Full wwPDB X-ray Structure Validation Report (i)

Oct 21, 2025 – 06:03 pm BST

PDB ID	:	9T1P / pdb_00009t1p
Title	:	HUMAN PI3KDELTA IN COMPLEX WITH IOA-244
Deposited on	:	2025-10-21
Resolution	:	2.97 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

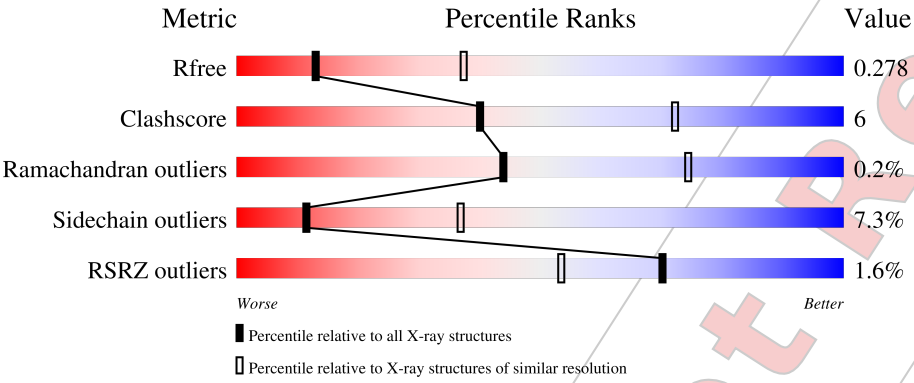
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

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 2.97 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}	164625	3360 (3.00-2.96)
Clashscore	180529	3751 (3.00-2.96)
Ramachandran outliers	177936	3628 (3.00-2.96)
Sidechain outliers	177891	3631 (3.00-2.96)
RSRZ outliers	164620	3372 (3.00-2.96)

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	1044	2% 69% 16% • 13%
2	B	169	80% 12% • 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8830 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.

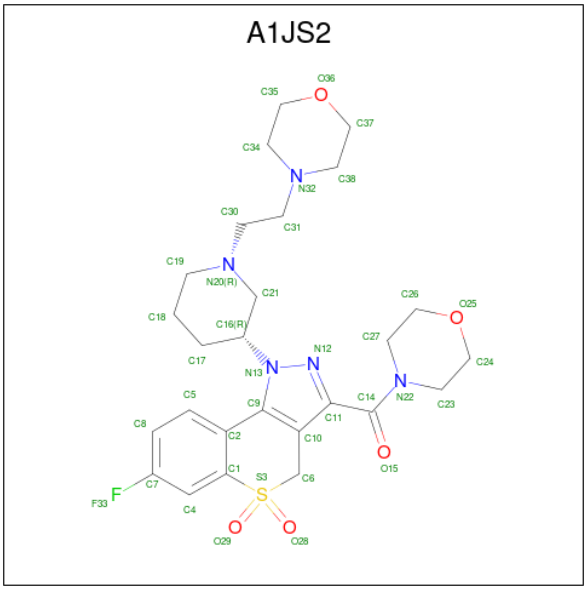
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	910	7362	4714	1254	1341	53	0	0	0

- Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	159	1381	863	251	262	5	0	0	0

- Molecule 3 is [7-fluoranyl-1-[(3 {R})-1-(2-morpholin-4-ylethyl)piperidin-3-yl]-5,5-bis(oxidanylidene)-4 {H}-thiochromeno[4,3-c]pyrazol-3-yl]-morpholin-4-yl-methanone (CCD ID: A1JS2) (formula: $C_{26}H_{34}FN_5O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
3	A	1	38	26	1	5	5	1	0	0

- Molecule 4 is water.

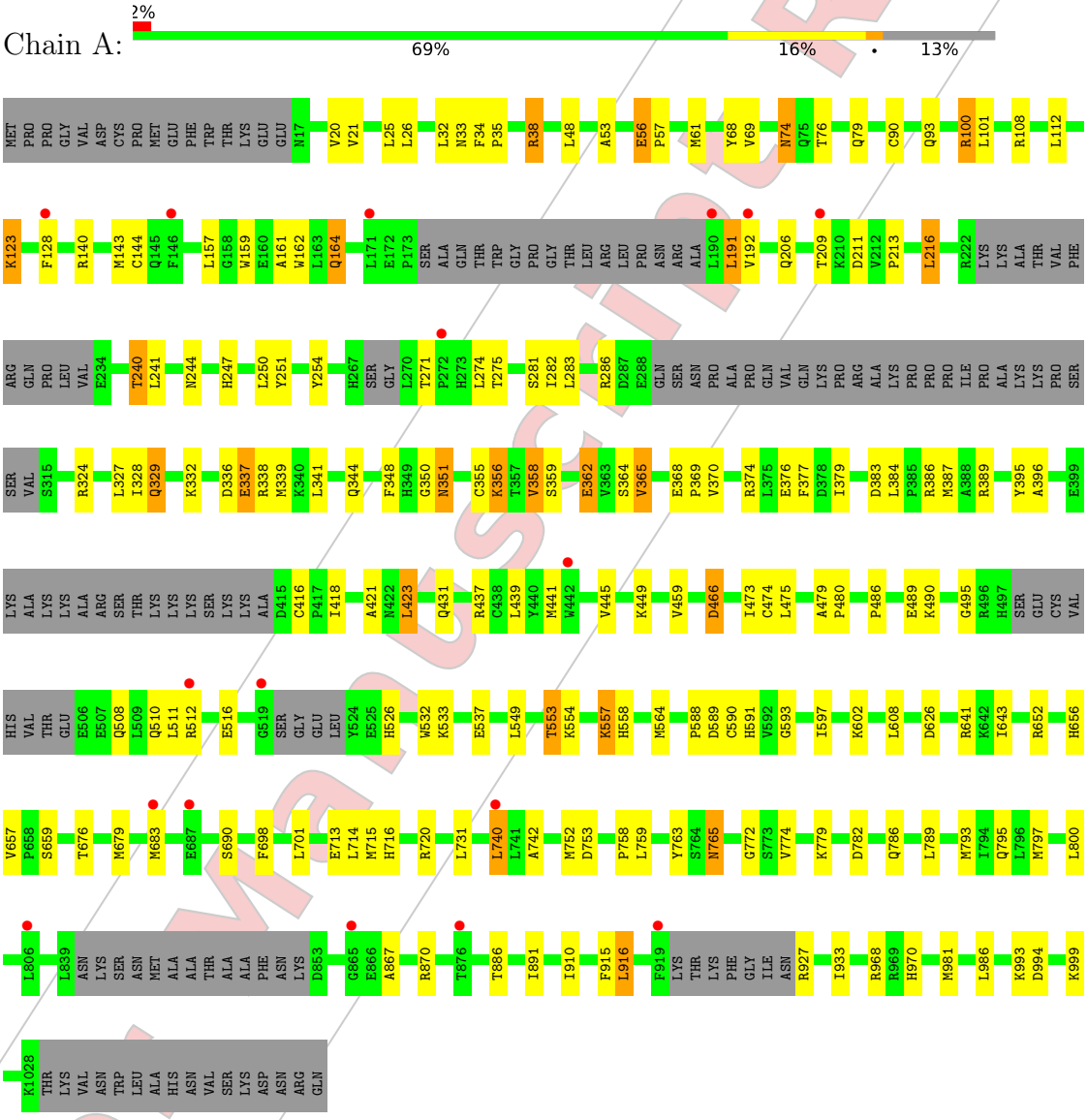
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	39	Total O 39 39	0	1
4	B	10	Total O 10 10	0	0

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 4,5-bisphosphate 3-kinase catalytic subunit delta isoform

Chain A:



• Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	93.23Å 113.34Å 144.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.43 – 2.97 48.43 – 2.97	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.43-2.97) 99.4 (48.43-2.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.96Å)	Xtriage
Refinement program	BUSTER 2.11.8 (17-JUL-2025)	Depositor
R, R_{free}	0.219 , 0.276 0.221 , 0.278	Depositor DCC
R_{free} test set	871 reflections (2.71%)	wwPDB-VP
Wilson B-factor (Å^2)	96.1	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 69.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8830	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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: A1JS2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.63	0/7523	1.03	0/10168
2	B	0.65	0/1399	1.14	0/1863
All	All	0.63	0/8922	1.05	0/12031

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7362	0	7331	100	0
2	B	1381	0	1390	12	0
3	A	38	0	0	1	0
4	A	39	0	0	0	0
4	B	10	0	0	0	0
All	All	8830	0	8721	113	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 (113) 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:549:LEU:HG	1:A:564:MET:HE1	1.42	0.97
1:A:867:ALA:HA	1:A:870:ARG:HD2	1.59	0.84
2:B:439:GLU:O	2:B:445:VAL:CG2	2.26	0.83
1:A:421:ALA:HB2	1:A:441:MET:HG2	1.63	0.80
2:B:440:ASP:OD1	2:B:440:ASP:N	2.15	0.77
1:A:140:ARG:O	1:A:144:CYS:SG	2.43	0.76
1:A:143:MET:HE2	1:A:626:ASP:OD1	1.86	0.75
1:A:554:LYS:HE3	1:A:557:LYS:HZ2	1.53	0.72
1:A:337:GLU:H	1:A:337:GLU:CD	1.96	0.72
1:A:332:LYS:NZ	1:A:466:ASP:C	2.48	0.72
1:A:554:LYS:CE	1:A:557:LYS:HZ2	2.04	0.71
1:A:589:ASP:OD2	1:A:591:HIS:ND1	2.24	0.71
1:A:74:ASN:HB3	1:A:76:THR:HG22	1.73	0.70
1:A:324:ARG:HE	1:A:374:ARG:NH1	1.91	0.69
1:A:927:ARG:HH12	1:A:993:LYS:HB3	1.56	0.69
1:A:244:ASN:ND2	1:A:275:THR:OG1	2.25	0.69
1:A:383:ASP:HA	1:A:558:HIS:HB3	1.74	0.69
1:A:387:MET:HE3	1:A:590:CYS:HB3	1.75	0.68
1:A:191:LEU:O	1:A:271:THR:HG23	1.95	0.66
1:A:324:ARG:HE	1:A:374:ARG:HH11	1.43	0.64
1:A:90:CYS:O	1:A:93:GLN:HG3	1.97	0.64
1:A:213:PRO:HD3	1:A:254:TYR:O	1.99	0.62
1:A:549:LEU:CG	1:A:564:MET:HE1	2.26	0.62
1:A:386:ARG:HG3	1:A:387:MET:HE2	1.83	0.60
1:A:800:LEU:HD22	1:A:970:HIS:CD2	2.36	0.59
1:A:332:LYS:NZ	1:A:466:ASP:O	2.36	0.59
1:A:800:LEU:HD22	1:A:970:HIS:CG	2.38	0.58
1:A:337:GLU:N	1:A:337:GLU:OE1	2.36	0.58
1:A:329:GLN:HG2	1:A:369:PRO:O	2.05	0.57
1:A:32:LEU:HD21	1:A:53:ALA:HA	1.88	0.56
1:A:20:VAL:HG23	1:A:38:ARG:HD2	1.86	0.56
1:A:192:VAL:HG11	1:A:216:LEU:HD11	1.87	0.56
1:A:396:ALA:HB2	1:A:418:ILE:HD11	1.88	0.55
1:A:69:VAL:HG11	1:A:108:ARG:HH12	1.72	0.55
1:A:698:PHE:HZ	1:A:714:LEU:HB3	1.73	0.54
2:B:441:ASN:O	2:B:445:VAL:HG23	2.08	0.54
1:A:532:TRP:HZ3	1:A:564:MET:HE2	1.73	0.53
1:A:479:ALA:HB1	1:A:480:PRO:HD2	1.91	0.53
1:A:247:HIS:CD2	1:A:740:LEU:HD11	2.44	0.52
1:A:241:LEU:HB2	1:A:250:LEU:HB2	1.92	0.52
1:A:512:ARG:HH21	1:A:537:GLU:HB3	1.73	0.52
1:A:608:LEU:HD23	1:A:643:ILE:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:VAL:HG13	1:A:377:PHE:CE1	2.45	0.52
1:A:61:MET:HA	1:A:61:MET:HE2	1.92	0.51
1:A:241:LEU:HB3	1:A:274:LEU:HD13	1.92	0.51
1:A:356:LYS:HG2	1:A:356:LYS:O	2.11	0.51
1:A:554:LYS:NZ	1:A:557:LYS:HZ2	2.09	0.51
1:A:508:GLN:HA	1:A:511:LEU:HD12	1.93	0.50
1:A:512:ARG:O	1:A:516:GLU:HG2	2.11	0.50
2:B:442:ILE:HD13	2:B:589:VAL:CG2	2.43	0.49
1:A:159:TRP:HB3	1:A:283:LEU:HG	1.94	0.49
1:A:789:LEU:HD13	1:A:981:MET:HE2	1.94	0.48
1:A:786:GLN:HG3	1:A:986:LEU:HD13	1.95	0.48
1:A:26:LEU:HD23	1:A:101:LEU:HD12	1.95	0.48
2:B:439:GLU:HB2	2:B:445:VAL:HG22	1.95	0.48
1:A:656:HIS:CD2	1:A:657:VAL:HG23	2.48	0.48
3:A:1101:A1JS2:N12	3:A:1101:A1JS2:C23	2.77	0.47
1:A:716:HIS:O	1:A:720:ARG:HG2	2.14	0.47
1:A:350:GLY:CA	1:A:588:PRO:HG3	2.44	0.47
1:A:423:LEU:HD13	1:A:439:LEU:HD21	1.96	0.47
1:A:886:THR:HA	1:A:891:ILE:HD12	1.96	0.47
1:A:191:LEU:HB3	1:A:206:GLN:HA	1.97	0.47
1:A:676:THR:HA	1:A:679:MET:HE2	1.97	0.47
1:A:348:PHE:O	1:A:389:ARG:HB3	2.15	0.47
1:A:715:MET:HE2	1:A:759:LEU:HD22	1.97	0.47
1:A:56:GLU:HG3	1:A:57:PRO:HD2	1.98	0.46
2:B:501:GLN:HG2	2:B:528:TYR:CD1	2.51	0.46
1:A:383:ASP:OD1	1:A:558:HIS:ND1	2.47	0.45
1:A:396:ALA:HB3	1:A:416:CYS:HB3	1.96	0.45
1:A:247:HIS:CD2	1:A:740:LEU:CD1	2.99	0.45
1:A:916:LEU:HD23	1:A:994:ASP:HB3	1.99	0.45
1:A:34:PHE:HB2	1:A:35:PRO:HD2	1.99	0.45
1:A:337:GLU:HA	1:A:365:VAL:CG1	2.46	0.45
1:A:793:MET:O	1:A:797:MET:HG3	2.16	0.45
1:A:329:GLN:HG3	1:A:370:VAL:HG22	1.98	0.45
1:A:486:PRO:HA	1:A:490:LYS:HE3	1.99	0.45
1:A:25:LEU:HB2	1:A:100:ARG:HG2	1.99	0.44
1:A:162:TRP:CD1	1:A:286:ARG:HG3	2.51	0.44
1:A:240:THR:HG21	1:A:282:ILE:HD11	1.99	0.44
2:B:439:GLU:O	2:B:445:VAL:HG23	2.12	0.44
1:A:698:PHE:CZ	1:A:714:LEU:HB3	2.53	0.44
1:A:341:LEU:HA	1:A:395:TYR:O	2.18	0.44
1:A:758:PRO:HB3	1:A:779:LYS:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:763:TYR:HB2	1:A:774:VAL:HG23	2.00	0.44
1:A:191:LEU:HA	1:A:206:GLN:HA	2.00	0.44
1:A:328:ILE:HD11	1:A:474:CYS:HB2	2.00	0.43
1:A:449:LYS:CE	1:A:993:LYS:NZ	2.81	0.43
1:A:123:LYS:NZ	1:A:128:PHE:CZ	2.83	0.43
1:A:164:GLN:HA	1:A:251:TYR:OH	2.17	0.43
2:B:555:GLU:O	2:B:559:ILE:HG12	2.17	0.43
2:B:439:GLU:O	2:B:445:VAL:HG21	2.14	0.43
1:A:157:LEU:HB3	1:A:161:ALA:HB3	2.00	0.42
1:A:21:VAL:CG1	1:A:33:ASN:HD21	2.32	0.42
1:A:362:GLU:H	1:A:362:GLU:HG3	1.59	0.42
1:A:742:ALA:HB3	1:A:765:ASN:HB3	2.01	0.42
1:A:765:ASN:OD1	1:A:772:GLY:O	2.38	0.42
1:A:68:TYR:HB3	1:A:101:LEU:HD22	2.01	0.42
1:A:379:ILE:HD13	1:A:384:LEU:HD23	2.02	0.42
1:A:752:MET:HB2	1:A:758:PRO:HG2	2.00	0.42
1:A:327:LEU:HA	1:A:473:ILE:HG22	2.01	0.42
1:A:387:MET:HG3	1:A:589:ASP:HA	2.01	0.42
1:A:593:GLY:O	1:A:597:ILE:HG12	2.19	0.41
1:A:74:ASN:C	1:A:76:THR:N	2.76	0.41
1:A:355:CYS:SG	1:A:377:PHE:HB3	2.61	0.41
2:B:477:ILE:HG23	2:B:549:LEU:HD11	2.01	0.41
1:A:351:ASN:HD22	1:A:351:ASN:HA	1.57	0.41
2:B:459:LYS:HE2	2:B:459:LYS:HB2	1.88	0.41
1:A:329:GLN:CG	1:A:370:VAL:HG22	2.51	0.41
1:A:244:ASN:HD21	1:A:275:THR:HG1	1.64	0.40
1:A:336:ASP:HB3	1:A:339:MET:HE2	2.02	0.40
2:B:483:ALA:HB3	2:B:545:LEU:HD21	2.02	0.40
1:A:508:GLN:HE21	1:A:533:LYS:NZ	2.19	0.40
1:A:553:THR:HG21	1:A:564:MET:HG2	2.04	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	890/1044 (85%)	852 (96%)	37 (4%)	1 (0%)	48	79
2	B	155/169 (92%)	152 (98%)	2 (1%)	1 (1%)	22	55
All	All	1045/1213 (86%)	1004 (96%)	39 (4%)	2 (0%)	44	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	513	LYS
1	A	495	GLY

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	813/927 (88%)	753 (93%)	60 (7%)	11	36
2	B	151/160 (94%)	141 (93%)	10 (7%)	14	41
All	All	964/1087 (89%)	894 (93%)	70 (7%)	11	37

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	48	LEU
1	A	56	GLU
1	A	74	ASN
1	A	79	GLN
1	A	100	ARG
1	A	112	LEU
1	A	123	LYS
1	A	164	GLN
1	A	191	LEU
1	A	209	THR

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Mol	Chain	Res	Type
1	A	211	ASP
1	A	216	LEU
1	A	240	THR
1	A	281	SER
1	A	329	GLN
1	A	337	GLU
1	A	338	ARG
1	A	344	GLN
1	A	351	ASN
1	A	356	LYS
1	A	358	VAL
1	A	359	SER
1	A	362	GLU
1	A	364	SER
1	A	365	VAL
1	A	368	GLU
1	A	376	GLU
1	A	423	LEU
1	A	431	GLN
1	A	437	ARG
1	A	445	VAL
1	A	459	VAL
1	A	466	ASP
1	A	475	LEU
1	A	489	GLU
1	A	510	GLN
1	A	526	HIS
1	A	553	THR
1	A	557	LYS
1	A	602	LYS
1	A	641	ARG
1	A	652	ARG
1	A	659	SER
1	A	683	MET
1	A	690	SER
1	A	701	LEU
1	A	713	GLU
1	A	731	LEU
1	A	740	LEU
1	A	753	ASP
1	A	765	ASN
1	A	782	ASP

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Mol	Chain	Res	Type
1	A	795	GLN
1	A	910	ILE
1	A	915	PHE
1	A	916	LEU
1	A	933	ILE
1	A	968	ARG
1	A	999	LYS
2	B	440	ASP
2	B	442	ILE
2	B	475	GLN
2	B	501	GLN
2	B	522	GLN
2	B	561	LYS
2	B	572	GLN
2	B	575	LYS
2	B	581	LEU
2	B	592	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	33	ASN
1	A	74	ASN
1	A	75	GLN
1	A	86	GLN
1	A	116	GLN
1	A	156	GLN
1	A	193	ASN
1	A	242	GLN
1	A	244	ASN
1	A	247	HIS
1	A	351	ASN
1	A	508	GLN
1	A	510	GLN
1	A	721	GLN
1	A	730	HIS
1	A	732	GLN
1	A	748	GLN
2	B	499	GLN
2	B	501	GLN
2	B	526	HIS

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

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	$\#\|Z\| > 2$
3	A1JS2	A	1101	-	40,43,43	1.41	2 (5%)	47,63,63	2.04	9 (19%)

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	A1JS2	A	1101	-	-	3/9/58/58	0/5/6/6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	A1JS2	N12-N13	-6.91	1.29	1.37
3	A	1101	A1JS2	C11-N12	-3.81	1.32	1.35

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1101	A1JS2	C11-N12-N13	6.70	110.52	105.17
3	A	1101	A1JS2	O28-S3-C1	-5.14	103.91	108.60
3	A	1101	A1JS2	O29-S3-C1	-4.38	104.61	108.60
3	A	1101	A1JS2	C7-C4-C1	4.36	119.83	116.86
3	A	1101	A1JS2	O29-S3-O28	4.03	121.17	117.75
3	A	1101	A1JS2	C23-N22-C27	2.84	118.09	112.62
3	A	1101	A1JS2	C9-N13-N12	-2.41	109.96	112.71
3	A	1101	A1JS2	C14-C11-N12	2.41	126.82	120.55
3	A	1101	A1JS2	C8-C7-C4	-2.29	120.31	123.29

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	A1JS2	C30-C31-N32-C34
3	A	1101	A1JS2	C31-C30-N20-C19
3	A	1101	A1JS2	C31-C30-N20-C21

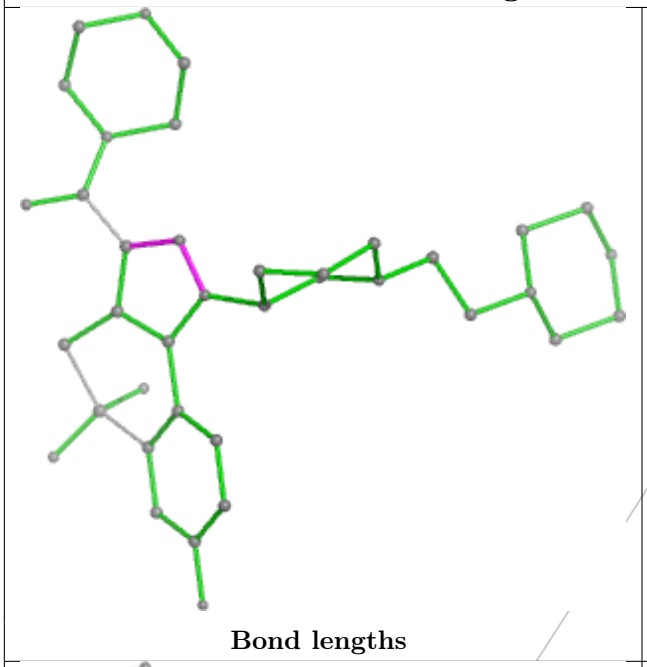
There are no ring outliers.

1 monomer is involved in 1 short contact:

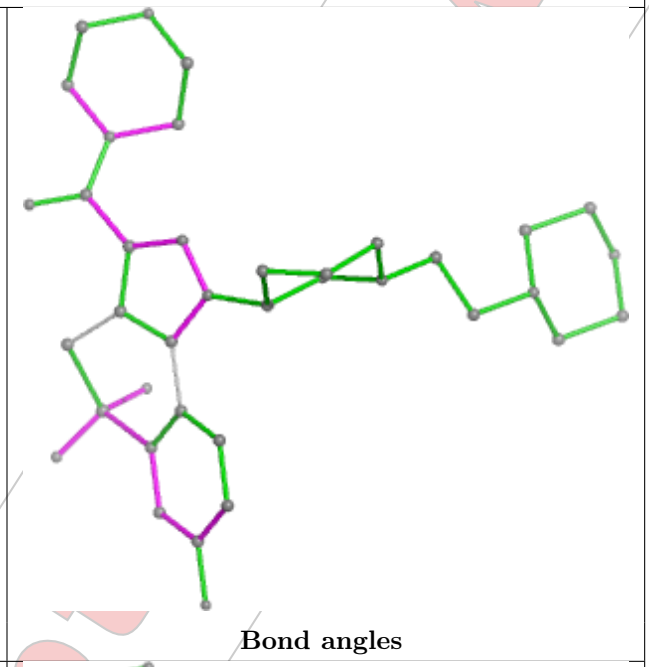
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	A1JS2	1	0

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.

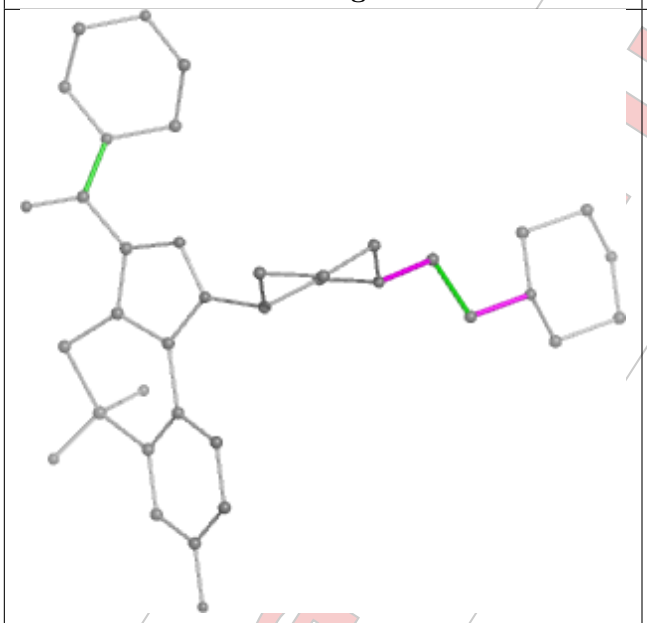
Ligand A1JS2 A 1101



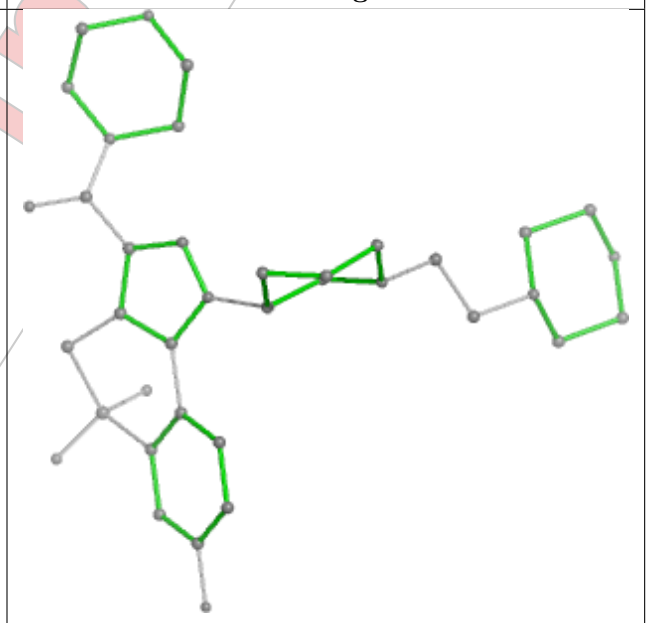
Bond lengths



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	910/1044 (87%)	0.01	17 (1%) 66 49	62, 111, 160, 188	3 (0%)
2	B	159/169 (94%)	-0.39	0 100 100	77, 96, 114, 139	0
All	All	1069/1213 (88%)	-0.05	17 (1%) 70 53	62, 106, 157, 188	3 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	190	LEU	3.2
1	A	171	LEU	3.0
1	A	442	TRP	2.7
1	A	519	GLY	2.7
1	A	192	VAL	2.6
1	A	683	MET	2.5
1	A	209	THR	2.4
1	A	865	GLY	2.3
1	A	512	ARG	2.3
1	A	272	PRO	2.3
1	A	687	GLU	2.2
1	A	876	THR	2.2
1	A	740	LEU	2.1
1	A	146	PHE	2.1
1	A	128	PHE	2.0
1	A	806	LEU	2.0
1	A	919	PHE	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 (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

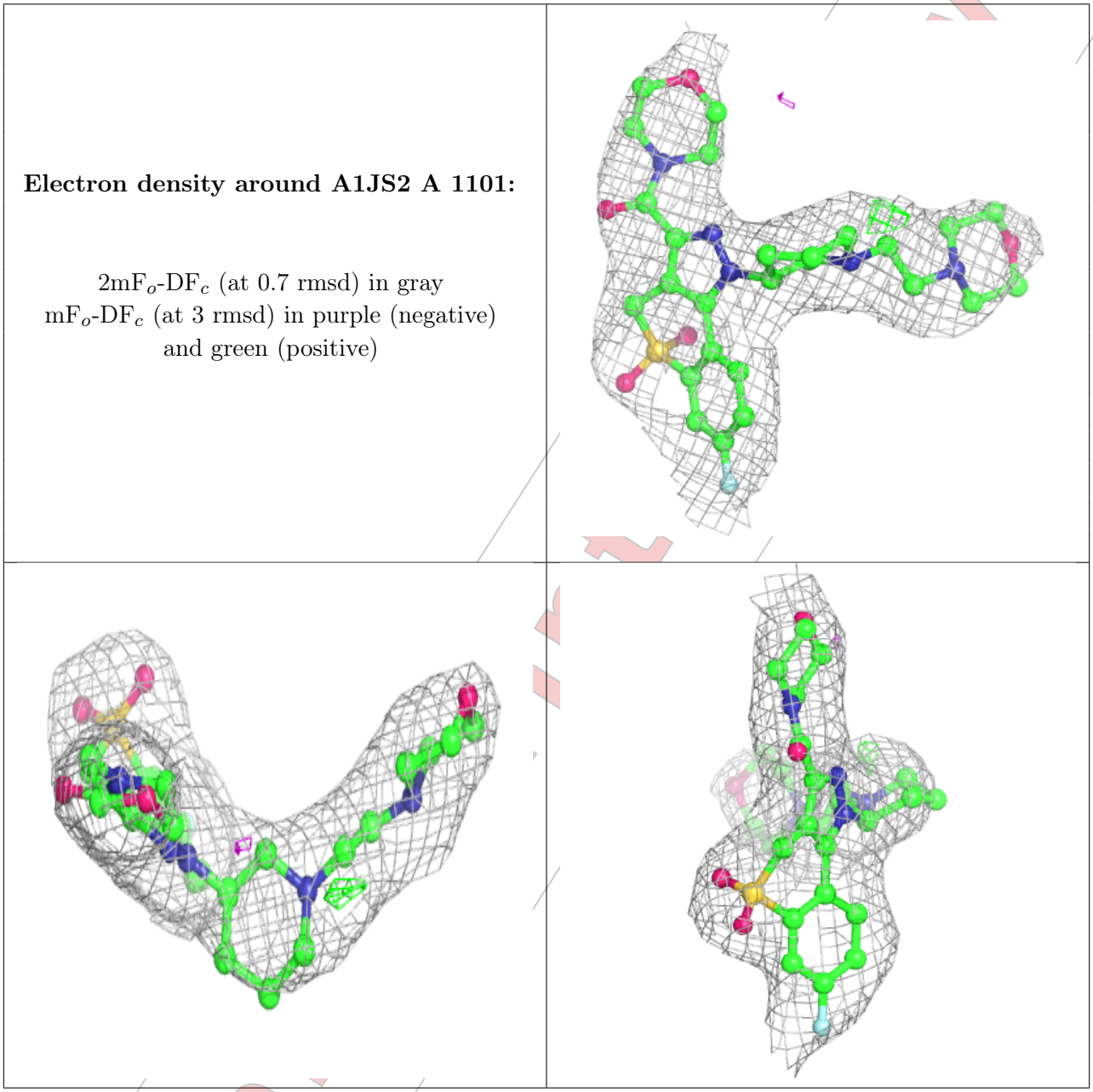
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	A1JS2	A	1101	38/38	0.92	0.10	116,117,122,122	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 A1JS2 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 (i)

There are no such residues in this entry.