



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:25 AM UTC

PDB ID : 7Z75 / pdb_00007z75
Title : PI3KC2a core in complex with PITCOIN3
Authors : Lo, W.T.; Roske, Y.; Daumke, O.; Haucke, V.
Deposited on : 2022-03-15
Resolution : 2.59 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

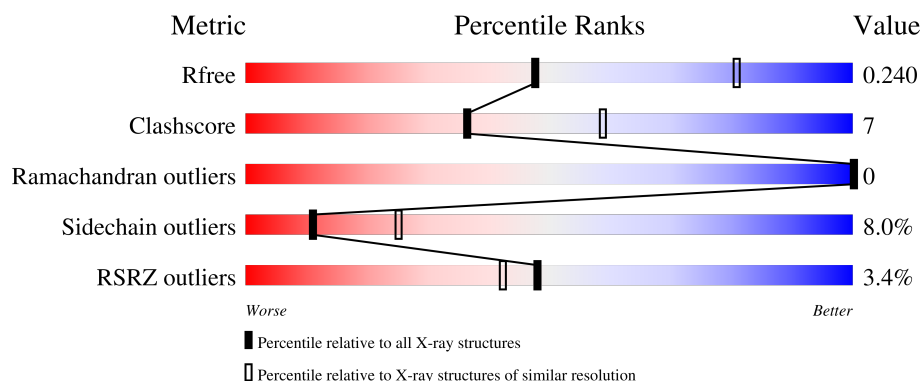
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	910	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6658 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.

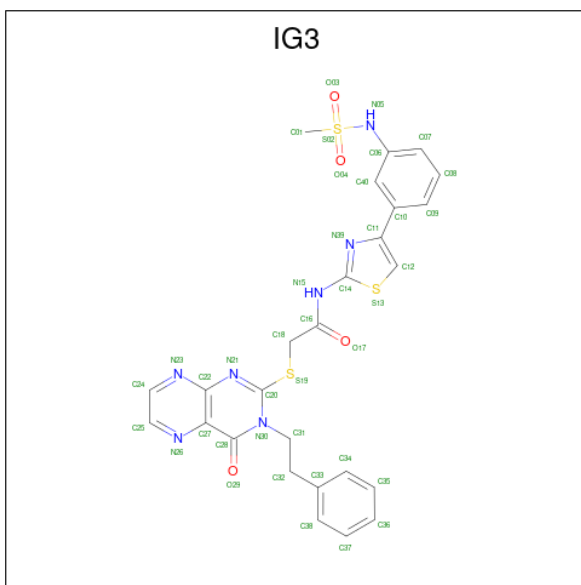
- Molecule 1 is a protein called Phosphatidylinositol 4-phosphate 3-kinase C2 domain-containing subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	827	Total	C	N	O	S	0	0	0
			6547	4209	1095	1203	40			

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 {N}-[4-[3-(methylsulfonylamino)phenyl]-1,3-thiazol-2-yl]-2-[4-oxidanylidene-3-(2-phenylethyl)pteridin-2-yl]sulfanyl-ethanamide (CCD ID: IG3) (formula: C₂₆H₂₃N₇O₄S₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			40	26	7	4	3		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- 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		

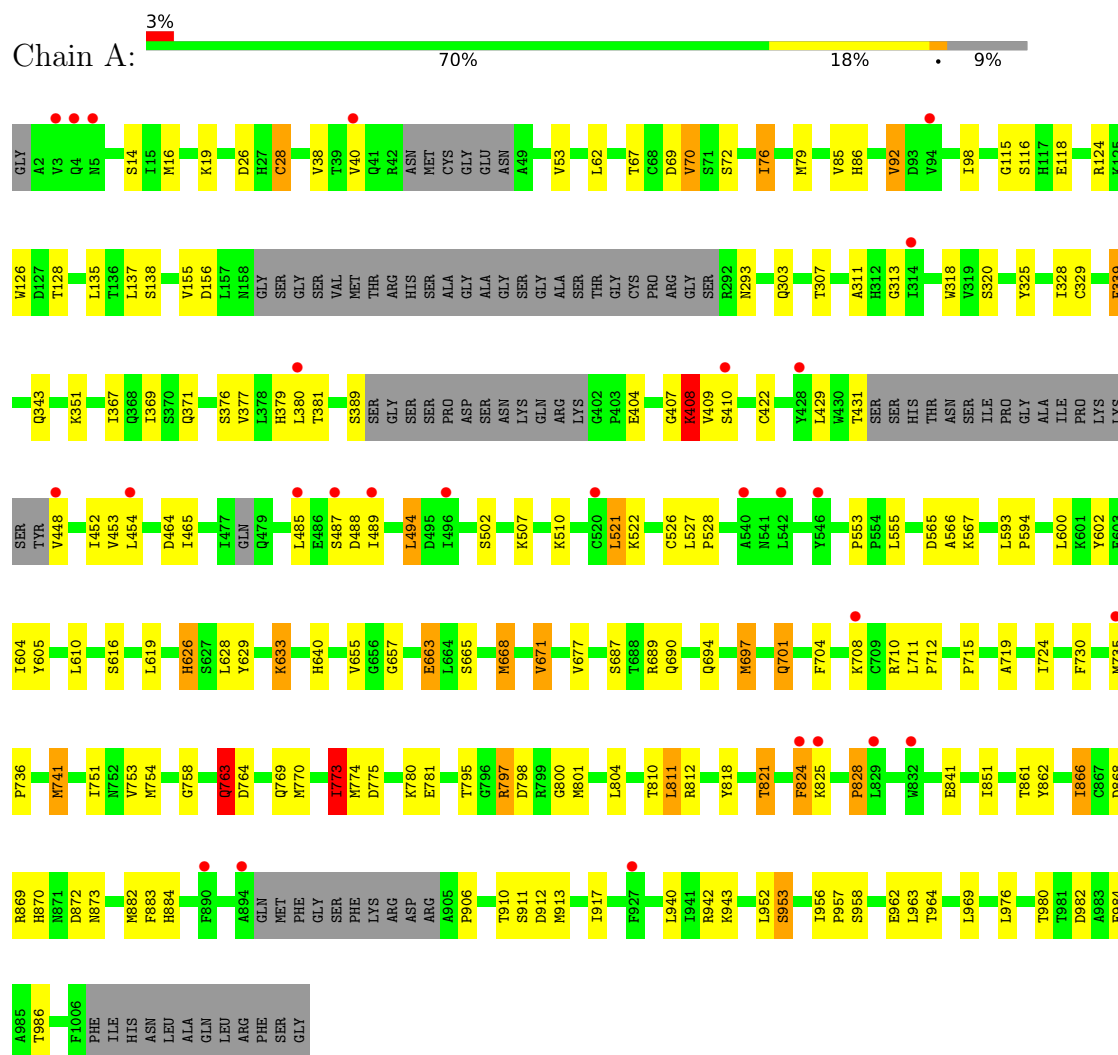
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	62	Total	O	0	0
			62	62		

3 Residue-property plots

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.06Å 134.41Å 152.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.01 – 2.59 49.01 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.01-2.59) 99.0 (49.01-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.223 , 0.267 (Not available) , 0.240	Depositor DCC
R_{free} test set	1811 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	77.1	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6658	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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, EDO, IG3

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	1.25	9/6681 (0.1%)	1.56	29/9048 (0.3%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	884	HIS	CE1-NE2	8.32	1.40	1.32
1	A	339	PHE	C-O	7.11	1.32	1.23
1	A	626	HIS	CE1-NE2	6.60	1.39	1.32
1	A	882	MET	C-O	6.08	1.30	1.23
1	A	626	HIS	CG-ND1	6.07	1.45	1.38
1	A	156	ASP	C-O	5.56	1.30	1.23
1	A	408	LYS	C-O	-5.28	1.17	1.23
1	A	116	SER	C-O	-5.17	1.17	1.24
1	A	118	GLU	C-O	5.01	1.29	1.24

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	824	PHE	CA-CB-CG	8.92	122.72	113.80
1	A	67	THR	CA-CB-OG1	-7.79	97.92	109.60
1	A	763	GLN	CB-CA-C	7.57	123.50	110.79
1	A	868	ASP	CA-CB-CG	7.19	119.79	112.60
1	A	303	GLN	CB-CG-CD	-7.18	100.39	112.60
1	A	488	ASP	CB-CA-C	6.67	116.43	109.83
1	A	763	GLN	CB-CG-CD	-6.51	101.54	112.60
1	A	657	GLY	CA-C-O	-6.24	117.59	122.52
1	A	964	THR	CA-CB-OG1	-6.10	100.45	109.60
1	A	487	SER	N-CA-C	-5.98	105.90	112.72
1	A	773	ILE	CA-C-O	-5.71	114.80	120.85
1	A	982	ASP	CA-CB-CG	5.70	118.30	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ASP	CB-CA-C	5.66	119.28	110.67
1	A	343	GLN	CA-C-O	-5.59	114.68	121.05
1	A	780	LYS	CB-CG-CD	5.54	124.05	111.30
1	A	828	PRO	CB-CA-C	-5.37	104.13	113.20
1	A	770	MET	N-CA-C	-5.34	105.54	111.36
1	A	328	ILE	CA-C-O	-5.29	114.60	120.74
1	A	687	SER	CA-C-O	-5.25	116.00	121.99
1	A	841	GLU	CB-CG-CD	5.20	121.44	112.60
1	A	320	SER	CA-C-N	5.17	127.17	120.44
1	A	320	SER	C-N-CA	5.17	127.17	120.44
1	A	741	MET	CA-C-N	5.17	128.80	121.66
1	A	741	MET	C-N-CA	5.17	128.80	121.66
1	A	657	GLY	CA-C-N	5.14	127.12	120.44
1	A	657	GLY	C-N-CA	5.14	127.12	120.44
1	A	883	PHE	CA-CB-CG	5.12	118.92	113.80
1	A	701	GLN	CA-C-O	-5.09	115.47	120.82
1	A	626	HIS	N-CA-C	-5.09	105.81	111.36

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	6547	0	6578	95	0
2	A	40	0	0	0	0
3	A	4	0	6	0	0
4	A	5	0	0	0	0
5	A	62	0	0	4	0
All	All	6658	0	6584	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 7.

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:A:72:SER:HB2	1:A:76:ILE:HD11	1.55	0.87
1:A:633:LYS:HE2	1:A:668:MET:SD	2.16	0.86
1:A:70:VAL:HG21	1:A:124:ARG:NH1	1.92	0.84
1:A:753:VAL:HG11	1:A:801:MET:HE1	1.61	0.82
1:A:753:VAL:HG21	1:A:801:MET:HE3	1.59	0.81
1:A:619:LEU:HD21	1:A:655:VAL:HG22	1.63	0.80
1:A:870:HIS:HA	5:A:1206:HOH:O	1.83	0.76
1:A:701:GLN:CD	1:A:724:ILE:HD11	2.11	0.76
1:A:754:MET:HB2	1:A:804:LEU:HD21	1.67	0.76
1:A:76:ILE:HA	1:A:79:MET:HE2	1.69	0.73
1:A:701:GLN:OE1	1:A:724:ILE:HD11	1.88	0.73
1:A:980:THR:HB	1:A:984:GLU:HG3	1.72	0.72
1:A:626:HIS:CE1	1:A:715:PRO:HG3	2.24	0.71
1:A:689:ARG:NH2	1:A:735:MET:HE2	2.06	0.70
1:A:565:ASP:OD2	1:A:953:SER:OG	2.12	0.68
1:A:869:ARG:NH2	1:A:873:ASN:HB3	2.09	0.67
1:A:753:VAL:HG21	1:A:801:MET:CE	2.23	0.67
1:A:861:THR:HA	1:A:866:ILE:HG13	1.76	0.66
1:A:567:LYS:HA	5:A:1202:HOH:O	1.99	0.61
1:A:795:THR:HG23	1:A:800:GLY:HA2	1.84	0.60
1:A:70:VAL:HG21	1:A:124:ARG:HH11	1.64	0.59
1:A:910:THR:OG1	1:A:912:ASP:OD1	2.20	0.59
1:A:313:GLY:O	1:A:452:ILE:CD1	2.51	0.58
1:A:85:VAL:HG13	1:A:86:HIS:CD2	2.39	0.58
1:A:719:ALA:CB	1:A:741:MET:HE2	2.33	0.58
1:A:16:MET:HG2	5:A:1238:HOH:O	2.06	0.56
1:A:711:LEU:HD11	1:A:801:MET:HE1	1.88	0.55
1:A:811:LEU:HD11	1:A:913:MET:HE2	1.87	0.55
1:A:953:SER:HB2	1:A:969:LEU:HD11	1.88	0.55
1:A:781:GLU:HG3	1:A:940:LEU:HD22	1.89	0.53
1:A:663:GLU:HG2	1:A:710:ARG:CD	2.38	0.53
1:A:824:PHE:O	1:A:828:PRO:HD3	2.07	0.53
1:A:711:LEU:HD12	1:A:712:PRO:HD2	1.91	0.53
1:A:812:ARG:NH1	1:A:872:ASP:HB2	2.24	0.53
1:A:663:GLU:HG2	1:A:710:ARG:HD2	1.91	0.53
1:A:677:VAL:HG21	1:A:697:MET:HE3	1.91	0.53
1:A:86:HIS:HE1	1:A:92:VAL:HG11	1.72	0.53
1:A:980:THR:HB	1:A:984:GLU:CG	2.38	0.52
1:A:126:TRP:HB2	1:A:128:THR:HG23	1.90	0.52
1:A:797:ARG:O	1:A:797:ARG:HG3	2.10	0.52
1:A:862:TYR:CD1	1:A:906:PRO:HG3	2.45	0.52
1:A:26:ASP:OD1	1:A:28:CYS:SG	2.52	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:952:LEU:O	1:A:963:LEU:HD21	2.10	0.51
1:A:753:VAL:HG11	1:A:801:MET:CE	2.34	0.51
1:A:629:TYR:OH	1:A:668:MET:HG3	2.11	0.50
1:A:690:GLN:O	1:A:694:GLN:HG2	2.12	0.50
1:A:769:GLN:O	1:A:773:ILE:HD12	2.12	0.50
1:A:910:THR:OG1	1:A:913:MET:HG3	2.12	0.50
1:A:604:ILE:HD12	1:A:605:TYR:CZ	2.47	0.50
1:A:98:ILE:HD13	1:A:137:LEU:HD23	1.94	0.49
1:A:753:VAL:CG2	1:A:801:MET:HE3	2.34	0.49
1:A:339:PHE:CE2	1:A:367:ILE:HB	2.47	0.49
1:A:318:TRP:CZ2	1:A:431:THR:HG21	2.49	0.48
1:A:593:LEU:N	1:A:594:PRO:CD	2.76	0.48
1:A:711:LEU:HD22	1:A:751:ILE:HG21	1.96	0.48
1:A:86:HIS:CE1	1:A:92:VAL:HG11	2.49	0.48
1:A:70:VAL:HG22	1:A:115:GLY:CA	2.44	0.48
1:A:600:LEU:HD23	1:A:610:LEU:HD23	1.95	0.48
1:A:942:ARG:NH2	1:A:980:THR:O	2.47	0.47
1:A:753:VAL:CB	1:A:801:MET:CE	2.92	0.47
1:A:758:GLY:N	1:A:798:ASP:O	2.40	0.47
1:A:19:LYS:CG	1:A:655:VAL:HG23	2.46	0.46
1:A:407:GLY:HA3	1:A:429:LEU:HD13	1.97	0.46
1:A:313:GLY:O	1:A:452:ILE:HD13	2.16	0.46
1:A:507:LYS:O	1:A:510:LYS:HB2	2.16	0.46
1:A:956:ILE:N	1:A:957:PRO:HD2	2.30	0.46
1:A:633:LYS:CE	1:A:668:MET:SD	2.96	0.45
1:A:763:GLN:O	1:A:764:ASP:C	2.59	0.45
1:A:369:ILE:HG21	1:A:465:ILE:HG21	1.98	0.45
1:A:604:ILE:HD12	1:A:605:TYR:CE1	2.52	0.44
1:A:753:VAL:CG2	1:A:801:MET:CE	2.93	0.44
1:A:851:ILE:HG12	1:A:917:ILE:HG23	1.99	0.44
1:A:671:VAL:HG21	1:A:795:THR:HB	1.98	0.44
1:A:730:PHE:HB2	1:A:736:PRO:HG2	2.00	0.44
1:A:818:TYR:O	1:A:821:THR:O	2.36	0.43
1:A:704:PHE:HZ	1:A:741:MET:HE3	1.83	0.43
1:A:774:MET:O	1:A:775:ASP:C	2.61	0.43
1:A:527:LEU:N	1:A:528:PRO:CD	2.82	0.43
1:A:521:LEU:HD23	1:A:553:PRO:HD3	2.00	0.42
1:A:311:ALA:HA	1:A:453:VAL:O	2.19	0.42
1:A:367:ILE:HG13	1:A:371:GLN:HB2	2.02	0.42
1:A:566:ALA:HB2	1:A:602:TYR:CZ	2.54	0.42
1:A:736:PRO:HB2	1:A:754:MET:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:HIS:HB3	1:A:408:LYS:HD3	2.01	0.42
1:A:753:VAL:HB	1:A:801:MET:CE	2.50	0.41
1:A:798:ASP:OD1	1:A:798:ASP:N	2.51	0.41
1:A:16:MET:CG	1:A:155:VAL:HG23	2.49	0.41
1:A:410:SER:HB2	1:A:640:HIS:CE1	2.55	0.41
1:A:494:LEU:HD13	1:A:494:LEU:HA	1.89	0.41
1:A:697:MET:HA	1:A:697:MET:HE2	2.03	0.40
1:A:862:TYR:HD1	1:A:906:PRO:HG3	1.83	0.40
1:A:16:MET:HG3	1:A:155:VAL:HG23	2.03	0.40
1:A:628:LEU:O	1:A:629:TYR:C	2.63	0.40
1:A:775:ASP:HB3	5:A:1205:HOH:O	2.21	0.40
1:A:942:ARG:HG2	1:A:976:LEU:O	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	813/910 (89%)	783 (96%)	30 (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	724/800 (90%)	666 (92%)	58 (8%)	11	25

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	28	CYS
1	A	38	VAL
1	A	40	VAL
1	A	53	VAL
1	A	62	LEU
1	A	70	VAL
1	A	76	ILE
1	A	92	VAL
1	A	135	LEU
1	A	138	SER
1	A	293	ASN
1	A	307	THR
1	A	325	TYR
1	A	329	CYS
1	A	351	LYS
1	A	376	SER
1	A	377	VAL
1	A	380	LEU
1	A	381	THR
1	A	389	SER
1	A	404	GLU
1	A	408	LYS
1	A	409	VAL
1	A	422	CYS
1	A	448	VAL
1	A	454	LEU
1	A	464	ASP
1	A	485	LEU
1	A	489	ILE
1	A	494	LEU
1	A	502	SER
1	A	521	LEU
1	A	522	LYS
1	A	526	CYS
1	A	555	LEU
1	A	616	SER
1	A	633	LYS

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Mol	Chain	Res	Type
1	A	663	GLU
1	A	665	SER
1	A	668	MET
1	A	671	VAL
1	A	697	MET
1	A	708	LYS
1	A	763	GLN
1	A	773	ILE
1	A	797	ARG
1	A	810	THR
1	A	811	LEU
1	A	821	THR
1	A	825	LYS
1	A	866	ILE
1	A	911	SER
1	A	943	LYS
1	A	953	SER
1	A	958	SER
1	A	962	GLU
1	A	986	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	HIS
1	A	104	GLN
1	A	293	ASN
1	A	352	ASN
1	A	475	ASN
1	A	640	HIS
1	A	667	GLN
1	A	690	GLN
1	A	694	GLN
1	A	815	GLN
1	A	870	HIS
1	A	871	ASN
1	A	946	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 ⓘ

3 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	SO4	A	1103	-	4,4,4	0.16	0	6,6,6	0.41	0
2	IG3	A	1101	-	44,44,44	3.17	16 (36%)	57,62,62	3.65	25 (43%)
3	EDO	A	1102	-	3,3,3	0.53	0	2,2,2	0.19	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
2	IG3	A	1101	-	-	11/23/23/23	0/5/5/5
3	EDO	A	1102	-	-	1/1/1/1	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	IG3	C20-N21	9.46	1.42	1.29
2	A	1101	IG3	C20-S19	7.28	1.86	1.74
2	A	1101	IG3	S02-N05	7.21	1.72	1.63
2	A	1101	IG3	C14-N15	7.10	1.48	1.38
2	A	1101	IG3	C16-N15	6.86	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	IG3	C12-C11	4.34	1.41	1.36
2	A	1101	IG3	C01-S02	4.32	1.85	1.75
2	A	1101	IG3	C18-C16	4.20	1.56	1.51
2	A	1101	IG3	C18-S19	4.05	1.87	1.80
2	A	1101	IG3	O03-S02	3.98	1.50	1.43
2	A	1101	IG3	C27-N26	2.62	1.39	1.34
2	A	1101	IG3	O04-S02	2.61	1.47	1.43
2	A	1101	IG3	C06-N05	2.46	1.47	1.43
2	A	1101	IG3	C14-N39	2.28	1.34	1.31
2	A	1101	IG3	C09-C10	2.26	1.42	1.39
2	A	1101	IG3	C12-S13	2.11	1.77	1.71

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	IG3	O04-S02-O03	-13.00	101.44	118.87
2	A	1101	IG3	C14-N39-C11	12.72	120.23	109.96
2	A	1101	IG3	S13-C14-N39	-8.33	106.94	115.69
2	A	1101	IG3	C08-C09-C10	6.87	127.11	120.36
2	A	1101	IG3	O03-S02-C01	6.47	118.50	108.26
2	A	1101	IG3	C12-S13-C14	5.88	92.98	88.40
2	A	1101	IG3	C09-C10-C40	-5.73	112.62	119.25
2	A	1101	IG3	N15-C14-N39	4.61	129.14	121.18
2	A	1101	IG3	C18-S19-C20	4.41	108.02	99.04
2	A	1101	IG3	N30-C20-N21	-3.72	121.37	124.93
2	A	1101	IG3	C40-C10-C11	3.63	126.59	120.43
2	A	1101	IG3	C07-C06-C40	3.37	123.73	119.66
2	A	1101	IG3	C01-S02-N05	3.37	110.35	106.56
2	A	1101	IG3	C18-C16-N15	3.28	119.36	114.53
2	A	1101	IG3	C24-C25-N26	-3.27	117.58	122.19
2	A	1101	IG3	C12-C11-N39	-2.73	111.39	114.53
2	A	1101	IG3	O17-C16-C18	-2.67	116.91	121.44
2	A	1101	IG3	C25-N26-C27	2.67	121.99	116.80
2	A	1101	IG3	C27-C22-N21	-2.53	119.64	123.19
2	A	1101	IG3	C24-N23-C22	2.41	121.36	115.14
2	A	1101	IG3	C11-C12-S13	-2.24	108.45	111.16
2	A	1101	IG3	C10-C11-N39	2.21	123.34	119.95
2	A	1101	IG3	C36-C35-C34	-2.16	117.57	120.24
2	A	1101	IG3	N23-C22-N21	2.08	122.44	116.41
2	A	1101	IG3	C37-C38-C33	-2.06	117.72	120.61

There are no chirality outliers.

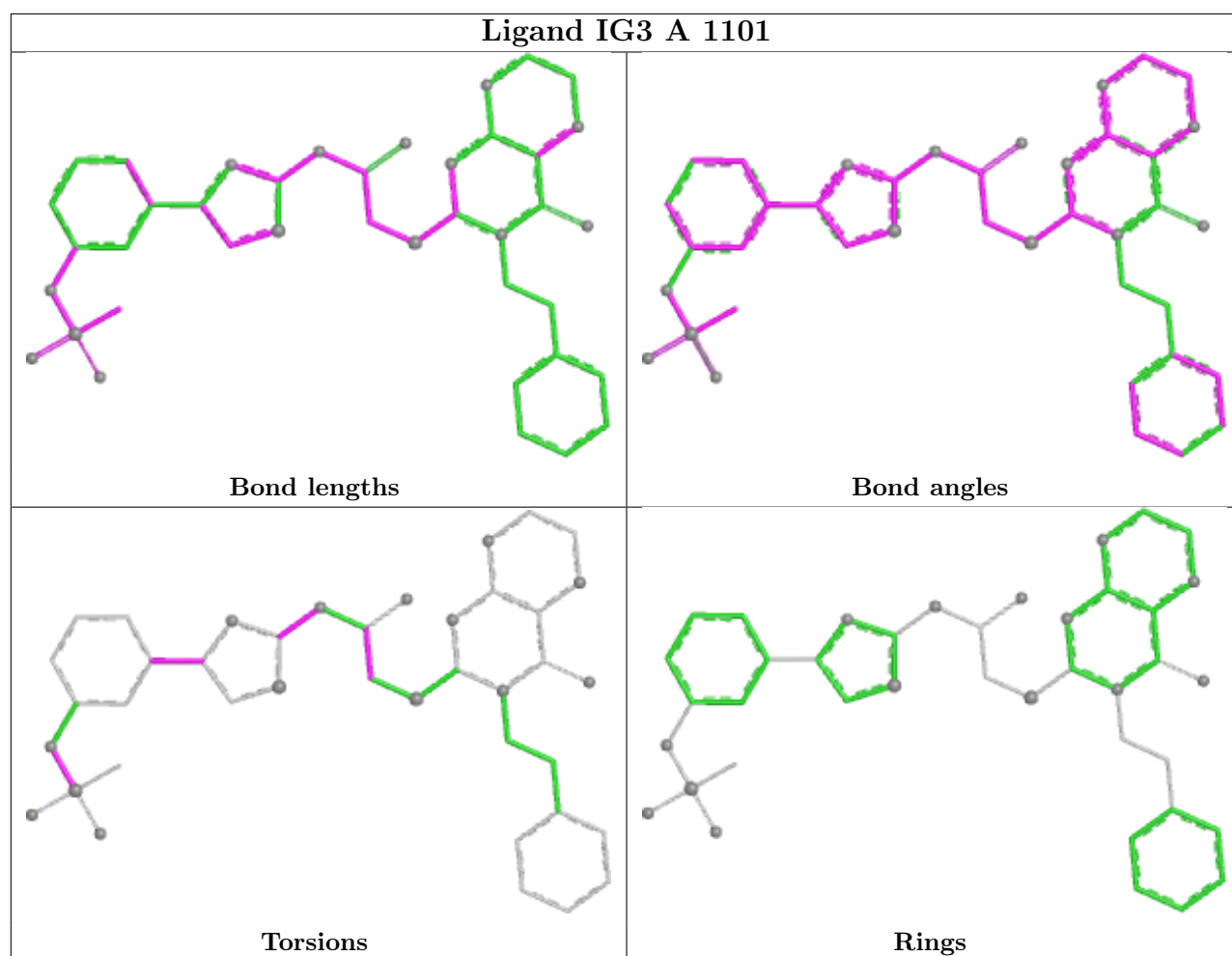
All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	IG3	C09-C10-C11-C12
2	A	1101	IG3	C09-C10-C11-N39
2	A	1101	IG3	C40-C10-C11-C12
2	A	1101	IG3	C40-C10-C11-N39
2	A	1101	IG3	C06-N05-S02-C01
2	A	1101	IG3	C06-N05-S02-O04
2	A	1101	IG3	S13-C14-N15-C16
2	A	1101	IG3	N39-C14-N15-C16
2	A	1101	IG3	N15-C16-C18-S19
2	A	1101	IG3	C06-N05-S02-O03
2	A	1101	IG3	O17-C16-C18-S19
3	A	1102	EDO	O1-C1-C2-O2

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	827/910 (90%)	0.17	28 (3%) 48 42	55, 88, 144, 207	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	894	ALA	4.1
1	A	40	VAL	3.3
1	A	520	CYS	3.0
1	A	489	ILE	2.9
1	A	542	LEU	2.9
1	A	487	SER	2.8
1	A	496	ILE	2.8
1	A	448	VAL	2.8
1	A	485	LEU	2.8
1	A	540	ALA	2.7
1	A	410	SER	2.7
1	A	3	VAL	2.7
1	A	890	PHE	2.6
1	A	5	ASN	2.5
1	A	454	LEU	2.5
1	A	380	LEU	2.3
1	A	735	MET	2.3
1	A	829	LEU	2.3
1	A	708	LYS	2.3
1	A	546	TYR	2.2
1	A	832	TRP	2.2
1	A	94	VAL	2.2
1	A	927	PHE	2.2
1	A	428	TYR	2.1
1	A	314	ILE	2.1
1	A	825	LYS	2.1
1	A	4	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	824	PHE	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](#)

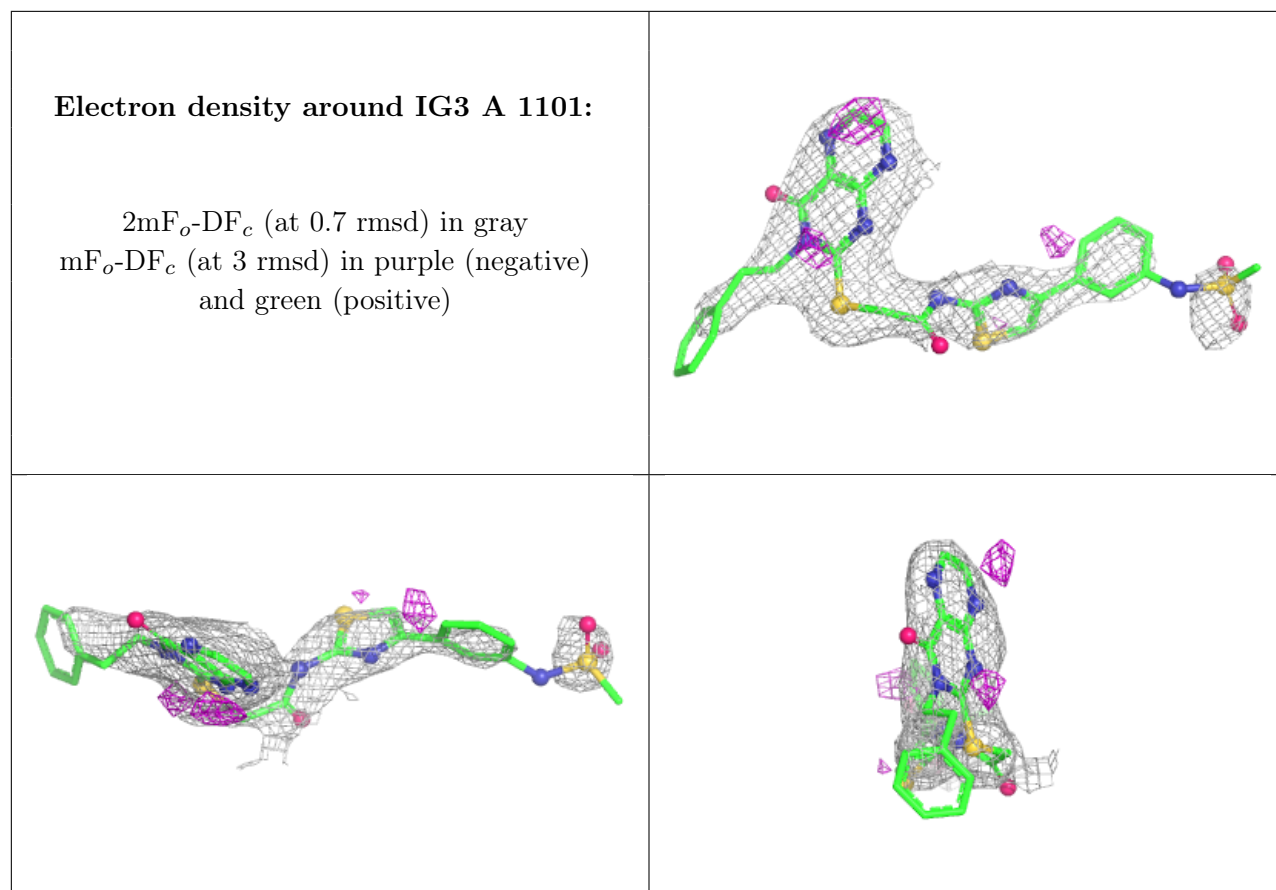
There are no oligosaccharides in this entry.

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
4	SO4	A	1103	5/5	0.56	0.11	146,153,167,167	0
2	IG3	A	1101	40/40	0.85	0.15	91,133,174,188	0
3	EDO	A	1102	4/4	0.94	0.18	98,101,101,104	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 ⓘ

There are no such residues in this entry.