



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:43 PM UTC

PDB ID : 9QFF / pdb_00009qff
Title : Structure of SOS1 in complex with compound 3
Authors : Breed, J.
Deposited on : 2025-03-11
Resolution : 1.88 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

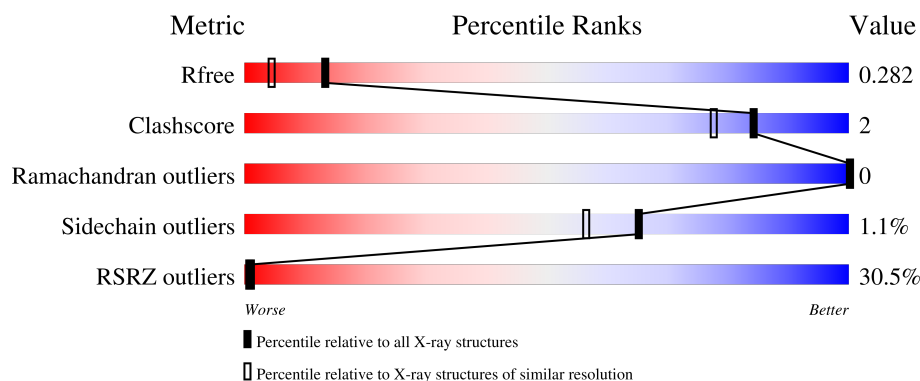
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	490	28% 83% 7% 10%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3585 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.

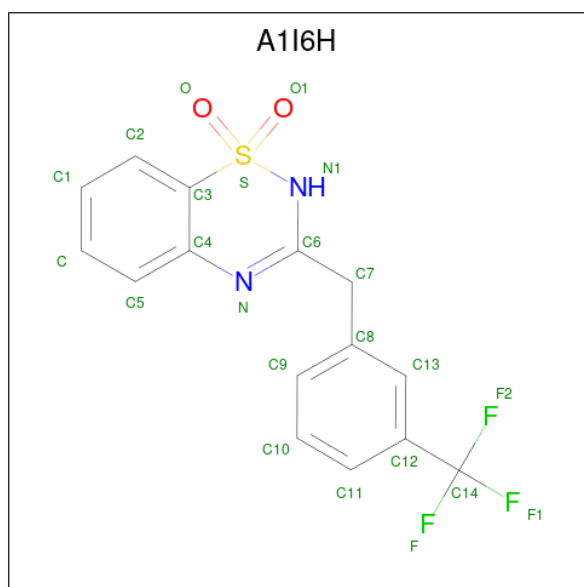
- Molecule 1 is a protein called Son of sevenless homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3492	2263	583	634	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	560	GLY	GLN	engineered mutation	UNP Q07889
A	561	ALA	GLU	engineered mutation	UNP Q07889
A	562	MET	GLU	engineered mutation	UNP Q07889
A	563	ALA	LYS	engineered mutation	UNP Q07889

- Molecule 2 is 3-[[3-(trifluoromethyl)phenyl]methyl]-2,4-benzothiadiazine 1,1-dioxide (CCD ID: A1I6H) (formula: C₁₅H₁₁F₃N₂O₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			23	15	3	2	2	1		

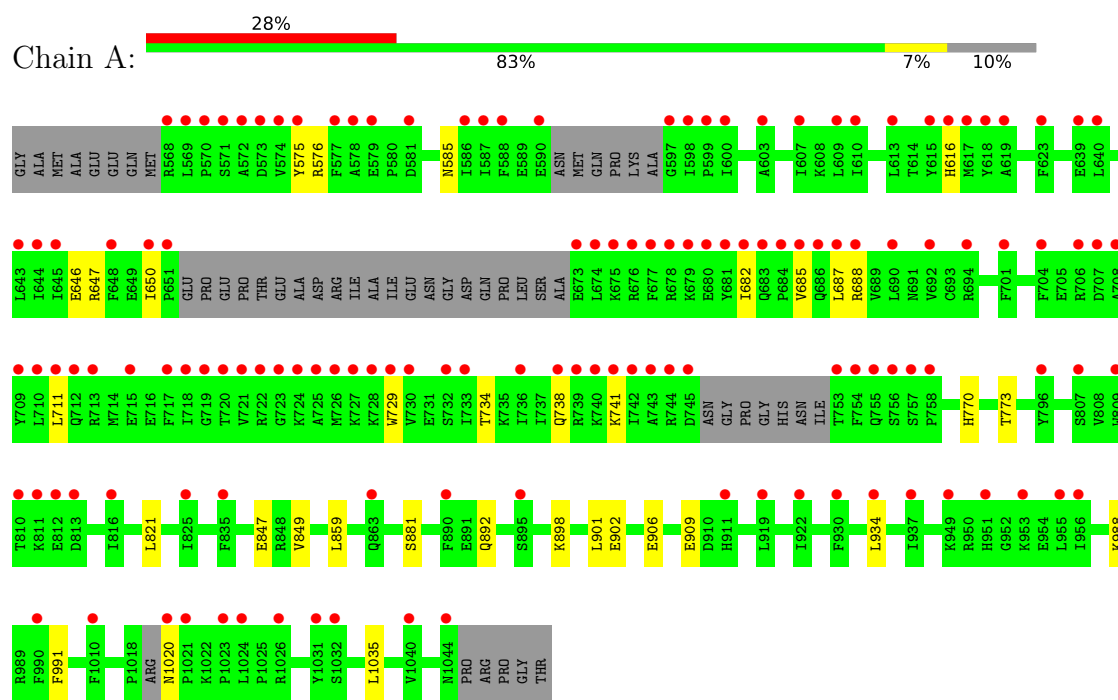
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	70	Total	O	0	0
			70	70		

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: Son of sevenless homolog 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	41.46Å 84.69Å 176.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.19 – 1.88 88.19 – 1.88	Depositor EDS
% Data completeness (in resolution range)	64.9 (88.19-1.88) 64.9 (88.19-1.88)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 1.88Å)	Xtriage
Refinement program	BUSTER 2.11.8 (24-FEB-2021)	Depositor
R, R_{free}	0.278 , 0.304 (Not available) , 0.282	Depositor DCC
R_{free} test set	1705 reflections (3.30%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3585	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.92% 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: A1I6H

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	0.77	0/3579	1.10	4/4873 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	991	PHE	CA-CB-CG	-6.36	107.44	113.80
1	A	988	LYS	CA-C-N	5.18	127.23	120.28
1	A	988	LYS	C-N-CA	5.18	127.23	120.28
1	A	585	ASN	CA-CB-CG	5.15	117.75	112.60

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	3492	0	3334	16	0
2	A	23	0	0	0	0
3	A	70	0	0	0	0
All	All	3585	0	3334	16	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 2.

All (16) 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:906:GLU:HA	1:A:909:GLU:HG3	1.46	0.98
1:A:770:HIS:HD2	1:A:773:THR:HG23	1.58	0.68
1:A:770:HIS:CD2	1:A:773:THR:HG23	2.29	0.67
1:A:616:HIS:HB3	1:A:685:VAL:HG23	1.81	0.62
1:A:847:GLU:HG2	1:A:1035:LEU:HD11	1.82	0.62
1:A:734:THR:O	1:A:738:GLN:HG2	2.03	0.59
1:A:821:LEU:HD11	1:A:934:LEU:HD21	1.85	0.57
1:A:687:LEU:HD22	1:A:729:TRP:CD1	2.42	0.54
1:A:650:ILE:HD12	1:A:682:ILE:HA	1.91	0.52
1:A:711:LEU:HD21	1:A:741:LYS:HE3	1.98	0.46
1:A:898:LYS:O	1:A:902:GLU:HG3	2.18	0.44
1:A:859:LEU:C	1:A:859:LEU:HD23	2.43	0.43
1:A:770:HIS:CD2	1:A:773:THR:CG2	3.01	0.43
1:A:575:TYR:OH	1:A:647:ARG:O	2.34	0.43
1:A:849:VAL:HG21	1:A:892:GLN:HB2	2.02	0.41
1:A:576:ARG:HD3	1:A:646:GLU:OE1	2.22	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	432/490 (88%)	417 (96%)	15 (4%)	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	365/452 (81%)	361 (99%)	4 (1%)	65 56

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	688	ARG
1	A	881	SER
1	A	901	LEU
1	A	1020	ASN

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

Mol	Chain	Res	Type
1	A	691	ASN
1	A	770	HIS
1	A	863	GLN
1	A	993	ASN
1	A	1020	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](#)

1 ligand is 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	A1I6H	A	1101	-	23,25,25	0.30	0	32,38,38	0.73	1 (3%)

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	A1I6H	A	1101	-	-	0/9/25/25	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	A1I6H	C8-C7-C6	-2.97	107.47	113.62

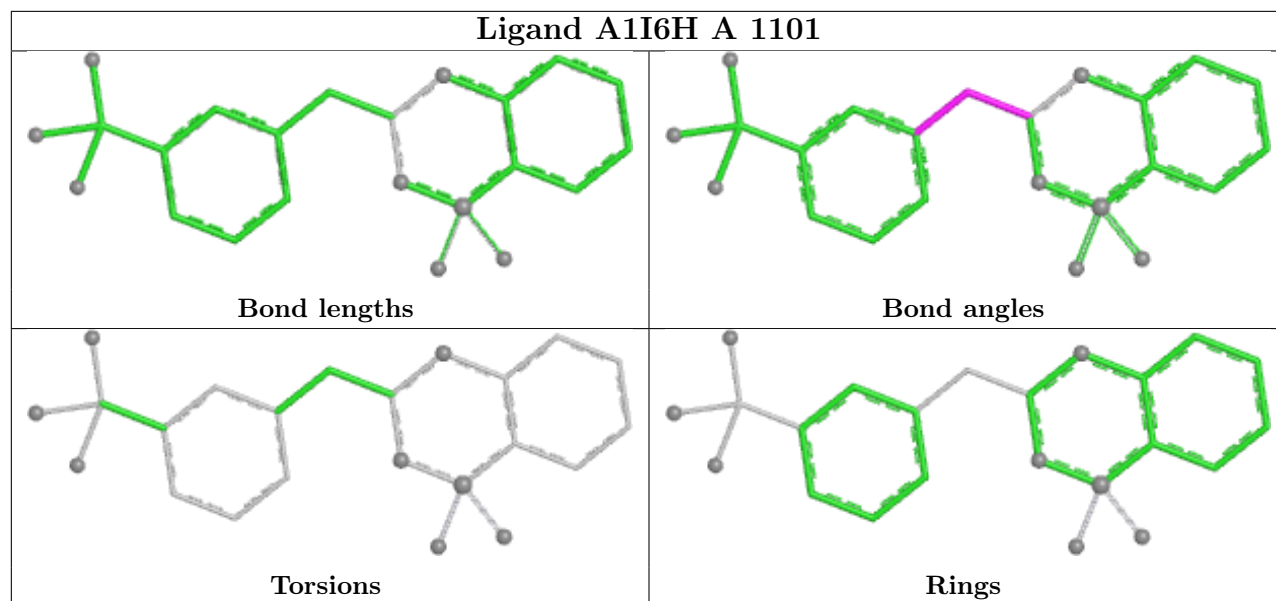
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	442/490 (90%)	1.62	135 (30%) 1 1	20, 39, 74, 94	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	722	ARG	6.9
1	A	674	LEU	6.5
1	A	742	ILE	6.2
1	A	675	LYS	6.0
1	A	721	VAL	5.7
1	A	681	TYR	5.5
1	A	574	VAL	5.4
1	A	673	GLU	5.2
1	A	677	PHE	5.2
1	A	709	TYR	5.0
1	A	678	ARG	5.0
1	A	725	ALA	4.9
1	A	743	ALA	4.8
1	A	568	ARG	4.8
1	A	717	PHE	4.8
1	A	644	ILE	4.6
1	A	812	GLU	4.5
1	A	679	LYS	4.5
1	A	720	THR	4.3
1	A	571	SER	4.2
1	A	680	GLU	4.2
1	A	738	GLN	4.1
1	A	676	ARG	4.1
1	A	718	ILE	4.1
1	A	753	THR	4.1
1	A	569	LEU	4.1
1	A	683	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	890	PHE	3.9
1	A	651	PRO	3.9
1	A	726	MET	3.9
1	A	1044	ASN	3.8
1	A	586	ILE	3.8
1	A	745	ASP	3.7
1	A	701	PHE	3.7
1	A	711	LEU	3.6
1	A	639	GLU	3.6
1	A	1020	ASN	3.6
1	A	809	TRP	3.6
1	A	1031	TYR	3.6
1	A	597	GLY	3.6
1	A	590	GLU	3.6
1	A	729	TRP	3.5
1	A	719	GLY	3.5
1	A	682	ILE	3.5
1	A	650	ILE	3.4
1	A	813	ASP	3.4
1	A	617	MET	3.4
1	A	710	LEU	3.4
1	A	911	HIS	3.3
1	A	930	PHE	3.3
1	A	616	HIS	3.3
1	A	724	LYS	3.3
1	A	684	PRO	3.3
1	A	740	LYS	3.2
1	A	609	LEU	3.2
1	A	587	ILE	3.2
1	A	643	LEU	3.2
1	A	600	ILE	3.2
1	A	757	SER	3.2
1	A	610	ILE	3.1
1	A	648	PHE	3.1
1	A	579	GLU	3.1
1	A	953	LYS	3.1
1	A	739	ARG	3.1
1	A	723	GLY	3.1
1	A	572	ALA	3.1
1	A	598	ILE	3.0
1	A	607	ILE	3.0
1	A	955	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	578	ALA	3.0
1	A	713	ARG	3.0
1	A	755	GLN	3.0
1	A	618	TYR	3.0
1	A	754	PHE	2.9
1	A	685	VAL	2.9
1	A	728	LYS	2.9
1	A	744	ARG	2.8
1	A	645	ILE	2.8
1	A	599	PRO	2.8
1	A	573	ASP	2.8
1	A	704	PHE	2.8
1	A	690	LEU	2.8
1	A	1024	LEU	2.8
1	A	708	ALA	2.8
1	A	588	PHE	2.8
1	A	623	PHE	2.7
1	A	863	GLN	2.7
1	A	1040	VAL	2.7
1	A	692	VAL	2.7
1	A	712	GLN	2.7
1	A	613	LEU	2.7
1	A	796	TYR	2.6
1	A	694	ARG	2.6
1	A	756	SER	2.6
1	A	990	PHE	2.6
1	A	1021	PRO	2.6
1	A	895	SER	2.6
1	A	577	PHE	2.6
1	A	732	SER	2.6
1	A	810	THR	2.6
1	A	581	ASP	2.5
1	A	741	LYS	2.5
1	A	951	HIS	2.5
1	A	1023	PRO	2.5
1	A	575	TYR	2.5
1	A	733	ILE	2.5
1	A	715	GLU	2.5
1	A	570	PRO	2.5
1	A	1032	SER	2.5
1	A	707	ASP	2.4
1	A	956	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	736	ILE	2.4
1	A	1026	ARG	2.4
1	A	619	ALA	2.4
1	A	835	PHE	2.3
1	A	937	ILE	2.3
1	A	640	LEU	2.3
1	A	687	LEU	2.3
1	A	949	LYS	2.3
1	A	727	LYS	2.2
1	A	706	ARG	2.2
1	A	686	GLN	2.2
1	A	615	TYR	2.2
1	A	825	ILE	2.2
1	A	1010	PHE	2.1
1	A	688	ARG	2.1
1	A	603	ALA	2.1
1	A	811	LYS	2.1
1	A	758	PRO	2.1
1	A	919	LEU	2.1
1	A	807	SER	2.0
1	A	816	ILE	2.0
1	A	934	LEU	2.0
1	A	922	ILE	2.0
1	A	730	VAL	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](#)

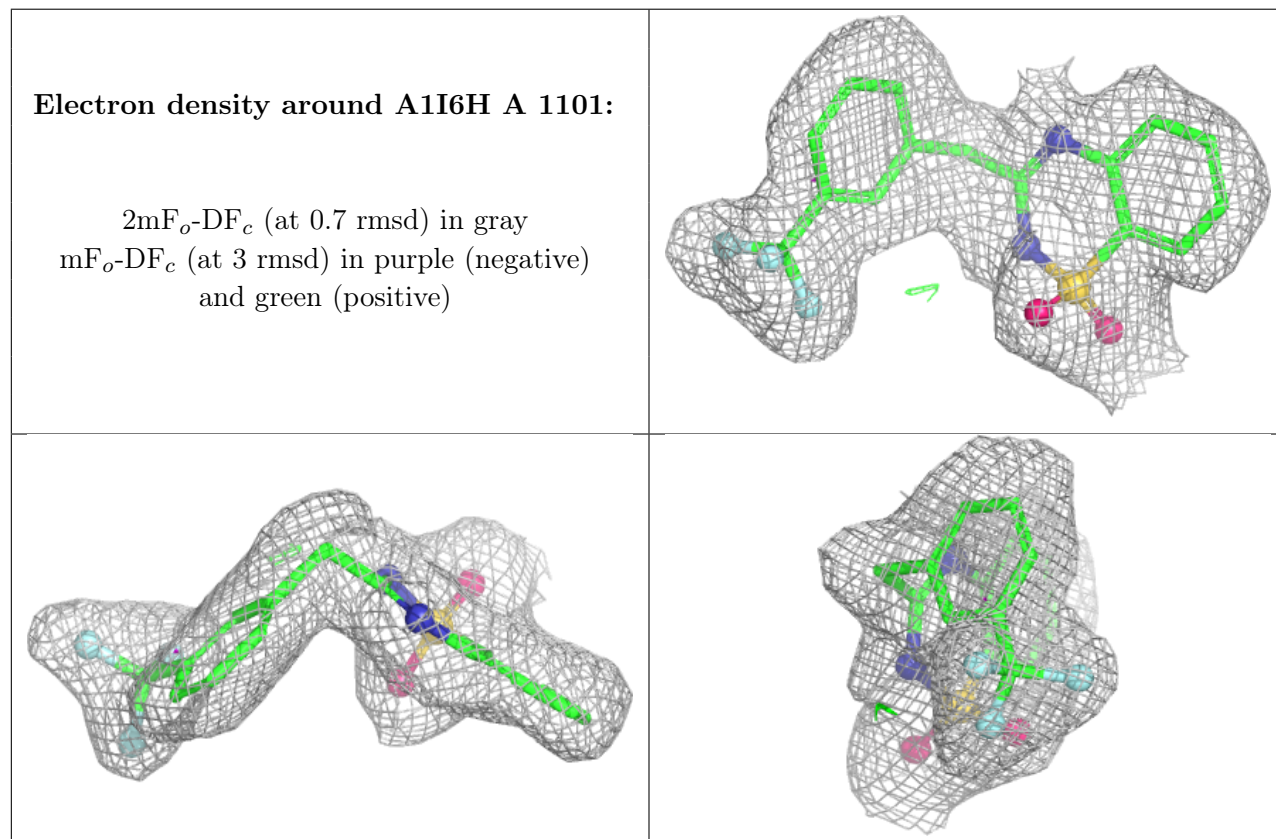
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	A1I6H	A	1101	23/23	0.91	0.10	33,36,40,41	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.