Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2026 – 05:26 PM UTC

PDB ID	:	8A9I / pdb_00008a9i
Title	:	PI3KC2a core in complex with PITCOIN1
Authors	:	Lo, W.T.; Roske, Y.; Daumke, O.; Haucke, V.
Deposited on	:	2022-06-28
Resolution	:	2.87 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 (i) 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 (i)) were used in the production of this report:

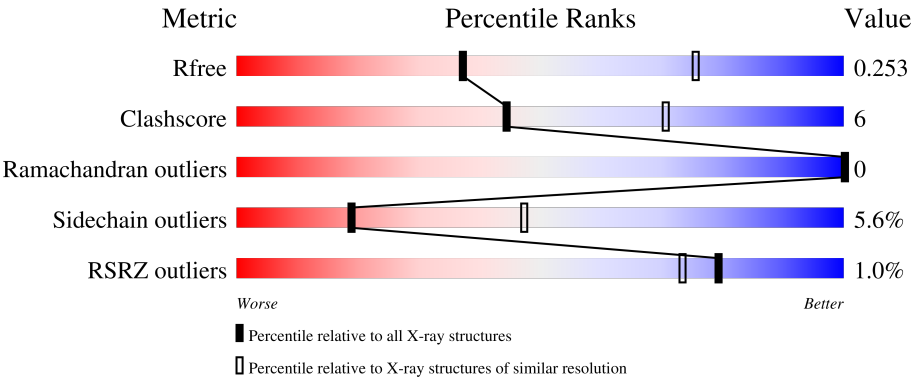
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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 <=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	910	% 76% 12% · 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6628 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.

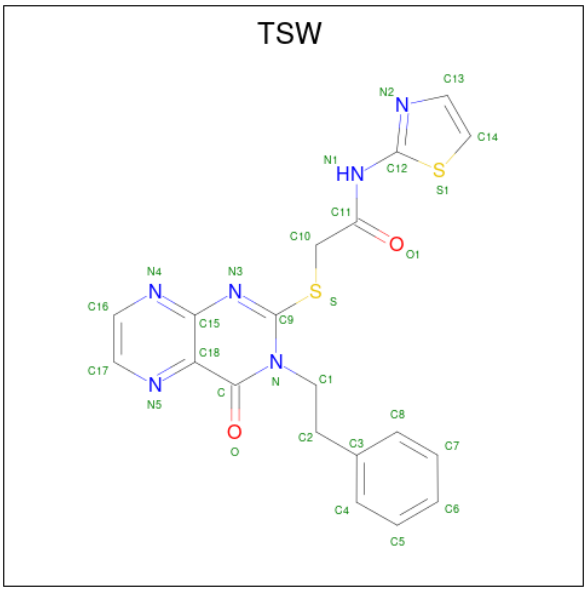
- Molecule 1 is a protein called Phosphatidylinositol 4-phosphate 3-kinase C2 domain-containing subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	822	6521	4192	1094	1195	40	0	2	0

There are 18 discrepancies between the modelled and reference sequences:

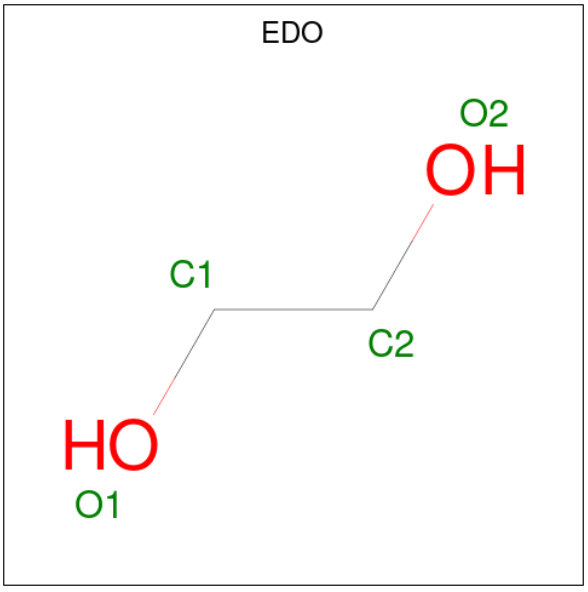
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	PHE	engineered mutation	UNP Q61194
A	2	ALA	GLU	engineered mutation	UNP Q61194
A	267	GLY	-	linker	UNP Q61194
A	268	SER	-	linker	UNP Q61194
A	269	GLY	-	linker	UNP Q61194
A	270	SER	-	linker	UNP Q61194
A	276	SER	-	linker	UNP Q61194
A	277	ALA	-	linker	UNP Q61194
A	278	GLY	-	linker	UNP Q61194
A	279	ALA	-	linker	UNP Q61194
A	280	GLY	-	linker	UNP Q61194
A	281	SER	-	linker	UNP Q61194
A	282	GLY	-	linker	UNP Q61194
A	283	ALA	-	linker	UNP Q61194
A	286	GLY	ALA	conflict	UNP Q61194
A	353	ALA	PHE	conflict	UNP Q61194
A	354	ALA	PHE	conflict	UNP Q61194
A	427	ALA	LEU	engineered mutation	UNP Q61194

- Molecule 2 is 2-[4-oxidanylidene-3-(2-phenylethyl)pteridin-2-yl]sulfanyl- {N}-(1,3-thiazol-2 -yl)ethanamide (CCD ID: TSW) (formula: $C_{19}H_{16}N_6O_2S_2$) (labeled as "Ligand of Interest" by depositor).



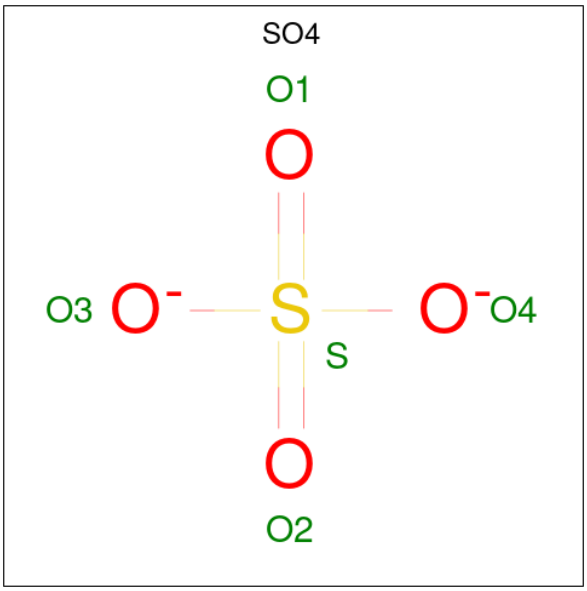
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			29	19	6	2	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

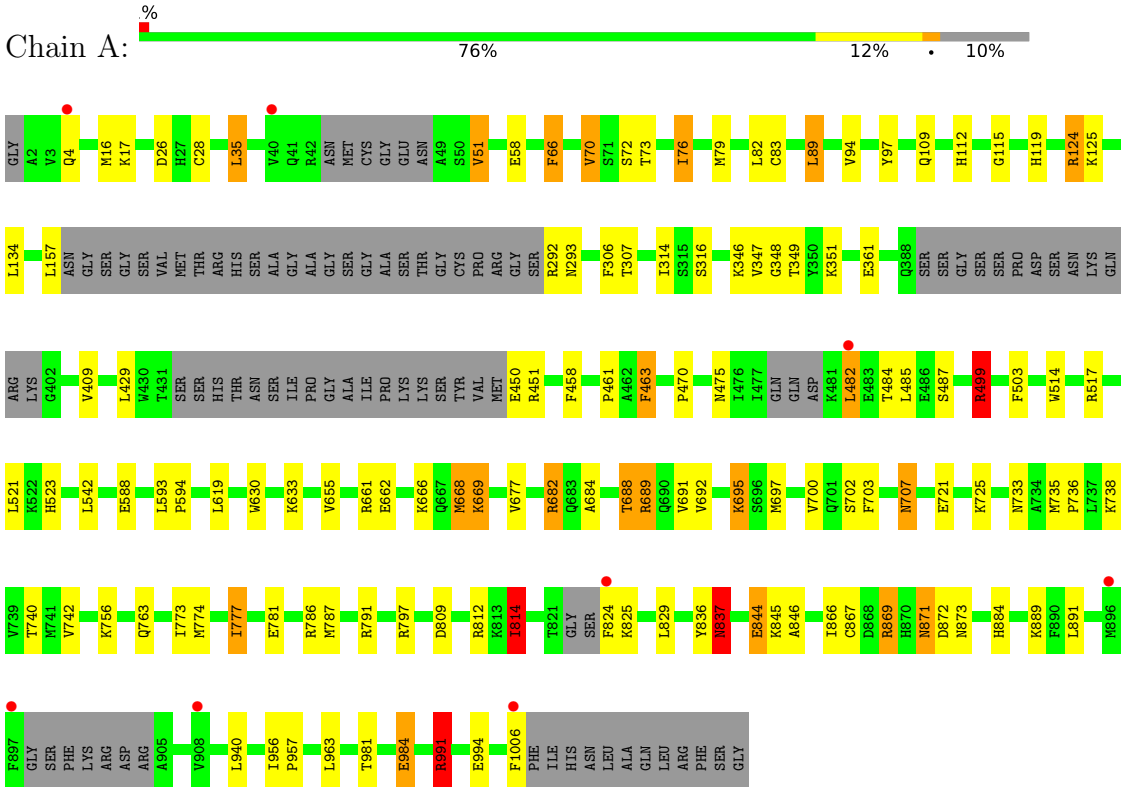
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	65	Total O 65 65	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: Phosphatidylinositol 4-phosphate 3-kinase C2 domain-containing subunit alpha



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	56.16Å 133.29Å 152.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.49 – 2.87 47.49 – 2.87	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.49-2.87) 98.7 (47.49-2.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.217 , 0.258 0.220 , 0.253	Depositor DCC
R_{free} test set	1334 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	77.2	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 57.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6628	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, SO4, TSW

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	0.62	4/6659 (0.1%)	1.22	12/9018 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	884	HIS	CE1-NE2	5.99	1.38	1.32
1	A	112	HIS	CE1-NE2	5.46	1.38	1.32
1	A	119	HIS	CE1-NE2	5.08	1.37	1.32
1	A	523	HIS	CE1-NE2	5.01	1.37	1.32

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	837	ASN	CA-CB-CG	8.84	121.44	112.60
1	A	499	ARG	CG-CD-NE	-8.05	94.28	112.00
1	A	293	ASN	CB-CA-C	7.94	122.82	109.80
1	A	4	GLN	CB-CA-C	7.87	126.43	110.38
1	A	361	GLU	CB-CG-CD	-7.77	99.40	112.60
1	A	814	ILE	CA-CB-CG1	6.17	120.88	110.40
1	A	293	ASN	CA-CB-CG	5.79	118.39	112.60
1	A	991	ARG	CB-CG-CD	5.70	124.42	111.30
1	A	994	GLU	CB-CG-CD	5.63	122.17	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	844	GLU	CB-CG-CD	5.34	121.67	112.60
1	A	1006	PHE	CA-CB-CG	5.27	119.07	113.80
1	A	824	PHE	CA-CB-CG	5.06	118.86	113.80

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	ARG	Sidechain
1	A	451	ARG	Sidechain
1	A	499	ARG	Sidechain
1	A	661	ARG	Sidechain
1	A	682	ARG	Sidechain
1	A	689	ARG	Sidechain
1	A	791	ARG	Sidechain
1	A	797	ARG	Sidechain
1	A	812	ARG	Sidechain
1	A	991	ARG	Sidechain

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	6521	0	6559	79	0
2	A	29	0	0	0	0
3	A	8	0	12	1	0
4	A	5	0	0	0	0
5	A	65	0	0	5	0
All	All	6628	0	6571	79	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 6.

All (79) 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:837:ASN:OD1	1:A:846:ALA:HB2	1.55	1.06
1:A:499:ARG:NH1	1:A:503:PHE:O	1.98	0.95
1:A:837:ASN:OD1	1:A:846:ALA:CB	2.16	0.94
1:A:461:PRO:HB2	1:A:463:PHE:CE1	2.16	0.81
1:A:669:LYS:NZ	5:A:1201:HOH:O	2.10	0.81
1:A:773:ILE:O	1:A:777:ILE:HG12	1.85	0.76
1:A:703:PHE:O	1:A:707:ASN:OD1	2.05	0.74
1:A:738:LYS:NZ	1:A:740:THR:OG1	2.20	0.74
1:A:809:ASP:HB2	1:A:814:ILE:HD11	1.71	0.72
1:A:668:MET:HA	1:A:668:MET:HE2	1.72	0.72
1:A:51:VAL:HG11	1:A:124:ARG:HD2	1.72	0.68
1:A:461:PRO:CB	1:A:463:PHE:CE1	2.77	0.67
1:A:461:PRO:CB	1:A:463:PHE:HE1	2.08	0.66
1:A:677:VAL:HG11	1:A:697:MET:HE3	1.77	0.66
1:A:72:SER:HB2	1:A:76:ILE:HD11	1.79	0.64
1:A:668:MET:HA	1:A:668:MET:CE	2.27	0.64
1:A:35:LEU:HD12	1:A:109:GLN:HG2	1.81	0.63
1:A:409:VAL:HG23	1:A:429:LEU:HB3	1.81	0.63
1:A:461:PRO:HB2	1:A:463:PHE:CD1	2.33	0.62
1:A:814:ILE:HG21	1:A:829:LEU:HD23	1.82	0.60
1:A:688:THR:HG22	1:A:692:VAL:HG23	1.86	0.58
1:A:837:ASN:CG	5:A:1205:HOH:O	2.45	0.58
1:A:314:ILE:HD11	1:A:349:THR:HG21	1.87	0.56
1:A:809:ASP:HB2	1:A:814:ILE:CD1	2.36	0.56
1:A:981:THR:HG22	1:A:984:GLU:CD	2.31	0.55
1:A:461:PRO:CG	1:A:463:PHE:HE1	2.20	0.55
1:A:682:ARG:HG2	1:A:735:MET:HB2	1.90	0.54
1:A:97:TYR:HB3	1:A:134:LEU:HD11	1.88	0.54
1:A:51:VAL:CG1	1:A:124:ARG:HD2	2.39	0.53
1:A:836:TYR:C	1:A:837:ASN:HD22	2.15	0.53
1:A:16:MET:HG2	5:A:1223:HOH:O	2.09	0.52
1:A:837:ASN:HD22	1:A:837:ASN:N	2.07	0.52
1:A:306:PHE:HB3	1:A:458:PHE:CD2	2.45	0.52
1:A:956:ILE:N	1:A:957:PRO:HD2	2.26	0.51
1:A:689:ARG:CD	1:A:735:MET:HE3	2.40	0.51
1:A:869:ARG:NH1	1:A:873:ASN:HB3	2.25	0.50
1:A:774:MET:HA	1:A:777:ILE:HG13	1.93	0.50
1:A:981:THR:H	1:A:984:GLU:HG3	1.76	0.50
1:A:630:TRP:CZ3	1:A:668:MET:HE3	2.46	0.49
1:A:514:TRP:O	1:A:517:ARG:NE	2.41	0.49
1:A:461:PRO:CG	1:A:463:PHE:CE1	2.95	0.49
1:A:871:ASN:HD22	1:A:872:ASP:N	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:PHE:H	1:A:463:PHE:HD1	1.59	0.49
1:A:82:LEU:HD13	1:A:94:VAL:HG12	1.95	0.49
1:A:26:ASP:OD1	1:A:28:CYS:SG	2.66	0.48
1:A:736:PRO:HG3	1:A:756:LYS:HE3	1.94	0.48
1:A:668:MET:HE2	1:A:668:MET:CA	2.43	0.47
1:A:763:GLN:HE21	1:A:763:GLN:HB2	1.53	0.46
1:A:630:TRP:CH2	1:A:668:MET:HE3	2.51	0.46
1:A:691:VAL:HG13	1:A:695:LYS:NZ	2.31	0.46
1:A:125:LYS:HB3	1:A:125:LYS:HE2	1.79	0.45
1:A:314:ILE:HD11	1:A:349:THR:CG2	2.47	0.45
1:A:619:LEU:HD21	1:A:655:VAL:HG22	1.97	0.45
1:A:866:ILE:HG23	1:A:889:LYS:O	2.17	0.45
1:A:79:MET:HA	1:A:82:LEU:HB2	1.98	0.44
1:A:684:ALA:HB1	1:A:688:THR:HB	1.98	0.44
1:A:73:THR:CG2	1:A:76:ILE:HG23	2.48	0.44
1:A:891:LEU:HD22	1:A:963:LEU:HD13	1.98	0.44
1:A:470:PRO:HG3	1:A:542:LEU:HB2	1.98	0.44
1:A:409:VAL:CG2	1:A:429:LEU:HB3	2.46	0.44
1:A:691:VAL:HG13	1:A:695:LYS:HZ3	1.83	0.43
1:A:781:GLU:HG3	1:A:940:LEU:HD22	2.00	0.43
1:A:588:GLU:HG3	3:A:1103:EDO:C1	2.49	0.43
1:A:593:LEU:N	1:A:594:PRO:CD	2.82	0.43
1:A:66:PHE:CD2	1:A:66:PHE:N	2.86	0.43
1:A:475:ASN:HD22	1:A:475:ASN:HA	1.72	0.43
1:A:697:MET:HE2	1:A:700:VAL:HG21	2.01	0.43
1:A:666:LYS:HD3	1:A:707:ASN:HB3	2.01	0.42
1:A:347:VAL:HG12	1:A:348:GLY:O	2.19	0.42
1:A:70:VAL:HG13	1:A:115:GLY:HA3	2.00	0.42
1:A:125:LYS:HD2	1:A:786:ARG:HA	2.01	0.42
1:A:83:CYS:SG	1:A:89:LEU:CD2	3.08	0.41
1:A:702:SER:CB	5:A:1206:HOH:O	2.69	0.41
1:A:482:LEU:HD13	1:A:482:LEU:HA	1.88	0.41
1:A:125:LYS:HE3	1:A:787:MET:O	2.20	0.41
1:A:346:LYS:HD2	5:A:1243:HOH:O	2.20	0.41
1:A:691:VAL:HG12	1:A:695:LYS:HD2	2.03	0.40
1:A:721:GLU:HB3	1:A:742:VAL:CG2	2.51	0.40
1:A:463:PHE:CD1	1:A:463:PHE:N	2.89	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	808/910 (89%)	785 (97%)	23 (3%)	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	722/800 (90%)	682 (94%)	40 (6%)	19 48

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	35	LEU
1	A	51	VAL
1	A	58	GLU
1	A	66	PHE
1	A	70	VAL
1	A	76	ILE
1	A	89	LEU
1	A	157	LEU
1	A	292	ARG
1	A	307	THR
1	A	316	SER
1	A	351	LYS

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Mol	Chain	Res	Type
1	A	450	GLU
1	A	463	PHE
1	A	482	LEU
1	A	484	THR
1	A	485	LEU
1	A	487	SER
1	A	521	LEU
1	A	633	LYS
1	A	662	GLU
1	A	668	MET
1	A	669	LYS
1	A	688	THR
1	A	695	LYS
1	A	707	ASN
1	A	725	LYS
1	A	733	ASN
1	A	777	ILE
1	A	814	ILE
1	A	825	LYS
1	A	837	ASN
1	A	844	GLU
1	A	845	LYS
1	A	867	CYS
1	A	869	ARG
1	A	871	ASN
1	A	984	GLU
1	A	991	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	104	GLN
1	A	133	GLN
1	A	305	GLN
1	A	475	ASN
1	A	523	HIS
1	A	536	ASN
1	A	683	GLN
1	A	690	GLN
1	A	763	GLN
1	A	815	GLN

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Mol	Chain	Res	Type
1	A	870	HIS
1	A	871	ASN
1	A	1005	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

4 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	EDO	A	1103	-	3,3,3	0.33	0	2,2,2	0.38	0
2	TSW	A	1101	-	32,32,32	4.04	11 (34%)	38,43,43	3.24	17 (44%)
4	SO4	A	1104	-	4,4,4	0.31	0	6,6,6	0.11	0
3	EDO	A	1102	-	3,3,3	0.06	0	2,2,2	0.11	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	EDO	A	1103	-	-	1/1/1/1	-
2	TSW	A	1101	-	-	7/14/14/14	0/4/4/4
3	EDO	A	1102	-	-	1/1/1/1	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	TSW	C12-S1	-13.03	1.56	1.74
2	A	1101	TSW	C13-N2	9.80	1.56	1.38
2	A	1101	TSW	C12-N2	8.02	1.44	1.31
2	A	1101	TSW	C9-N3	6.06	1.38	1.29
2	A	1101	TSW	C12-N1	6.00	1.47	1.38
2	A	1101	TSW	C11-N1	5.15	1.46	1.37
2	A	1101	TSW	C13-C14	4.72	1.45	1.34
2	A	1101	TSW	C9-S	4.20	1.81	1.74
2	A	1101	TSW	C14-S1	-3.77	1.53	1.70
2	A	1101	TSW	C10-C11	3.15	1.55	1.51
2	A	1101	TSW	C18-C	-2.72	1.39	1.47

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1101	TSW	C14-S1-C12	13.88	105.96	90.07
2	A	1101	TSW	C10-C11-N1	6.54	124.16	114.53
2	A	1101	TSW	C14-C13-N2	-5.53	108.14	116.12
2	A	1101	TSW	S-C9-N3	-4.78	114.21	120.16
2	A	1101	TSW	S1-C12-N2	-3.26	108.44	114.59
2	A	1101	TSW	C1-C2-C3	-3.06	103.52	112.15
2	A	1101	TSW	C11-N1-C12	-2.90	118.73	123.69
2	A	1101	TSW	C10-S-C9	2.86	104.86	99.04
2	A	1101	TSW	C18-C15-N3	-2.80	119.25	123.19
2	A	1101	TSW	N-C9-N3	-2.60	122.44	124.93
2	A	1101	TSW	C11-C10-S	2.56	121.28	111.55
2	A	1101	TSW	C15-C18-N5	-2.45	118.32	122.95
2	A	1101	TSW	O1-C11-N1	-2.38	117.92	122.44
2	A	1101	TSW	C9-N-C	-2.26	117.80	122.08
2	A	1101	TSW	C-C18-N5	2.20	120.75	116.23
2	A	1101	TSW	O1-C11-C10	-2.13	117.83	121.44
2	A	1101	TSW	S1-C12-N1	2.11	127.06	123.29

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	TSW	N2-C12-N1-C11
2	A	1101	TSW	S1-C12-N1-C11
2	A	1101	TSW	C11-C10-S-C9
3	A	1102	EDO	O1-C1-C2-O2
3	A	1103	EDO	O1-C1-C2-O2
2	A	1101	TSW	S-C10-C11-O1
2	A	1101	TSW	C2-C1-N-C
2	A	1101	TSW	C2-C1-N-C9
2	A	1101	TSW	S-C10-C11-N1

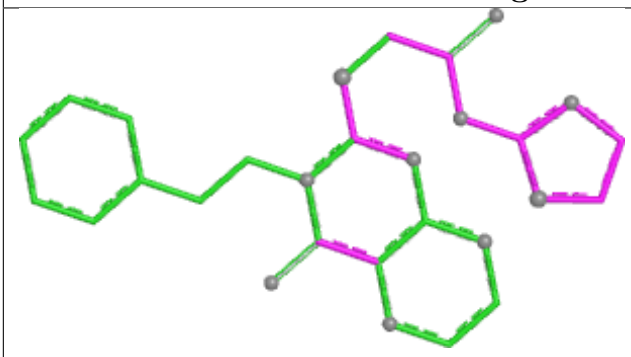
There are no ring outliers.

1 monomer is involved in 1 short contact:

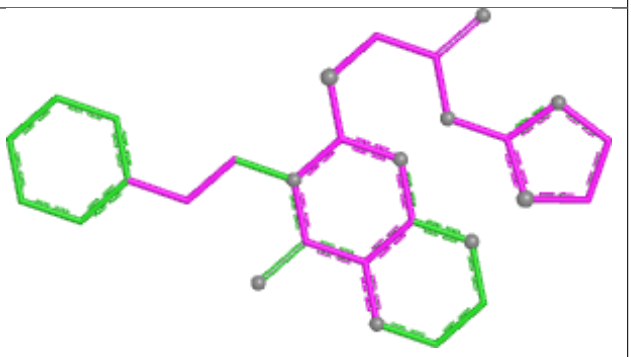
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1103	EDO	1	0

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 then 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.

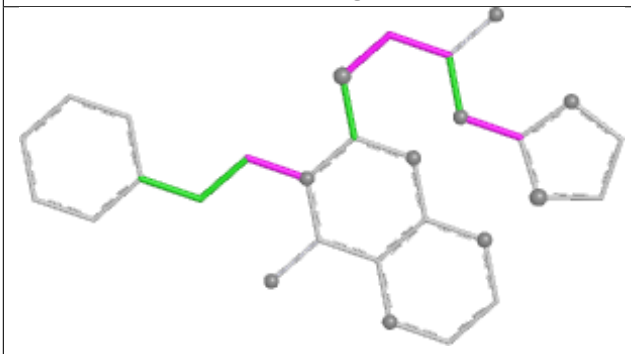
Ligand TSW A 1101



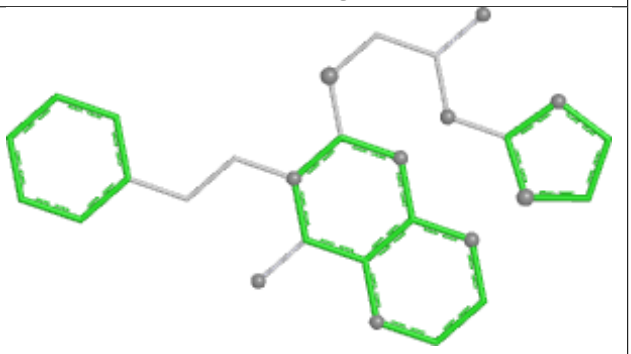
Bond lengths



Bond angles



Torsions



Rings

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

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, 95^{th} 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	822/910 (90%)	0.00	8 (0%) 79 73	49, 85, 134, 174	2 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	482	LEU	3.6
1	A	897	PHE	3.3
1	A	1006	PHE	3.0
1	A	908	VAL	2.9
1	A	824	PHE	2.6
1	A	40	VAL	2.2
1	A	4	GLN	2.2
1	A	896	MET	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

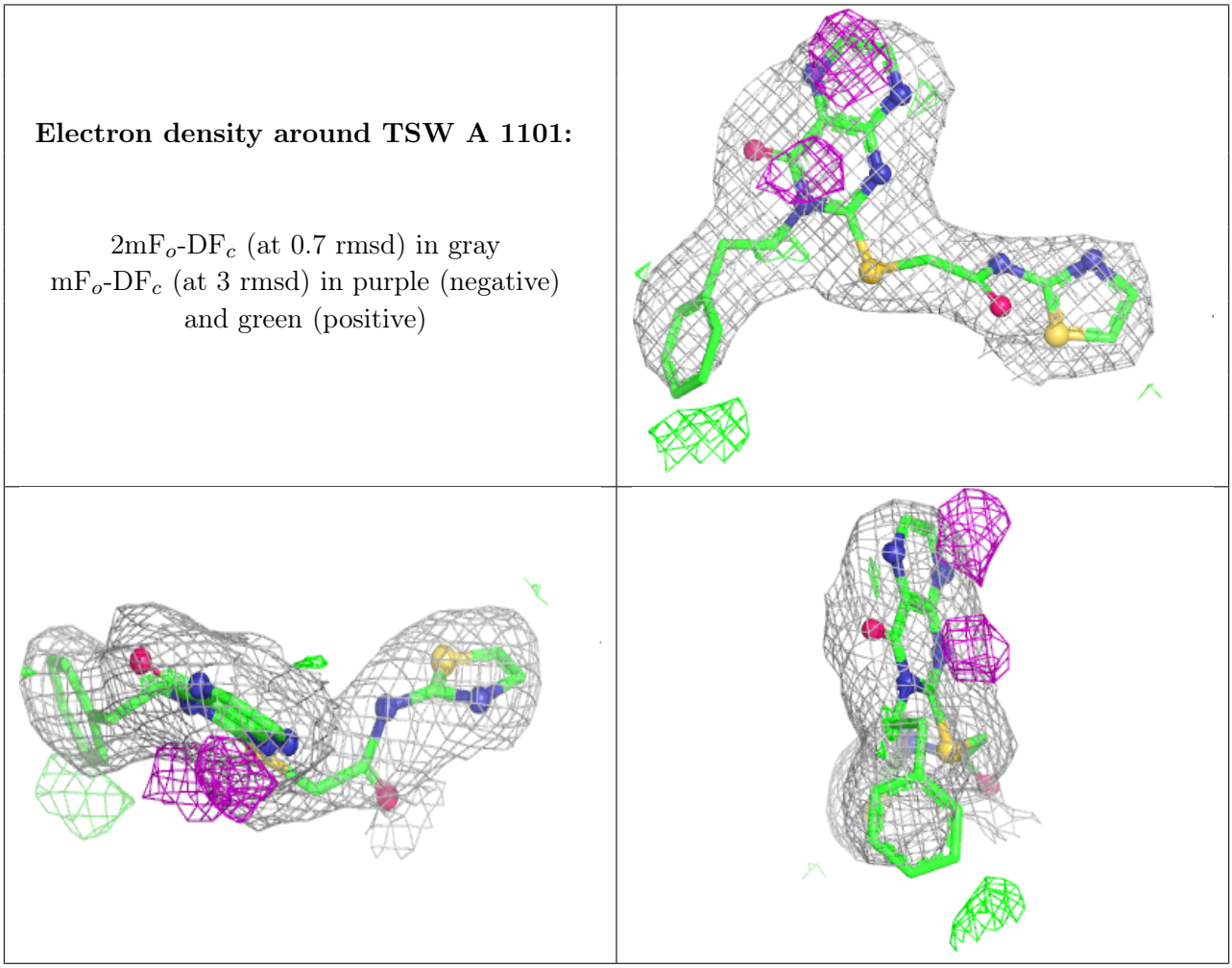
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	SO4	A	1104	5/5	0.86	0.06	127,143,152,154	0
2	TSW	A	1101	29/29	0.90	0.14	68,87,109,113	0
3	EDO	A	1103	4/4	0.92	0.14	82,84,87,88	0
3	EDO	A	1102	4/4	0.93	0.08	81,82,85,88	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 TSW A 1101:

$2mF_o$-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

There are no such residues in this entry.