



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:50 PM UTC

PDB ID : 1W3Y / pdb_00001w3y
Title : Crystal structure of S. pneumoniae hyaluronate lyase in complex with
palmitoyl-vitamin C
Authors : Rigden, D.J.; Jedrzejewski, M.J.
Deposited on : 2004-07-21
Resolution : 1.65 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

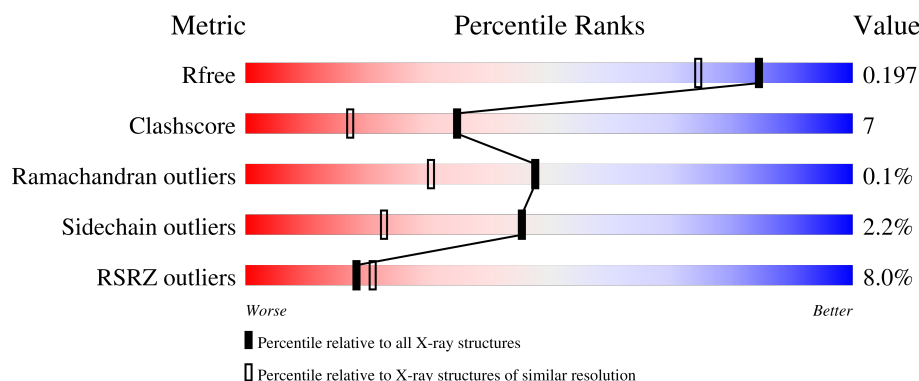
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	731	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6471 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.

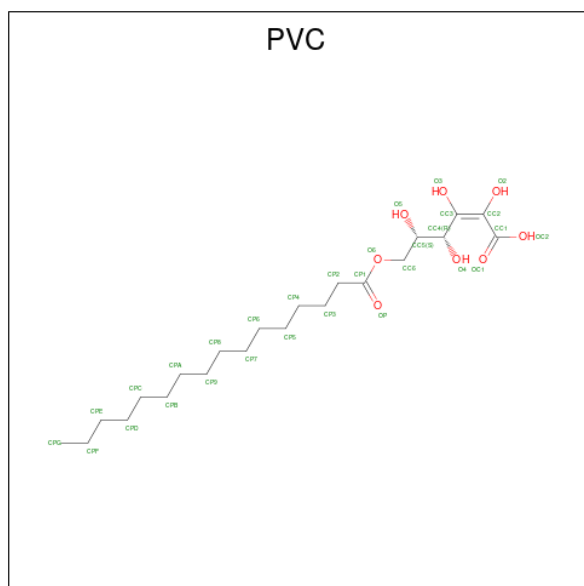
- Molecule 1 is a protein called HYALURONATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	721	Total	C	N	O	S	0	5	0
			5835	3671	979	1162	23			

There is a discrepancy between the modelled and reference sequences:

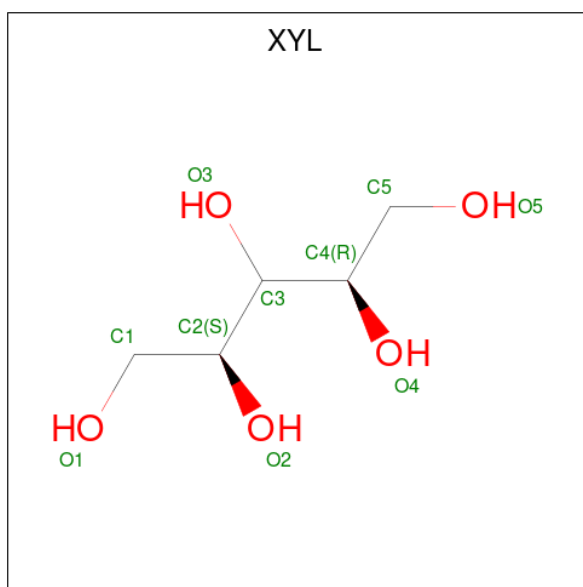
Chain	Residue	Modelled	Actual	Comment	Reference
A	196	ASP	GLU	conflict	UNP Q54873

- Molecule 2 is (2E,4R,5S)-2,3,4,5-TETRAHYDROXY-6-(PALMITOYLOXY)HEX-2-ENOIC ACID (CCD ID: PVC) (formula: $C_{22}H_{40}O_8$).



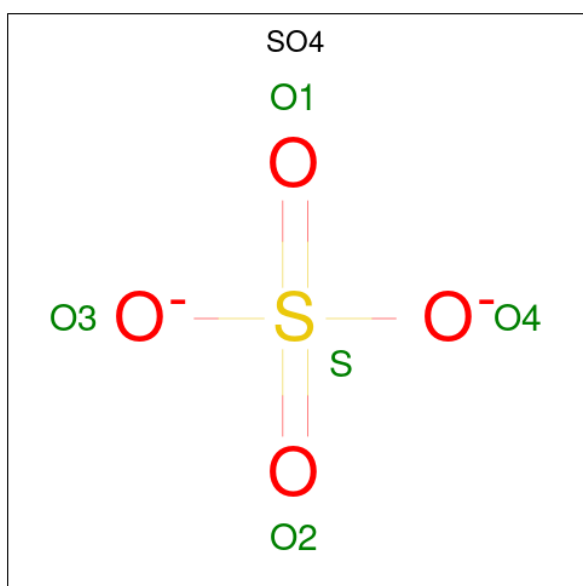
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			27	19	8		

- Molecule 3 is Xylitol (CCD ID: XYL) (formula: $C_5H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	A	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is SULFATE ION (CCD ID: SO₄) (formula: O₄S).



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

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

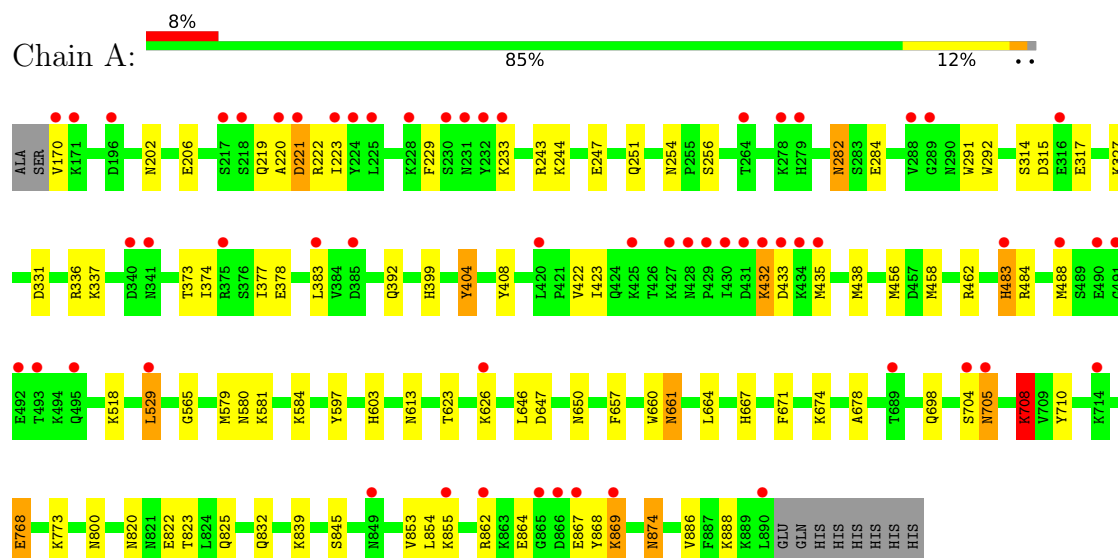
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	564	Total	O	0	0
			564	564		

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: HYALURONATE LYASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.13Å 102.71Å 102.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.91 – 1.65 45.91 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.91-1.65) 99.7 (45.91-1.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.65Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.192 , 0.210 0.196 , 0.197	Depositor DCC
R_{free} test set	5318 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6471	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: SO4, XYL, PVC

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	0.33	0/5956	0.85	12/8042 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	433	ASP	N-CA-C	-7.57	105.21	114.75
1	A	518	LYS	N-CA-C	7.36	121.11	112.72
1	A	800	ASN	N-CA-C	7.02	121.23	112.24
1	A	657	PHE	N-CA-C	6.92	121.13	110.20
1	A	854	LEU	N-CA-C	6.67	122.40	113.72
1	A	233	LYS	N-CA-C	-6.30	104.30	112.23
1	A	603	HIS	N-CA-C	5.97	118.27	111.11
1	A	660	TRP	N-CA-C	5.74	119.10	111.75
1	A	623	THR	N-CA-C	-5.51	102.59	110.59
1	A	404	TYR	N-CA-C	5.45	119.17	112.03
1	A	768	GLU	N-CA-C	5.39	117.86	111.33
1	A	708	LYS	N-CA-C	-5.16	100.32	108.73

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	5835	0	5655	83	0
2	A	27	0	28	18	0
3	A	20	0	24	0	0
4	A	25	0	0	1	0
5	A	564	0	0	7	0
All	All	6471	0	5707	87	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 7.

All (87) 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)
2:A:1891:PVC:HC5	2:A:1891:PVC:CC1	1.71	1.18
2:A:1891:PVC:HC5	2:A:1891:PVC:OC2	1.56	1.06
1:A:613:ASN:H	1:A:698:GLN:HE22	1.08	0.97
2:A:1891:PVC:CC1	2:A:1891:PVC:CC5	2.51	0.88
1:A:392:GLN:HG2	5:A:2181:HOH:O	1.74	0.86
1:A:869:LYS:HE3	1:A:869:LYS:N	1.94	0.83
1:A:336:ARG:HH12	2:A:1891:PVC:HP42	1.47	0.78
1:A:855:LYS:HD3	1:A:886:VAL:HG12	1.66	0.78
1:A:456:MET:HE1	1:A:565:GLY:HA3	1.66	0.76
1:A:399:HIS:HA	2:A:1891:PVC:HP91	1.67	0.74
1:A:282:ASN:HD22	1:A:284:GLU:H	1.37	0.73
1:A:462:ARG:NH2	2:A:1891:PVC:HC61	2.03	0.72
1:A:868:TYR:C	1:A:869:LYS:HE3	2.17	0.70
1:A:456:MET:HE3	1:A:597:TYR:HE2	1.58	0.69
1:A:435:MET:HG2	1:A:438:MET:HE2	1.76	0.68
1:A:874:ASN:C	1:A:874:ASN:HD22	2.04	0.66
1:A:580:ASN:HD21	2:A:1891:PVC:HC62	1.60	0.65
1:A:462:ARG:HH22	2:A:1891:PVC:HC61	1.61	0.65
1:A:864:GLU:HB2	1:A:869:LYS:NZ	2.12	0.65
1:A:864:GLU:HB2	1:A:869:LYS:HZ3	1.63	0.62
1:A:458:MET:HE1	1:A:565:GLY:C	2.25	0.62
2:A:1891:PVC:HC4	5:A:2553:HOH:O	2.01	0.60
1:A:292:TRP:CB	2:A:1891:PVC:O5	2.50	0.59
1:A:483[B]:HIS:CE1	1:A:529:LEU:HD12	2.37	0.58
1:A:580:ASN:ND2	2:A:1891:PVC:HC62	2.18	0.58
1:A:581:LYS:HB3	1:A:768:GLU:HB2	1.87	0.57
1:A:704:SER:C	1:A:705:ASN:HD22	2.14	0.55
1:A:291:TRP:HE1	2:A:1891:PVC:HP21	1.72	0.55
1:A:529:LEU:C	1:A:529:LEU:HD23	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:MET:SD	2:A:1891:PVC:OP	2.64	0.55
1:A:650:ASN:HD21	1:A:832:GLN:HE22	1.54	0.55
1:A:867:GLU:HB3	1:A:869:LYS:HZ1	1.72	0.55
1:A:254:ASN:C	1:A:254:ASN:HD22	2.14	0.54
1:A:867:GLU:CB	1:A:869:LYS:HZ1	2.20	0.54
1:A:705:ASN:HD22	1:A:705:ASN:N	2.05	0.53
1:A:336:ARG:NH1	2:A:1891:PVC:HP42	2.21	0.53
1:A:456:MET:HE1	1:A:565:GLY:CA	2.35	0.53
1:A:383:LEU:HD11	1:A:392:GLN:N	2.24	0.53
1:A:456:MET:CE	1:A:565:GLY:HA3	2.38	0.53
1:A:282:ASN:ND2	1:A:284:GLU:H	2.06	0.52
1:A:820:ASN:HD22	1:A:825:GLN:HG2	1.75	0.52
1:A:483[A]:HIS:HD2	1:A:484:ARG:N	2.09	0.51
1:A:822:GLU:H	1:A:822:GLU:CD	2.19	0.51
1:A:292:TRP:HB2	2:A:1891:PVC:O5	2.11	0.50
1:A:373:THR:O	1:A:377:ILE:HG12	2.11	0.50
1:A:399:HIS:HA	2:A:1891:PVC:CP9	2.37	0.50
1:A:243:ARG:O	1:A:247:GLU:HG3	2.12	0.50
1:A:768:GLU:HG3	5:A:2559:HOH:O	2.11	0.50
1:A:336:ARG:HH22	2:A:1891:PVC:HP62	1.77	0.49
1:A:647:ASP:OD2	1:A:862[A]:ARG:NH2	2.45	0.49
1:A:584:LYS:NZ	1:A:768:GLU:HG2	2.28	0.48
1:A:664:LEU:C	1:A:664:LEU:HD23	2.39	0.48
1:A:483[B]:HIS:CE1	5:A:2244:HOH:O	2.67	0.48
1:A:282:ASN:HD22	1:A:282:ASN:C	2.22	0.47
1:A:839:LYS:HD2	1:A:853:VAL:HG23	1.96	0.47
1:A:374:ILE:O	1:A:378:GLU:HG3	2.14	0.47
1:A:282:ASN:HD22	1:A:284:GLU:N	2.09	0.47
1:A:220:ALA:O	1:A:221:ASP:C	2.57	0.47
1:A:708:LYS:HE3	1:A:710:TYR:OH	2.16	0.46
1:A:671:PHE:HB2	1:A:678:ALA:HB3	1.98	0.46
1:A:435:MET:HE1	1:A:488[A]:MET:HG3	1.98	0.46
1:A:170:VAL:HG23	1:A:315:ASP:OD2	2.16	0.45
1:A:646:LEU:HD21	1:A:862[A]:ARG:HB2	1.98	0.45
1:A:327:LYS:HD3	1:A:327:LYS:C	2.42	0.45
1:A:229:PHE:HE2	1:A:244:LYS:HE2	1.81	0.45
1:A:456:MET:HE3	1:A:597:TYR:CE2	2.44	0.44
1:A:661:ASN:C	1:A:661:ASN:HD22	2.24	0.44
1:A:202:ASN:ND2	1:A:251:GLN:HE22	2.14	0.44
1:A:483[A]:HIS:C	1:A:483[A]:HIS:CD2	2.96	0.43
1:A:432:LYS:O	1:A:432:LYS:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ILE:HG22	1:A:223:ILE:O	2.18	0.43
1:A:822:GLU:HG2	1:A:823:THR:HG23	2.00	0.43
1:A:674[A]:LYS:HE3	5:A:2407:HOH:O	2.19	0.42
1:A:254:ASN:C	1:A:254:ASN:ND2	2.75	0.42
1:A:584:LYS:HE2	4:A:1895:SO4:O1	2.20	0.42
1:A:222:ARG:H	1:A:222:ARG:HG2	1.59	0.42
1:A:254:ASN:ND2	1:A:256:SER:H	2.18	0.42
1:A:314:SER:OG	1:A:317:GLU:HG3	2.20	0.42
1:A:202:ASN:O	1:A:206:GLU:HG2	2.19	0.42
1:A:408:TYR:OH	2:A:1891:PVC:OC1	2.23	0.42
1:A:584:LYS:HZ2	1:A:768:GLU:HG2	1.85	0.42
1:A:646:LEU:HD21	1:A:862[B]:ARG:HB2	2.00	0.41
1:A:374:ILE:HD13	1:A:423:ILE:HG23	2.02	0.41
1:A:331:ASP:CB	1:A:337:LYS:HE3	2.51	0.41
1:A:845:SER:HB2	1:A:853:VAL:HG23	2.01	0.41
1:A:422:VAL:HA	5:A:2008:HOH:O	2.21	0.40
1:A:667:HIS:HD2	5:A:2512:HOH:O	2.04	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	724/731 (99%)	692 (96%)	31 (4%)	1 (0%)	48	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	ASP

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	645/649 (99%)	630 (98%)	15 (2%)	44 21

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	219	GLN
1	A	282	ASN
1	A	404	TYR
1	A	432	LYS
1	A	483[A]	HIS
1	A	483[B]	HIS
1	A	529	LEU
1	A	626	LYS
1	A	661	ASN
1	A	705	ASN
1	A	708	LYS
1	A	773	LYS
1	A	869	LYS
1	A	874	ASN
1	A	888	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	202	ASN
1	A	203	GLN
1	A	237	ASN
1	A	254	ASN
1	A	261	GLN
1	A	277	HIS
1	A	282	ASN
1	A	349	ASN
1	A	368	GLN

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Mol	Chain	Res	Type
1	A	418	GLN
1	A	495	GLN
1	A	580	ASN
1	A	661	ASN
1	A	667	HIS
1	A	683	ASN
1	A	698	GLN
1	A	705	ASN
1	A	759	GLN
1	A	788	GLN
1	A	820	ASN
1	A	825	GLN
1	A	832	GLN
1	A	850	GLN
1	A	874	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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
3	XYL	A	1892	-	9,9,9	0.62	0	11,11,11	1.49	2 (18%)
4	SO4	A	1898	-	4,4,4	0.22	0	6,6,6	0.08	0
4	SO4	A	1899	-	4,4,4	0.22	0	6,6,6	0.10	0
3	XYL	A	1893	-	9,9,9	0.58	0	11,11,11	1.51	3 (27%)
4	SO4	A	1896	-	4,4,4	0.24	0	6,6,6	0.08	0
2	PVC	A	1891	-	26,26,29	2.22	4 (15%)	24,31,34	1.31	2 (8%)
4	SO4	A	1897	-	4,4,4	0.23	0	6,6,6	0.10	0
4	SO4	A	1895	-	4,4,4	0.23	0	6,6,6	0.06	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
3	XYL	A	1892	-	-	0/12/12/12	-
2	PVC	A	1891	-	-	16/26/33/36	-
3	XYL	A	1893	-	-	5/12/12/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1891	PVC	CC4-CC3	7.87	1.55	1.49
2	A	1891	PVC	CC2-CC3	6.31	1.39	1.35
2	A	1891	PVC	O6-CP1	3.10	1.42	1.33
2	A	1891	PVC	CC2-CC1	2.09	1.54	1.49

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1891	PVC	CC5-CC4-CC3	4.33	117.02	109.64
2	A	1891	PVC	O3-CC3-CC2	3.17	125.77	121.50
3	A	1893	XYL	O5-C5-C4	2.77	116.97	111.16
3	A	1892	XYL	O5-C5-C4	2.77	116.96	111.16
3	A	1893	XYL	O1-C1-C2	-2.25	106.42	111.16
3	A	1892	XYL	O1-C1-C2	-2.12	106.71	111.16
3	A	1893	XYL	O3-C3-C2	2.01	113.50	108.93

There are no chirality outliers.

All (21) torsion outliers are listed below:

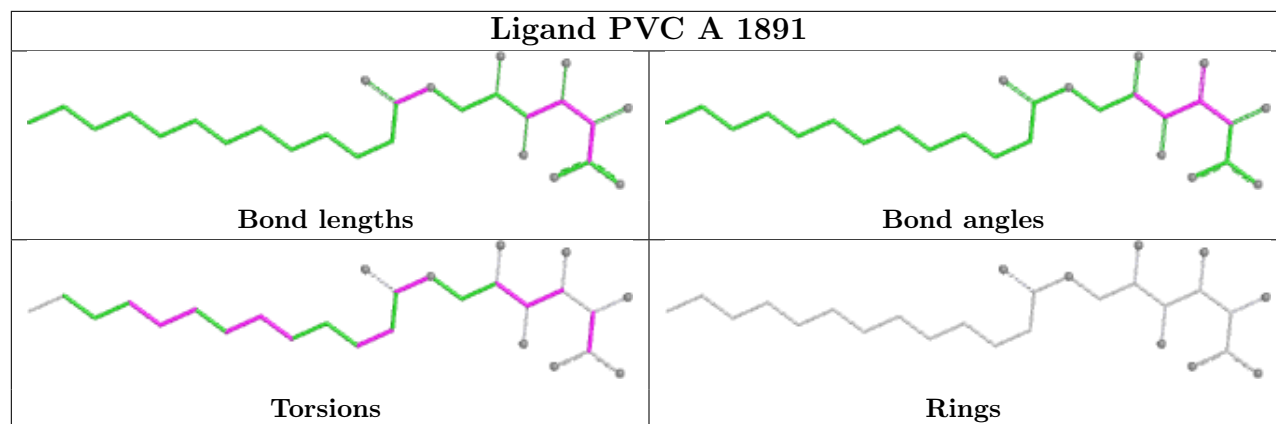
Mol	Chain	Res	Type	Atoms
2	A	1891	PVC	CC3-CC4-CC5-CC6
2	A	1891	PVC	O4-CC4-CC5-CC6
2	A	1891	PVC	CC3-CC4-CC5-O5
2	A	1891	PVC	O4-CC4-CC5-O5
2	A	1891	PVC	OC1-CC1-CC2-CC3
2	A	1891	PVC	OC1-CC1-CC2-O2
2	A	1891	PVC	O3-CC3-CC4-CC5
2	A	1891	PVC	CP2-CP1-O6-CC6
2	A	1891	PVC	OP-CP1-O6-CC6
2	A	1891	PVC	O3-CC3-CC4-O4
2	A	1891	PVC	OC2-CC1-CC2-O2
2	A	1891	PVC	CP7-CP8-CP9-CPA
3	A	1893	XYL	C1-C2-C3-O3
3	A	1893	XYL	O2-C2-C3-O3
2	A	1891	PVC	CP5-CP6-CP7-CP8
3	A	1893	XYL	C1-C2-C3-C4
3	A	1893	XYL	O4-C4-C5-O5
3	A	1893	XYL	O2-C2-C3-C4
2	A	1891	PVC	CP1-CP2-CP3-CP4
2	A	1891	PVC	CP4-CP5-CP6-CP7
2	A	1891	PVC	CP8-CP9-CPA-CPB

There are no ring outliers.

2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1891	PVC	18	0
4	A	1895	SO4	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

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	721/731 (98%)	0.26	58 (8%)	18 21	7, 21, 38, 60	5 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	435	MET	6.0
1	A	223	ILE	5.7
1	A	340	ASP	5.0
1	A	221	ASP	4.6
1	A	224	TYR	4.5
1	A	170	VAL	4.4
1	A	430	ILE	4.4
1	A	432	LYS	4.3
1	A	427	LYS	4.2
1	A	433	ASP	4.0
1	A	529	LEU	3.9
1	A	434	LYS	3.8
1	A	429	PRO	3.8
1	A	431	ASP	3.7
1	A	428	ASN	3.6
1	A	196	ASP	3.4
1	A	492	GLU	3.3
1	A	689	THR	3.2
1	A	865	GLY	3.2
1	A	491	GLY	3.1
1	A	279	HIS	3.1
1	A	341	ASN	3.1
1	A	220	ALA	3.1
1	A	232	TYR	3.0
1	A	420	LEU	3.0
1	A	890	LEU	2.9
1	A	493	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	375	ARG	2.8
1	A	862[A]	ARG	2.8
1	A	217	SER	2.8
1	A	490	GLU	2.7
1	A	233	LYS	2.7
1	A	225	LEU	2.7
1	A	316	GLU	2.7
1	A	385	ASP	2.6
1	A	383	LEU	2.6
1	A	869	LYS	2.6
1	A	218	SER	2.5
1	A	855	LYS	2.5
1	A	705	ASN	2.5
1	A	171	LYS	2.5
1	A	626	LYS	2.5
1	A	704	SER	2.5
1	A	289	GLY	2.5
1	A	230	SER	2.4
1	A	488[A]	MET	2.4
1	A	264	THR	2.4
1	A	867	GLU	2.3
1	A	288	VAL	2.3
1	A	483[A]	HIS	2.3
1	A	714	LYS	2.3
1	A	231	ASN	2.2
1	A	278	LYS	2.1
1	A	866	ASP	2.1
1	A	228	LYS	2.1
1	A	849	ASN	2.1
1	A	495	GLN	2.0
1	A	425	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

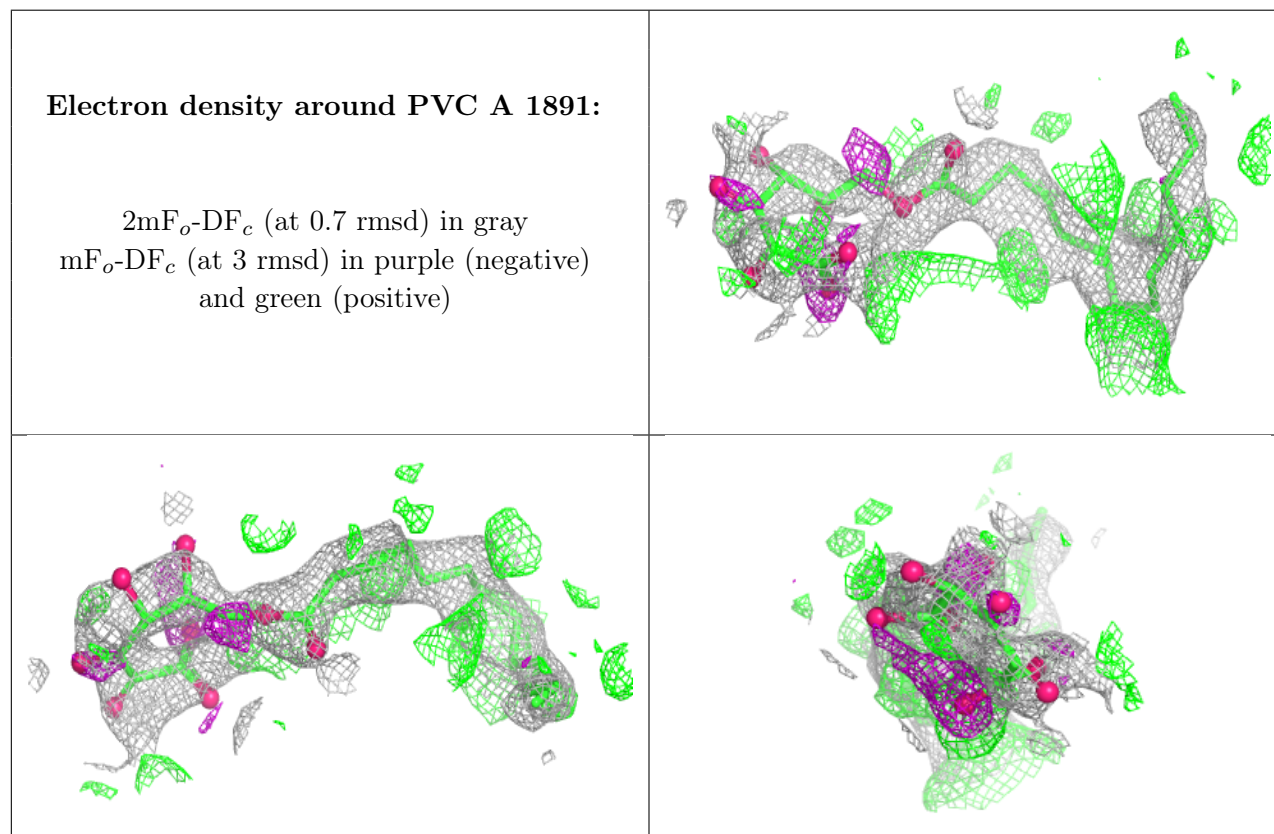
There are no oligosaccharides in this entry.

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
2	PVC	A	1891	27/30	0.50	0.26	50,52,60,61	0
4	SO4	A	1899	5/5	0.83	0.14	50,50,50,51	0
4	SO4	A	1898	5/5	0.87	0.12	59,59,59,60	0
4	SO4	A	1897	5/5	0.89	0.11	49,49,50,50	0
3	XYL	A	1892	10/10	0.90	0.11	24,32,34,35	0
4	SO4	A	1896	5/5	0.92	0.10	34,35,37,37	0
4	SO4	A	1895	5/5	0.93	0.09	34,35,37,38	0
3	XYL	A	1893	10/10	0.94	0.07	17,21,26,26	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.