



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 11:47 AM UTC

PDB ID : 6FCS / pdb_00006fcs
Title : The X-ray Structure of Lytic Transglycosylase Slr inactive mutant E503Q from *Pseudomonas aeruginosa* in complex with NAG-NAMpentapeptide-NAG-NAMpentapeptide
Authors : Batuecas, M.T.; Dominguez-Gil, T.; Hermoso, J.A.
Deposited on : 2017-12-21
Resolution : 2.90 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
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

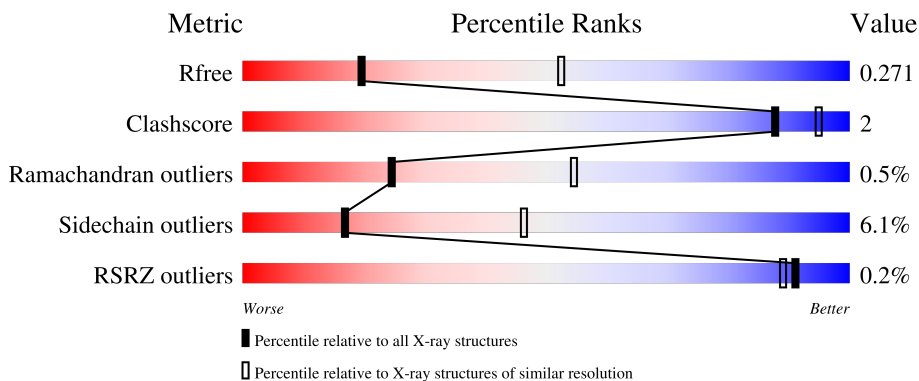
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

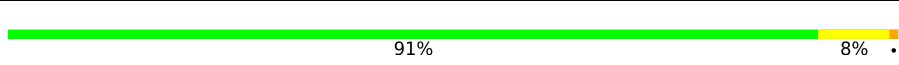

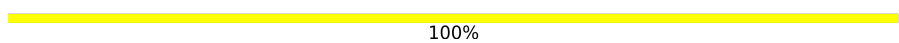

The reported resolution of this entry is 2.90 Å.

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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	613	
2	B	5	
3	C	4	
4	D	4	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5210 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 Soluble lytic murein transglycosylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	613	4977	3157	914	895	11	0	1	0

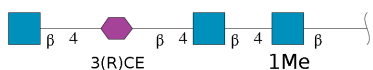
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	503	GLN	GLU	engineered mutation	UNP A0A069QJX4

- Molecule 2 is a protein (with D amino acids) called ALA-DGL-API-DAL-DAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	5	36	21	6	9	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-beta-muramic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-methyl 2-acetamido-2-deoxy-beta-D-glucopyranoside.

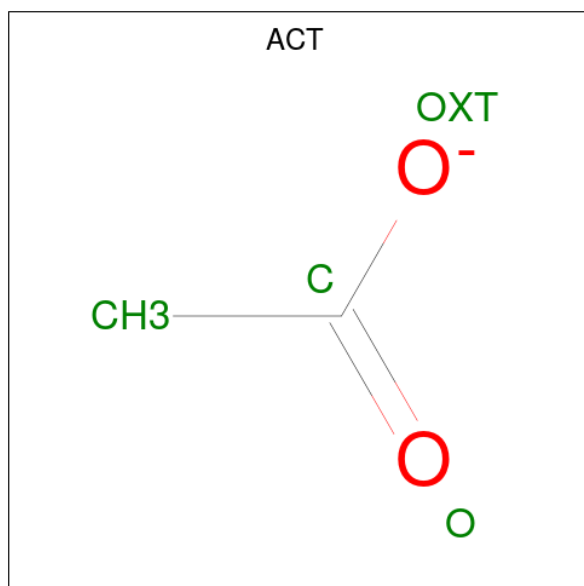


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	4	62	36	4	22	0	0	0

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-3-O-[(2R)-1-amino-1-oxopropan-2-yl]-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-methyl 2-acetamido-3-O-[(1R)-1-carboxyethyl]-2-deoxy-beta-D-glucopyranoside.

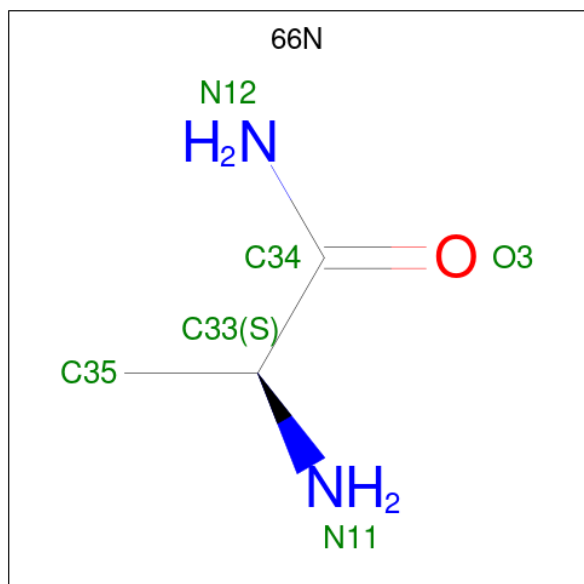
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	4	67	39	5	23	0	0	0

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0

- Molecule 6 is L-alaninamide (CCD ID: 66N) (formula: $C_3H_8N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			6	3	2	1		

- Molecule 7 is water.

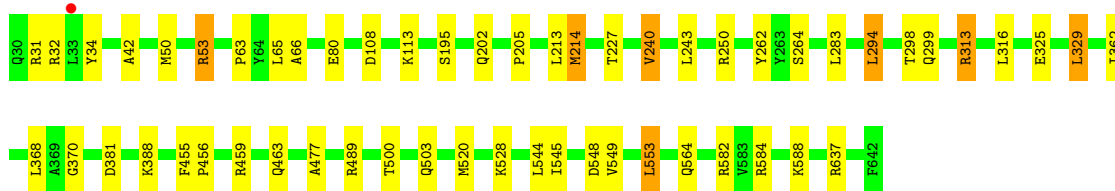
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	53	Total	O	0	0
			53	53		
7	B	1	Total	O	0	0
			1	1		

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: Soluble lytic murein transglycosylase

Chain A:  91% 8%



- Molecule 2: ALA-DGL-API-DAL-DAL

Chain B:  60% 40%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-beta-muramic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-methyl 2-acetamido-2-deoxy-beta-D-glucopyranoside

Chain C:  100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-3-O-[(2R)-1-amino-1-oxopropan-2-yl]-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-methyl 2-acetamido-3-O-[(1R)-1-carboxyethyl]-2-deoxy-beta-D-glucopyranoside

Chain D:  50% 50%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	166.87Å 166.87Å 54.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	144.52 – 2.90 144.52 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (144.52-2.90) 99.9 (144.52-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.91Å)	Xtrriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.193 , 0.269 0.201 , 0.271	Depositor DCC
R_{free} test set	972 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	70.2	Xtrriage
Anisotropy	0.009	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5210	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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: NM6, 66N, ACT, API, MAG, NAG, AMV, DAL, DGL, AMU

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	0.58	0/5104	0.91	0/6920
2	B	0.93	0/4	0.97	0/4
All	All	0.58	0/5108	0.91	0/6924

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	4977	0	4909	19	0
2	B	36	0	29	1	0
3	C	62	0	56	0	0
4	D	67	0	50	2	0
5	A	8	0	6	0	0
6	A	6	0	0	0	0
7	A	53	0	0	4	2
7	B	1	0	0	0	0
All	All	5210	0	5050	20	2

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 2.

All (20) 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:66:ALA:N	7:A:801:HOH:O	2.06	0.89
1:A:63:PRO:C	7:A:801:HOH:O	2.23	0.80
1:A:294:LEU:HD13	1:A:316:LEU:HD23	1.79	0.64
1:A:500:THR:HG22	1:A:520:MET:HG2	1.83	0.61
1:A:214:MET:HE3	1:A:240:VAL:HA	1.83	0.60
1:A:313:ARG:HG2	1:A:329:LEU:HD11	1.82	0.59
1:A:214:MET:HE2	1:A:243:LEU:HD22	1.90	0.53
1:A:503:GLN:NE2	4:D:1:AMV:O6	2.42	0.53
1:A:500:THR:HG22	1:A:520:MET:CG	2.39	0.52
1:A:50:MET:SD	1:A:53:ARG:NH1	2.85	0.50
1:A:370:GLY:HA2	1:A:388:LYS:HD2	1.97	0.46
1:A:564:GLN:HE21	1:A:584:ARG:NH2	2.14	0.45
1:A:549:VAL:O	1:A:553:LEU:HD23	2.16	0.45
1:A:582:ARG:NH1	2:B:1:ALA:O	2.51	0.43
1:A:65:LEU:N	7:A:801:HOH:O	2.51	0.43
4:D:1:AMV:H112	4:D:2:NAG:H62	2.01	0.42
1:A:250:ARG:NH2	7:A:804:HOH:O	2.51	0.42
1:A:455:PHE:HB3	1:A:456:PRO:HD3	2.02	0.41
1:A:227:THR:HB	1:A:262:TYR:CE2	2.55	0.41
1:A:381:ASP:OD2	1:A:637:ARG:NH2	2.54	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:824:HOH:O	7:A:842:HOH:O[6_655]	1.17	1.03
7:A:805:HOH:O	7:A:828:HOH:O[6_654]	1.91	0.29

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	612/613 (100%)	594 (97%)	15 (2%)	3 (0%)	24 54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ALA
1	A	477	ALA
1	A	205	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	508/507 (100%)	477 (94%)	31 (6%)	17 46

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ARG
1	A	32	ARG
1	A	34	TYR
1	A	53	ARG
1	A	80	GLU
1	A	108	ASP
1	A	113	LYS
1	A	195	SER
1	A	202	GLN
1	A	213	LEU
1	A	214	MET
1	A	240	VAL
1	A	264	SER
1	A	283	LEU
1	A	294	LEU
1	A	298	THR
1	A	299	GLN
1	A	313	ARG

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Mol	Chain	Res	Type
1	A	325	GLU
1	A	329	LEU
1	A	362	ILE
1	A	368	LEU
1	A	459	ARG
1	A	463	GLN
1	A	489	ARG
1	A	528	LYS
1	A	544	LEU
1	A	545	ILE
1	A	548	ASP
1	A	553	LEU
1	A	588	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	A	219	GLN
1	A	418	ASN
1	A	452	GLN
1	A	502	GLN
1	A	503	GLN
1	A	560	GLN
1	A	564	GLN
1	A	577	ASN
1	A	592	HIS
1	A	613	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](#)

4 non-standard protein/DNA/RNA residues 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	API	B	3	2	9,11,12	2.66	2 (22%)	5,13,15	1.26	1 (20%)

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	API	B	3	2	-	3/11/12/14	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	API	O3-C7	7.24	1.43	1.22
2	B	3	API	O4-C7	-2.92	1.21	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	API	O4-C7-O3	-2.05	119.42	124.08

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3	API	C4-C3-CA-C
2	B	3	API	C4-C3-CA-N
2	B	3	API	C3-C4-C5-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

8 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	MAG	C	1	3	16,16,16	1.94	5 (31%)	22,22,22	2.27	6 (27%)
3	NAG	C	2	3	14,14,15	1.24	1 (7%)	17,19,21	1.46	3 (17%)
3	AMU	C	3	6,3	17,18,20	1.05	1 (5%)	20,24,28	2.22	9 (45%)
3	NAG	C	4	3	14,14,15	0.85	0	17,19,21	1.61	3 (17%)
4	AMV	D	1	2,4	19,20,21	1.59	2 (10%)	22,27,29	1.77	6 (27%)
4	NAG	D	2	4	14,14,15	1.17	2 (14%)	17,19,21	1.48	4 (23%)
4	NM6	D	3	4	19,19,20	1.79	2 (10%)	23,26,28	2.02	8 (34%)
4	NAG	D	4	4	14,14,15	0.73	0	17,19,21	1.21	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
3	MAG	C	1	3	-	4/8/28/28	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	AMU	C	3	6,3	-	2/11/29/34	0/1/1/1
3	NAG	C	4	3	-	4/6/23/26	0/1/1/1
4	AMV	D	1	2,4	-	3/13/34/36	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NM6	D	3	4	-	1/14/31/34	0/1/1/1
4	NAG	D	4	4	-	2/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3	NM6	C3C-N3A	6.30	1.47	1.32
3	C	1	MAG	C7-N2	4.64	1.49	1.34
4	D	1	AMV	C7-N2	4.32	1.48	1.34
3	C	2	NAG	C1-C2	3.52	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2	NAG	C1-C2	3.02	1.56	1.52
3	C	1	MAG	O1-C1	2.96	1.45	1.40
3	C	1	MAG	C2-N2	2.89	1.50	1.45
4	D	1	AMV	O1-C1	2.49	1.44	1.40
4	D	2	NAG	O5-C1	-2.46	1.39	1.43
3	C	1	MAG	C1-C2	2.39	1.56	1.53
4	D	3	NM6	C4-C5	2.32	1.58	1.53
3	C	3	AMU	C11-C9	2.24	1.56	1.51
3	C	1	MAG	O5-C1	2.11	1.47	1.41

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	MAG	C1-O5-C5	7.59	128.54	113.72
3	C	3	AMU	O5-C1-C2	-4.79	103.88	111.29
4	D	3	NM6	O3-C3-C2	4.39	119.14	108.85
4	D	3	NM6	O3B-C3C-C3A	4.24	121.99	118.93
4	D	1	AMV	C3-C2-N2	3.98	117.26	110.91
3	C	4	NAG	C4-C3-C2	3.94	116.79	111.02
4	D	3	NM6	O5-C1-C2	-3.61	105.70	111.29
3	C	3	AMU	O3-C3-C4	3.56	116.29	107.23
3	C	3	AMU	C2-N2-C7	3.55	127.66	122.90
4	D	1	AMV	O1-C1-C2	3.50	113.44	108.13
3	C	4	NAG	C2-N2-C7	3.45	127.53	122.90
3	C	2	NAG	O5-C1-C2	-3.44	105.97	111.29
3	C	3	AMU	C3-C2-N2	3.29	115.95	110.57
3	C	1	MAG	C1-C2-N2	3.20	116.29	110.92
4	D	4	NAG	C2-N2-C7	3.07	127.02	122.90
4	D	2	NAG	O5-C5-C4	-2.88	103.83	110.83
4	D	1	AMV	O5-C5-C6	2.74	113.23	106.44
4	D	1	AMV	O5-C1-C2	-2.72	105.44	110.59
3	C	1	MAG	CM-O1-C1	2.66	117.30	113.26
3	C	3	AMU	O4-C4-C5	-2.65	102.80	109.32
4	D	1	AMV	C2-N2-C7	-2.50	117.26	123.11
4	D	3	NM6	O3-C3-C4	2.46	113.49	107.23
3	C	1	MAG	O7-C7-C8	-2.43	117.72	122.05
4	D	4	NAG	C1-O5-C5	2.42	115.43	112.19
3	C	1	MAG	O3-C3-C2	-2.37	104.86	109.58
3	C	1	MAG	O5-C5-C6	2.36	112.29	106.44
3	C	2	NAG	C1-O5-C5	2.31	115.29	112.19
3	C	3	AMU	C4-C3-C2	2.31	115.21	111.18
3	C	2	NAG	O3-C3-C2	-2.24	104.75	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	NAG	C2-N2-C7	2.23	125.89	122.90
4	D	2	NAG	O7-C7-C8	-2.21	118.12	122.05
4	D	3	NM6	C3-C2-N2	2.18	114.13	110.57
4	D	3	NM6	C3A-C3C-N3A	2.15	118.59	117.31
4	D	2	NAG	C1-O5-C5	2.14	115.06	112.19
3	C	3	AMU	C1-O5-C5	-2.13	109.33	112.19
3	C	4	NAG	O7-C7-C8	-2.12	118.29	122.05
4	D	3	NM6	O4-C4-C5	2.06	114.39	109.32
3	C	3	AMU	C1-C2-N2	-2.05	107.20	110.43
4	D	3	NM6	O3B-C3C-N3A	-2.05	119.42	123.04
4	D	1	AMV	O5-C1-O1	2.03	115.67	110.94
3	C	3	AMU	C6-C5-C4	2.02	117.98	113.02

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	MAG	O5-C1-O1-CM
4	D	3	NM6	C2-C3-O3-C3A
4	D	2	NAG	C4-C5-C6-O6
3	C	3	AMU	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
3	C	4	NAG	C4-C5-C6-O6
3	C	4	NAG	O5-C5-C6-O6
3	C	3	AMU	O5-C5-C6-O6
4	D	4	NAG	O5-C5-C6-O6
3	C	1	MAG	O5-C5-C6-O6
4	D	4	NAG	C4-C5-C6-O6
3	C	4	NAG	C3-C2-N2-C7
4	D	1	AMV	C3-C2-N2-C7
3	C	1	MAG	C3-C2-N2-C7
3	C	4	NAG	C1-C2-N2-C7
3	C	1	MAG	C1-C2-N2-C7
4	D	1	AMV	C1-C2-N2-C7
4	D	1	AMV	C10-C9-O3-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

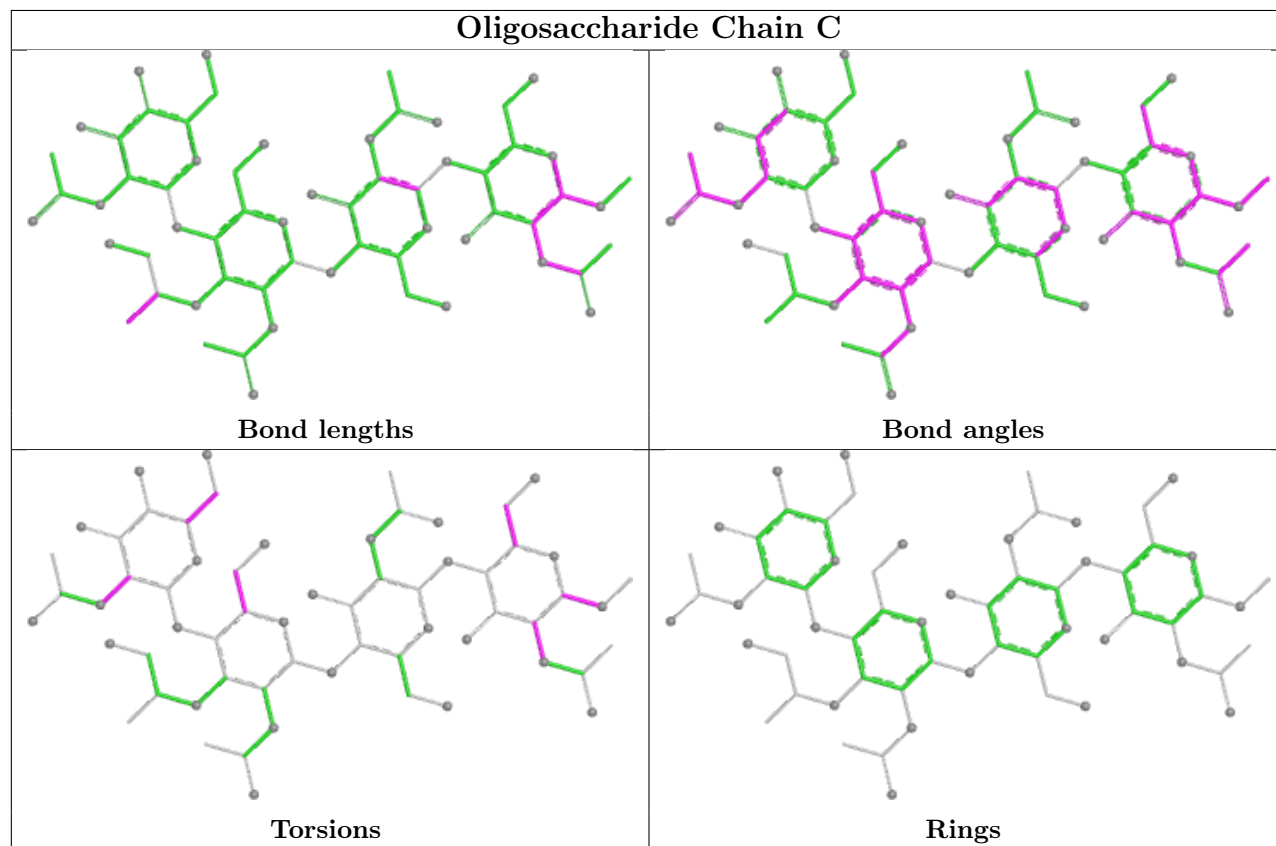
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2	NAG	1	0

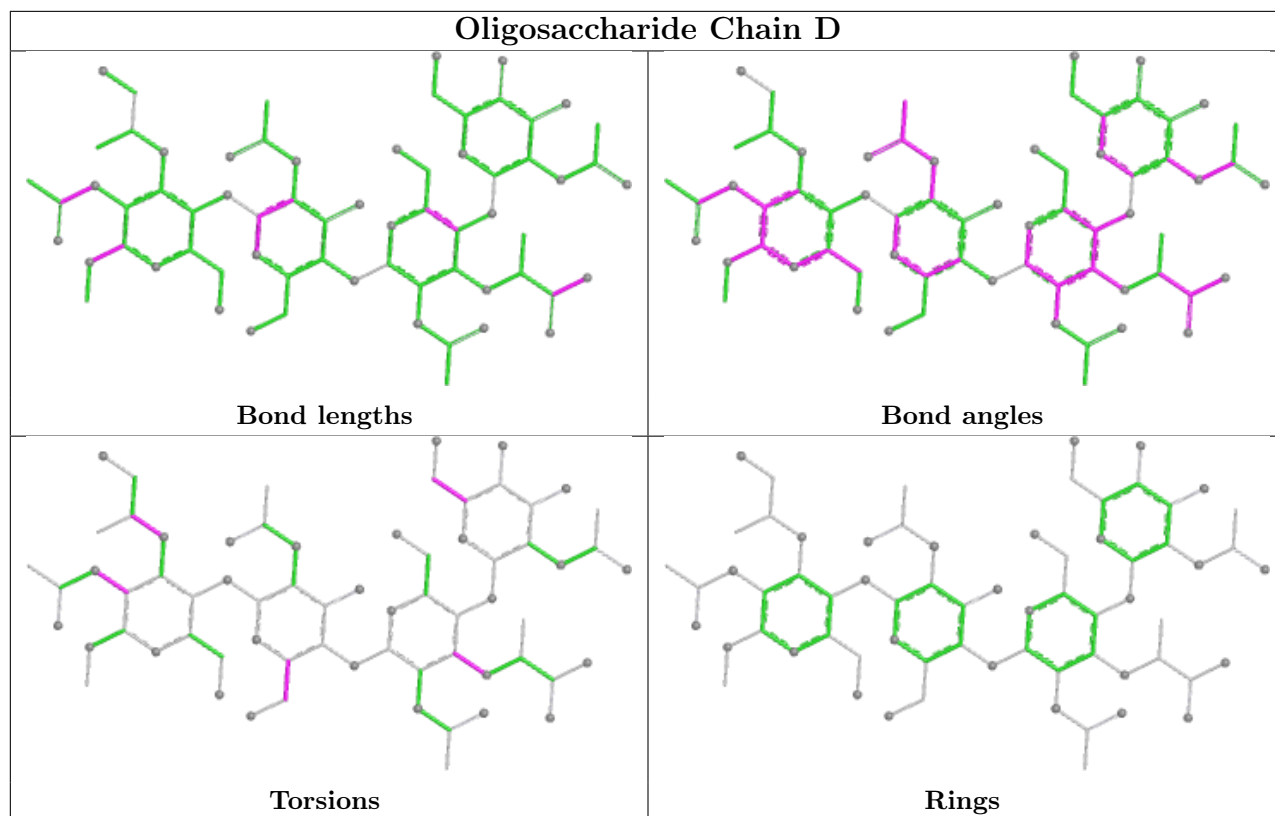
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	AMV	2	0

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](#)

3 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	ACT	A	701	-	3,3,3	0.77	0	3,3,3	0.86	0
6	66N	A	707	3	5,5,5	2.78	1 (20%)	6,6,6	1.16	1 (16%)
5	ACT	A	702	-	3,3,3	0.79	0	3,3,3	0.82	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	66N	A	707	3	-	0/3/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	707	66N	C34-N12	6.01	1.47	1.32

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	707	66N	O3-C34-N12	-2.65	118.37	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	613/613 (100%)	-0.25	1 (0%) 91 89	39, 74, 102, 121	1 (0%)
2	B	1/5 (20%)	-0.17	0 100 100	81, 81, 81, 81	0
All	All	614/618 (99%)	-0.25	1 (0%) 91 89	39, 74, 102, 121	1 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	33	LEU	2.8

6.2 Non-standard residues in protein, DNA, RNA chains [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.

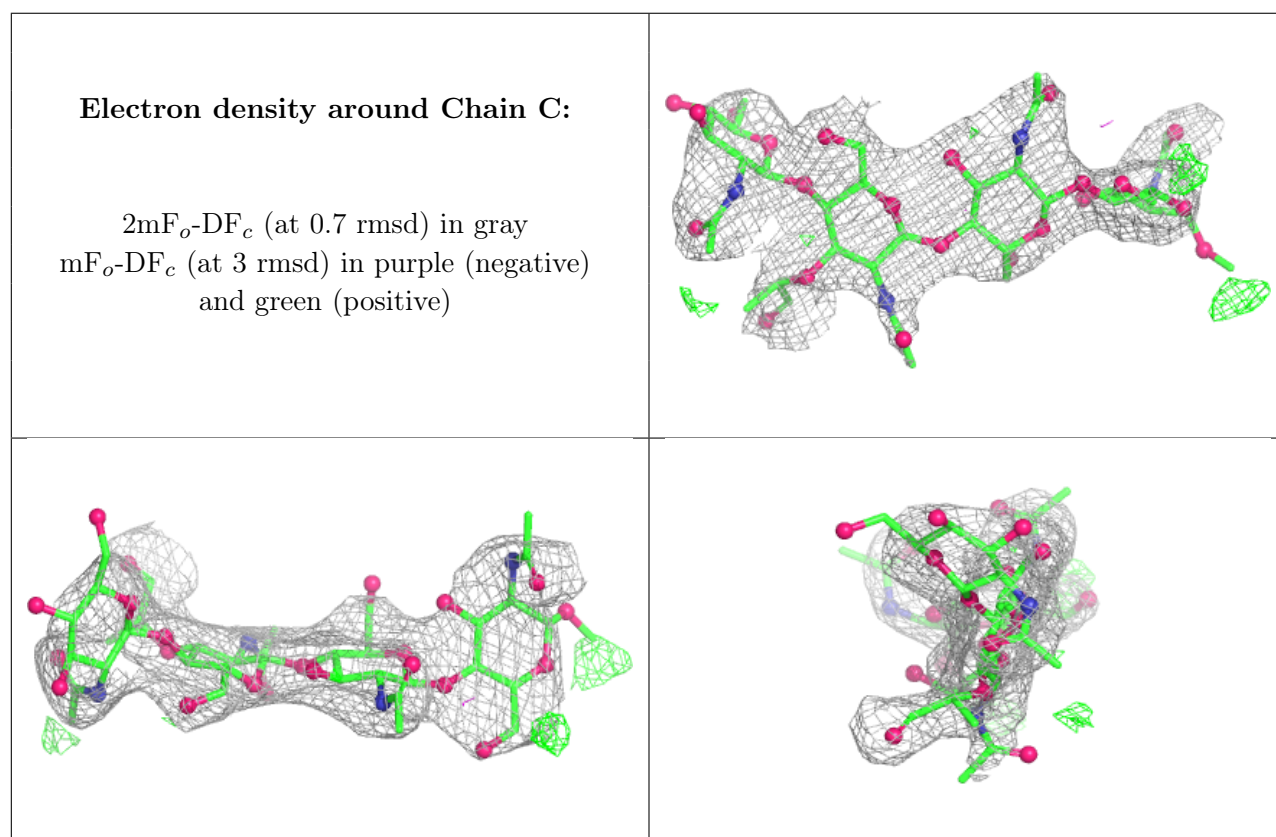
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	DAL	B	4	5/6	0.77	0.23	118,122,125,127	0
2	DAL	B	5	6/6	0.82	0.16	118,122,122,123	0
2	DGL	B	2	8/10	0.84	0.12	90,100,102,104	0
2	API	B	3	12/13	0.87	0.15	104,106,110,112	0

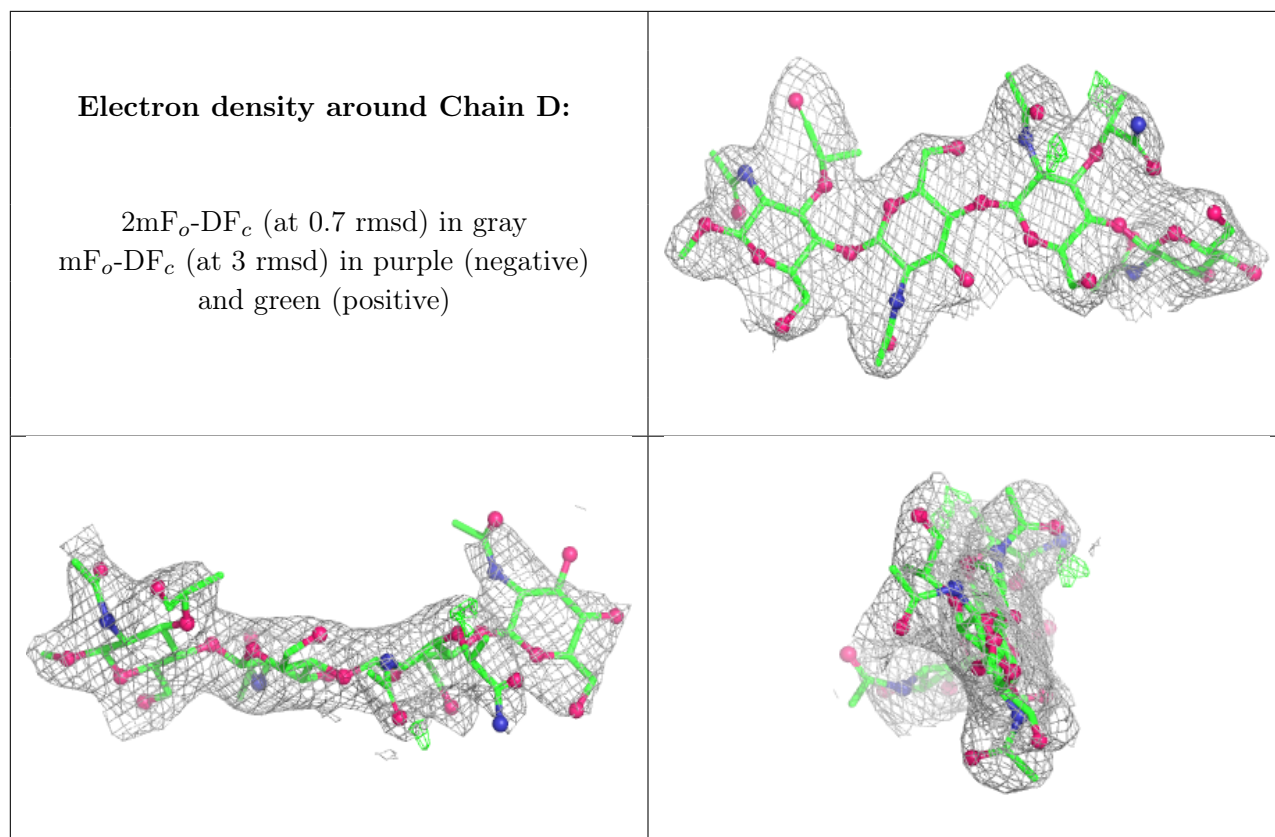
6.3 Carbohydrates [i](#)

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)	$Q < 0.9$
3	MAG	C	1	16/16	0.68	0.15	104,119,124,124	0
3	NAG	C	4	14/15	0.75	0.12	107,119,123,127	0
4	NAG	D	4	14/15	0.85	0.10	88,100,108,108	0
3	AMU	C	3	18/20	0.88	0.13	97,115,123,125	0
4	NM6	D	3	19/20	0.89	0.10	76,81,89,89	0
3	NAG	C	2	14/15	0.89	0.11	98,110,116,117	0
4	AMV	D	1	20/21	0.95	0.09	67,72,79,79	0
4	NAG	D	2	14/15	0.97	0.07	63,65,70,74	0

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ACT	A	702	4/4	0.27	0.22	88,89,92,92	0
5	ACT	A	701	4/4	0.68	0.15	79,82,82,84	0
6	66N	A	707	6/6	0.71	0.15	104,106,109,113	0

6.5 Other polymers [i](#)

There are no such residues in this entry.