



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 12:36 AM EDT

PDB ID : 3ET7
Title : Crystal structure of PYK2 complexed with PF-2318841
Authors : Han, S.
Deposited on : 2008-10-07
Resolution : 2.70 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

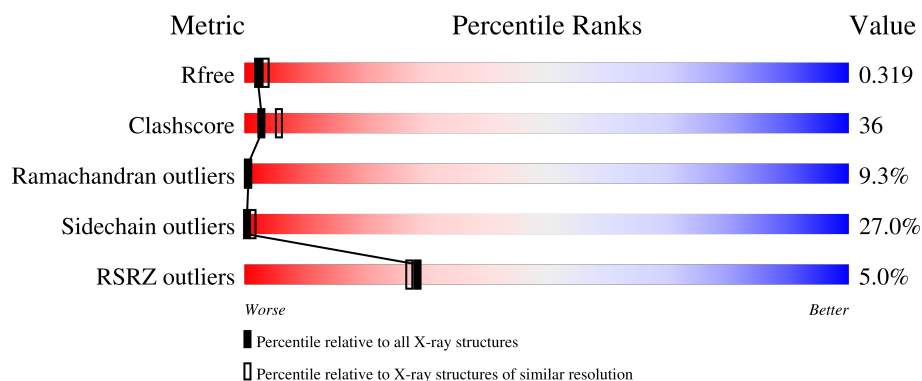
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	277	

2 Entry composition [i](#)

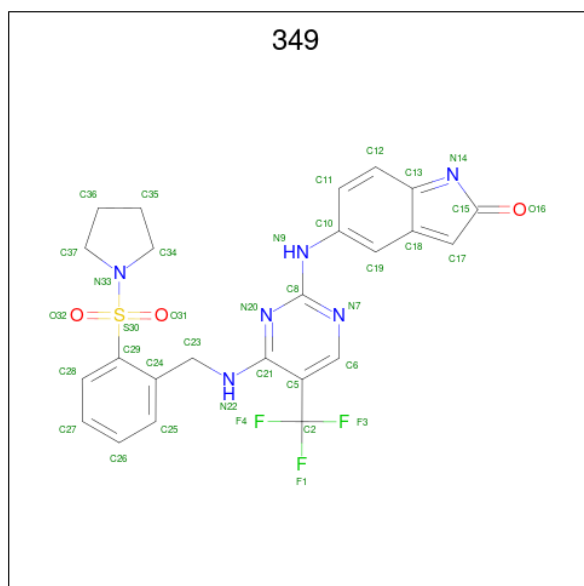
There are 4 unique types of molecules in this entry. The entry contains 2168 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Protein tyrosine kinase 2 beta.

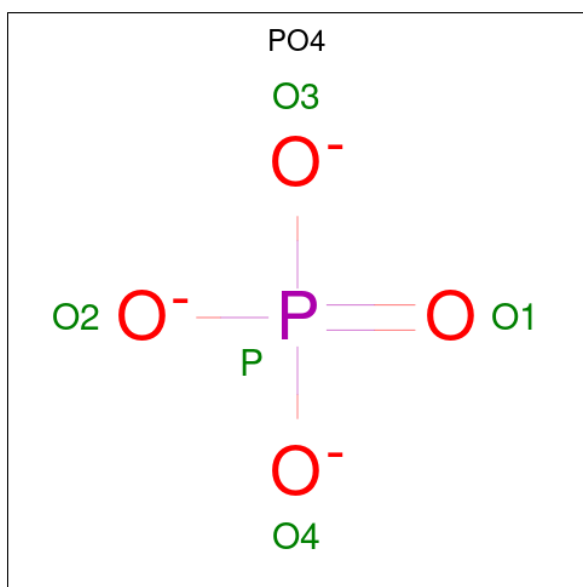
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			2114	1365	349	381	19			

- Molecule 2 is 5-{{4-{{2-(pyrrolidin-1-ylsulfonyl)benzyl}amino}-5-(trifluoromethyl)pyrimidin-2-yl}amino}-1,3-dihydro-2H-indol-2-one (three-letter code: 349) (formula: C₂₄H₂₁F₃N₆O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			37	24	3	6	3		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

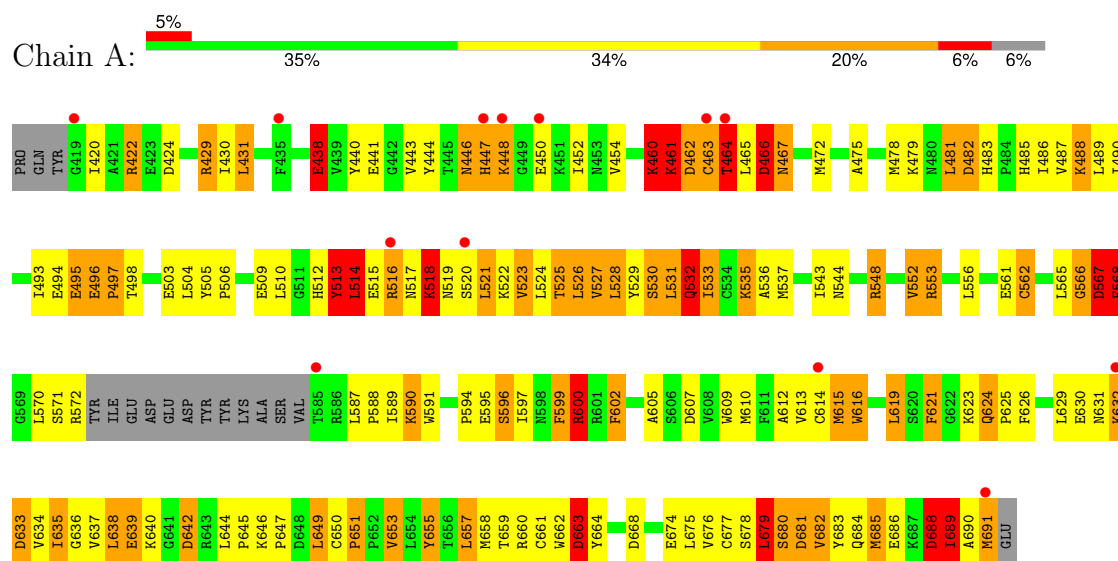
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	O	0	0
			12	12		

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: Protein tyrosine kinase 2 beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.82Å 106.82Å 75.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 29.63 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.9 (30.00-2.70) 97.9 (29.63-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.80 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.1	Depositor
R, R_{free}	0.247 , 0.328 0.238 , 0.319	Depositor DCC
R_{free} test set	587 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	68.9	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2168	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 349, PO4

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	1.42	12/2163 (0.6%)	1.48	28/2926 (1.0%)

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	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	658	MET	CG-SD	7.39	2.00	1.81
1	A	655	TYR	CD2-CE2	6.67	1.49	1.39
1	A	605	ALA	CA-CB	6.36	1.65	1.52
1	A	616	TRP	CB-CG	-6.26	1.39	1.50
1	A	621	PHE	CE1-CZ	6.09	1.49	1.37
1	A	685	MET	SD-CE	5.75	2.10	1.77
1	A	532	GLN	CG-CD	5.16	1.62	1.51
1	A	591	TRP	CB-CG	-5.15	1.41	1.50
1	A	561	GLU	CD-OE2	5.08	1.31	1.25
1	A	561	GLU	CG-CD	5.08	1.59	1.51
1	A	527	VAL	CA-CB	5.07	1.65	1.54
1	A	676	VAL	CB-CG1	-5.02	1.42	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	567	ASP	CB-CG-OD2	12.01	129.10	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	568	PHE	N-CA-C	-8.21	88.85	111.00
1	A	556	LEU	CA-CB-CG	-7.79	97.39	115.30
1	A	607	ASP	CB-CG-OD2	7.79	125.31	118.30
1	A	653	VAL	CB-CA-C	-7.66	96.85	111.40
1	A	681	ASP	CB-CG-OD1	7.55	125.10	118.30
1	A	528	LEU	CB-CG-CD2	-7.37	98.47	111.00
1	A	466	ASP	CB-CG-OD2	7.33	124.90	118.30
1	A	431	LEU	CA-CB-CG	-7.29	98.55	115.30
1	A	552	VAL	CB-CA-C	7.25	125.17	111.40
1	A	568	PHE	N-CA-CB	6.68	122.63	110.60
1	A	514	LEU	CA-CB-CG	6.52	130.31	115.30
1	A	514	LEU	CB-CG-CD2	6.49	122.03	111.00
1	A	688	ASP	CB-CG-OD2	6.41	124.06	118.30
1	A	478	MET	CG-SD-CE	6.28	110.25	100.20
1	A	462	ASP	CB-CG-OD2	6.25	123.92	118.30
1	A	424	ASP	CB-CG-OD2	6.13	123.82	118.30
1	A	553	ARG	CB-CA-C	-5.94	98.52	110.40
1	A	679	LEU	CB-CG-CD2	-5.85	101.05	111.00
1	A	531	LEU	CB-CG-CD1	5.69	120.67	111.00
1	A	642	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	658	MET	CA-CB-CG	5.37	122.43	113.30
1	A	567	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	A	680	SER	CB-CA-C	5.24	120.05	110.10
1	A	663	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	568	PHE	CB-CA-C	-5.20	99.99	110.40
1	A	614	CYS	CA-CB-SG	5.18	123.33	114.00
1	A	668	ASP	CB-CG-OD2	5.14	122.93	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	460	LYS	Peptide
1	A	461	LYS	Peptide
1	A	496	GLU	Peptide
1	A	513	TYR	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	2114	0	2129	151	0
2	A	37	0	21	3	0
3	A	5	0	0	0	0
4	A	12	0	0	2	0
All	All	2168	0	2150	153	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 36.

All (153) 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:685:MET:SD	1:A:685:MET:CE	2.10	1.40
1:A:429:ARG:HH11	1:A:429:ARG:HB2	0.96	1.08
1:A:566:GLY:O	1:A:567:ASP:HB3	1.53	1.07
2:A:999:349:N20	2:A:999:349:H11	1.60	1.07
1:A:513:TYR:HD2	1:A:513:TYR:O	1.36	1.05
1:A:513:TYR:O	1:A:513:TYR:CD2	2.09	1.05
1:A:429:ARG:HB2	1:A:429:ARG:NH1	1.73	1.01
1:A:528:LEU:O	1:A:532:GLN:HG3	1.61	1.00
1:A:429:ARG:HH11	1:A:429:ARG:CB	1.80	0.94
1:A:537:MET:HE1	1:A:565:LEU:HD21	1.54	0.90
1:A:635:ILE:O	1:A:639:GLU:HG2	1.74	0.88
2:A:999:349:N20	2:A:999:349:C11	2.25	0.87
1:A:460:LYS:HE3	1:A:462:ASP:HA	1.61	0.82
1:A:688:ASP:O	1:A:690:ALA:N	2.12	0.82
1:A:682:VAL:HG12	1:A:682:VAL:O	1.78	0.82
1:A:485:HIS:HE1	1:A:532:GLN:NE2	1.77	0.81
1:A:522:LYS:O	1:A:524:LEU:N	2.17	0.78
1:A:448:LYS:HE3	1:A:450:GLU:OE2	1.85	0.77
1:A:682:VAL:O	1:A:682:VAL:CG1	2.34	0.76
1:A:646:LYS:HE2	4:A:1010:HOH:O	1.87	0.75
1:A:522:LYS:O	1:A:523:VAL:C	2.25	0.74
1:A:689:ILE:HG13	1:A:689:ILE:O	1.88	0.73
1:A:485:HIS:CE1	1:A:532:GLN:NE2	2.56	0.73
1:A:448:LYS:HG2	1:A:448:LYS:O	1.87	0.73
1:A:567:ASP:HA	1:A:570:LEU:HD12	1.72	0.72
1:A:527:VAL:HG12	1:A:683:TYR:HB2	1.72	0.72
1:A:485:HIS:HE1	1:A:532:GLN:HE21	1.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:LEU:O	1:A:524:LEU:HG	1.89	0.71
1:A:524:LEU:HD11	1:A:683:TYR:CE1	2.26	0.70
1:A:675:LEU:O	1:A:679:LEU:HB2	1.92	0.70
1:A:619:LEU:HD23	1:A:619:LEU:N	2.06	0.69
1:A:523:VAL:HG22	1:A:649:LEU:HB3	1.74	0.69
1:A:527:VAL:CG1	1:A:683:TYR:HB2	2.24	0.68
1:A:537:MET:HE1	1:A:565:LEU:CD2	2.23	0.68
1:A:465:LEU:O	1:A:467:ASN:N	2.29	0.66
1:A:636:GLY:HA2	1:A:639:GLU:HG3	1.79	0.65
1:A:612:ALA:HB3	1:A:662:TRP:HE1	1.61	0.65
1:A:612:ALA:HB3	1:A:662:TRP:NE1	2.12	0.65
1:A:646:LYS:HE3	1:A:650:CYS:O	1.97	0.64
1:A:567:ASP:O	1:A:567:ASP:CG	2.35	0.64
1:A:514:LEU:HD13	1:A:621:PHE:HA	1.78	0.64
1:A:537:MET:CE	1:A:565:LEU:CD2	2.77	0.63
1:A:532:GLN:HE22	1:A:562:CYS:HA	1.64	0.62
1:A:631:ASN:O	1:A:634:VAL:HG23	1.99	0.62
1:A:522:LYS:O	1:A:525:THR:N	2.30	0.61
1:A:660:ARG:O	1:A:663:ASP:HB2	2.00	0.61
1:A:446:ASN:HB2	1:A:450:GLU:H	1.65	0.61
1:A:486:ILE:HG22	1:A:487:VAL:N	2.16	0.60
1:A:567:ASP:HA	1:A:570:LEU:CD1	2.32	0.60
1:A:517:ASN:O	1:A:519:ASN:N	2.35	0.59
1:A:681:ASP:O	1:A:683:TYR:N	2.35	0.59
1:A:634:VAL:O	1:A:637:VAL:HB	2.03	0.59
1:A:624:GLN:CA	1:A:624:GLN:HE21	2.16	0.59
1:A:537:MET:CE	1:A:565:LEU:HD21	2.30	0.58
1:A:472:MET:O	1:A:475:ALA:HB3	2.03	0.58
1:A:446:ASN:HB2	1:A:450:GLU:N	2.18	0.58
1:A:488:LYS:HB2	1:A:505:TYR:OH	2.03	0.58
1:A:517:ASN:C	1:A:519:ASN:H	2.06	0.57
1:A:485:HIS:CE1	1:A:532:GLN:HE21	2.17	0.57
1:A:587:LEU:O	1:A:589:ILE:N	2.36	0.57
1:A:430:ILE:HG12	1:A:440:TYR:HE2	1.70	0.57
1:A:683:TYR:HA	1:A:686:GLU:HB2	1.88	0.56
1:A:422:ARG:NH1	1:A:497:PRO:O	2.33	0.56
1:A:462:ASP:OD2	1:A:462:ASP:O	2.25	0.55
1:A:624:GLN:HE21	1:A:624:GLN:HA	1.73	0.54
1:A:496:GLU:HG3	1:A:497:PRO:CD	2.38	0.54
1:A:619:LEU:HD23	1:A:619:LEU:H	1.73	0.54
1:A:567:ASP:O	1:A:568:PHE:CB	2.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:GLU:HG2	1:A:553:ARG:O	2.09	0.53
1:A:465:LEU:O	1:A:466:ASP:C	2.47	0.52
1:A:635:ILE:HD12	1:A:635:ILE:H	1.74	0.52
1:A:674:GLU:O	1:A:678:SER:HB3	2.09	0.52
1:A:688:ASP:C	1:A:690:ALA:H	2.13	0.52
1:A:681:ASP:C	1:A:683:TYR:H	2.12	0.52
1:A:461:LYS:O	1:A:461:LYS:HG3	2.09	0.51
1:A:613:VAL:HG12	1:A:613:VAL:O	2.10	0.51
1:A:513:TYR:CD2	1:A:513:TYR:C	2.84	0.51
1:A:493:ILE:O	1:A:498:THR:HA	2.10	0.51
1:A:537:MET:HA	1:A:537:MET:HE2	1.93	0.51
1:A:616:TRP:CZ3	1:A:625:PRO:HA	2.46	0.51
1:A:678:SER:O	1:A:681:ASP:HB2	2.12	0.49
1:A:533:ILE:O	1:A:536:ALA:N	2.46	0.49
1:A:631:ASN:O	1:A:633:ASP:N	2.45	0.49
1:A:463:CYS:SG	1:A:466:ASP:HB2	2.52	0.49
1:A:429:ARG:HD3	1:A:441:GLU:HB3	1.95	0.48
1:A:463:CYS:O	1:A:464:THR:C	2.51	0.48
1:A:490:ILE:HD12	1:A:503:GLU:N	2.28	0.48
1:A:594:PRO:HG2	1:A:664:TYR:CE1	2.48	0.48
1:A:523:VAL:O	1:A:525:THR:N	2.47	0.48
1:A:510:LEU:HB3	1:A:552:VAL:HG22	1.95	0.48
1:A:530:SER:O	1:A:531:LEU:C	2.51	0.48
1:A:602:PHE:CD1	1:A:602:PHE:N	2.82	0.48
1:A:657:LEU:HD12	4:A:1012:HOH:O	2.13	0.48
1:A:609:TRP:CE3	1:A:662:TRP:HA	2.49	0.47
1:A:512:HIS:HD2	1:A:515:GLU:OE1	1.97	0.47
1:A:505:TYR:HA	1:A:506:PRO:HD3	1.73	0.47
1:A:535:LYS:HB3	1:A:535:LYS:HE3	1.46	0.47
1:A:609:TRP:CD1	1:A:609:TRP:C	2.88	0.47
1:A:443:VAL:HG12	1:A:444:TYR:O	2.14	0.47
1:A:486:ILE:CG2	1:A:487:VAL:N	2.78	0.47
1:A:517:ASN:C	1:A:519:ASN:N	2.69	0.46
1:A:619:LEU:N	1:A:619:LEU:CD2	2.77	0.46
1:A:430:ILE:HG12	1:A:440:TYR:CE2	2.50	0.46
1:A:533:ILE:O	1:A:536:ALA:HB3	2.16	0.46
1:A:567:ASP:C	1:A:567:ASP:OD1	2.53	0.46
1:A:691:MET:SD	1:A:691:MET:N	2.89	0.46
1:A:529:TYR:O	1:A:532:GLN:N	2.49	0.45
1:A:655:TYR:O	1:A:655:TYR:CG	2.69	0.45
1:A:481:LEU:HD21	1:A:543:ILE:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:LYS:HB3	1:A:518:LYS:HE3	1.39	0.45
1:A:553:ARG:CZ	1:A:553:ARG:HB2	2.46	0.45
1:A:587:LEU:O	1:A:589:ILE:HG12	2.17	0.45
1:A:521:LEU:HD23	1:A:525:THR:HG21	1.99	0.45
1:A:438:GLU:H	1:A:438:GLU:HG2	1.57	0.44
1:A:487:VAL:HG21	1:A:567:ASP:HB3	1.99	0.44
1:A:524:LEU:CD1	1:A:683:TYR:CD1	3.00	0.44
1:A:590:LYS:HG3	1:A:626:PHE:HB2	1.99	0.44
1:A:599:PHE:CD2	1:A:599:PHE:N	2.85	0.44
1:A:438:GLU:HB2	1:A:440:TYR:CZ	2.53	0.44
1:A:447:HIS:HD2	1:A:447:HIS:O	2.00	0.44
1:A:430:ILE:HA	1:A:440:TYR:HD2	1.83	0.43
1:A:596:SER:O	1:A:600:ARG:HA	2.18	0.43
1:A:650:CYS:HA	1:A:651:PRO:HD2	1.77	0.43
1:A:516:ARG:O	1:A:517:ASN:CG	2.56	0.43
1:A:646:LYS:HG3	1:A:655:TYR:CG	2.53	0.43
1:A:441:GLU:HG2	1:A:504:LEU:HD22	2.00	0.43
1:A:635:ILE:HA	1:A:638:LEU:HD12	2.01	0.43
1:A:524:LEU:HD12	1:A:683:TYR:CD1	2.53	0.43
1:A:422:ARG:HE	1:A:422:ARG:HB2	1.49	0.43
1:A:527:VAL:HG11	1:A:683:TYR:HB2	2.00	0.43
1:A:646:LYS:CE	1:A:650:CYS:O	2.66	0.42
1:A:661:CYS:SG	1:A:675:LEU:HD11	2.59	0.42
1:A:496:GLU:OE2	1:A:496:GLU:HA	2.20	0.42
1:A:594:PRO:O	1:A:597:ILE:HB	2.20	0.42
1:A:553:ARG:O	2:A:999:349:H27	2.19	0.42
1:A:431:LEU:HA	1:A:431:LEU:HD23	1.73	0.42
1:A:487:VAL:HG13	1:A:565:LEU:O	2.20	0.42
1:A:465:LEU:C	1:A:467:ASN:N	2.73	0.41
1:A:679:LEU:HA	1:A:679:LEU:HD23	1.22	0.41
1:A:467:ASN:HD22	1:A:467:ASN:HA	1.59	0.41
1:A:548:ARG:HH11	1:A:571:SER:HB3	1.86	0.41
1:A:526:LEU:HD11	1:A:621:PHE:CZ	2.56	0.41
1:A:524:LEU:CD1	1:A:683:TYR:CE1	3.00	0.41
1:A:566:GLY:O	1:A:567:ASP:CB	2.34	0.41
1:A:637:VAL:HG13	1:A:642:ASP:HB2	2.03	0.41
1:A:688:ASP:O	1:A:689:ILE:C	2.56	0.41
1:A:482:ASP:O	1:A:483:HIS:HB2	2.21	0.40
1:A:624:GLN:CA	1:A:624:GLN:NE2	2.84	0.40
1:A:644:LEU:HD23	1:A:644:LEU:HA	1.71	0.40
1:A:646:LYS:HA	1:A:647:PRO:HD3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:HIS:O	1:A:516:ARG:HG2	2.21	0.40
1:A:447:HIS:O	1:A:447:HIS:CD2	2.74	0.40
1:A:530:SER:HB3	1:A:615: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	257/277 (93%)	197 (77%)	36 (14%)	24 (9%)	0 0

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	460	LYS
1	A	497	PRO
1	A	514	LEU
1	A	523	VAL
1	A	526	LEU
1	A	568	PHE
1	A	632	LYS
1	A	651	PRO
1	A	682	VAL
1	A	689	ILE
1	A	464	THR
1	A	466	ASP
1	A	495	GLU
1	A	518	LYS
1	A	566	GLY
1	A	688	ASP
1	A	482	ASP
1	A	567	ASP

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Mol	Chain	Res	Type
1	A	447	HIS
1	A	562	CYS
1	A	600	ARG
1	A	438	GLU
1	A	588	PRO
1	A	645	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	237/252 (94%)	173 (73%)	64 (27%)	0 1

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	420	ILE
1	A	422	ARG
1	A	429	ARG
1	A	438	GLU
1	A	446	ASN
1	A	448	LYS
1	A	452	ILE
1	A	454	VAL
1	A	461	LYS
1	A	463	CYS
1	A	464	THR
1	A	466	ASP
1	A	467	ASN
1	A	479	LYS
1	A	481	LEU
1	A	488	LYS
1	A	489	LEU
1	A	494	GLU
1	A	495	GLU
1	A	513	TYR

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Mol	Chain	Res	Type
1	A	514	LEU
1	A	516	ARG
1	A	518	LYS
1	A	520	SER
1	A	521	LEU
1	A	525	THR
1	A	530	SER
1	A	532	GLN
1	A	533	ILE
1	A	535	LYS
1	A	544	ASN
1	A	548	ARG
1	A	567	ASP
1	A	572	ARG
1	A	590	LYS
1	A	595	GLU
1	A	596	SER
1	A	599	PHE
1	A	600	ARG
1	A	602	PHE
1	A	610	MET
1	A	615	MET
1	A	619	LEU
1	A	623	LYS
1	A	624	GLN
1	A	629	LEU
1	A	630	GLU
1	A	632	LYS
1	A	633	ASP
1	A	635	ILE
1	A	638	LEU
1	A	639	GLU
1	A	640	LYS
1	A	649	LEU
1	A	653	VAL
1	A	657	LEU
1	A	659	THR
1	A	663	ASP
1	A	677	CYS
1	A	679	LEU
1	A	680	SER
1	A	684	GLN

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Mol	Chain	Res	Type
1	A	689	ILE
1	A	691	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	447	HIS
1	A	467	ASN
1	A	485	HIS
1	A	512	HIS
1	A	532	GLN
1	A	554	ASN
1	A	598	ASN
1	A	624	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	PO4	A	1001	-	4,4,4	0.93	0	6,6,6	2.25	2 (33%)
2	349	A	999	-	39,41,41	2.16	11 (28%)	51,61,61	2.92	23 (45%)

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	349	A	999	-	-	10/27/42/42	0/5/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	999	349	C17-C18	6.07	1.53	1.39
2	A	999	349	S30-N33	5.03	1.70	1.63
2	A	999	349	C28-C29	3.76	1.43	1.39
2	A	999	349	C21-N22	3.64	1.40	1.34
2	A	999	349	C17-C15	3.61	1.54	1.41
2	A	999	349	C12-C13	-3.19	1.36	1.42
2	A	999	349	C8-N9	-3.01	1.34	1.38
2	A	999	349	C19-C18	-2.69	1.38	1.43
2	A	999	349	F3-C2	2.24	1.41	1.33
2	A	999	349	C13-N14	2.16	1.41	1.36
2	A	999	349	C35-C34	2.08	1.58	1.51

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	999	349	C12-C13-C18	-8.47	115.43	120.56
2	A	999	349	O31-S30-O32	6.48	129.70	119.59
2	A	999	349	C5-C6-N7	-6.36	115.62	124.18
2	A	999	349	C27-C26-C25	5.74	127.32	120.24
2	A	999	349	F1-C2-F4	4.50	122.00	105.77
2	A	999	349	C8-N9-C10	-4.40	119.02	127.69
2	A	999	349	F1-C2-C5	-4.39	104.86	112.65
2	A	999	349	C11-C12-C13	4.25	128.04	119.75
2	A	999	349	C28-C29-C24	4.13	125.01	121.40
3	A	1001	PO4	O4-P-O3	-4.05	95.33	107.91
2	A	999	349	C26-C27-C28	-3.99	115.31	120.24
2	A	999	349	C34-N33-S30	3.94	126.15	119.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	999	349	C37-N33-S30	3.67	125.71	119.81
2	A	999	349	F4-C2-C5	-3.59	106.28	112.65
2	A	999	349	O16-C15-C17	-3.53	120.47	130.26
3	A	1001	PO4	O4-P-O2	3.27	118.08	107.91
2	A	999	349	C5-C21-N20	-3.24	117.15	122.02
2	A	999	349	C24-C23-N22	-3.06	103.56	113.35
2	A	999	349	C36-C37-N33	3.01	108.91	103.52
2	A	999	349	C2-C5-C21	-2.83	116.44	120.06
2	A	999	349	O32-S30-C29	-2.71	102.10	107.35
2	A	999	349	C37-N33-C34	-2.46	107.81	111.22
2	A	999	349	O16-C15-N14	2.33	129.00	124.28
2	A	999	349	C26-C25-C24	-2.25	117.58	120.88
2	A	999	349	C19-C10-N9	-2.17	121.23	126.42

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	999	349	C28-C29-S30-N33
2	A	999	349	C24-C29-S30-N33
2	A	999	349	C37-N33-S30-O31
2	A	999	349	C37-N33-S30-C29
2	A	999	349	C37-N33-S30-O32
2	A	999	349	C24-C29-S30-O32
2	A	999	349	C24-C29-S30-O31
2	A	999	349	C34-N33-S30-O32
2	A	999	349	C28-C29-S30-O32
2	A	999	349	C28-C29-S30-O31

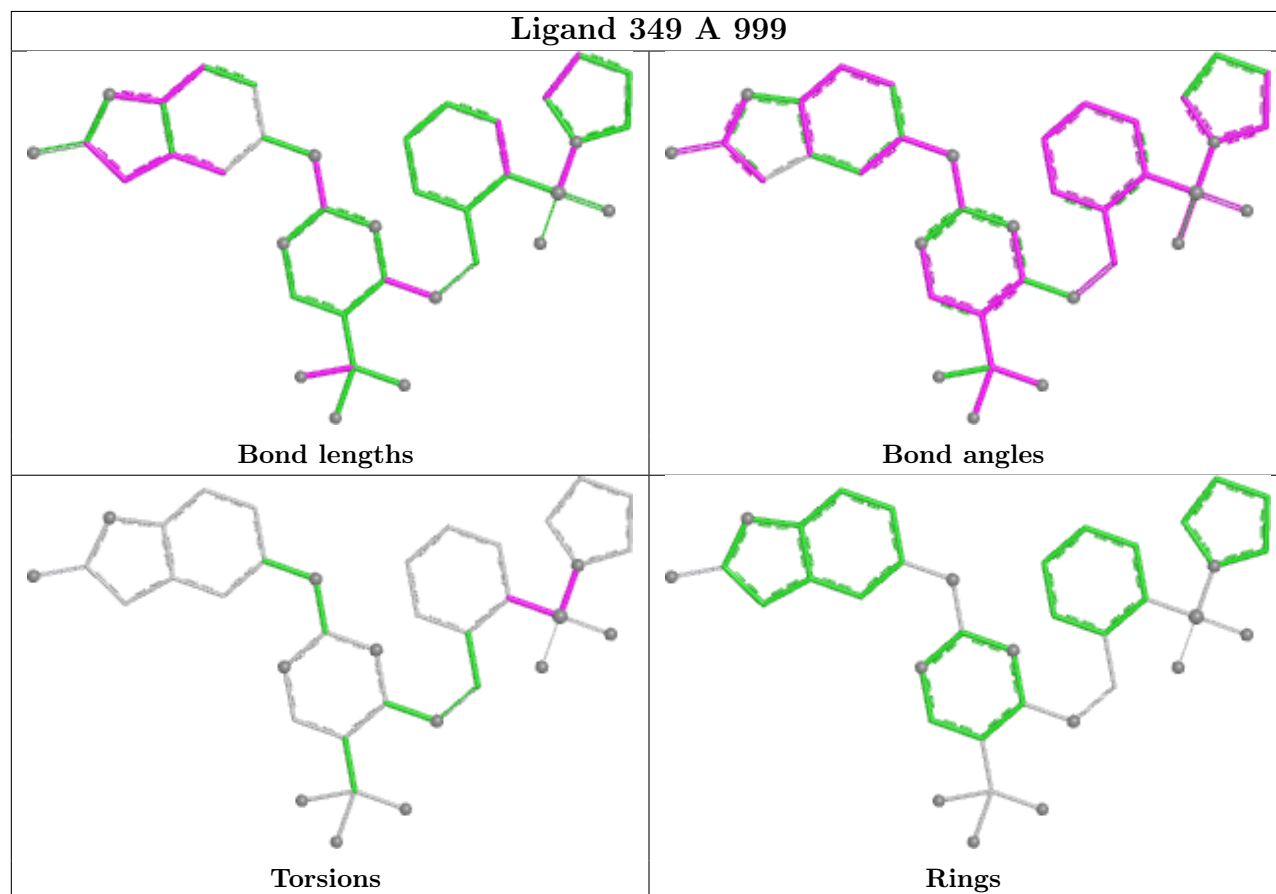
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	999	349	3	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 [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 [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	261/277 (94%)	0.15	13 (4%) 28 27	35, 60, 88, 97	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	447	HIS	4.9
1	A	585	THR	4.4
1	A	448	LYS	3.3
1	A	419	GLY	3.2
1	A	450	GLU	2.8
1	A	464	THR	2.7
1	A	463	CYS	2.6
1	A	691	MET	2.4
1	A	520	SER	2.3
1	A	435	PHE	2.3
1	A	614	CYS	2.2
1	A	516	ARG	2.2
1	A	632	LYS	2.2

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 monosaccharides in this entry.

6.4 Ligands [i](#)

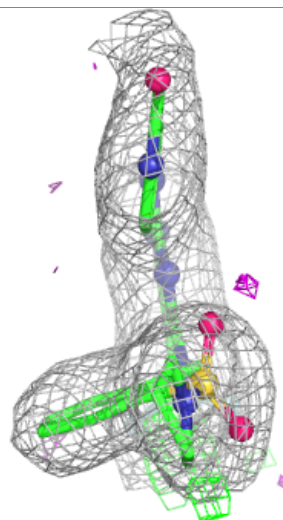
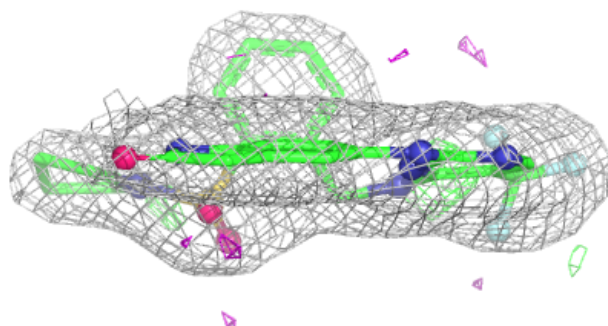
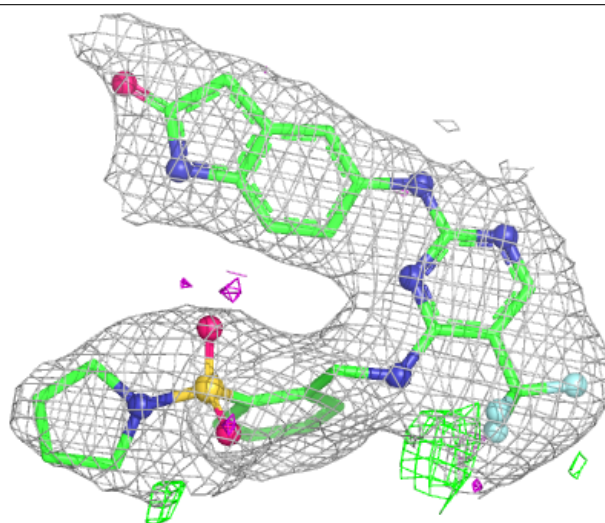
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PO4	A	1001	5/5	0.90	0.15	73,78,80,80	0
2	349	A	999	37/37	0.93	0.17	31,40,65,66	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 349 A 999:

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.