



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 11:14 AM UTC

PDB ID : 8DV4 / pdb_00008dv4
Title : Crystal structure of the BC8B TCR-CD1b-PI complex
Authors : Farquhar, R.; Rossjohn, J.; Shahine, A.
Deposited on : 2022-07-28
Resolution : 2.40 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

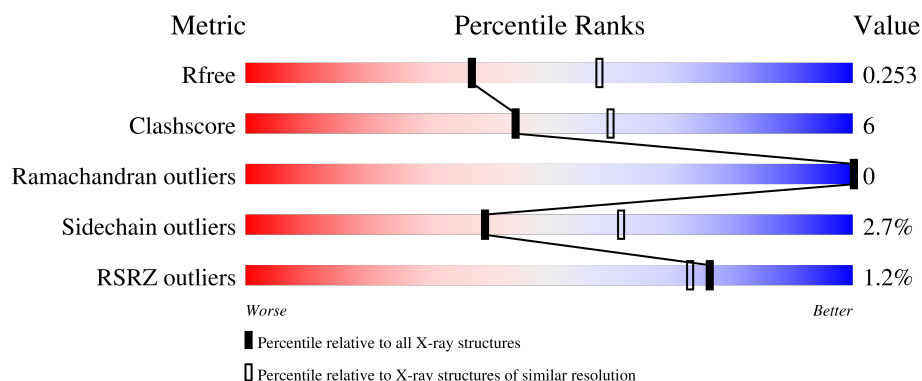
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	300	2% 75% 16% 9%
2	B	99	84% 15% .
3	D	207	2% 74% 16% 9%
4	E	245	2% 88% 11%
5	C	3	67% 33%

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Mol	Chain	Length	Quality of chain
6	F	4	 25% 75%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 6742 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 T-cell surface glycoprotein CD1b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2107	1354	356	387	10			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	GLY	-	expression tag	UNP P29016
A	280	SER	-	expression tag	UNP P29016
A	281	GLY	-	expression tag	UNP P29016
A	282	LEU	-	expression tag	UNP P29016
A	283	ASN	-	expression tag	UNP P29016
A	284	ASP	-	expression tag	UNP P29016
A	285	ILE	-	expression tag	UNP P29016
A	286	PHE	-	expression tag	UNP P29016
A	287	GLU	-	expression tag	UNP P29016
A	288	ALA	-	expression tag	UNP P29016
A	289	GLN	-	expression tag	UNP P29016
A	290	LYS	-	expression tag	UNP P29016
A	291	ILE	-	expression tag	UNP P29016
A	292	GLU	-	expression tag	UNP P29016
A	293	TRP	-	expression tag	UNP P29016
A	294	HIS	-	expression tag	UNP P29016
A	295	GLU	-	expression tag	UNP P29016
A	296	HIS	-	expression tag	UNP P29016
A	297	HIS	-	expression tag	UNP P29016
A	298	HIS	-	expression tag	UNP P29016
A	299	HIS	-	expression tag	UNP P29016
A	300	HIS	-	expression tag	UNP P29016
A	301	HIS	-	expression tag	UNP P29016

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	1	0
			807	515	138	152	2			

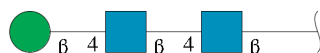
- Molecule 3 is a protein called T-cell receptor alpha variable TRAV9-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	189	Total	C	N	O	S	0	0	0
			1409	888	224	290	7			

- Molecule 4 is a protein called T-cell receptor beta variable TRBV6-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	244	Total	C	N	O	S	0	2	0
			1921	1220	329	362	10			

- Molecule 5 is an oligosaccharide called 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
5	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
6	F	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



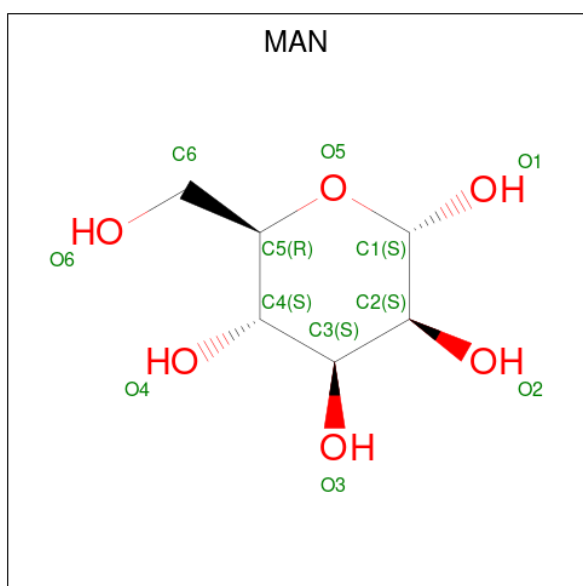
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		

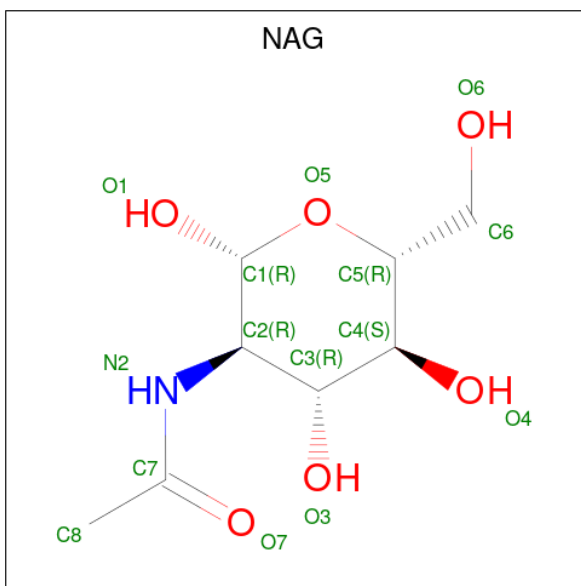
- Molecule 9 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			11	6	5		

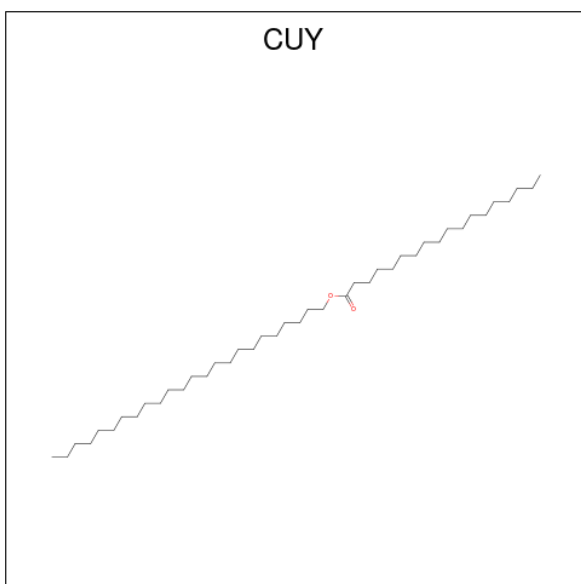
- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆).



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

- Molecule 11 is tetracosyl octadecanoate (CCD ID: CUY) (formula: C₄₂H₈₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			38	36	2		

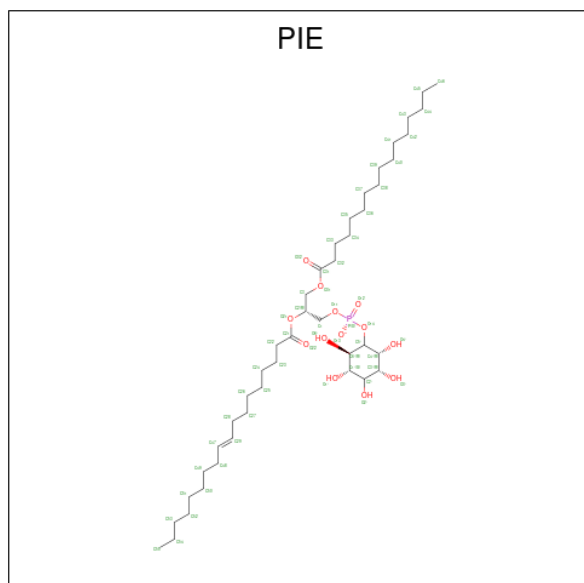
- Molecule 12 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total Cl 1 1	0	0
12	E	2	Total Cl 2 2	0	0

- Molecule 13 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	2	Total Na 2 2	0	0
13	B	1	Total Na 1 1	0	0

- Molecule 14 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphoinositol (CCD ID: PIE) (formula: C₄₃H₈₀O₁₃P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	D	1	Total C O P 57 43 13 1	4	0

- Molecule 15 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	82	Total O 82 82	0	0

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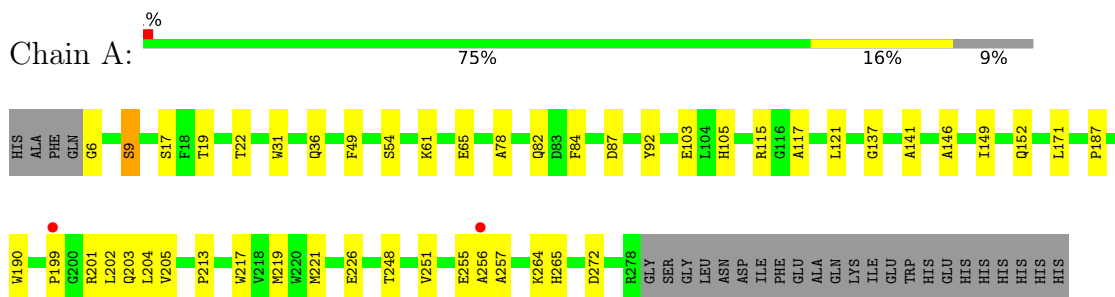
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	B	41	Total 41	O 41	0	0
15	D	43	Total 43	O 43	0	0
15	E	81	Total 81	O 81	0	0

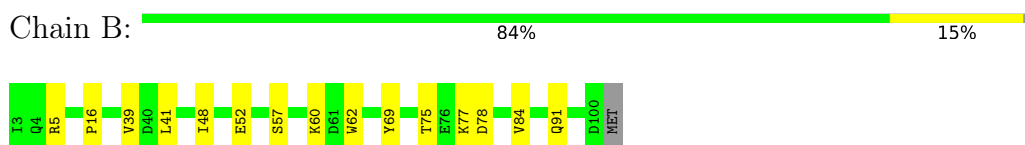
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

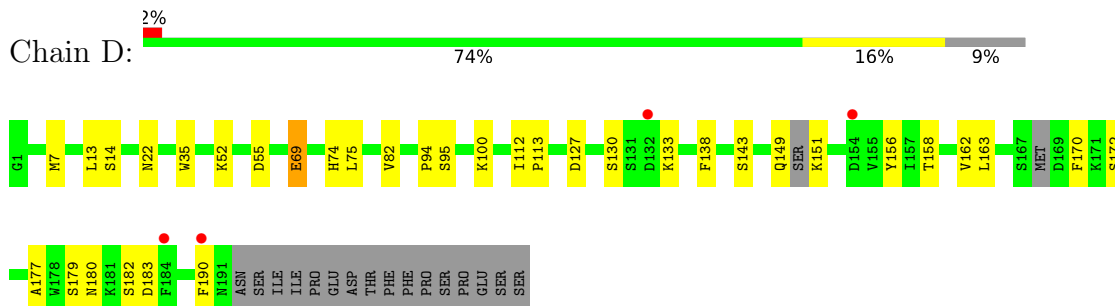
- Molecule 1: T-cell surface glycoprotein CD1b



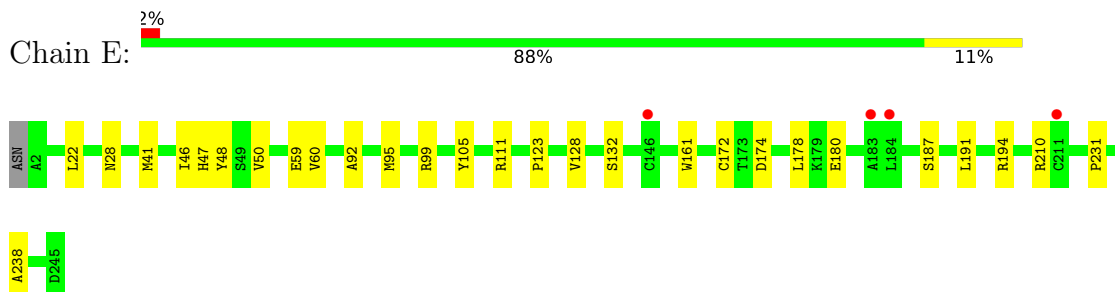
- Molecule 2: Beta-2-microglobulin



- Molecule 3: T-cell receptor alpha variable TRAV9-2



- Molecule 4: T-cell receptor beta variable TRBV6-2



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  67% 33%

NAG1
NAG2
BMA3

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

Chain F:  25% 75%

NAG1
NAG2
BMA3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.09Å 65.43Å 101.58Å 90.00° 102.26° 90.00°	Depositor
Resolution (Å)	46.07 – 2.40 46.07 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.07-2.40) 99.9 (46.07-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.192 , 0.255 0.193 , 0.253	Depositor DCC
R_{free} test set	1863 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.872	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.6	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	0.96	EDS
Total number of atoms	6742	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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: MAN, EDO, CL, GOL, NA, PIE, BMA, CUY, 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	0.34	0/2166	0.50	0/2945
2	B	0.34	0/833	0.49	0/1133
3	D	0.31	0/1437	0.54	0/1955
4	E	0.35	0/1977	0.56	0/2693
All	All	0.34	0/6413	0.53	0/8726

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 [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	2107	0	2007	34	0
2	B	807	0	749	9	0
3	D	1409	0	1297	23	0
4	E	1921	0	1829	17	0
5	C	39	0	34	0	0
6	F	50	0	43	1	0
7	A	8	0	12	1	0
7	D	8	0	12	0	0
7	E	8	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	12	0	16	0	0
9	A	11	0	10	0	0
10	A	14	0	13	1	0
11	A	38	0	0	0	0
12	A	1	0	0	0	0
12	E	2	0	0	0	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
14	D	57	0	80	2	0
15	A	82	0	0	7	0
15	B	41	0	0	0	0
15	D	43	0	0	1	0
15	E	81	0	0	2	0
All	All	6742	0	6114	76	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 (76) 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:221:MET:HE1	1:A:226:GLU:HG2	1.59	0.83
3:D:163:LEU:HB3	4:E:172:CYS:HB2	1.64	0.77
2:B:75:THR:HG22	2:B:77:LYS:H	1.54	0.71
1:A:6:GLY:N	15:A:702:HOH:O	2.23	0.70
1:A:187:PRO:HD3	15:A:709:HOH:O	1.93	0.68
1:A:257:ALA:O	15:A:701:HOH:O	2.11	0.67
1:A:264:LYS:HB3	7:A:601:EDO:H21	1.77	0.67
4:E:161:TRP:HB2	4:E:210:ARG:HB3	1.80	0.64
10:A:604:NAG:H3	10:A:604:NAG:H83	1.81	0.62
3:D:158:THR:HA	4:E:178[A]:LEU:HD21	1.82	0.62
3:D:170:PHE:CE1	3:D:172:SER:HB3	2.36	0.61
1:A:251:VAL:HG11	1:A:256:ALA:HB2	1.82	0.60
3:D:170:PHE:HE1	3:D:172:SER:HB3	1.66	0.60
4:E:111:ARG:HG3	7:E:302:EDO:H12	1.84	0.59
3:D:7:MET:HE3	3:D:22:ASN:H	1.68	0.59
4:E:174:ASP:HB2	4:E:191:LEU:HD12	1.86	0.57
3:D:94:PRO:HG3	14:D:501:PIE:H4'1	1.87	0.56
3:D:95:SER:O	15:D:601:HOH:O	2.18	0.56
3:D:149:GLN:O	3:D:151:LYS:N	2.38	0.56
3:D:35:TRP:CE2	3:D:75:LEU:HB2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ARG:NH1	15:A:706:HOH:O	2.34	0.54
1:A:205:VAL:HG22	1:A:248:THR:HG22	1.90	0.53
1:A:251:VAL:HG22	1:A:255:GLU:HB3	1.89	0.53
3:D:127:ASP:HB3	3:D:130:SER:O	2.08	0.53
1:A:9:SER:HB2	1:A:103:GLU:HB3	1.91	0.52
3:D:69:GLU:H	3:D:69:GLU:CD	2.17	0.51
2:B:75:THR:HB	2:B:78:ASP:OD2	2.11	0.51
4:E:210:ARG:HD3	15:E:460:HOH:O	2.11	0.51
4:E:46:ILE:HG22	4:E:47:HIS:CD2	2.47	0.50
1:A:49:PHE:HB3	1:A:54:SER:HB2	1.93	0.49
1:A:202:LEU:HD12	1:A:203:GLN:H	1.76	0.49
1:A:19:THR:O	1:A:92:TYR:HB3	2.13	0.49
1:A:84:PHE:CZ	4:E:99:ARG:HD2	2.47	0.49
1:A:87:ASP:CG	4:E:99:ARG:HH22	2.21	0.48
4:E:123:PRO:HD3	4:E:231:PRO:HB3	1.95	0.48
1:A:199:PRO:C	1:A:201:ARG:H	2.22	0.47
4:E:41:MET:HB3	15:E:411:HOH:O	2.15	0.46
1:A:190:TRP:CD2	2:B:16:PRO:HG3	2.50	0.46
3:D:113:PRO:HG3	3:D:162:VAL:HG11	1.97	0.46
1:A:219:MET:HB3	1:A:221:MET:HE3	1.98	0.45
4:E:128:VAL:HG23	4:E:238:ALA:HB3	1.97	0.45
1:A:213:PRO:HG2	15:A:761:HOH:O	2.17	0.45
1:A:265:HIS:CG	15:A:709:HOH:O	2.69	0.45
2:B:39:VAL:HG22	2:B:84:VAL:HG22	1.99	0.44
3:D:100:LYS:HD3	4:E:48:TYR:CE1	2.53	0.44
14:D:501:PIE:H6'1	14:D:501:PIE:H12	1.99	0.44
3:D:7:MET:HE3	3:D:7:MET:HB2	1.79	0.44
3:D:138:PHE:HB2	3:D:190:PHE:CE2	2.53	0.43
2:B:41:LEU:O	2:B:48:ILE:HG13	2.19	0.43
4:E:60:VAL:O	4:E:60:VAL:HG13	2.18	0.43
4:E:28:ASN:O	4:E:95:MET:HE1	2.19	0.43
1:A:204:LEU:HD11	1:A:256:ALA:HB1	2.00	0.43
3:D:133:LYS:HB2	3:D:133:LYS:HE2	1.62	0.43
1:A:137:GLY:HA3	1:A:141:ALA:HB2	2.01	0.43
1:A:171:LEU:HD12	6:F:2:NAG:H82	2.00	0.43
2:B:52:GLU:HB2	2:B:69:TYR:CZ	2.54	0.43
1:A:264:LYS:NZ	1:A:272:ASP:OD2	2.49	0.42
1:A:204:LEU:O	1:A:248:THR:HA	2.19	0.42
3:D:52:LYS:O	3:D:55:ASP:HB2	2.19	0.42
1:A:78:ALA:O	1:A:82:GLN:HG2	2.20	0.42
1:A:31:TRP:CZ2	2:B:57:SER:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5[B]:ARG:HE	2:B:5[B]:ARG:HB3	1.43	0.42
1:A:117:ALA:HB2	2:B:62:TRP:CE2	2.55	0.42
1:A:103:GLU:OE2	1:A:105:HIS:NE2	2.48	0.42
1:A:61:LYS:NZ	1:A:65:GLU:OE2	2.53	0.41
3:D:156:TYR:O	3:D:177:ALA:HA	2.20	0.41
3:D:179:SER:HB2	3:D:182:SER:HB3	2.03	0.41
1:A:146:ALA:O	1:A:149:ILE:HG22	2.21	0.41
1:A:217:TRP:CZ2	1:A:219:MET:HG3	2.56	0.41
3:D:156:TYR:HE1	4:E:180:GLU:O	2.03	0.41
3:D:22:ASN:HA	3:D:74:HIS:ND1	2.36	0.40
1:A:31:TRP:CZ3	1:A:36:GLN:HB2	2.55	0.40
1:A:265:HIS:ND1	15:A:709:HOH:O	2.37	0.40
3:D:156:TYR:HE2	3:D:180:ASN:HD21	1.69	0.40
3:D:112:ILE:HG22	3:D:143:SER:HB3	2.04	0.40
4:E:92:ALA:HA	4:E:105:TYR:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	271/300 (90%)	263 (97%)	8 (3%)	0	100	100
2	B	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
3	D	183/207 (88%)	176 (96%)	7 (4%)	0	100	100
4	E	244/245 (100%)	239 (98%)	5 (2%)	0	100	100
All	All	795/851 (93%)	773 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	216/247 (87%)	211 (98%)	5 (2%)	44	66
2	B	88/94 (94%)	86 (98%)	2 (2%)	44	66
3	D	151/182 (83%)	146 (97%)	5 (3%)	33	55
4	E	205/211 (97%)	199 (97%)	6 (3%)	37	60
All	All	660/734 (90%)	642 (97%)	18 (3%)	39	62

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	17	SER
1	A	22	THR
1	A	121	LEU
1	A	152	GLN
2	B	60	LYS
2	B	91	GLN
3	D	13	LEU
3	D	14	SER
3	D	69	GLU
3	D	82	VAL
3	D	183	ASP
4	E	22	LEU
4	E	50	VAL
4	E	59	GLU
4	E	132	SER
4	E	187	SER
4	E	194	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN

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Mol	Chain	Res	Type
2	B	10	GLN
2	B	26	ASN
3	D	110	GLN
4	E	73	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

7 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$
5	NAG	C	1	5,1	14,14,15	0.58	0	17,19,21	0.61	0
5	NAG	C	2	5	14,14,15	0.31	0	17,19,21	0.66	0
5	BMA	C	3	5	11,11,12	1.02	1 (9%)	15,15,17	1.05	2 (13%)
6	NAG	F	1	1,6	14,14,15	0.54	0	17,19,21	0.59	0
6	NAG	F	2	6	14,14,15	0.34	0	17,19,21	0.50	0
6	BMA	F	3	6	11,11,12	1.24	1 (9%)	15,15,17	1.10	1 (6%)
6	MAN	F	4	6	11,11,12	0.99	0	15,15,17	1.35	1 (6%)

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	NAG	C	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	2/6/23/26	0/1/1/1
5	BMA	C	3	5	-	0/2/19/22	0/1/1/1
6	NAG	F	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	0/1/1/1
6	BMA	F	3	6	-	2/2/19/22	0/1/1/1
6	MAN	F	4	6	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	3	BMA	C2-C3	2.96	1.57	1.52
5	C	3	BMA	C1-C2	2.24	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	4	MAN	C1-O5-C5	4.44	118.14	112.19
5	C	3	BMA	C1-O5-C5	2.54	115.59	112.19
6	F	3	BMA	C1-C2-C3	2.47	113.23	109.64
5	C	3	BMA	O2-C2-C3	-2.08	105.85	110.15

There are no chirality outliers.

All (8) torsion outliers are listed below:

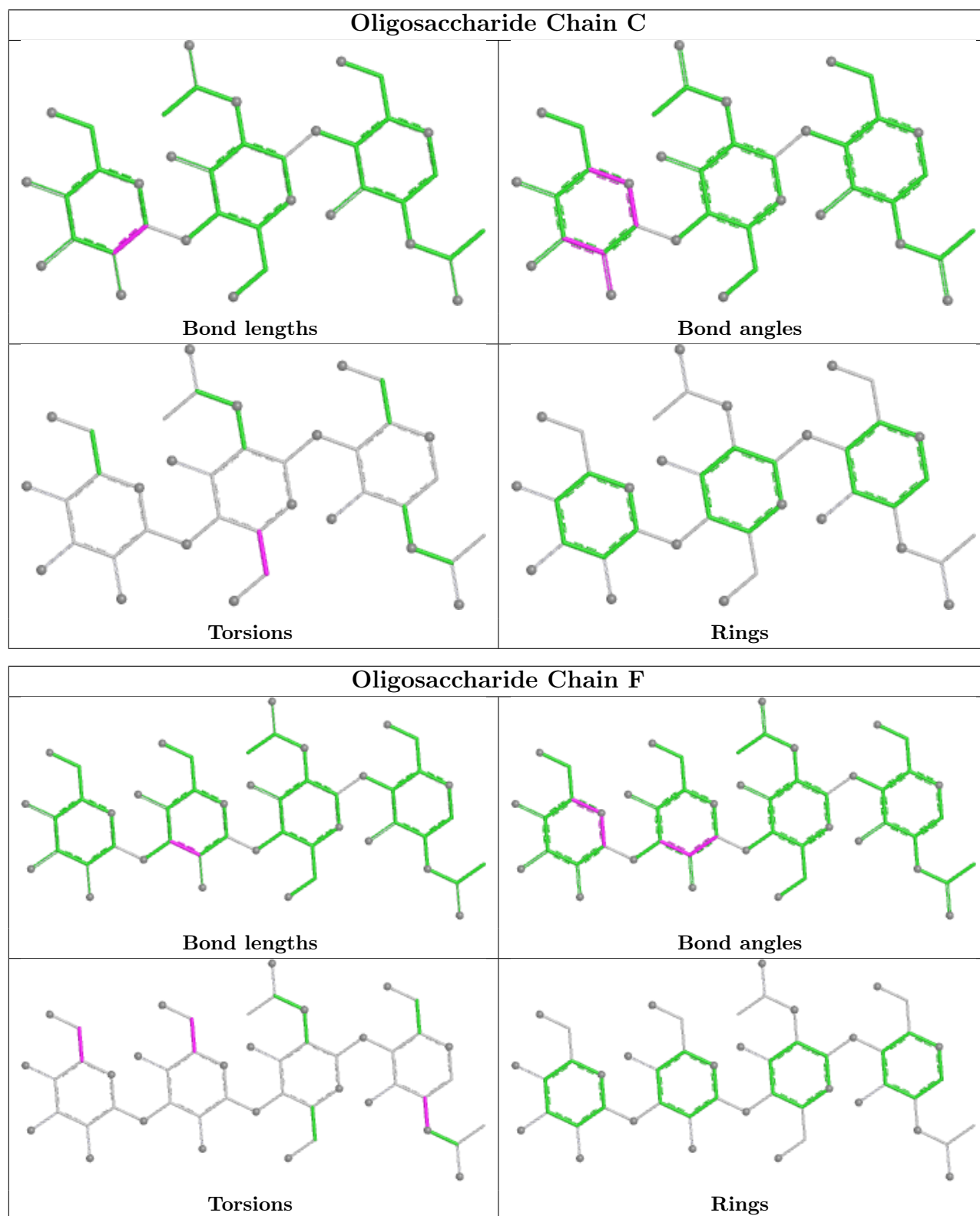
Mol	Chain	Res	Type	Atoms
6	F	3	BMA	O5-C5-C6-O6
6	F	3	BMA	C4-C5-C6-O6
5	C	2	NAG	O5-C5-C6-O6
6	F	4	MAN	C4-C5-C6-O6
6	F	4	MAN	O5-C5-C6-O6
5	C	2	NAG	C4-C5-C6-O6
6	F	1	NAG	C3-C2-N2-C7
6	F	1	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	2	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

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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
8	GOL	A	602	-	5,5,5	1.24	0	5,5,5	0.97	0
7	EDO	E	301	-	3,3,3	0.65	0	2,2,2	0.14	0
8	GOL	A	609	-	5,5,5	0.95	0	5,5,5	1.03	0
9	MAN	A	603	-	11,11,12	1.76	3 (27%)	15,15,17	1.37	2 (13%)
14	PIE	D	501	-	57,57,57	0.34	0	66,69,69	0.60	1 (1%)
7	EDO	A	607	-	3,3,3	0.45	0	2,2,2	0.36	0
7	EDO	D	503	-	3,3,3	0.47	0	2,2,2	0.30	0
7	EDO	A	601	-	3,3,3	0.58	0	2,2,2	0.18	0
10	NAG	A	604	1	14,14,15	0.76	1 (7%)	17,19,21	1.54	3 (17%)
7	EDO	E	302	-	3,3,3	0.54	0	2,2,2	0.26	0
7	EDO	D	502	-	3,3,3	0.39	0	2,2,2	0.26	0
11	CUY	A	605	-	37,37,43	0.26	0	37,37,43	0.58	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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	A	602	-	-	2/4/4/4	-
7	EDO	E	301	-	-	0/1/1/1	-
8	GOL	A	609	-	-	0/4/4/4	-
9	MAN	A	603	-	-	2/2/19/22	0/1/1/1
14	PIE	D	501	-	-	18/52/76/76	0/1/1/1
7	EDO	A	607	-	-	0/1/1/1	-
7	EDO	D	503	-	-	0/1/1/1	-
7	EDO	A	601	-	-	0/1/1/1	-
10	NAG	A	604	1	-	5/6/23/26	0/1/1/1
7	EDO	E	302	-	-	1/1/1/1	-
7	EDO	D	502	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CUY	A	605	-	-	9/36/36/42	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	603	MAN	C2-C3	3.77	1.58	1.52
9	A	603	MAN	O5-C5	2.86	1.49	1.43
10	A	604	NAG	C1-C2	2.56	1.55	1.52
9	A	603	MAN	O5-C1	-2.07	1.40	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	604	NAG	C2-N2-C7	4.67	129.16	122.90
9	A	603	MAN	C1-O5-C5	2.96	116.16	112.19
10	A	604	NAG	C1-O5-C5	2.82	115.97	112.19
10	A	604	NAG	C1-C2-N2	2.46	114.31	110.43
14	D	501	PIE	O21-C2-C3	-2.42	99.66	108.34
9	A	603	MAN	C2-C3-C4	2.08	114.51	110.86

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	602	GOL	C1-C2-C3-O3
14	D	501	PIE	C4'-C5'-O14-P
14	D	501	PIE	C6'-C5'-O14-P
14	D	501	PIE	O32-C31-O31-C3
14	D	501	PIE	C32-C31-O31-C3
9	A	603	MAN	O5-C5-C6-O6
10	A	604	NAG	C8-C7-N2-C2
10	A	604	NAG	O7-C7-N2-C2
9	A	603	MAN	C4-C5-C6-O6
10	A	604	NAG	O5-C5-C6-O6
11	A	605	CUY	CAT-CAU-CAV-CAW
11	A	605	CUY	CAD-CAE-CAF-CAG
11	A	605	CUY	CAI-CAJ-CAK-CAL
11	A	605	CUY	CBH-CBI-CBJ-CBK
11	A	605	CUY	CBF-CBG-CBH-CBI
14	D	501	PIE	C31-C32-C33-C34
14	D	501	PIE	C33-C34-C35-C36

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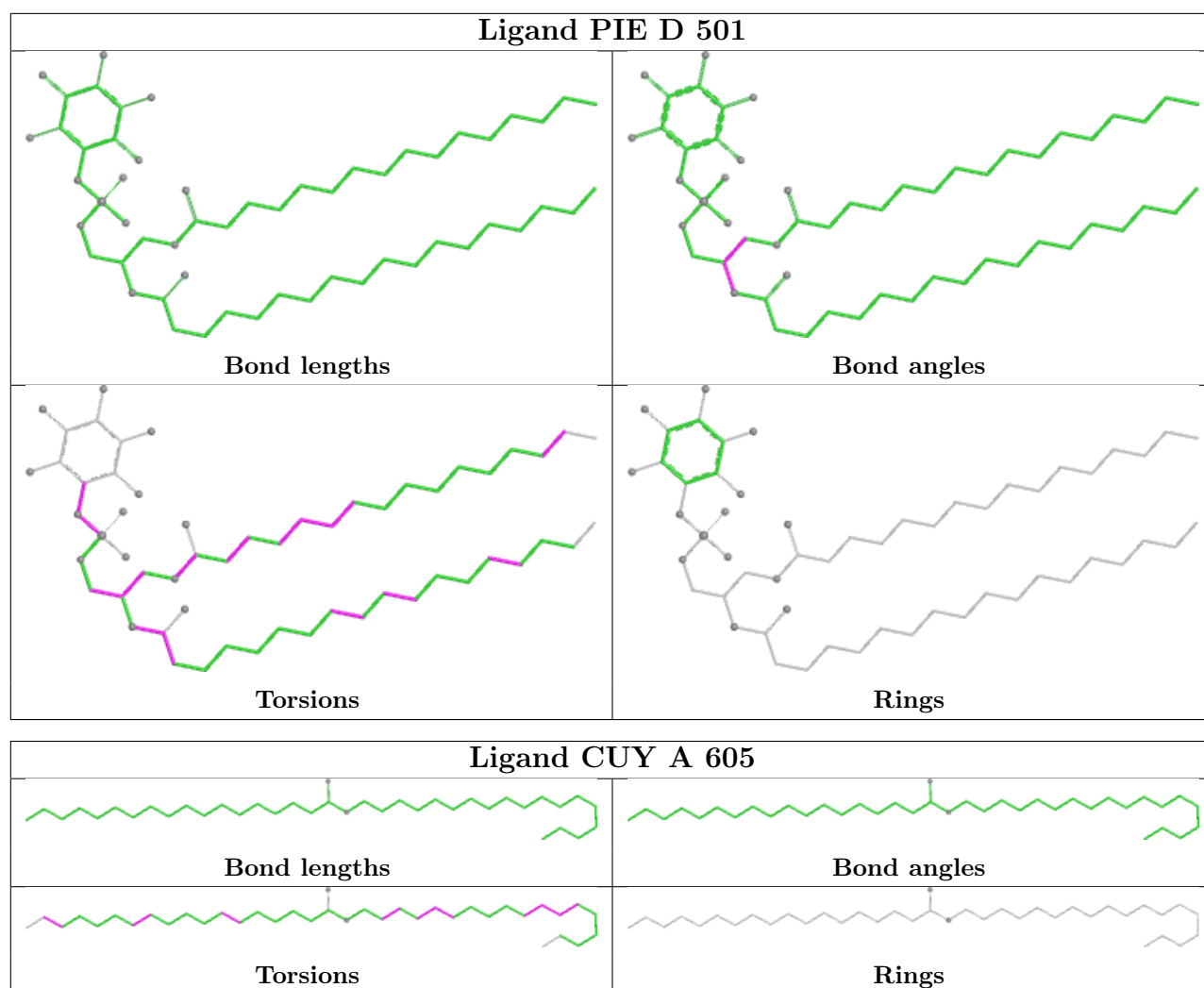
Mol	Chain	Res	Type	Atoms
8	A	602	GOL	O2-C2-C3-O3
11	A	605	CUY	CBG-CBH-CBI-CBJ
11	A	605	CUY	CAU-CAV-CAW-CBM
11	A	605	CUY	C41-C40-CAA-CAB
10	A	604	NAG	C4-C5-C6-O6
7	E	302	EDO	O1-C1-C2-O2
14	D	501	PIE	C34-C35-C36-C37
14	D	501	PIE	C27-C28-C29-C47
14	D	501	PIE	C50-C51-C52-C53
10	A	604	NAG	C3-C2-N2-C7
14	D	501	PIE	C5'-O14-P-O11
14	D	501	PIE	C43-C44-C45-C46
14	D	501	PIE	O21-C21-C22-C23
14	D	501	PIE	O11-C1-C2-O21
14	D	501	PIE	C22-C21-O21-C2
14	D	501	PIE	C29-C47-C48-C49
14	D	501	PIE	C5'-O14-P-O13
14	D	501	PIE	O21-C2-C3-O31
14	D	501	PIE	C35-C36-C37-C38
11	A	605	CUY	CAR-CAS-CAT-CAU

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	D	501	PIE	2	0
7	A	601	EDO	1	0
10	A	604	NAG	1	0
7	E	302	EDO	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 [i](#)

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	273/300 (91%)	-0.13	2 (0%) 84 81	33, 48, 88, 111	0
2	B	98/99 (98%)	-0.18	0 100 100	24, 47, 73, 81	1 (1%)
3	D	189/207 (91%)	0.07	4 (2%) 63 59	33, 56, 100, 130	0
4	E	244/245 (99%)	-0.25	4 (1%) 70 66	21, 45, 66, 84	2 (0%)
All	All	804/851 (94%)	-0.13	10 (1%) 76 73	21, 48, 86, 130	3 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	146	CYS	4.1
1	A	199	PRO	3.1
4	E	211	CYS	2.6
4	E	183	ALA	2.6
3	D	154	ASP	2.4
4	E	184	LEU	2.3
3	D	184	PHE	2.2
3	D	190	PHE	2.2
3	D	132	ASP	2.1
1	A	256	ALA	2.0

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

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

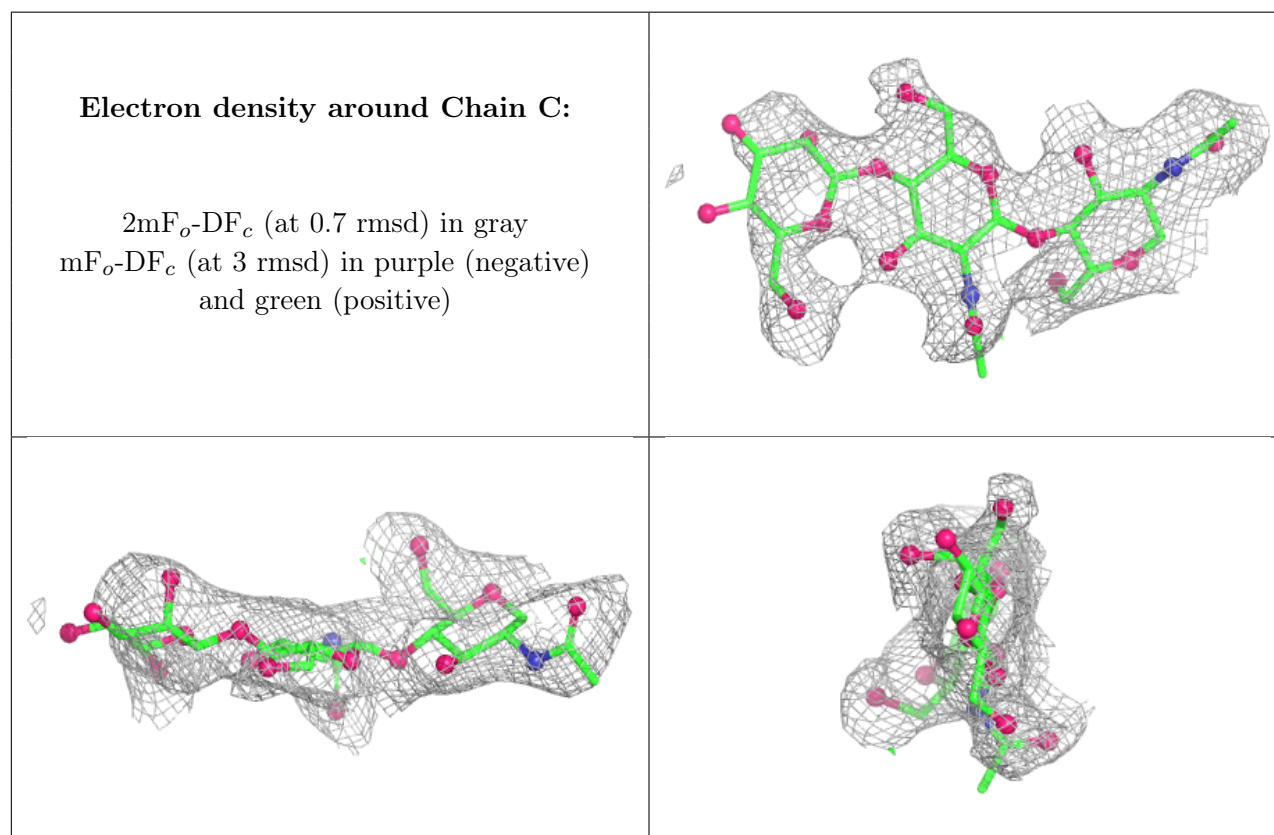
6.3 Carbohydrates [i](#)

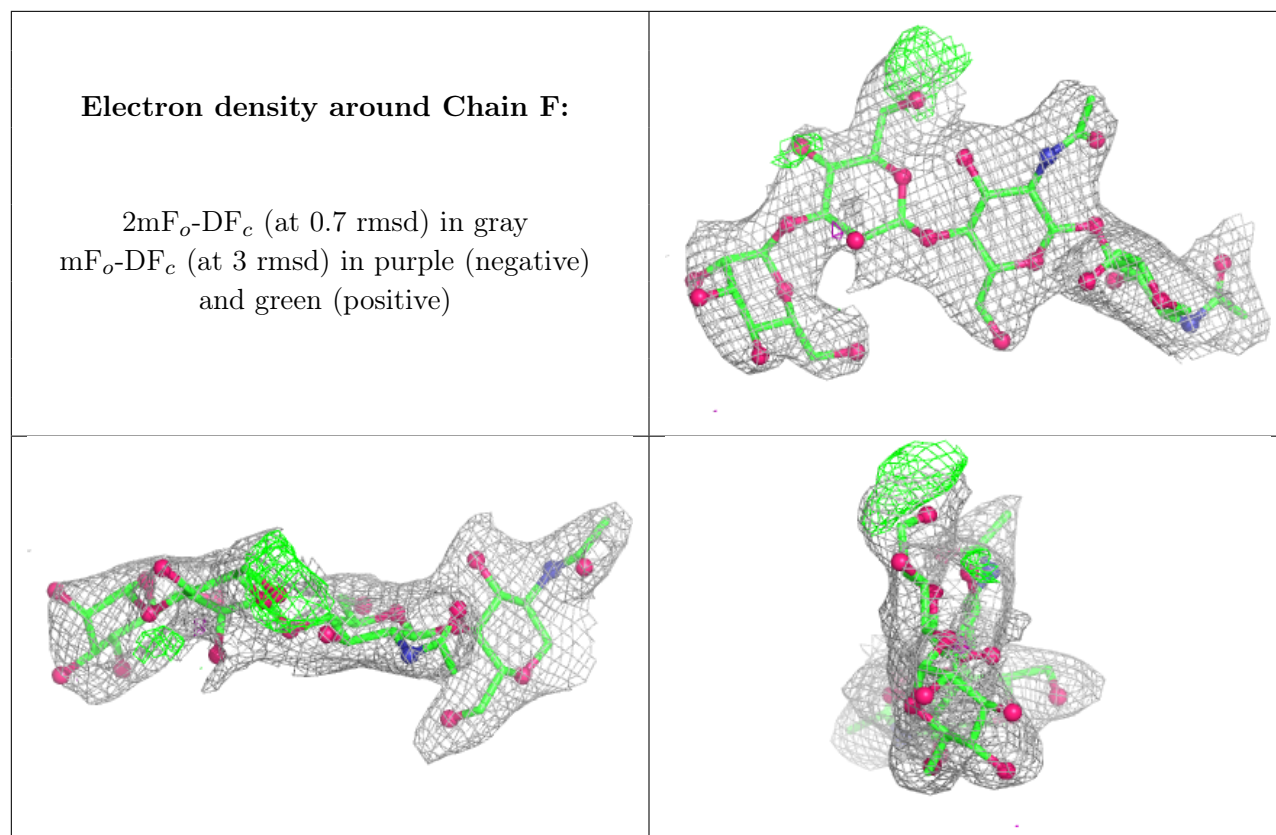
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	C	1	14/15	-	-	57,70,74,77	0
5	NAG	C	2	14/15	-	-	80,89,94,95	0
5	BMA	C	3	11/12	-	-	92,102,108,111	0
6	BMA	F	3	11/12	0.52	0.15	75,90,94,94	0
6	MAN	F	4	11/12	0.71	0.12	89,94,99,99	0
6	NAG	F	2	14/15	0.85	0.10	55,69,77,84	0
6	NAG	F	1	14/15	0.90	0.09	44,50,58,66	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($\text{\AA}^2$)	Q<0.9
7	EDO	D	503	4/4	0.39	0.18	72,80,88,90	0
10	NAG	A	604	14/15	0.41	0.13	91,105,115,116	0
8	GOL	A	609	6/6	0.64	0.15	80,86,92,92	0
9	MAN	A	603	11/12	0.66	0.17	72,88,97,97	0
8	GOL	A	602	6/6	0.75	0.13	73,84,88,89	0
13	NA	A	608	1/1	0.77	0.18	68,68,68,68	0
13	NA	A	610	1/1	0.79	0.18	66,66,66,66	0
7	EDO	E	301	4/4	0.84	0.16	44,48,49,57	0
13	NA	B	201	1/1	0.84	0.21	63,63,63,63	0
14	PIE	D	501	57/57	0.84	0.15	34,53,81,86	4
7	EDO	A	601	4/4	0.86	0.14	60,60,61,64	0
7	EDO	E	302	4/4	0.89	0.10	48,50,53,54	0
12	CL	E	303	1/1	0.89	0.09	83,83,83,83	0
12	CL	A	606	1/1	0.90	0.10	64,64,64,64	0

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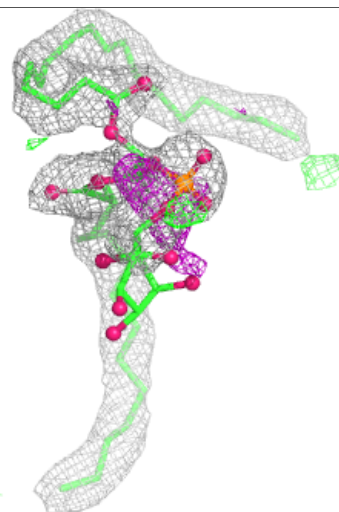
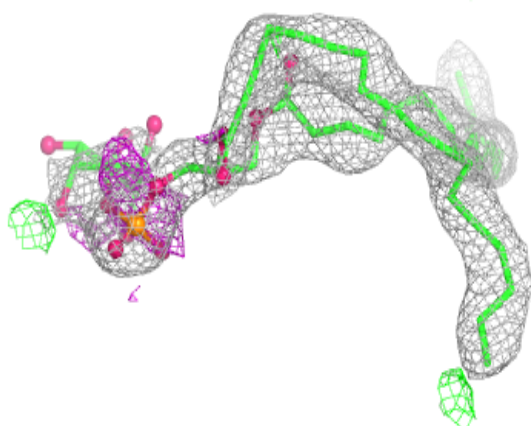
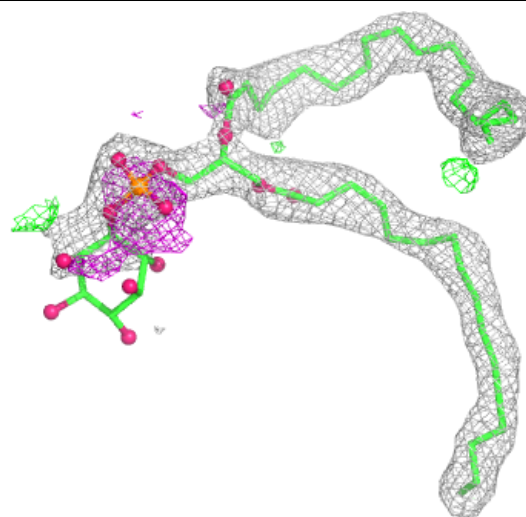
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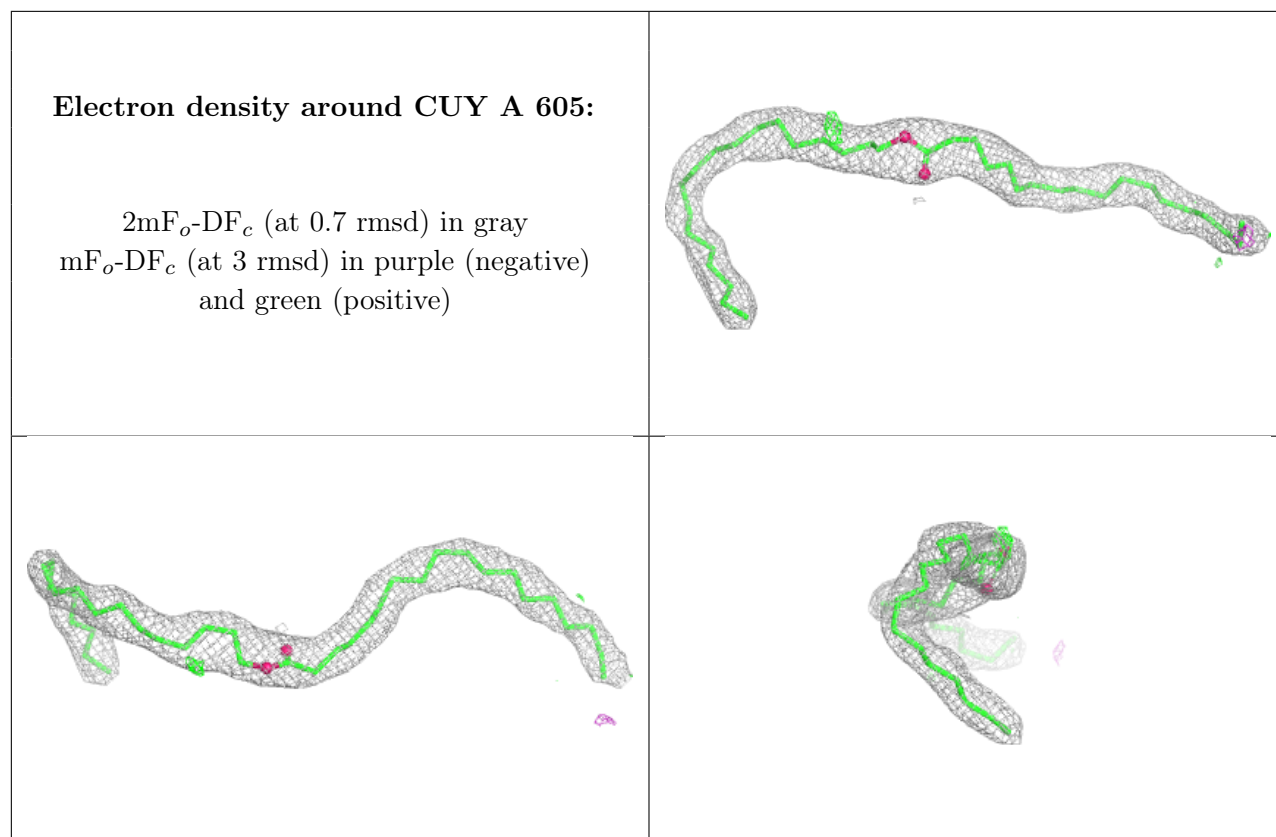
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	A	607	4/4	0.91	0.09	43,44,46,46	0
11	CUY	A	605	38/44	0.93	0.10	37,47,54,59	0
12	CL	E	304	1/1	0.93	0.08	62,62,62,62	0
7	EDO	D	502	4/4	0.95	0.11	47,48,57,57	0

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 PIE D 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.