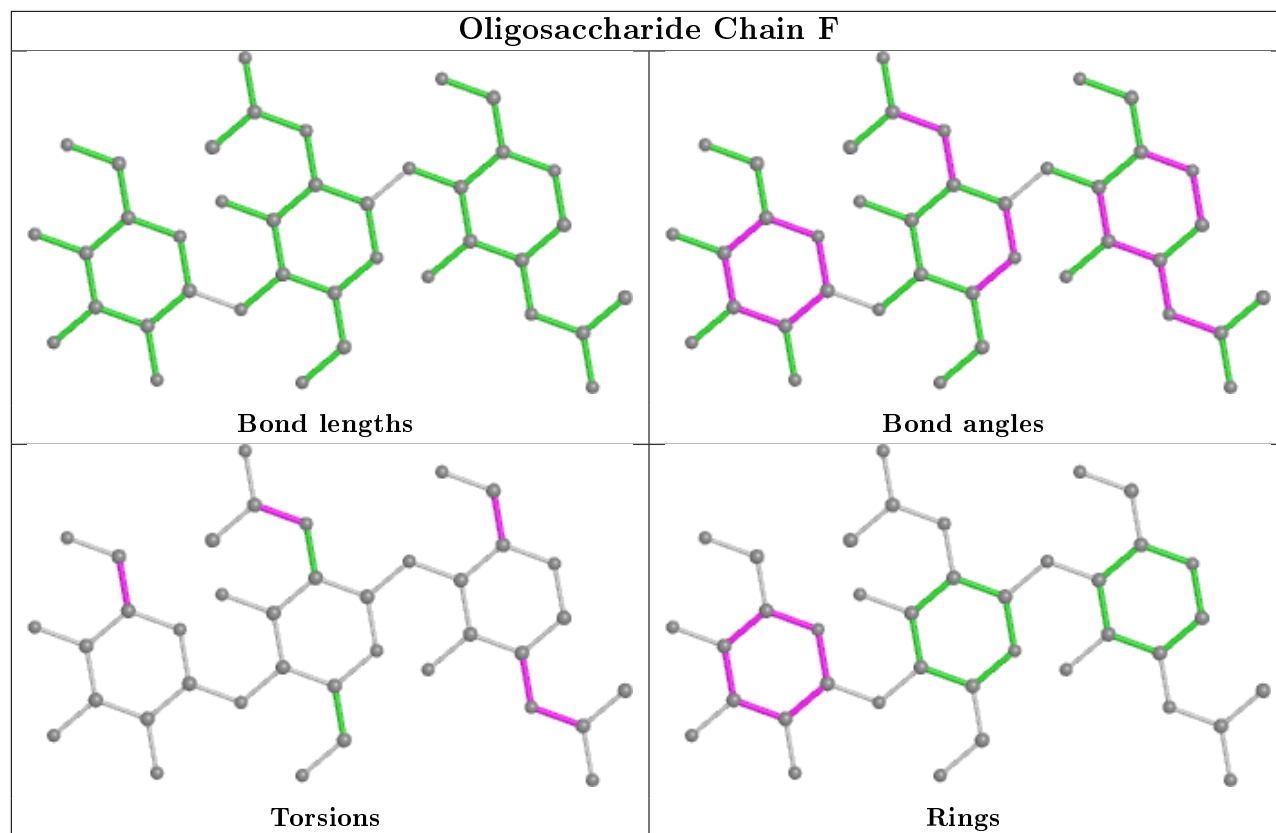
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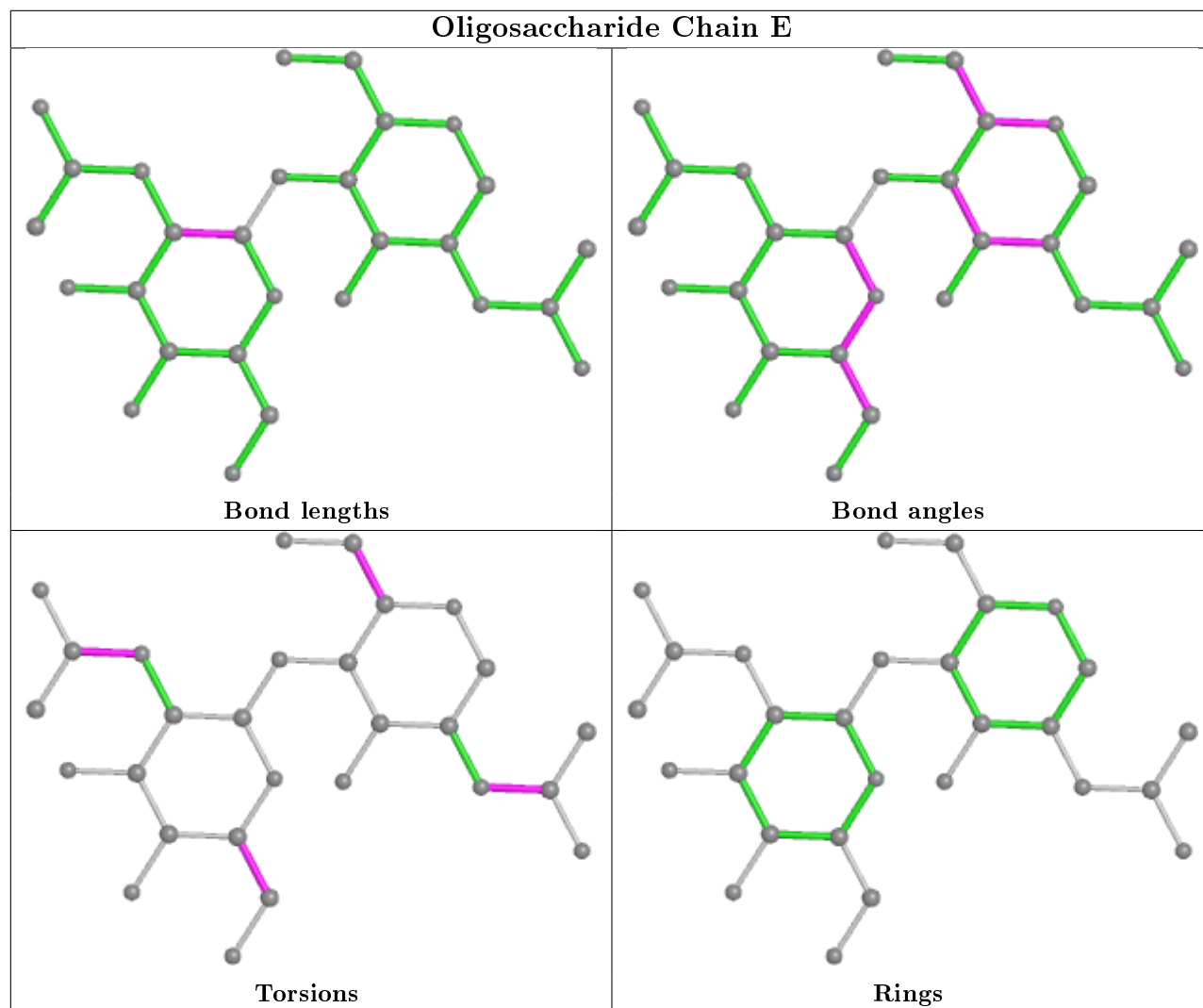
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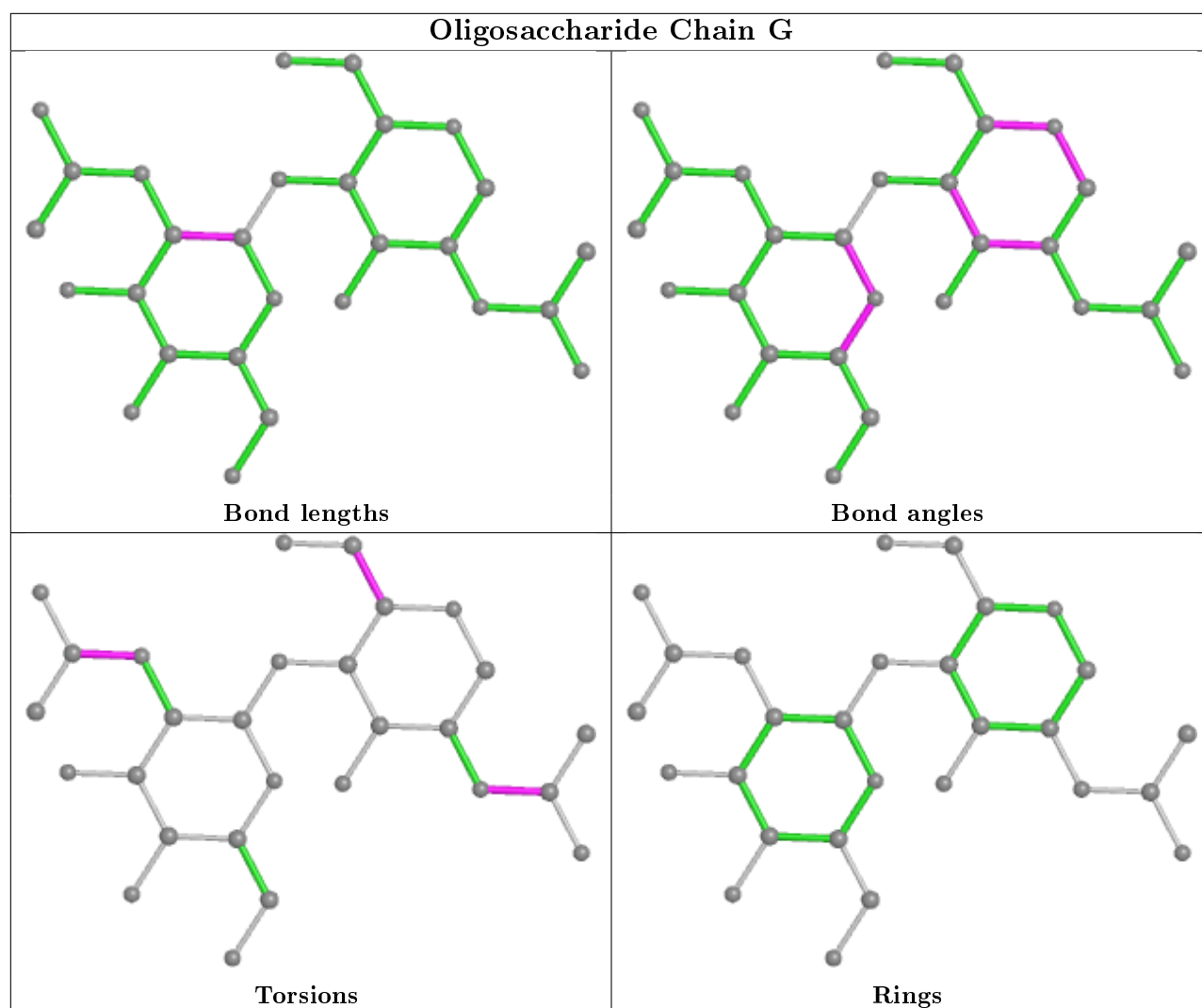
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	1	0
2	F	1	NAG	4	0
3	E	1	NAG	1	0

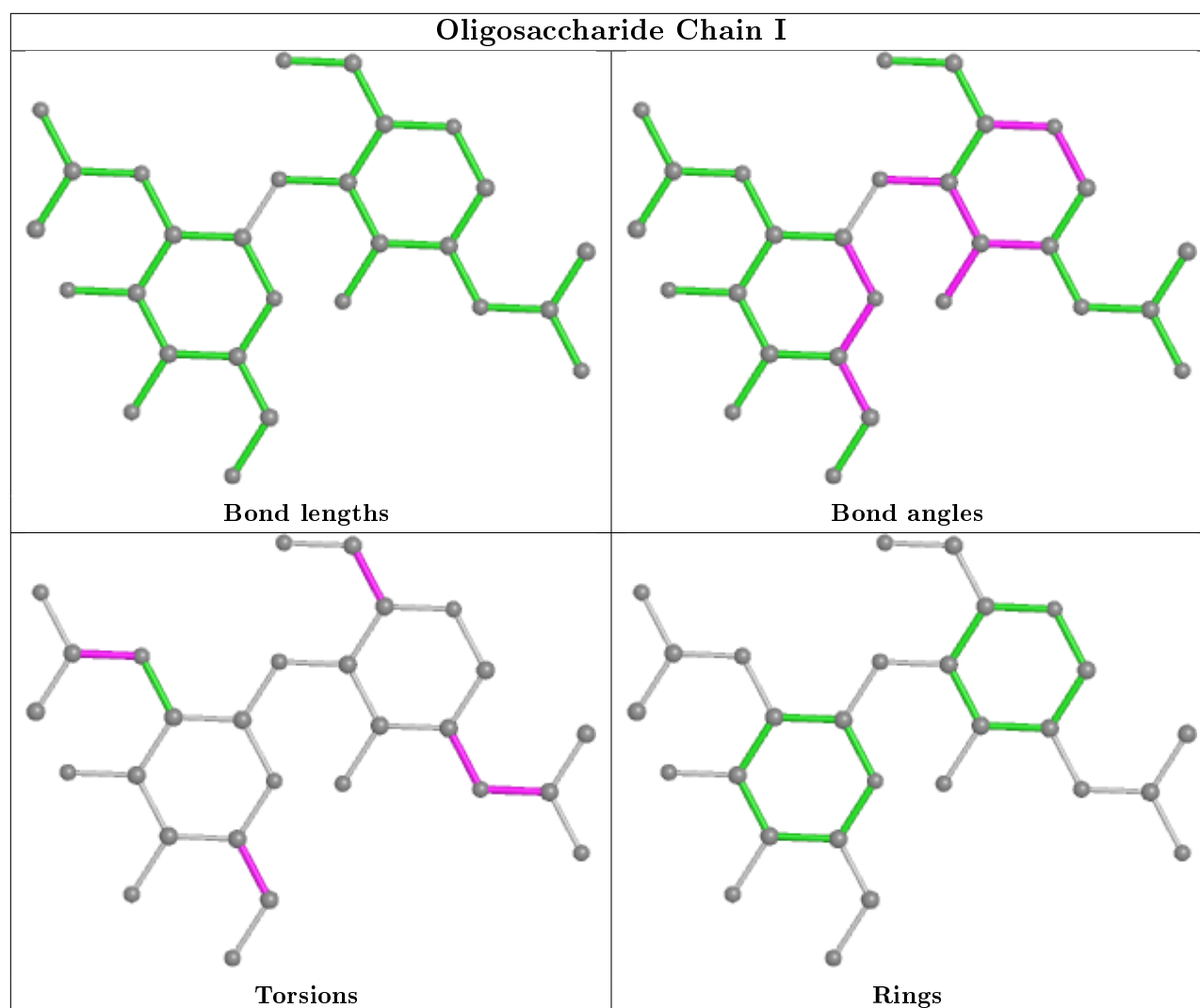
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

1 ligand is 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	PLM	A	401	1	16,16,17	0.28	0	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
4	PLM	A	401	1	-	5/13/14/15	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

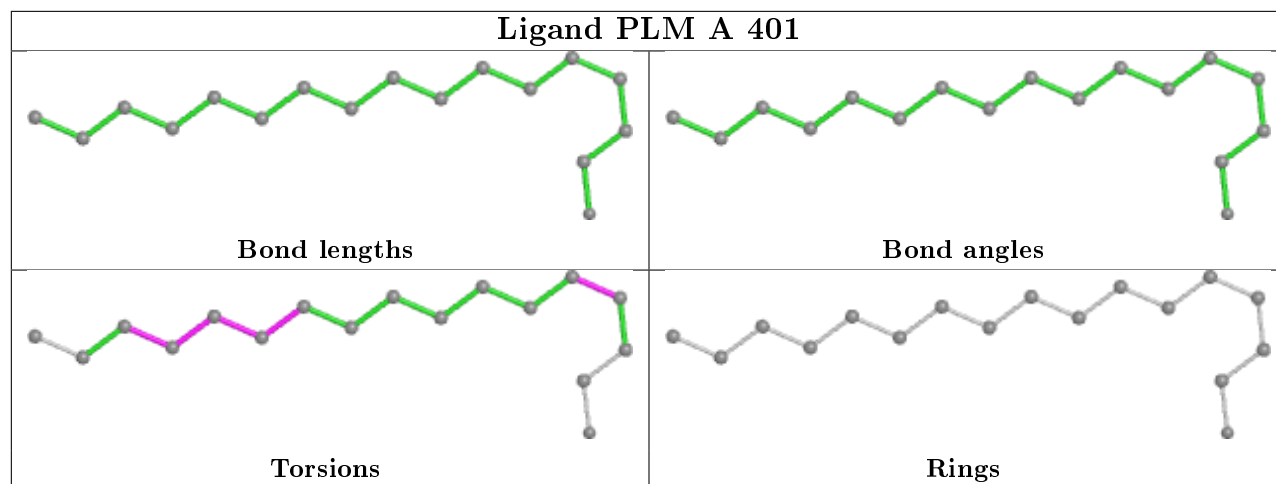
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	401	PLM	C9-CA-CB-CC
4	A	401	PLM	CC-CD-CE-CF
4	A	401	PLM	CB-CC-CD-CE
4	A	401	PLM	C2-C3-C4-C5
4	A	401	PLM	CA-CB-CC-CD

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	326/349 (93%)	-0.31	7 (2%) 63 54	185, 185, 185, 185	0
1	B	314/349 (89%)	-0.19	14 (4%) 33 27	185, 185, 185, 185	0
1	C	322/349 (92%)	-0.36	3 (0%) 84 77	185, 185, 185, 185	0
All	All	962/1047 (91%)	-0.29	24 (2%) 57 47	185, 185, 185, 185	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	239	GLU	4.3
1	B	243	THR	4.2
1	B	240	SER	4.1
1	B	232	GLU	3.8
1	B	244	GLN	3.5
1	B	231	LYS	3.4
1	B	185	CYS	3.2
1	B	242	THR	3.1
1	A	67	LYS	2.9
1	A	74	TYR	2.8
1	B	241	ALA	2.7
1	B	230	VAL	2.6
1	B	315	ASN	2.6
1	A	29	TYR	2.5
1	A	239	GLU	2.5
1	A	69	ARG	2.4
1	C	138	VAL	2.3
1	B	234	ALA	2.3
1	A	185	CYS	2.3
1	C	1	MET	2.2
1	C	25	GLU	2.2
1	B	151	ASN	2.2
1	B	235	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	228	PHE	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](#)

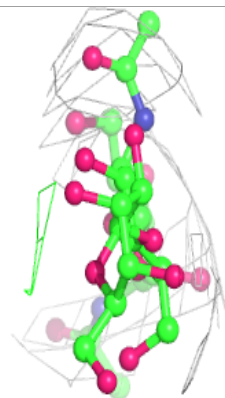
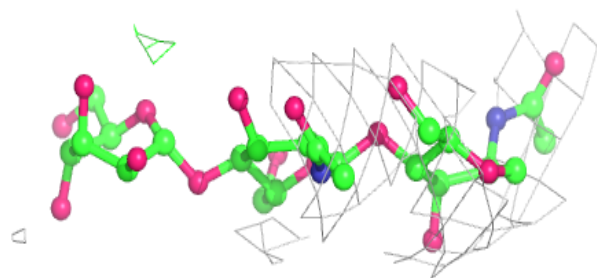
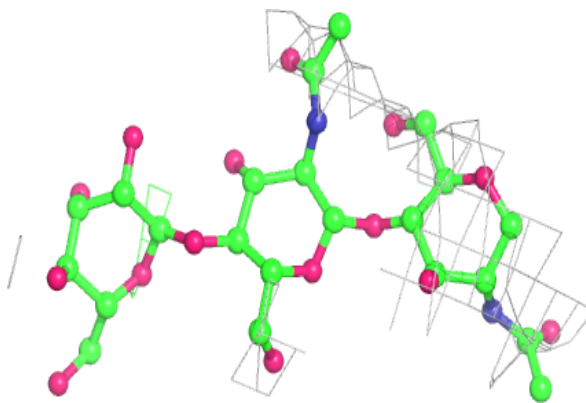
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	F	3	11/12	0.64	0.24	185,185,185,185	0
2	MAN	H	3	11/12	0.80	0.17	185,185,185,185	0
3	NAG	E	1	14/15	0.82	0.25	185,185,185,185	0
3	NAG	E	2	14/15	0.82	0.30	185,185,185,185	0
3	NAG	G	2	14/15	0.83	0.65	185,185,185,185	0
2	NAG	F	2	14/15	0.84	0.17	185,185,185,185	0
3	NAG	I	2	14/15	0.84	0.33	185,185,185,185	0
3	NAG	G	1	14/15	0.85	0.45	185,185,185,185	0
2	NAG	H	2	14/15	0.88	0.25	185,185,185,185	0
2	MAN	D	3	11/12	0.91	0.18	185,185,185,185	0
2	NAG	H	1	14/15	0.92	0.18	185,185,185,185	0
3	NAG	I	1	14/15	0.93	0.21	185,185,185,185	0
2	NAG	D	1	14/15	0.93	0.18	185,185,185,185	0
2	NAG	D	2	14/15	0.95	0.08	185,185,185,185	0
2	NAG	F	1	14/15	0.97	0.19	185,185,185,185	0

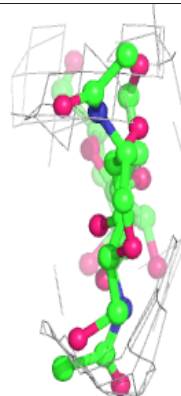
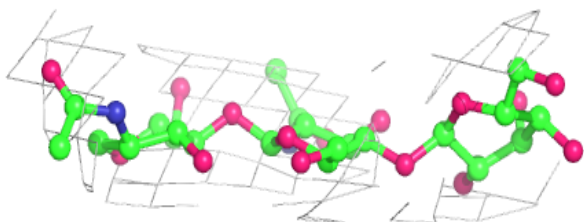
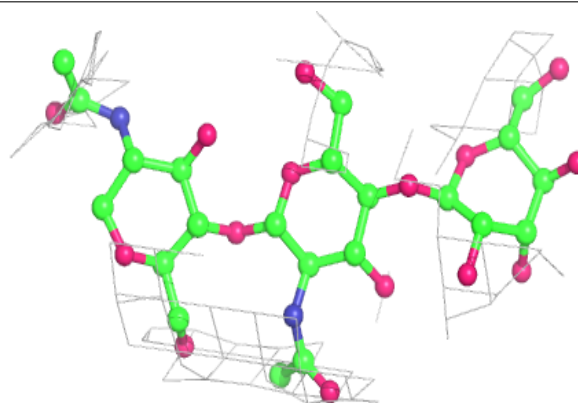
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

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

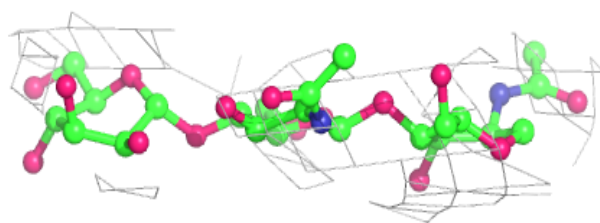
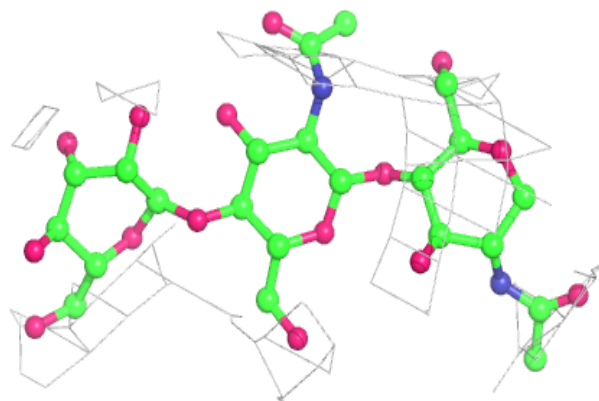
**Electron density around Chain F:**

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



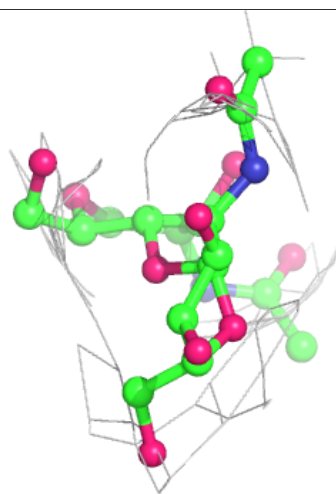
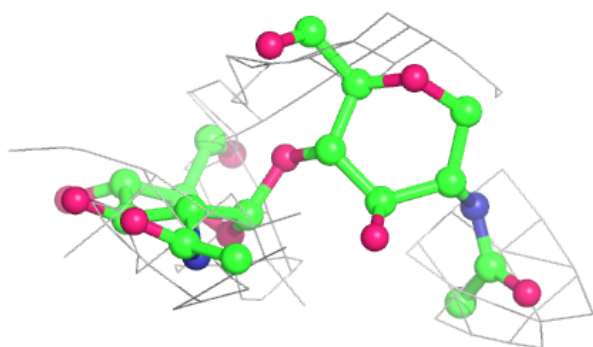
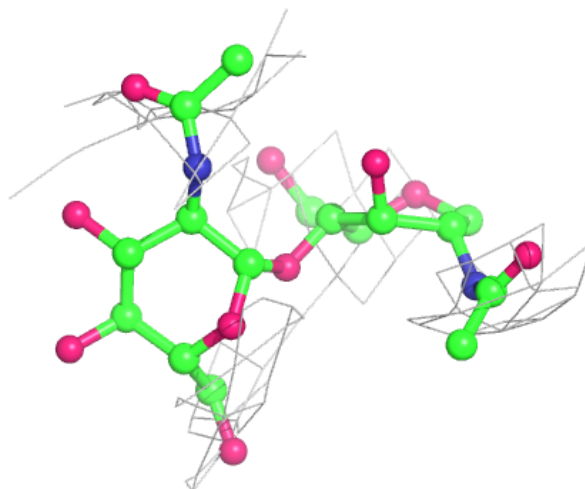
Electron density around Chain H:

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



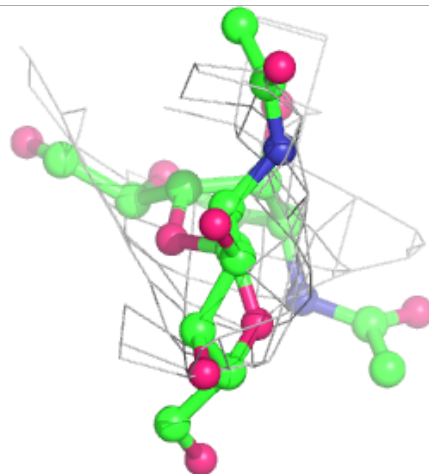
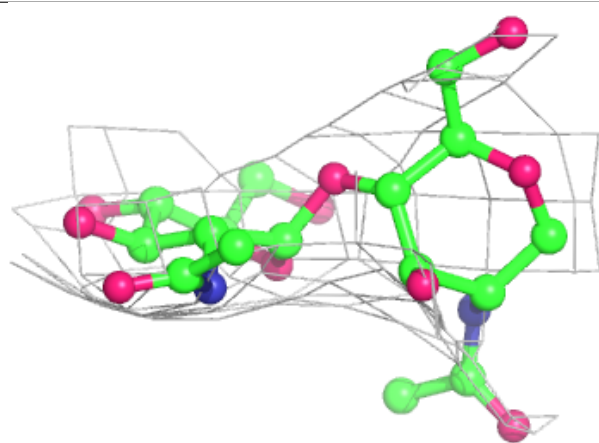
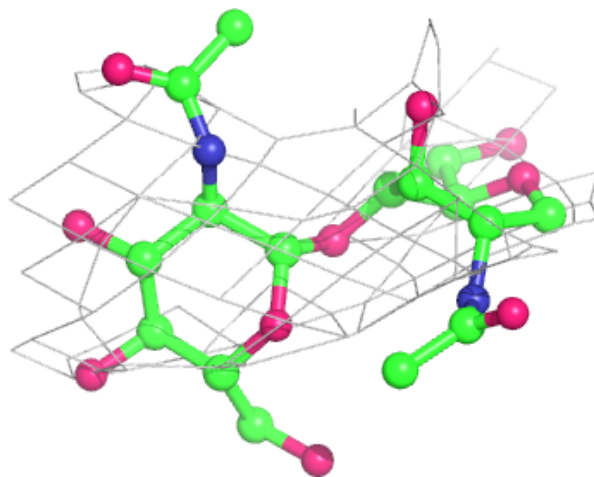
Electron density around Chain E:

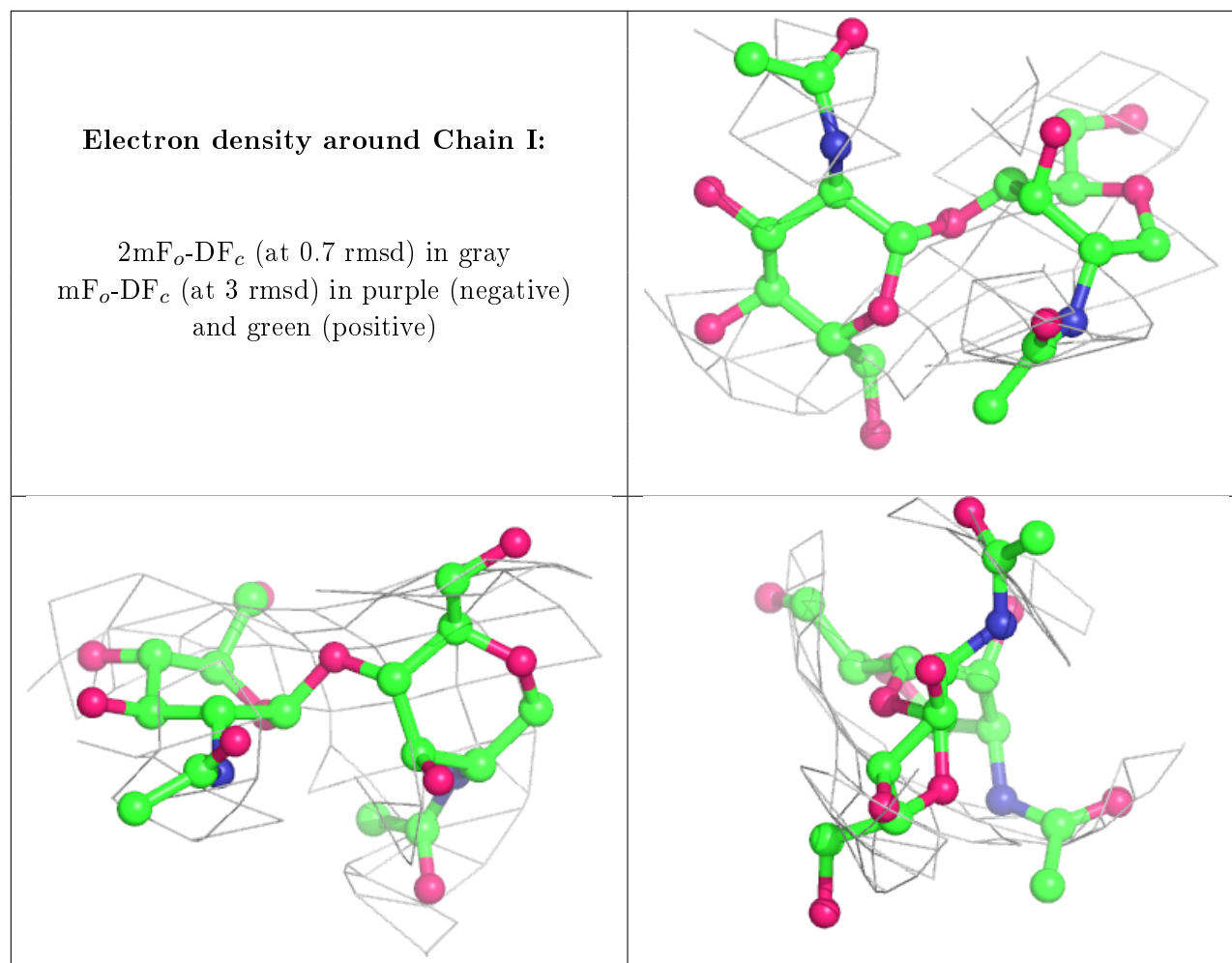
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

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



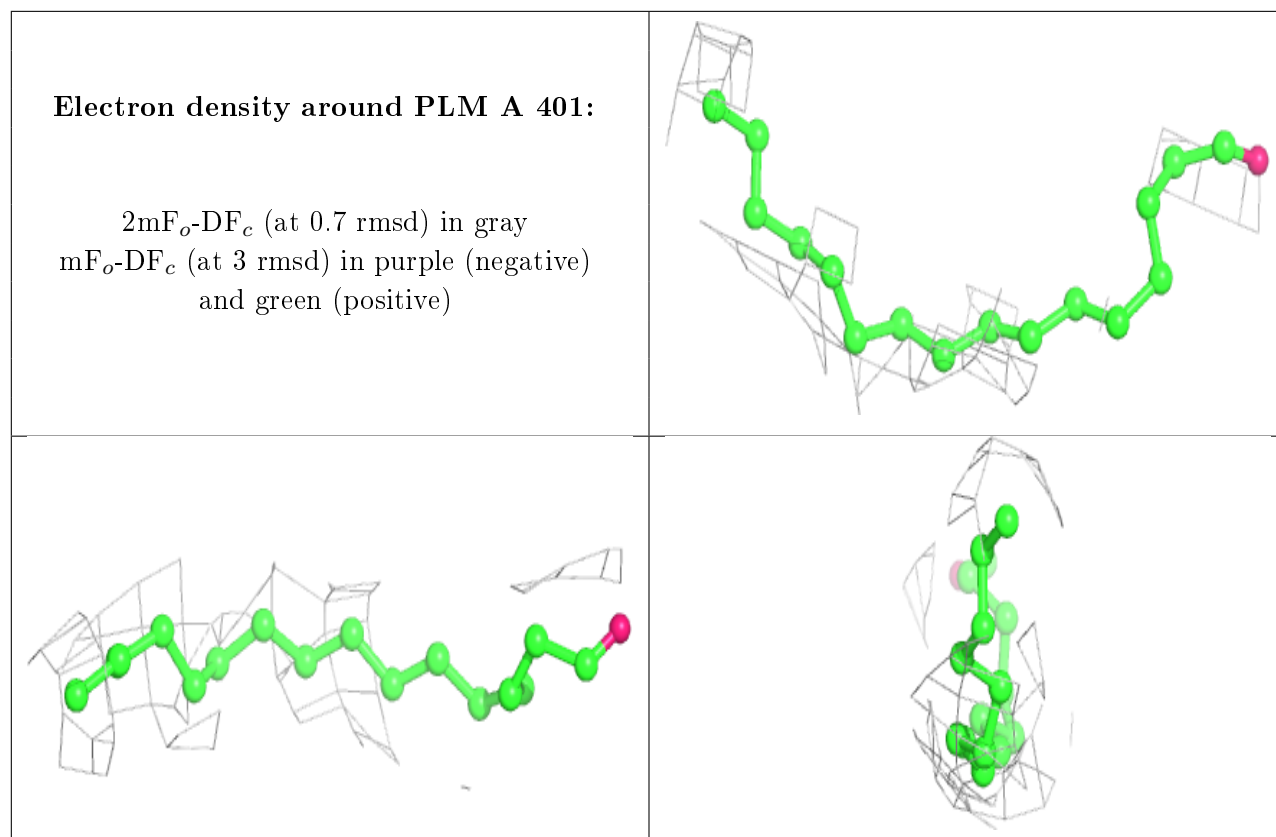


6.4 Ligands ⓘ

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	PLM	A	401	17/18	0.58	0.21	185,185,185,185	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.