



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:29 PM UTC

PDB ID : 5OA6 / pdb_00005oa6
Title : Crystal structure of ScGas2 in complex with compound 12
Authors : Delso, I.; Valero-Gonzalez, J.; Gomollon-Bel, F.; Castro-Lopez, J.; Fang, W.;
Navratilova, I.; Van Aalten, D.; Tejero, T.; Merino, P.; Hurtado-Guerrero, R.
Deposited on : 2017-06-21
Resolution : 1.94 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

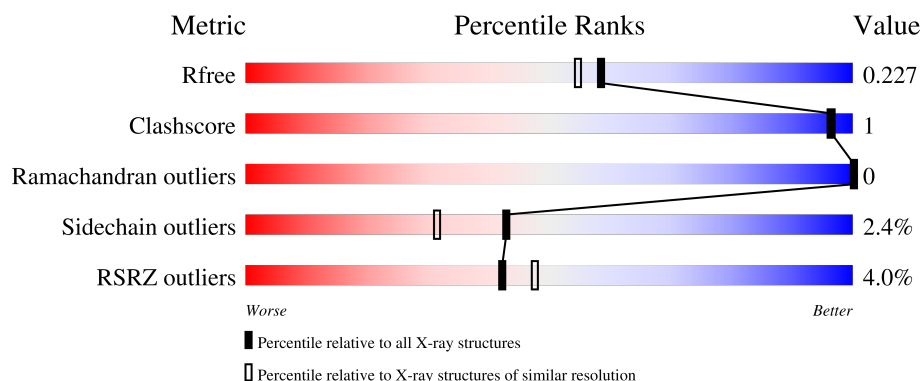
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	555	

2 Entry composition [i](#)

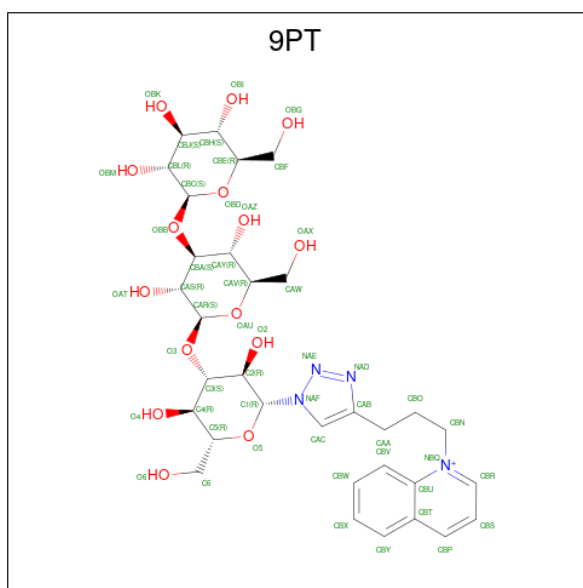
There are 5 unique types of molecules in this entry. The entry contains 3824 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1,3-beta-glucanosyltransferase GAS2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	2	0
			3434	2189	552	670	23			

- Molecule 2 is (2 {R},3 {S},4 {S},5 {R},6 {S})-2-(hydroxymethyl)-6-[(2 {R},3 {R},4 {S},5 {R},6 {S})-2-(hydroxymethyl)-6-[(2 {R},3 {R},4 {S},5 {R},6 {R})-2-(hydroxymethyl)-3,5-bis(oxidanyl)-6-[4-(3-quinolin-1-ium-1-ylpropyl)-1,2,3-triazol-1-yl]oxan-4-yl]oxy-3,5-bis(oxidanyl)oxan-4-yl]oxy-oxane-3,4,5-triol (CCD ID: 9PT) (formula: C₃₂H₄₅N₄O₁₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O		0	0
			51	32	4	15			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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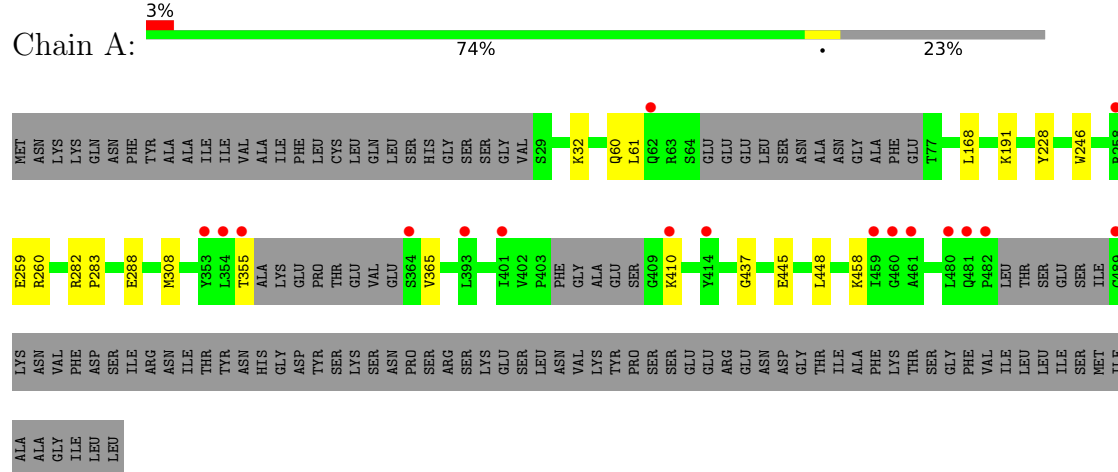
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	318	Total	O	0	0
			318	318		

- Molecule 1: 1,3-beta-glucanosyltransferase GAS2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.75Å 70.59Å 150.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.21 – 1.94 75.20 – 1.94	Depositor EDS
% Data completeness (in resolution range)	91.9 (75.21-1.94) 92.0 (75.20-1.94)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.41 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.189 , 0.219 0.196 , 0.227	Depositor DCC
R_{free} test set	1091 reflections (2.72%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3824	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% 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: EDO, 9PT, SO4

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	0.63	0/3522	0.78	0/4763

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	3434	0	3275	6	0
2	A	51	0	0	0	0
3	A	5	0	0	0	0
4	A	16	0	24	2	0
5	A	318	0	0	1	0
All	All	3824	0	3299	7	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 1.

All (7) 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)
4:A:605:EDO:C1	5:A:701:HOH:O	2.51	0.57
1:A:60:GLN:O	1:A:308:MET:HE1	2.13	0.49
1:A:282:ARG:HA	1:A:283:PRO:C	2.39	0.47
1:A:259:GLU:HG3	1:A:260:ARG:NH2	2.30	0.45
1:A:246:TRP:CG	1:A:288:GLU:HB3	2.54	0.42
1:A:437:GLY:HA2	4:A:605:EDO:H22	2.01	0.41
1:A:191:LYS:HD2	1:A:228:TYR:CE2	2.57	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	423/555 (76%)	413 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	380/485 (78%)	371 (98%)	9 (2%)	43	31

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	61	LEU
1	A	168	LEU
1	A	355	THR
1	A	365	VAL
1	A	410	LYS
1	A	445	GLU
1	A	448	LEU
1	A	458	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	HIS
1	A	205	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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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
4	EDO	A	603	-	3,3,3	0.44	0	2,2,2	0.25	0
2	9PT	A	601	-	56,56,56	1.55	5 (8%)	80,81,81	1.43	15 (18%)
4	EDO	A	605	-	3,3,3	0.31	0	2,2,2	0.69	0
3	SO4	A	602	-	4,4,4	0.44	0	6,6,6	0.10	0
4	EDO	A	606	-	3,3,3	0.44	0	2,2,2	0.29	0
4	EDO	A	604	-	3,3,3	0.43	0	2,2,2	0.37	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	603	-	-	1/1/1/1	-
2	9PT	A	601	-	-	8/24/84/84	0/6/6/6
4	EDO	A	605	-	-	0/1/1/1	-
4	EDO	A	606	-	-	1/1/1/1	-
4	EDO	A	604	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	9PT	CBR-NBQ	6.16	1.44	1.33
2	A	601	9PT	NAD-NAE	-5.90	1.22	1.32
2	A	601	9PT	NAF-NAE	-4.89	1.29	1.35
2	A	601	9PT	CAA-CAB	2.48	1.55	1.50
2	A	601	9PT	CAC-CAB	-2.16	1.33	1.36

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	9PT	NAF-NAE-NAD	4.57	110.95	107.09
2	A	601	9PT	CBO-CAA-CAB	-4.55	104.37	113.56
2	A	601	9PT	CBR-NBQ-CBU	-3.50	118.05	121.05
2	A	601	9PT	O5-C1-NAF	-3.28	98.19	107.20
2	A	601	9PT	OBD-CBE-CBF	3.07	114.04	106.44
2	A	601	9PT	CBN-NBQ-CBR	3.06	121.58	117.86
2	A	601	9PT	CAC-NAF-NAE	-2.52	108.25	110.63
2	A	601	9PT	CBY-CBT-CBP	-2.42	117.49	123.01
2	A	601	9PT	CBT-CBU-NBQ	2.38	120.04	117.90
2	A	601	9PT	C1-NAF-NAE	2.20	123.56	119.98
2	A	601	9PT	CBY-CBT-CBU	2.14	121.33	118.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	9PT	O5-C5-C6	-2.04	101.39	106.44
2	A	601	9PT	CBP-CBT-CBU	2.03	121.18	118.55
2	A	601	9PT	C6-C5-C4	2.02	117.99	113.02
2	A	601	9PT	CBC-OB-OB-CBA	-2.01	113.22	117.98

There are no chirality outliers.

All (11) torsion outliers are listed below:

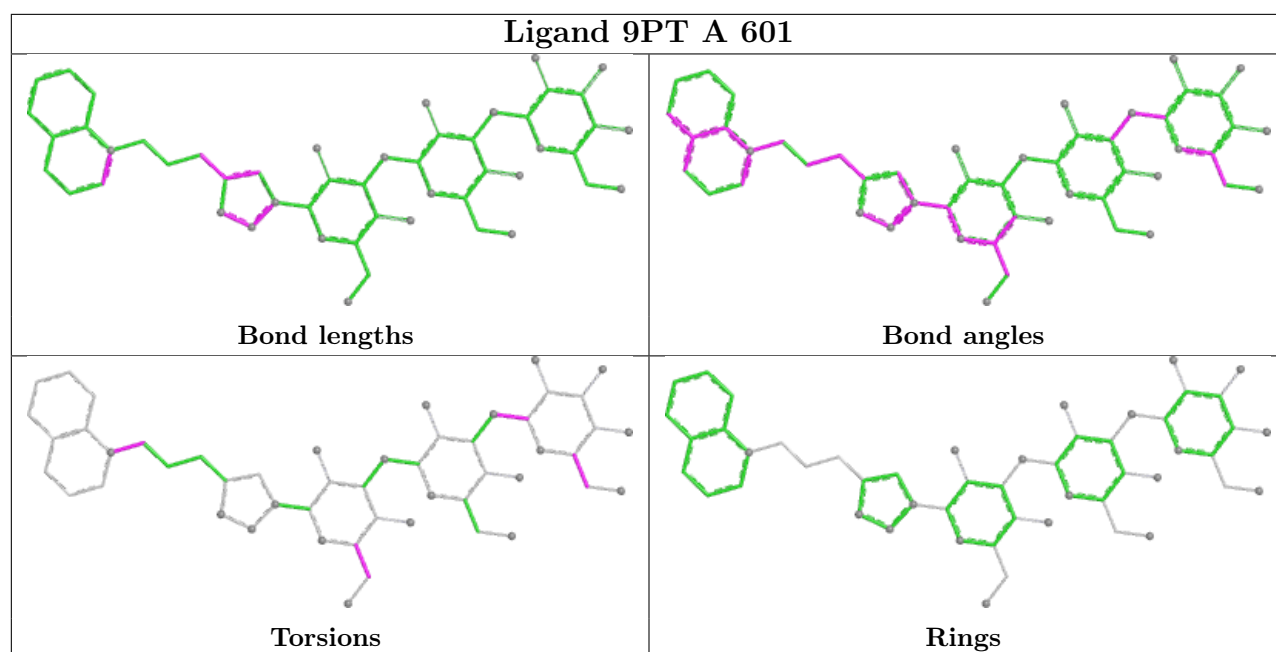
Mol	Chain	Res	Type	Atoms
2	A	601	9PT	CBO-CBN-NBQ-CBR
2	A	601	9PT	CBO-CBN-NBQ-CBU
2	A	601	9PT	C4-C5-C6-O6
2	A	601	9PT	O5-C5-C6-O6
4	A	606	EDO	O1-C1-C2-O2
2	A	601	9PT	CBH-CBE-CBF-OBG
2	A	601	9PT	CBL-CBC-OB-OB-CBA
2	A	601	9PT	OB-OB-CBC-OB-OB-CBA
4	A	603	EDO	O1-C1-C2-O2
2	A	601	9PT	OB-OB-CBE-CBF-OBG
4	A	604	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	605	EDO	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 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	430/555 (77%)	0.13	17 (3%)	42 47	20, 32, 56, 75	2 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	489	CYS	4.2
1	A	482	PRO	3.4
1	A	354	LEU	3.1
1	A	410	LYS	3.0
1	A	364	SER	2.8
1	A	258	ARG	2.5
1	A	480	LEU	2.5
1	A	353	TYR	2.4
1	A	355	THR	2.4
1	A	460	GLY	2.3
1	A	62	GLN	2.2
1	A	481	GLN	2.2
1	A	459	ILE	2.1
1	A	461	ALA	2.1
1	A	401	ILE	2.1
1	A	393	LEU	2.1
1	A	414	TYR	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](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

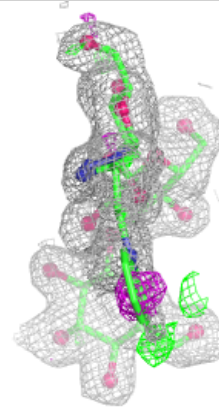
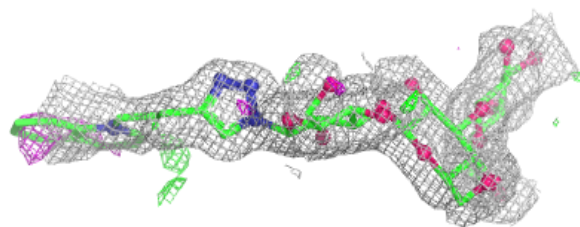
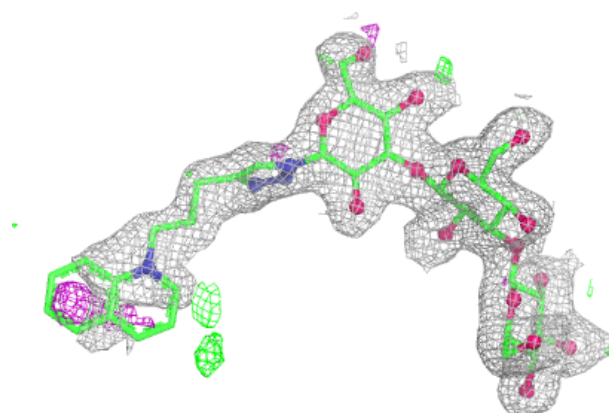
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	A	604	4/4	0.72	0.15	52,54,56,58	0
4	EDO	A	603	4/4	0.75	0.14	43,46,47,49	0
4	EDO	A	606	4/4	0.75	0.21	50,52,54,57	0
4	EDO	A	605	4/4	0.80	0.28	36,40,42,46	0
3	SO4	A	602	5/5	0.80	0.09	84,85,85,86	0
2	9PT	A	601	51/51	0.90	0.11	24,32,63,63	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 9PT A 601:

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.