



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:28 AM UTC

PDB ID : 5I6U / pdb_00005i6u
Title : The crystal structure of PI3Kdelta with compound 32
Authors : Somoza, J.R.; Villasenor, A.G.
Deposited on : 2016-02-16
Resolution : 2.84 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

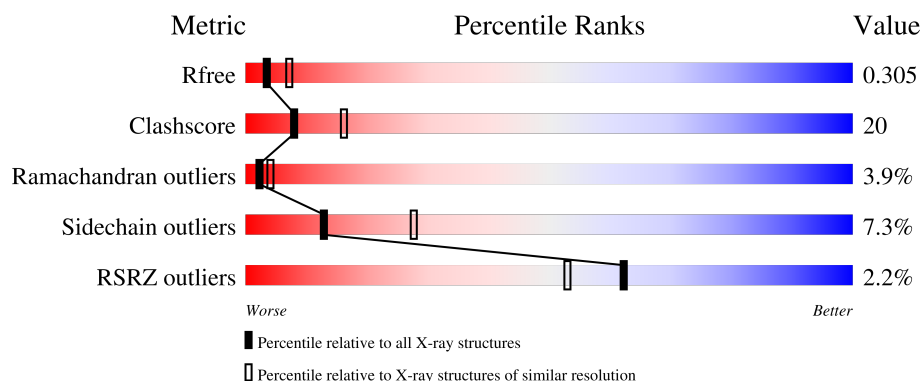
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	939	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6622 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.

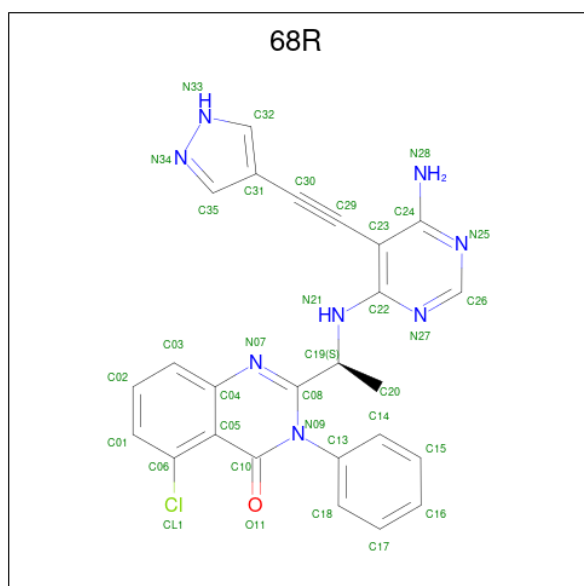
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	816	6587	4224	1118	1191	54	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	508	GLN	-	insertion	UNP O35904

- Molecule 2 is 2-[(1S)-1-({6-amino-5-[(1H-pyrazol-4-yl)ethynyl]pyrimidin-4-yl}amino)ethyl]-5-chloro-3-phenylquinazolin-4(3H)-one (CCD ID: 68R) (formula: C₂₅H₁₉ClN₈O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
2	A	1	35	25	1	8	1	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.84Å 64.93Å 117.06Å 90.00° 103.17° 90.00°	Depositor
Resolution (Å)	29.66 – 2.84 29.66 – 2.84	Depositor EDS
% Data completeness (in resolution range)	96.9 (29.66-2.84) 89.9 (29.66-2.84)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.85Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.212 , 0.307 0.217 , 0.305	Depositor DCC
R_{free} test set	1999 reflections (8.02%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 28.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6622	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.05% 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: 68R

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	0.82	0/6727	1.15	31/9071 (0.3%)

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	8

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	GLU	N-CA-C	11.42	124.35	110.19
1	A	491	ILE	N-CA-C	-8.96	104.19	112.43
1	A	489	GLU	N-CA-C	-8.15	103.34	113.20
1	A	488	LEU	N-CA-C	8.03	124.98	113.02
1	A	252	GLY	N-CA-C	7.94	120.27	111.85
1	A	239	TYR	N-CA-C	7.24	119.93	109.14
1	A	442	TRP	CA-C-N	6.33	127.75	119.84
1	A	442	TRP	C-N-CA	6.33	127.75	119.84
1	A	953	PHE	N-CA-C	6.32	118.25	111.36
1	A	112	LEU	N-CA-C	-6.28	104.12	110.97
1	A	526	HIS	N-CA-C	-5.92	106.11	113.15
1	A	367	SER	CA-C-N	5.87	132.26	121.70
1	A	367	SER	C-N-CA	5.87	132.26	121.70
1	A	906	GLN	N-CA-C	-5.80	101.69	110.28
1	A	667	ILE	CB-CA-C	-5.79	104.47	111.88
1	A	483	VAL	N-CA-C	5.67	115.72	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	708	LYS	CA-C-N	-5.56	113.30	119.19
1	A	708	LYS	C-N-CA	-5.56	113.30	119.19
1	A	946	LYS	N-CA-C	5.53	118.09	110.35
1	A	1015	PHE	N-CA-C	-5.49	105.30	111.28
1	A	994	ASP	N-CA-C	-5.29	105.96	112.90
1	A	783	ASP	N-CA-C	-5.25	102.09	109.96
1	A	367	SER	N-CA-C	5.20	116.97	108.55
1	A	939	VAL	N-CA-C	-5.18	105.49	110.72
1	A	475	LEU	CA-C-N	5.16	125.88	120.11
1	A	475	LEU	C-N-CA	5.16	125.88	120.11
1	A	744	VAL	N-CA-C	5.14	115.63	108.84
1	A	360	SER	N-CA-C	5.04	115.81	108.14
1	A	657	VAL	CA-C-N	5.01	125.29	119.47
1	A	657	VAL	C-N-CA	5.01	125.29	119.47
1	A	814	GLY	N-CA-C	5.01	117.22	111.36

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	444	SER	Peptide
1	A	490	LYS	Peptide
1	A	514	ILE	Peptide
1	A	516	GLU	Peptide
1	A	523	LEU	Peptide
1	A	525	GLU	Peptide
1	A	537	GLU	Peptide
1	A	914	HIS	Peptide

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	6587	0	6572	259	0
2	A	35	0	0	4	0
All	All	6622	0	6572	259	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 20.

All (259) 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:525:GLU:HB3	1:A:528:LYS:HB3	1.38	1.02
1:A:387:MET:HE3	1:A:590:CYS:H	1.36	0.87
1:A:355:CYS:SG	1:A:356:LYS:N	2.47	0.84
1:A:241:LEU:HD13	1:A:274:LEU:HD13	1.58	0.83
1:A:957:ARG:NH1	1:A:1020:ASN:OD1	2.12	0.83
1:A:383:ASP:OD1	1:A:558:HIS:ND1	2.13	0.82
1:A:982:ARG:HH12	1:A:992:SER:HA	1.47	0.80
1:A:547:ALA:HA	1:A:550:LEU:HD12	1.65	0.78
1:A:245:GLY:HA3	1:A:768:ALA:HB2	1.65	0.78
1:A:887:TYR:OH	1:A:929:ARG:NH2	2.17	0.77
1:A:216:LEU:HD22	1:A:241:LEU:HD11	1.67	0.77
1:A:267:HIS:CD2	1:A:809:ARG:NH1	2.53	0.76
1:A:192:VAL:HG12	1:A:272:PRO:HB2	1.68	0.76
1:A:517:ARG:NH1	1:A:544:GLU:OE1	2.18	0.74
1:A:904:SER:OG	1:A:906:GLN:HG3	1.86	0.74
1:A:533:LYS:HG2	1:A:534:MET:HG3	1.70	0.72
1:A:843:ASN:OD1	1:A:844:MET:N	2.23	0.71
1:A:359:SER:OG	1:A:360:SER:N	2.23	0.71
1:A:154:ARG:NH2	1:A:674:GLY:O	2.25	0.69
1:A:356:LYS:HD3	1:A:378:ASP:OD2	1.92	0.69
1:A:826:GLU:O	2:A:1101:68R:N28	2.26	0.68
1:A:891:ILE:HG22	1:A:894:ARG:HD3	1.74	0.68
1:A:533:LYS:HE2	1:A:534:MET:HE3	1.76	0.68
1:A:371:TRP:O	1:A:373:GLN:N	2.27	0.67
1:A:380:SER:HB3	1:A:557:LYS:NZ	2.09	0.67
1:A:696:ASN:HB2	1:A:759:LEU:HD11	1.76	0.67
1:A:155:GLN:NE2	1:A:286:ARG:O	2.26	0.66
1:A:894:ARG:NH2	1:A:910:ILE:O	2.29	0.65
1:A:512:ARG:HD3	1:A:530:LEU:HD22	1.78	0.64
1:A:116:GLN:HA	1:A:119:LEU:HD12	1.78	0.64
1:A:765:SER:HB3	1:A:768:ALA:HB3	1.78	0.64
1:A:513:GLU:HA	1:A:515:LEU:HB2	1.80	0.64
1:A:191:LEU:O	1:A:272:PRO:HD2	1.98	0.64
1:A:512:ARG:HH11	1:A:530:LEU:CD2	2.11	0.64
1:A:199:SER:OG	1:A:200:GLU:N	2.28	0.63
1:A:341:LEU:HB2	1:A:363:VAL:HG23	1.79	0.63
1:A:435:GLY:HA2	1:A:475:LEU:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:PHE:HZ	1:A:220:ALA:HA	1.62	0.63
1:A:701:VAL:O	1:A:704:GLN:HB2	1.98	0.63
1:A:355:CYS:C	1:A:356:LYS:HD2	2.24	0.63
1:A:453:LEU:HD12	1:A:454:ASN:H	1.63	0.63
1:A:614:GLN:HG3	1:A:981:MET:HG2	1.80	0.63
1:A:110:LYS:O	1:A:114:ASN:ND2	2.32	0.63
1:A:917:GLY:HA3	1:A:997:TYR:CE1	2.34	0.62
1:A:982:ARG:NH1	1:A:992:SER:HA	2.14	0.62
1:A:488:LEU:HD21	1:A:491:ILE:HB	1.81	0.62
1:A:936:TYR:HD1	1:A:1026:SER:HB3	1.64	0.61
1:A:138:ASP:OD1	1:A:142:LYS:HB2	2.00	0.61
1:A:652:ARG:O	1:A:652:ARG:NH1	2.31	0.60
1:A:693:LYS:NZ	1:A:697:ASP:OD2	2.34	0.60
1:A:120:LEU:HD13	1:A:683:MET:HG3	1.82	0.60
1:A:435:GLY:O	1:A:475:LEU:N	2.34	0.60
1:A:706:THR:OG1	1:A:707:THR:N	2.34	0.60
1:A:263:CYS:HA	1:A:266:LEU:HG	1.83	0.60
1:A:656:HIS:CD2	1:A:820:ASP:OD2	2.55	0.60
1:A:329:GLU:HG3	1:A:370:VAL:HG22	1.84	0.59
1:A:136:VAL:HG13	1:A:666:LEU:HD11	1.84	0.59
1:A:982:ARG:HH12	1:A:992:SER:CA	2.14	0.59
1:A:192:VAL:HG23	1:A:205:PHE:HB2	1.84	0.59
1:A:488:LEU:CD2	1:A:491:ILE:HB	2.32	0.59
1:A:360:SER:OG	1:A:373:GLN:OE1	2.22	0.58
1:A:383:ASP:CG	1:A:557:LYS:HD2	2.28	0.58
1:A:789:LEU:HD13	1:A:981:MET:HE2	1.85	0.58
1:A:971:GLY:HA3	1:A:1004:LEU:HD11	1.83	0.58
1:A:875:PHE:CE2	1:A:938:PHE:HB3	2.39	0.58
1:A:693:LYS:NZ	1:A:697:ASP:CG	2.62	0.58
1:A:356:LYS:N	1:A:356:LYS:HD2	2.19	0.57
1:A:525:GLU:C	1:A:527:GLU:H	2.13	0.57
1:A:1010:GLU:O	1:A:1013:LYS:HB2	2.04	0.57
1:A:371:TRP:C	1:A:373:GLN:H	2.12	0.57
1:A:154:ARG:HG2	1:A:154:ARG:HH11	1.70	0.57
1:A:267:HIS:CD2	1:A:809:ARG:HH11	2.23	0.57
1:A:157:LEU:O	1:A:286:ARG:NH1	2.38	0.56
1:A:389:ARG:HB3	1:A:424:MET:CE	2.35	0.56
1:A:621:TYR:CZ	1:A:983:ALA:HB2	2.40	0.56
1:A:255:PRO:HG2	1:A:258:HIS:HB2	1.87	0.56
1:A:129:ASP:C	1:A:131:LEU:H	2.14	0.56
1:A:187:ASN:OD1	1:A:187:ASN:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:LEU:HD22	1:A:441:MET:HE1	1.88	0.55
1:A:431:GLN:HA	1:A:484:TYR:HA	1.88	0.55
1:A:128:PHE:HB2	1:A:140:ARG:NH1	2.22	0.55
1:A:367:SER:HA	1:A:368:GLU:C	2.32	0.54
1:A:352:GLU:OE2	1:A:353:MET:HG2	2.08	0.54
1:A:493:GLU:HG2	1:A:494:LEU:N	2.23	0.54
1:A:512:ARG:HG3	1:A:513:GLU:N	2.23	0.53
1:A:693:LYS:HE2	1:A:780:ASN:HD21	1.73	0.53
1:A:380:SER:HB3	1:A:557:LYS:HZ2	1.73	0.53
1:A:693:LYS:NZ	1:A:697:ASP:OD1	2.41	0.53
1:A:935:THR:HG22	1:A:937:ASP:H	1.72	0.53
1:A:1017:VAL:O	1:A:1021:GLU:HG3	2.08	0.53
1:A:205:PHE:CZ	1:A:220:ALA:HA	2.43	0.53
1:A:326:GLU:HG2	1:A:327:LEU:O	2.09	0.53
1:A:390:LEU:HD12	1:A:391:CYS:H	1.74	0.53
1:A:424:MET:HG3	1:A:624:TYR:CE1	2.44	0.52
1:A:571:TRP:CD1	1:A:572:PRO:HD2	2.44	0.52
1:A:271:THR:O	1:A:273:HIS:ND1	2.42	0.52
1:A:367:SER:OG	1:A:369:PRO:HD3	2.09	0.52
1:A:397:VAL:HG22	1:A:398:VAL:H	1.73	0.52
1:A:493:GLU:HG2	1:A:494:LEU:HB3	1.92	0.52
1:A:129:ASP:O	1:A:131:LEU:N	2.42	0.52
1:A:383:ASP:CG	1:A:558:HIS:HD1	2.15	0.52
1:A:270:LEU:HD12	1:A:271:THR:H	1.75	0.52
1:A:209:THR:HB	1:A:257:CYS:HB3	1.93	0.51
1:A:529:ASP:OD1	1:A:530:LEU:N	2.40	0.51
1:A:609:PHE:CD2	1:A:642:LYS:NZ	2.76	0.51
1:A:114:ASN:CG	1:A:673:ARG:HH22	2.18	0.51
1:A:381:VAL:C	1:A:383:ASP:H	2.19	0.51
1:A:329:GLU:HG2	1:A:330:GLY:H	1.74	0.51
1:A:343:VAL:HG22	1:A:394:LEU:HD12	1.93	0.51
1:A:996:GLN:O	1:A:996:GLN:HG3	2.09	0.51
1:A:242:GLN:HG2	1:A:243:VAL:O	2.11	0.51
1:A:147:CYS:SG	1:A:638:LEU:HD11	2.50	0.50
1:A:530:LEU:HA	1:A:533:LYS:HB3	1.94	0.50
1:A:419:ALA:HB3	1:A:441:MET:HE3	1.94	0.50
1:A:592:VAL:O	1:A:596:ALA:N	2.36	0.50
1:A:532:TRP:HZ3	1:A:564:MET:HE2	1.76	0.50
1:A:593:GLY:O	1:A:597:ILE:HG12	2.11	0.50
1:A:389:ARG:HB3	1:A:424:MET:HE1	1.93	0.49
1:A:424:MET:O	1:A:433:LYS:HD2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:PHE:O	1:A:149:GLU:HG2	2.12	0.49
1:A:491:ILE:HG23	1:A:562:ALA:HB1	1.94	0.49
1:A:431:GLN:HG3	1:A:432:LEU:O	2.12	0.49
1:A:394:LEU:O	1:A:418:ILE:HB	2.13	0.49
1:A:239:TYR:CZ	1:A:278:HIS:HD2	2.31	0.49
1:A:114:ASN:HD22	1:A:114:ASN:H	1.60	0.49
1:A:825:ILE:HD13	2:A:1101:68R:C35	2.43	0.49
1:A:243:VAL:HA	1:A:274:LEU:HD23	1.95	0.49
1:A:330:GLY:C	1:A:331:ARG:HG3	2.38	0.49
1:A:549:LEU:O	1:A:552:VAL:HG22	2.13	0.49
1:A:944:GLN:OE1	1:A:952:LYS:HE3	2.13	0.49
1:A:420:TRP:CH2	1:A:457:GLY:HA3	2.48	0.48
1:A:453:LEU:HD12	1:A:454:ASN:N	2.29	0.48
1:A:617:GLN:HG3	1:A:981:MET:SD	2.53	0.48
1:A:218:ALA:O	1:A:222:ARG:HG3	2.14	0.48
1:A:617:GLN:HB3	1:A:983:ALA:HB3	1.96	0.48
1:A:807:ASP:OD1	1:A:807:ASP:C	2.54	0.48
1:A:936:TYR:CD1	1:A:1026:SER:HB3	2.48	0.48
1:A:419:ALA:HA	1:A:443:PRO:HA	1.95	0.48
1:A:862:LYS:HD2	1:A:903:GLU:HG2	1.95	0.48
1:A:397:VAL:HG22	1:A:398:VAL:HG13	1.95	0.48
1:A:358:VAL:HG21	1:A:377:PHE:CD1	2.49	0.48
1:A:371:TRP:C	1:A:373:GLN:N	2.71	0.48
1:A:380:SER:HB3	1:A:557:LYS:HZ1	1.78	0.48
1:A:525:GLU:C	1:A:527:GLU:N	2.72	0.48
1:A:246:ARG:NH1	1:A:248:GLU:OE1	2.47	0.47
1:A:512:ARG:O	1:A:514:ILE:N	2.47	0.47
1:A:330:GLY:C	1:A:369:PRO:HD2	2.40	0.47
1:A:804:GLU:OE2	1:A:966:ILE:HG23	2.14	0.47
1:A:968:ARG:NH1	1:A:968:ARG:HB3	2.30	0.47
1:A:427:ASP:HB3	1:A:431:GLN:O	2.14	0.47
1:A:690:SER:O	1:A:693:LYS:HB3	2.14	0.47
1:A:112:LEU:O	1:A:115:SER:HB3	2.14	0.47
1:A:387:MET:HE3	1:A:590:CYS:N	2.19	0.46
1:A:224:LYS:C	1:A:226:THR:H	2.23	0.46
1:A:237:GLU:OE1	1:A:237:GLU:N	2.43	0.46
1:A:284:ALA:O	1:A:288:GLU:HG3	2.16	0.46
1:A:110:LYS:HE2	1:A:110:LYS:HB3	1.51	0.46
1:A:424:MET:CE	1:A:459:VAL:HG11	2.46	0.46
1:A:574:LEU:HG	1:A:595:PHE:HE2	1.81	0.46
1:A:875:PHE:CZ	1:A:938:PHE:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:LYS:HD2	1:A:936:TYR:CE2	2.51	0.45
1:A:953:PHE:O	1:A:956:PHE:HB3	2.16	0.45
1:A:613:LEU:O	1:A:617:GLN:HG2	2.16	0.45
1:A:860:LYS:HG2	1:A:868:LEU:HD22	1.97	0.45
1:A:389:ARG:HB3	1:A:424:MET:HE2	1.98	0.45
1:A:424:MET:HE3	1:A:459:VAL:HG11	1.99	0.45
1:A:628:GLU:OE2	1:A:631:LYS:HE3	2.16	0.45
1:A:652:ARG:HA	1:A:652:ARG:HD2	1.68	0.45
1:A:870:ARG:O	1:A:873:GLU:HB3	2.16	0.45
1:A:129:ASP:C	1:A:131:LEU:N	2.74	0.45
1:A:535:ARG:O	1:A:538:VAL:HB	2.16	0.45
1:A:163:LEU:HG	1:A:282:ILE:HG21	1.98	0.45
1:A:609:PHE:HE1	1:A:646:PHE:CD2	2.34	0.45
1:A:811:THR:HG23	1:A:902:ARG:HH21	1.81	0.45
1:A:415:ASP:OD1	1:A:415:ASP:N	2.48	0.45
1:A:113:ILE:HD12	1:A:679:MET:HE1	1.98	0.45
1:A:167:PHE:CZ	1:A:285:MET:HE1	2.52	0.45
1:A:428:TYR:CE2	1:A:429:LYS:HG2	2.51	0.45
1:A:135:GLU:HG3	1:A:428:TYR:CG	2.52	0.44
1:A:383:ASP:HB3	1:A:556:ASN:O	2.17	0.44
1:A:126:HIS:O	1:A:130:SER:HB3	2.18	0.44
1:A:136:VAL:O	1:A:140:ARG:HG3	2.17	0.44
1:A:714:MET:HE2	1:A:714:MET:HB2	1.85	0.44
1:A:327:LEU:O	1:A:372:LYS:HA	2.18	0.44
1:A:436:GLU:HB2	1:A:474:TYR:HD1	1.83	0.44
1:A:728:LEU:O	1:A:763:TYR:OH	2.33	0.44
1:A:886:THR:HG22	1:A:891:ILE:HD12	1.99	0.44
1:A:932:PHE:HE2	1:A:934:LEU:CD2	2.31	0.44
1:A:729:SER:OG	1:A:744:VAL:HG12	2.18	0.44
1:A:325:ILE:HG22	1:A:475:LEU:HD23	2.00	0.44
1:A:142:LYS:O	1:A:143:MET:HE2	2.18	0.43
1:A:731:LEU:HD23	1:A:731:LEU:H	1.82	0.43
1:A:491:ILE:HG23	1:A:562:ALA:CB	2.48	0.43
1:A:462:ASN:HA	1:A:463:PRO:HD2	1.81	0.43
1:A:167:PHE:CE2	1:A:285:MET:HE1	2.53	0.43
1:A:267:HIS:C	1:A:269:GLY:H	2.26	0.43
1:A:589:ASP:OD2	1:A:591:TYR:HD2	2.01	0.43
1:A:982:ARG:HH12	1:A:991:CYS:C	2.27	0.43
1:A:239:TYR:CD1	1:A:278:HIS:HA	2.53	0.43
1:A:837:ILE:HD13	1:A:858:TRP:CD2	2.53	0.43
1:A:266:LEU:HD12	1:A:267:HIS:ND1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:GLU:HA	1:A:528:LYS:H	1.83	0.43
1:A:825:ILE:HD13	2:A:1101:68R:C31	2.49	0.42
1:A:982:ARG:HH12	1:A:992:SER:N	2.17	0.42
1:A:224:LYS:C	1:A:226:THR:N	2.78	0.42
1:A:393:ALA:HB2	1:A:453:LEU:HD13	2.01	0.42
1:A:514:ILE:O	1:A:514:ILE:HG13	2.19	0.42
1:A:656:HIS:CG	1:A:820:ASP:HB2	2.55	0.42
1:A:702:SER:O	1:A:706:THR:HG22	2.19	0.42
1:A:169:LEU:HD21	1:A:251:TYR:CE2	2.55	0.42
1:A:139:PHE:CD1	1:A:625:LEU:HB3	2.55	0.42
1:A:460:ARG:HE	1:A:460:ARG:HB2	1.50	0.42
1:A:326:GLU:O	1:A:474:TYR:N	2.47	0.42
1:A:383:ASP:OD1	1:A:558:HIS:N	2.29	0.42
1:A:829:LEU:HA	1:A:829:LEU:HD23	1.83	0.42
1:A:918:ASN:HB2	1:A:988:GLU:OE2	2.20	0.42
1:A:513:GLU:HA	1:A:515:LEU:HD12	2.01	0.41
1:A:619:LEU:HA	1:A:619:LEU:HD23	1.84	0.41
1:A:902:ARG:HG3	1:A:908:PHE:HE2	1.85	0.41
1:A:1024:ARG:NH1	1:A:1024:ARG:HG3	2.35	0.41
1:A:328:ILE:HD12	1:A:472:VAL:HG12	2.02	0.41
1:A:143:MET:HE2	1:A:143:MET:HA	2.03	0.41
1:A:241:LEU:O	1:A:250:LEU:N	2.48	0.41
1:A:323:PHE:O	1:A:377:PHE:HB2	2.20	0.41
1:A:858:TRP:CZ2	1:A:862:LYS:HE3	2.55	0.41
1:A:676:THR:O	1:A:679:MET:HB3	2.20	0.41
1:A:428:TYR:CZ	1:A:429:LYS:HG2	2.55	0.41
1:A:525:GLU:O	1:A:528:LYS:HG2	2.20	0.41
1:A:970:HIS:O	1:A:971:GLY:C	2.63	0.41
1:A:426:PHE:C	1:A:433:LYS:HE3	2.46	0.41
1:A:492:LEU:HD23	1:A:492:LEU:O	2.20	0.41
1:A:600:LEU:HD23	1:A:600:LEU:HA	1.85	0.41
1:A:632:PHE:O	1:A:636:ARG:HG2	2.20	0.41
1:A:750:THR:HG23	2:A:1101:68R:CL1	2.57	0.41
1:A:790:THR:HG21	1:A:912:PHE:CD1	2.56	0.41
1:A:898:ASN:HB2	1:A:910:ILE:O	2.20	0.41
1:A:139:PHE:CD2	1:A:139:PHE:C	2.99	0.41
1:A:316:LEU:HB2	1:A:317:TRP:H	1.69	0.41
1:A:319:LEU:O	1:A:382:CYS:HB3	2.21	0.41
1:A:360:SER:OG	1:A:361:SER:N	2.54	0.41
1:A:585:PHE:C	1:A:587:PHE:H	2.29	0.41
1:A:557:LYS:HD2	1:A:557:LYS:HA	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:GLU:O	1:A:717:MET:HG3	2.21	0.41
1:A:491:ILE:O	1:A:491:ILE:CG2	2.69	0.41
1:A:191:LEU:HD12	1:A:206:GLN:HG2	2.03	0.40
1:A:340:LYS:HD3	1:A:398:VAL:C	2.46	0.40
1:A:935:THR:HB	1:A:938:PHE:CE2	2.57	0.40
1:A:365:VAL:O	1:A:367:SER:N	2.54	0.40
1:A:567:LEU:O	1:A:571:TRP:HE3	2.05	0.40
1:A:145:GLN:O	1:A:149:GLU:OE2	2.39	0.40
1:A:564:MET:HE2	1:A:564:MET:HA	2.03	0.40
1:A:750:THR:OG1	1:A:751:PHE:N	2.53	0.40
1:A:795:GLN:HE21	1:A:812:PRO:HB2	1.87	0.40
1:A:427:ASP:CG	1:A:429:LYS:H	2.28	0.40
1:A:525:GLU:HA	1:A:527:GLU:H	1.87	0.40
1:A:1014:HIS:NE2	1:A:1018:LYS:HE2	2.37	0.40
1:A:242:GLN:HB2	1:A:249:TYR:CZ	2.57	0.40
1:A:271:THR:O	1:A:273:HIS:CE1	2.75	0.40
1:A:429:LYS:C	1:A:430:ASP:OD2	2.64	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	792/939 (84%)	682 (86%)	79 (10%)	31 (4%)	2 4

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	SER
1	A	253	ASN
1	A	264	SER
1	A	366	CYS

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Mol	Chain	Res	Type
1	A	372	LYS
1	A	465	THR
1	A	843	ASN
1	A	844	MET
1	A	944	GLN
1	A	359	SER
1	A	388	ALA
1	A	397	VAL
1	A	478	VAL
1	A	487	ALA
1	A	893	ASP
1	A	387	MET
1	A	427	ASP
1	A	430	ASP
1	A	493	GLU
1	A	268	SER
1	A	513	GLU
1	A	589	ASP
1	A	129	ASP
1	A	368	GLU
1	A	464	ASN
1	A	586	SER
1	A	867	ALA
1	A	514	ILE
1	A	328	ILE
1	A	113	ILE
1	A	931	PRO

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	724/827 (88%)	671 (93%)	53 (7%)	13	28

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	VAL
1	A	110	LYS
1	A	166	SER
1	A	187	ASN
1	A	190	LEU
1	A	191	LEU
1	A	199	SER
1	A	200	GLU
1	A	210	LYS
1	A	250	LEU
1	A	256	LEU
1	A	291	ASN
1	A	316	LEU
1	A	325	ILE
1	A	359	SER
1	A	375	LEU
1	A	398	VAL
1	A	415	ASP
1	A	423	LEU
1	A	460	ARG
1	A	471	LEU
1	A	488	LEU
1	A	515	LEU
1	A	517	ARG
1	A	525	GLU
1	A	528	LYS
1	A	550	LEU
1	A	551	LEU
1	A	594	SER
1	A	628	GLU
1	A	631	LYS
1	A	676	THR
1	A	681	VAL
1	A	687	GLU
1	A	707	THR
1	A	744	VAL
1	A	747	GLU
1	A	767	GLU
1	A	792	GLN
1	A	811	THR
1	A	822	THR
1	A	852	LYS
1	A	855	LEU

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Mol	Chain	Res	Type
1	A	859	LEU
1	A	863	ASN
1	A	944	GLN
1	A	965	THR
1	A	972	LEU
1	A	986	LEU
1	A	988	GLU
1	A	998	LEU
1	A	1000	ASP
1	A	1024	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	258	HIS
1	A	656	HIS
1	A	773	ASN
1	A	786	GLN
1	A	795	GLN

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	68R	A	1101	-	39,39,39	1.18	3 (7%)	44,55,55	1.84	8 (18%)

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	68R	A	1101	-	-	1/11/17/17	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	68R	C23-C22	-3.66	1.37	1.42
2	A	1101	68R	C22-N21	3.10	1.40	1.35
2	A	1101	68R	C05-C06	2.37	1.43	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	68R	C20-C19-C08	-5.41	103.83	111.43
2	A	1101	68R	C05-C06-CL1	4.74	125.73	119.62
2	A	1101	68R	C18-C13-N09	3.94	124.36	119.65
2	A	1101	68R	C26-N25-C24	-3.22	113.44	118.73
2	A	1101	68R	C01-C06-CL1	-2.75	113.00	118.42
2	A	1101	68R	C24-C23-C29	2.40	122.86	118.71
2	A	1101	68R	C15-C14-C13	2.39	122.52	119.68
2	A	1101	68R	N28-C24-N25	-2.32	113.20	118.38

There are no chirality outliers.

All (1) torsion outliers are listed below:

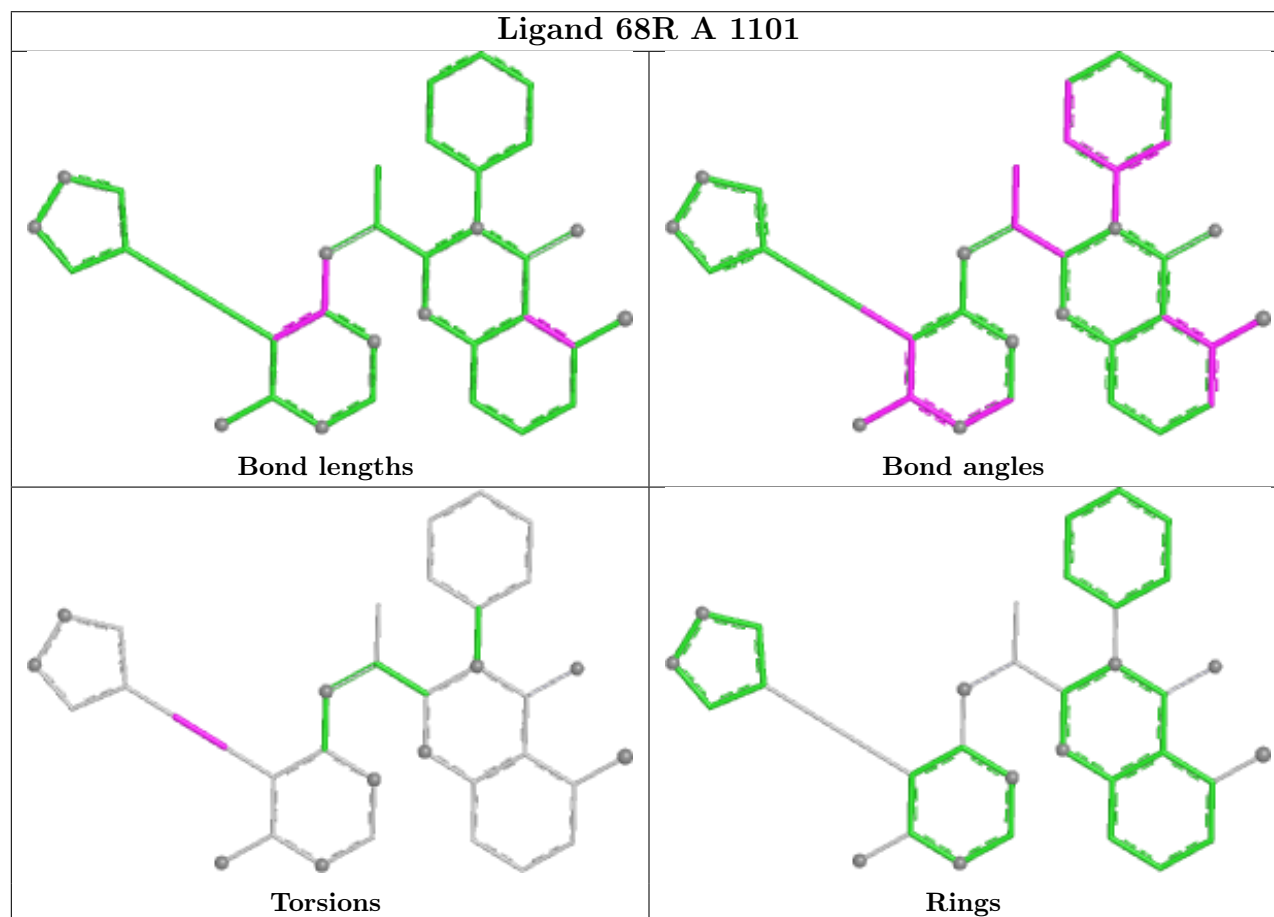
Mol	Chain	Res	Type	Atoms
2	A	1101	68R	C23-C29-C30-C31

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	68R	4	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

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 [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	816/939 (86%)	0.00	18 (2%) 62 53	23, 52, 88, 141	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	316	LEU	6.4
1	A	332	LYS	5.9
1	A	845	ALA	4.1
1	A	494	LEU	4.1
1	A	488	LEU	3.9
1	A	511	LEU	3.5
1	A	591	TYR	2.9
1	A	347	LEU	2.9
1	A	393	ALA	2.8
1	A	317	TRP	2.7
1	A	377	PHE	2.6
1	A	365	VAL	2.5
1	A	491	ILE	2.5
1	A	767	GLU	2.4
1	A	395	TYR	2.2
1	A	513	GLU	2.1
1	A	487	ALA	2.0
1	A	445	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](#)

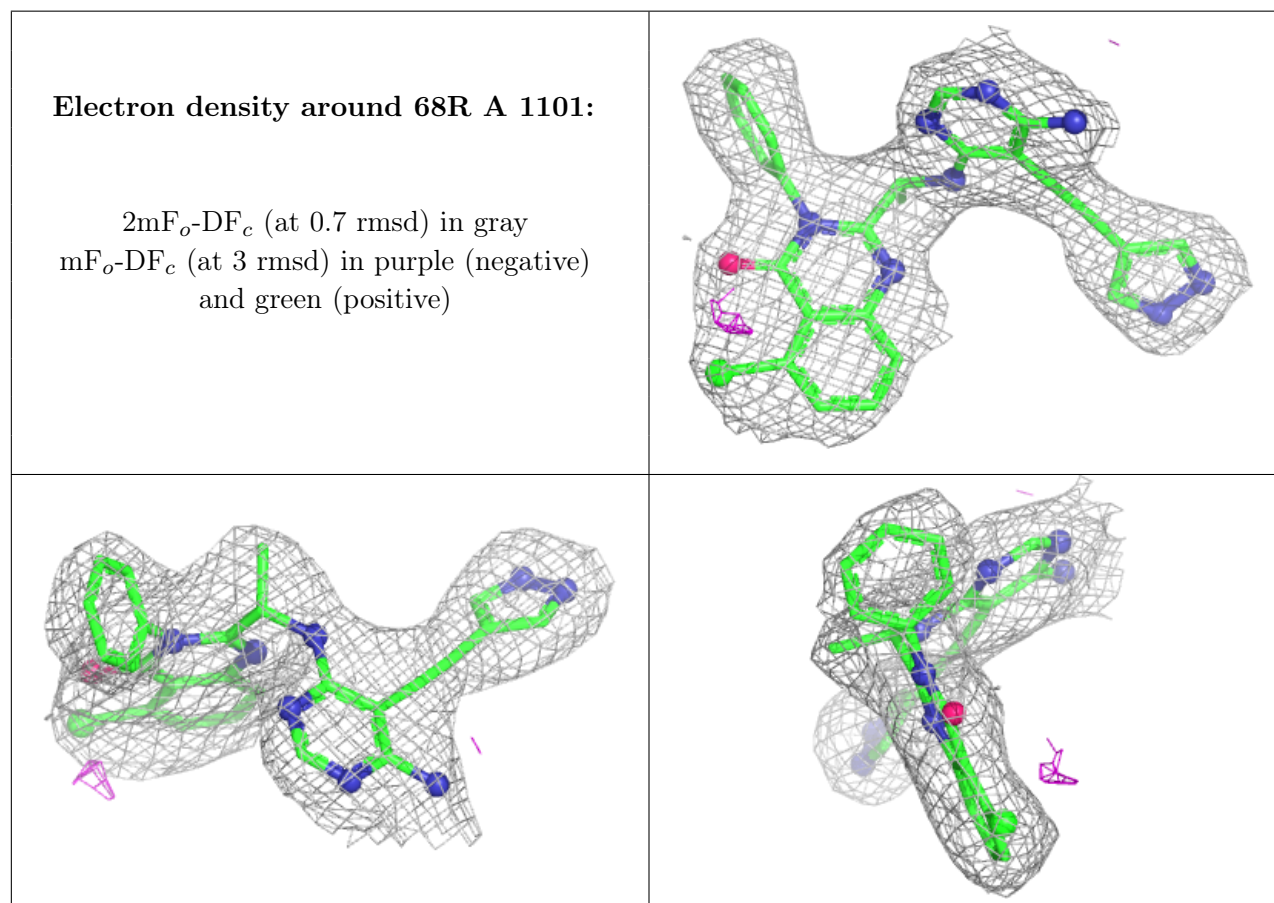
There are no oligosaccharides in this entry.

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	68R	A	1101	35/35	0.95	0.07	18,31,37,73	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.