



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:25 PM UTC

PDB ID : 1O75 / pdb_00001o75
Title : Tp47, the 47-Kilodalton Lipoprotein of Treponema pallidum
Authors : Deka, R.K.; Machius, M.; Norgard, M.V.; Tomchick, D.R.
Deposited on : 2002-10-23
Resolution : 1.95 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

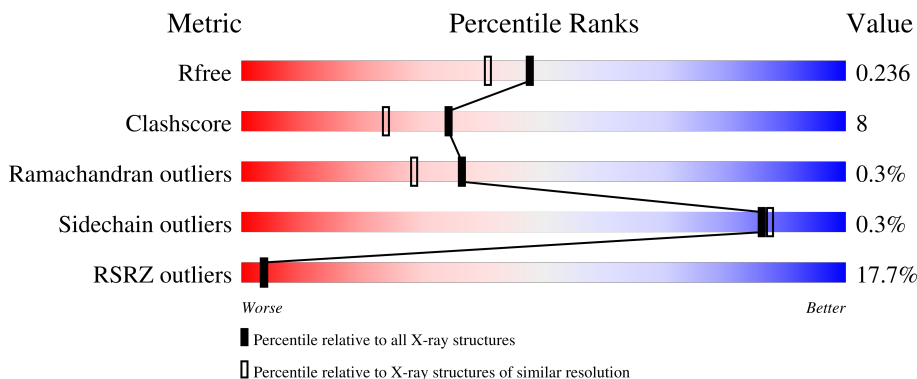
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	415	 15% 85% 11%
1	B	415	 19% 77% 19%
2	C	2	 50% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	XE	A	1416	-	-	X	-
3	XE	B	1415	-	-	X	-
3	XE	B	1417	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7017 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.

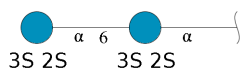
- Molecule 1 is a protein called 47 KDA MEMBRANE ANTIGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	399	Total 3175	C 1993	N 539	O 630	S 13	0	9	0
1	B	402	Total 3179	C 1998	N 542	O 626	S 13	0	5	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	SER	HIS	engineered mutation	UNP P29723
A	9	SER	HIS	engineered mutation	UNP P29273
B	5	SER	HIS	engineered mutation	UNP P29723
B	9	SER	HIS	engineered mutation	UNP P29273

- Molecule 2 is an oligosaccharide called 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-2,3-di-O-sulfo-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	O	S			
2	C	2	Total 39	C 12	O 23	S 4	0	0	0

- Molecule 3 is XENON (CCD ID: XE) (formula: Xe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total 2 Xe 2	0	0
3	B	3	Total 3 Xe 3	0	0

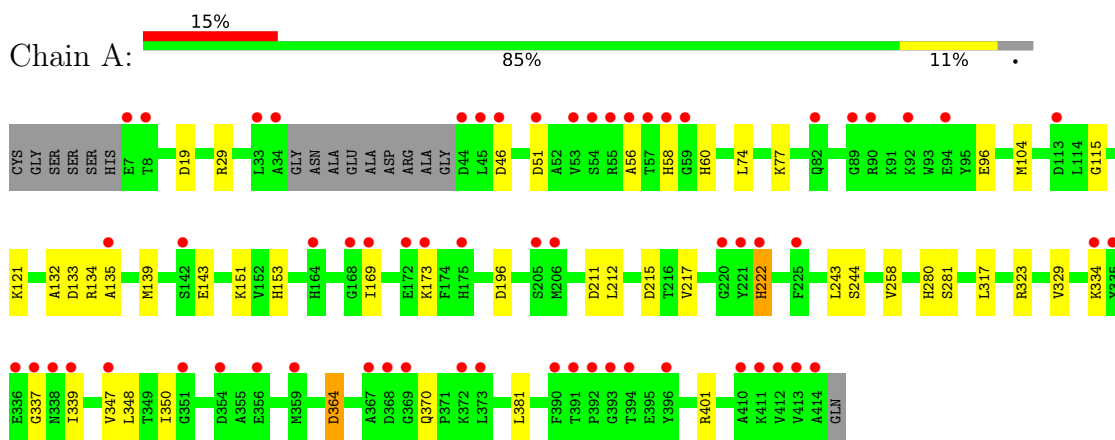
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	311	Total 311	O 311	0	0
4	B	308	Total 308	O 308	0	0

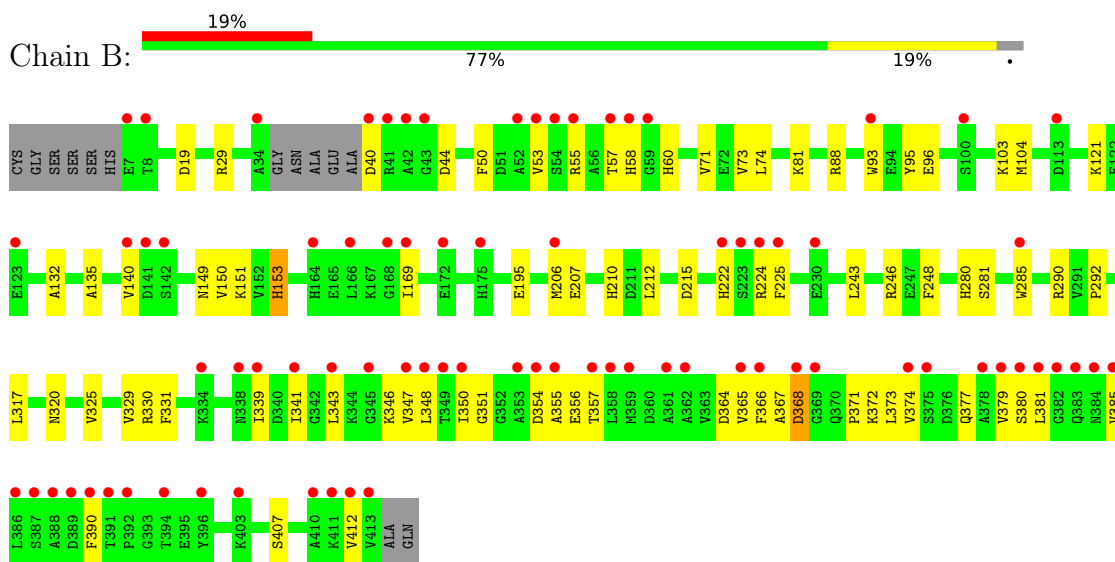
3 Residue-property plots [i](#)

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: 47 KDA MEMBRANE ANTIGEN



- Molecule 1: 47 KDA MEMBRANE ANTIGEN



- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-2,3-di-O-sulfo-alpha-D-glucopyranos e



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.93Å 128.93Å 151.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.20 – 1.95 28.20 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (28.20-1.95) 94.1 (28.20-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 1.95Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.228 0.213 , 0.236	Depositor DCC
R_{free} test set	5036 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtrriage
Anisotropy	0.034	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7017	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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: XE, PDX

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	2/3239 (0.1%)	0.93	10/4372 (0.2%)
1	B	0.57	2/3245 (0.1%)	0.95	11/4380 (0.3%)
All	All	0.57	4/6484 (0.1%)	0.94	21/8752 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	153	HIS	ND1-CE1	5.49	1.38	1.32
1	A	222	HIS	ND1-CE1	5.39	1.38	1.32
1	B	320	ASN	CG-OD1	5.34	1.33	1.23
1	A	153	HIS	ND1-CE1	5.16	1.37	1.32

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	HIS	CB-CG-CD2	-6.75	122.42	131.20
1	B	215	ASP	N-CA-C	-6.60	102.65	111.96
1	B	153	HIS	CB-CG-CD2	-6.58	122.64	131.20
1	A	153	HIS	CB-CG-CD2	-6.50	122.75	131.20
1	A	56	ALA	N-CA-C	-6.37	98.83	108.96
1	B	95	TYR	N-CA-C	6.10	119.14	109.81
1	A	96	GLU	N-CA-C	-6.03	98.69	108.52
1	B	55	ARG	N-CA-C	5.87	119.24	110.14
1	B	364	ASP	N-CA-C	-5.82	100.41	109.72
1	A	215	ASP	N-CA-C	-5.76	99.38	110.56
1	A	222	HIS	CB-CG-ND1	5.72	131.29	122.70
1	B	50	PHE	N-CA-C	5.62	119.45	112.59
1	B	153	HIS	CB-CG-ND1	5.60	131.10	122.70
1	A	347	VAL	N-CA-C	5.59	116.35	108.36
1	A	153	HIS	CB-CG-ND1	5.58	131.07	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	347	VAL	N-CA-C	5.57	115.91	108.11
1	A	364	ASP	N-CA-C	-5.41	100.21	109.24
1	A	244	SER	N-CA-C	-5.25	103.76	110.53
1	B	373	LEU	N-CA-C	-5.22	106.06	112.90
1	B	96	GLU	N-CA-C	-5.13	100.08	108.76
1	B	71	VAL	N-CA-C	5.04	115.73	108.48

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	3175	0	3036	30	0
1	B	3179	0	3042	68	0
2	C	39	0	19	1	0
3	A	2	0	0	2	0
3	B	3	0	0	6	0
4	A	311	0	0	2	0
4	B	308	0	0	1	0
All	All	7017	0	6097	95	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 8.

All (95) 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:B:339:ILE:HD11	1:B:350:ILE:HG23	1.44	0.98
1:B:151:LYS:HE2	1:B:153:HIS:CE1	2.06	0.91
1:B:169:ILE:HD13	1:B:195:GLU:HB2	1.54	0.88
1:B:350:ILE:HD12	1:B:379:VAL:HG11	1.57	0.85
1:B:19:ASP:OD1	1:B:29:ARG:HD3	1.79	0.83
1:A:211:ASP:OD2	1:A:323[A]:ARG:HD3	1.80	0.79
1:B:350:ILE:HD12	1:B:379:VAL:CG1	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104[A]:MET:HE2	3:B:1416:XE:XE	2.71	0.69
1:B:350:ILE:CD1	1:B:379:VAL:HG11	2.27	0.64
1:B:169:ILE:CD1	1:B:195:GLU:HB2	2.25	0.64
1:A:222:HIS:O	1:B:371:PRO:HG3	1.97	0.63
1:B:339:ILE:HD12	1:B:351:GLY:O	1.98	0.63
1:B:53:VAL:O	1:B:151:LYS:HA	2.00	0.62
1:B:58:HIS:CD2	1:B:60:HIS:H	2.18	0.61
1:B:212:LEU:HD22	1:B:243:LEU:HD21	1.83	0.60
1:A:212:LEU:HD22	1:A:243:LEU:HD21	1.84	0.60
1:B:57:THR:CG2	1:B:150:VAL:HG23	2.32	0.60
1:A:370:GLN:HG2	1:B:225:PHE:CE1	2.37	0.59
1:A:217:VAL:HG21	1:A:329[A]:VAL:CG1	2.35	0.57
1:B:29:ARG:HH11	1:B:29:ARG:HG2	1.71	0.56
1:A:258:VAL:HG13	1:A:317:LEU:HD23	1.88	0.55
1:A:173:LYS:NZ	1:A:196:ASP:HB3	2.21	0.55
1:B:222:HIS:HE1	1:B:407:SER:C	2.14	0.55
1:B:81:LYS:HE3	3:B:1417:XE:XE	2.85	0.54
1:A:169:ILE:HG13	4:A:2139:HOH:O	2.07	0.54
1:A:58:HIS:HD2	1:A:60:HIS:CG	2.25	0.54
1:A:77:LYS:HZ3	1:A:143:GLU:CD	2.14	0.53
1:B:331:PHE:CZ	3:B:1415:XE:XE	3.39	0.53
1:B:88:ARG:NH2	2:C:2:PDX:H4	2.22	0.53
1:B:103:LYS:HG2	1:B:140:VAL:HG21	1.91	0.53
1:B:246:ARG:CZ	4:B:2209:HOH:O	2.57	0.53
1:B:350:ILE:O	1:B:381:LEU:HD12	2.08	0.53
1:A:19:ASP:OD1	1:A:29:ARG:HD3	2.09	0.51
1:B:379:VAL:CG1	1:B:380:SER:N	2.74	0.51
1:B:341:ILE:HG23	1:B:348:LEU:HD11	1.92	0.51
1:B:73:VAL:HG12	1:B:150:VAL:HG22	1.93	0.50
1:A:74:LEU:HD13	1:A:104[A]:MET:HE3	1.93	0.49
1:B:354:ASP:OD1	1:B:355:ALA:N	2.44	0.49
1:A:104[A]:MET:HE2	3:A:1416:XE:XE	2.90	0.49
1:B:354:ASP:O	1:B:357:THR:HG22	2.12	0.49
1:B:224:ARG:NH1	1:B:285:TRP:CG	2.81	0.49
1:B:343:LEU:HD22	1:B:390:PHE:CE2	2.47	0.49
1:A:334:LYS:HE3	4:A:2097:HOH:O	2.12	0.48
1:B:354:ASP:C	1:B:357:THR:HG22	2.38	0.48
1:A:350:ILE:O	1:A:381:LEU:HD12	2.13	0.48
1:B:354:ASP:OD1	1:B:356:GLU:N	2.42	0.48
1:A:173:LYS:HZ3	1:A:196:ASP:HB3	1.76	0.48
1:B:93[A]:TRP:CD1	3:B:1417:XE:XE	3.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ASP:HB3	1:B:44:ASP:HB2	1.96	0.48
1:B:151:LYS:HE2	1:B:153:HIS:HE1	1.72	0.48
1:A:46[B]:ASP:OD2	1:A:46[B]:ASP:N	2.46	0.47
1:B:331:PHE:HZ	3:B:1415:XE:XE	2.75	0.47
1:B:331:PHE:CE2	3:B:1415:XE:XE	3.45	0.47
1:B:58:HIS:CD2	1:B:60:HIS:HB2	2.50	0.47
1:B:248:PHE:CD1	1:B:292:PRO:HA	2.50	0.47
1:A:115:GLY:HA3	1:A:121:LYS:HE3	1.96	0.47
1:A:370:GLN:HG2	1:B:225:PHE:CZ	2.50	0.46
1:B:224:ARG:NH2	1:B:281:SER:O	2.48	0.46
1:B:367:ALA:O	1:B:368:ASP:C	2.59	0.46
1:B:374:VAL:HG13	1:B:377:GLN:CG	2.46	0.46
1:B:57:THR:HG23	1:B:150:VAL:HG23	1.98	0.46
1:B:222:HIS:CE1	1:B:407:SER:C	2.94	0.46
1:A:280:HIS:O	1:A:281:SER:HB3	2.15	0.45
1:A:348:LEU:C	1:A:348:LEU:HD23	2.41	0.45
1:B:210:HIS:C	1:B:210:HIS:CD2	2.94	0.45
1:B:280:HIS:O	1:B:281:SER:HB3	2.17	0.45
1:B:248:PHE:CE1	1:B:292:PRO:HA	2.52	0.45
1:B:206:MET:HE2	1:B:207:GLU:O	2.17	0.45
1:B:74:LEU:HD23	1:B:149:ASN:HD22	1.82	0.44
1:A:339:ILE:HG23	1:A:339:ILE:O	2.16	0.44
1:B:132:ALA:O	1:B:135:ALA:HB2	2.17	0.44
1:A:151:LYS:HB2	3:A:1416:XE:XE	2.96	0.44
1:A:339:ILE:HD11	1:A:350:ILE:CG2	2.48	0.44
1:A:58:HIS:CD2	1:A:60:HIS:CG	3.05	0.44
1:B:74:LEU:HD23	1:B:149:ASN:ND2	2.33	0.43
1:B:341:ILE:HG23	1:B:348:LEU:CD1	2.48	0.43
1:A:132:ALA:O	1:A:135:ALA:HB2	2.18	0.43
1:B:212:LEU:CD2	1:B:243:LEU:HD21	2.48	0.43
1:B:366:PHE:HB3	1:B:372:LYS:HA	2.01	0.43
1:B:317:LEU:HB2	1:B:325:VAL:HB	2.00	0.42
1:A:364:ASP:CG	1:A:401:ARG:HH12	2.27	0.42
1:A:133:ASP:O	1:A:134:ARG:HB2	2.19	0.42
1:B:365:VAL:HG11	1:B:390:PHE:CE1	2.55	0.42
1:A:217:VAL:HG21	1:A:329[B]:VAL:HG22	2.01	0.42
1:B:121:LYS:HA	1:B:121:LYS:HD3	1.88	0.42
1:B:222:HIS:CE1	1:B:407:SER:O	2.73	0.41
1:B:29:ARG:HG2	1:B:29:ARG:NH1	2.34	0.41
1:B:290:ARG:NH1	1:B:290:ARG:HG2	2.35	0.41
1:B:329:VAL:HG22	1:B:330:ARG:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:VAL:HG21	1:A:329[B]:VAL:CG2	2.50	0.41
1:B:88:ARG:HG2	1:B:88:ARG:O	2.20	0.41
1:B:346:LYS:O	1:B:385:VAL:HA	2.21	0.41
1:B:104[B]:MET:SD	1:B:104[B]:MET:C	3.05	0.40
1:B:343:LEU:HG	1:B:412:VAL:HG11	2.03	0.40
1:B:290:ARG:HG2	1:B:290:ARG:HH11	1.86	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	404/415 (97%)	391 (97%)	12 (3%)	1 (0%)	43	36
1	B	403/415 (97%)	389 (96%)	13 (3%)	1 (0%)	43	36
All	All	807/830 (97%)	780 (97%)	25 (3%)	2 (0%)	36	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	368	ASP
1	A	337	GLY

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	336/337 (100%)	334 (99%)	2 (1%)	78	79
1	B	334/337 (99%)	334 (100%)	0	100	100
All	All	670/674 (99%)	668 (100%)	2 (0%)	86	87

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

Mol	Chain	Res	Type
1	A	51	ASP
1	A	139	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	112	GLN
1	A	370	GLN
1	B	112	GLN
1	B	149	ASN
1	B	153	HIS
1	B	222	HIS
1	B	383	GLN

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](#)

2 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	PDX	C	1	2	20,20,20	1.69	5 (25%)	26,31,31	1.49	5 (19%)
2	PDX	C	2	2	19,19,20	1.59	5 (26%)	22,29,31	1.23	1 (4%)

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	PDX	C	1	2	-	0/12/32/32	0/1/1/1
2	PDX	C	2	2	-	2/12/29/32	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	PDX	O2S-S	4.08	1.63	1.45
2	C	2	PDX	O2-S	-3.19	1.47	1.57
2	C	1	PDX	C1-C2	2.93	1.55	1.52
2	C	2	PDX	O5-C5	2.72	1.48	1.43
2	C	2	PDX	O1S-S	-2.51	1.34	1.45
2	C	1	PDX	O1S-S	-2.43	1.34	1.45
2	C	2	PDX	O3-S'	-2.25	1.50	1.57
2	C	1	PDX	O3-S'	-2.24	1.50	1.57
2	C	1	PDX	O2-S	-2.21	1.50	1.57
2	C	2	PDX	O2X-S'	-2.09	1.36	1.45

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	PDX	C3-O3-S'	4.50	129.83	119.04
2	C	2	PDX	O2-C2-C3	4.21	111.31	106.65
2	C	1	PDX	O3S-S-O2	3.23	113.80	106.37
2	C	1	PDX	O4-C4-C5	2.88	116.41	109.32
2	C	1	PDX	O2-C2-C1	2.31	110.68	107.58
2	C	1	PDX	O3S-S-O2S	-2.02	101.47	108.56

There are no chirality outliers.

All (2) torsion outliers are listed below:

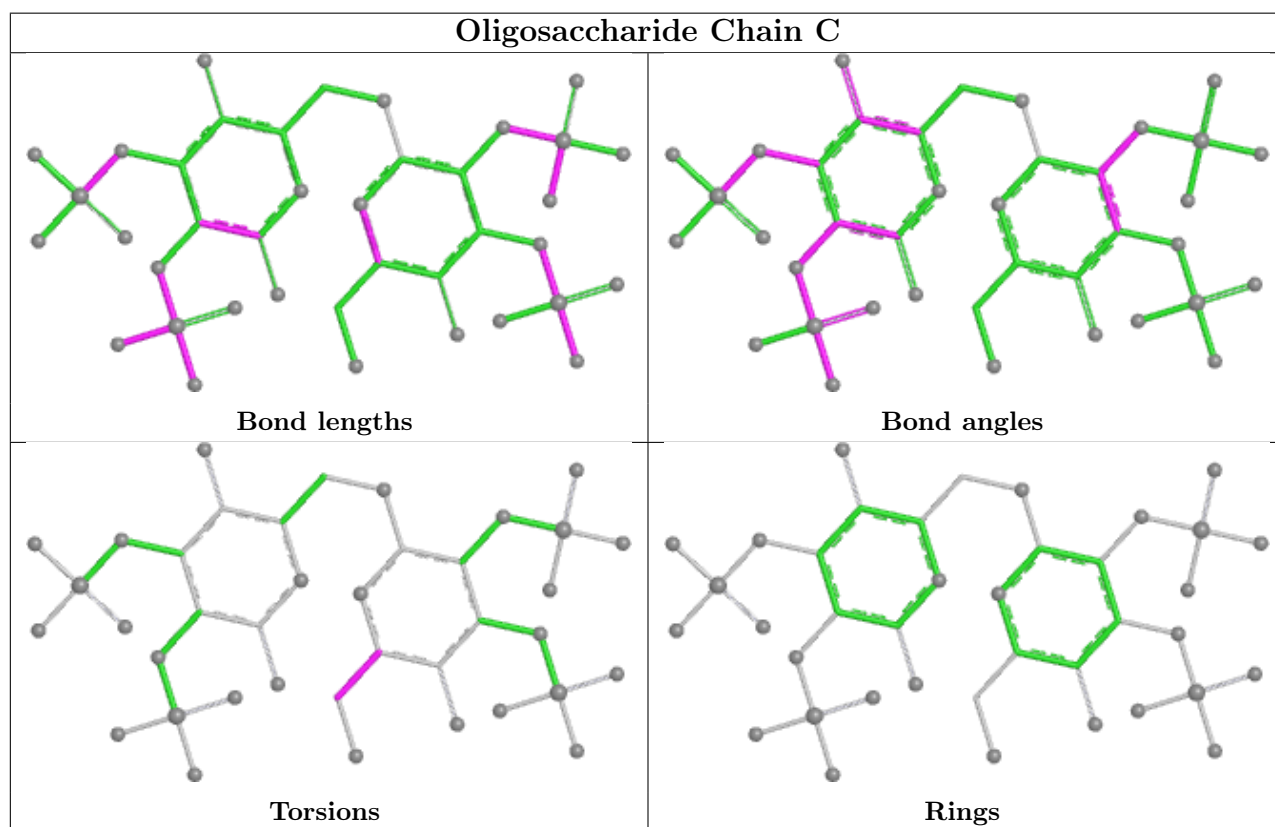
Mol	Chain	Res	Type	Atoms
2	C	2	PDX	O5-C5-C6-O6
2	C	2	PDX	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	PDX	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](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	399/415 (96%)	0.73	62 (15%) 5 5	14, 38, 68, 76	9 (2%)
1	B	402/415 (96%)	0.87	80 (19%) 3 3	16, 38, 76, 89	5 (1%)
All	All	801/830 (96%)	0.80	142 (17%) 4 4	14, 38, 74, 89	14 (1%)

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	413	VAL	7.3
1	B	53	VAL	6.5
1	A	414	ALA	6.0
1	A	58	HIS	5.8
1	B	93[A]	TRP	5.0
1	B	368	ASP	5.0
1	A	34	ALA	4.9
1	B	381	LEU	4.8
1	B	412	VAL	4.8
1	A	412	VAL	4.8
1	B	359	MET	4.7
1	B	42	ALA	4.6
1	B	58	HIS	4.5
1	A	413	VAL	4.5
1	B	230	GLU	4.3
1	B	358	LEU	4.2
1	B	34	ALA	4.1
1	B	41	ARG	4.1
1	A	57	THR	4.1
1	B	222	HIS	4.1
1	A	221	TYR	3.9
1	A	45	LEU	3.9
1	B	7	GLU	3.8
1	A	142	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	59	GLY	3.7
1	B	390	PHE	3.7
1	B	223	SER	3.6
1	B	57	THR	3.6
1	A	7	GLU	3.5
1	B	345	GLY	3.5
1	B	285	TRP	3.5
1	B	347	VAL	3.5
1	B	52	ALA	3.5
1	A	56	ALA	3.5
1	A	337	GLY	3.5
1	B	350	ILE	3.4
1	A	54[A]	SER	3.4
1	B	394	THR	3.4
1	A	46[A]	ASP	3.4
1	B	385	VAL	3.4
1	B	355	ALA	3.4
1	B	380	SER	3.4
1	B	54	SER	3.3
1	A	55	ARG	3.3
1	A	390	PHE	3.3
1	A	356	GLU	3.3
1	B	341	ILE	3.3
1	A	369	GLY	3.3
1	B	349	THR	3.2
1	A	172	GLU	3.2
1	B	168	GLY	3.2
1	A	44	ASP	3.2
1	B	357	THR	3.1
1	B	142	SER	3.1
1	A	351	GLY	3.1
1	A	391	THR	3.1
1	B	348	LEU	3.0
1	A	90	ARG	3.0
1	A	367	ALA	3.0
1	B	113	ASP	3.0
1	A	394	THR	3.0
1	A	359	MET	3.0
1	B	339	ILE	3.0
1	A	410	ALA	2.9
1	B	353	ALA	2.9
1	B	392	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	175	HIS	2.8
1	B	338	ASN	2.8
1	A	51	ASP	2.8
1	B	366	PHE	2.8
1	A	59	GLY	2.8
1	B	396	TYR	2.8
1	B	387	SER	2.8
1	A	338	ASN	2.8
1	B	343	LEU	2.7
1	A	206	MET	2.7
1	A	89	GLY	2.7
1	A	164	HIS	2.7
1	B	40	ASP	2.7
1	B	141	ASP	2.7
1	A	82	GLN	2.6
1	A	53	VAL	2.6
1	B	206	MET	2.6
1	A	411	LYS	2.6
1	B	375	SER	2.6
1	B	164	HIS	2.6
1	A	33	LEU	2.6
1	A	169	ILE	2.6
1	A	396	TYR	2.6
1	B	166	LEU	2.6
1	B	43	GLY	2.6
1	B	382	GLY	2.5
1	B	140	VAL	2.5
1	B	365	VAL	2.5
1	B	374	VAL	2.5
1	A	392	PRO	2.5
1	B	386	LEU	2.5
1	B	175	HIS	2.5
1	B	379	VAL	2.5
1	A	220	GLY	2.5
1	A	222	HIS	2.5
1	B	378	ALA	2.5
1	B	410	ALA	2.5
1	A	173	LYS	2.5
1	A	373	LEU	2.4
1	B	172	GLU	2.4
1	B	100	SER	2.4
1	B	369	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	388	ALA	2.4
1	A	347	VAL	2.4
1	A	354	ASP	2.4
1	A	368	ASP	2.4
1	A	339	ILE	2.4
1	B	169	ILE	2.4
1	B	224	ARG	2.4
1	B	123	GLU	2.4
1	B	391	THR	2.3
1	B	384	ASN	2.3
1	A	393	GLY	2.3
1	B	411	LYS	2.3
1	B	8	THR	2.3
1	A	225	PHE	2.3
1	A	168	GLY	2.3
1	A	205	SER	2.3
1	B	354	ASP	2.2
1	B	383	GLN	2.2
1	B	55	ARG	2.2
1	A	135	ALA	2.2
1	B	362	ALA	2.2
1	B	403	LYS	2.2
1	A	336	GLU	2.1
1	B	334	LYS	2.1
1	A	113	ASP	2.1
1	A	334	LYS	2.1
1	B	361	ALA	2.1
1	A	335	TYR	2.1
1	A	94	GLU	2.1
1	A	372	LYS	2.1
1	B	389	ASP	2.1
1	A	92	LYS	2.0
1	B	225	PHE	2.0
1	A	8	THR	2.0

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

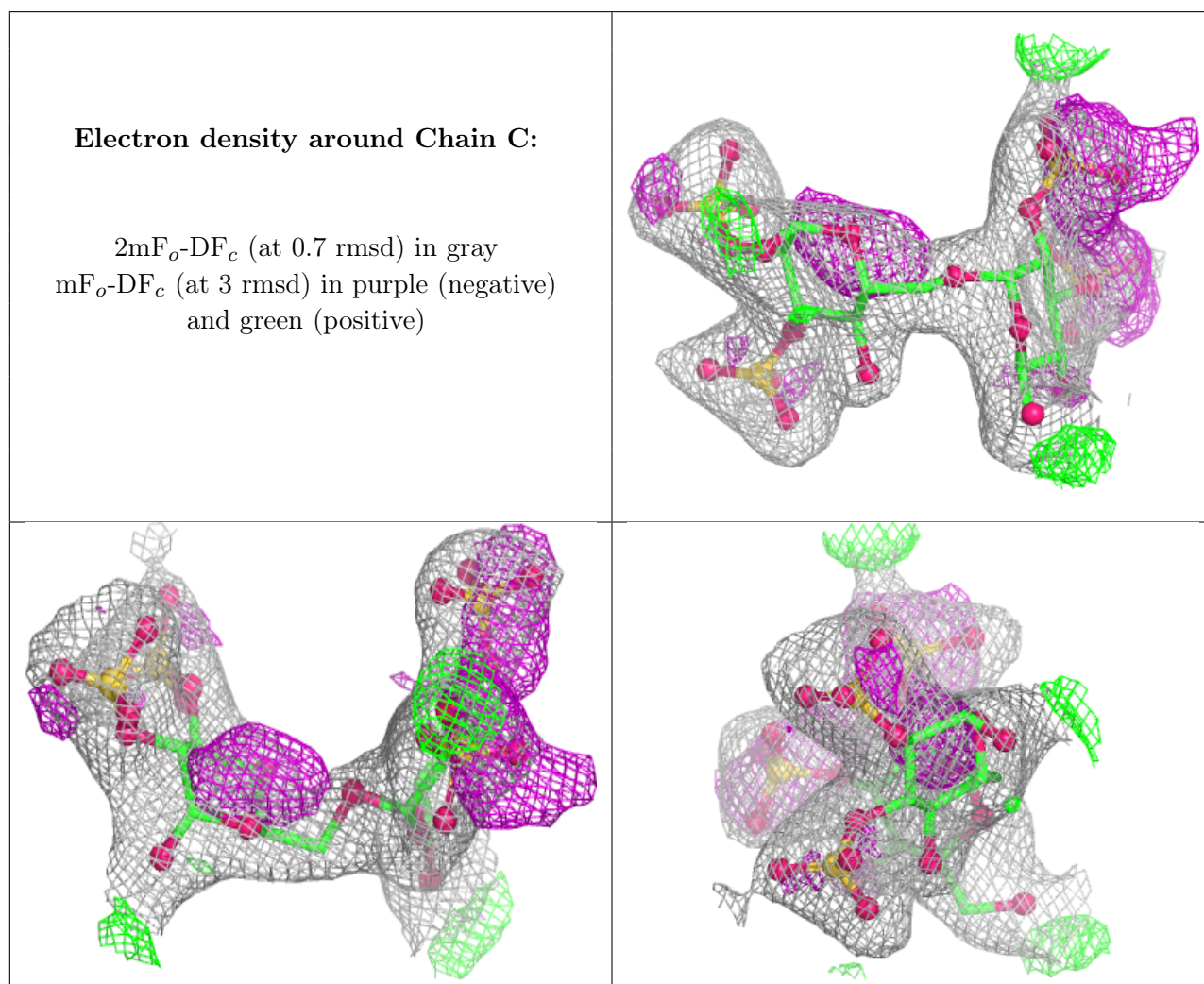
There are no non-standard protein/DNA/RNA residues in this entry.

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	PDX	C	2	19/20	0.85	0.15	53,56,60,60	0
2	PDX	C	1	20/20	0.91	0.11	52,55,57,58	0

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



6.4 Ligands [i](#)

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	XE	B	1417	1/1	0.94	0.10	58,58,58,58	1
3	XE	A	1416	1/1	0.95	0.12	56,56,56,56	1
3	XE	B	1416	1/1	0.97	0.07	45,45,45,45	1
3	XE	B	1415	1/1	0.98	0.03	34,34,34,34	1
3	XE	A	1415	1/1	1.00	0.04	35,35,35,35	1

6.5 Other polymers [i](#)

There are no such residues in this entry.