



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:27 PM UTC

PDB ID : 3ET7 / pdb_00003et7
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 : 4-5-2 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

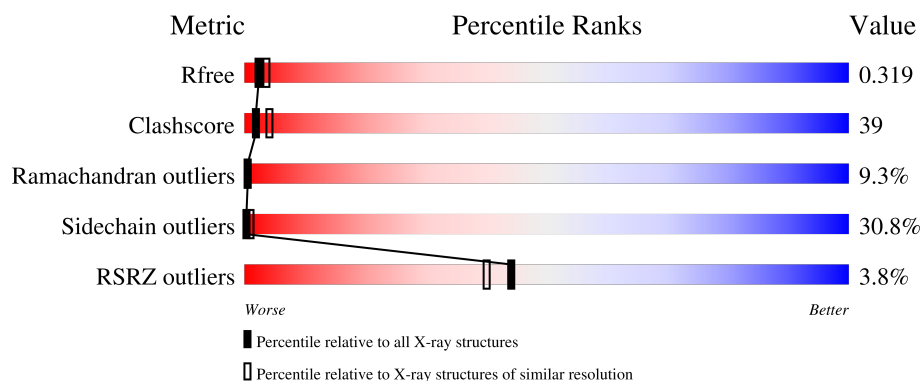
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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](#)

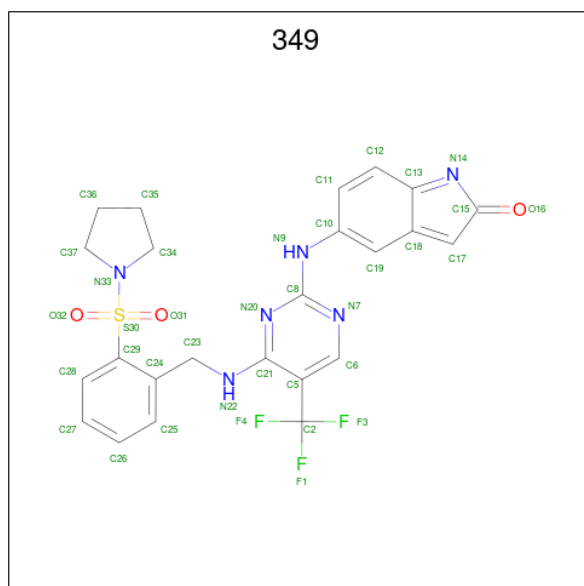
There are 4 unique types of molecules in this entry. The entry contains 2168 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	261	2114	1365	349	381	19	0	0	0

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



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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

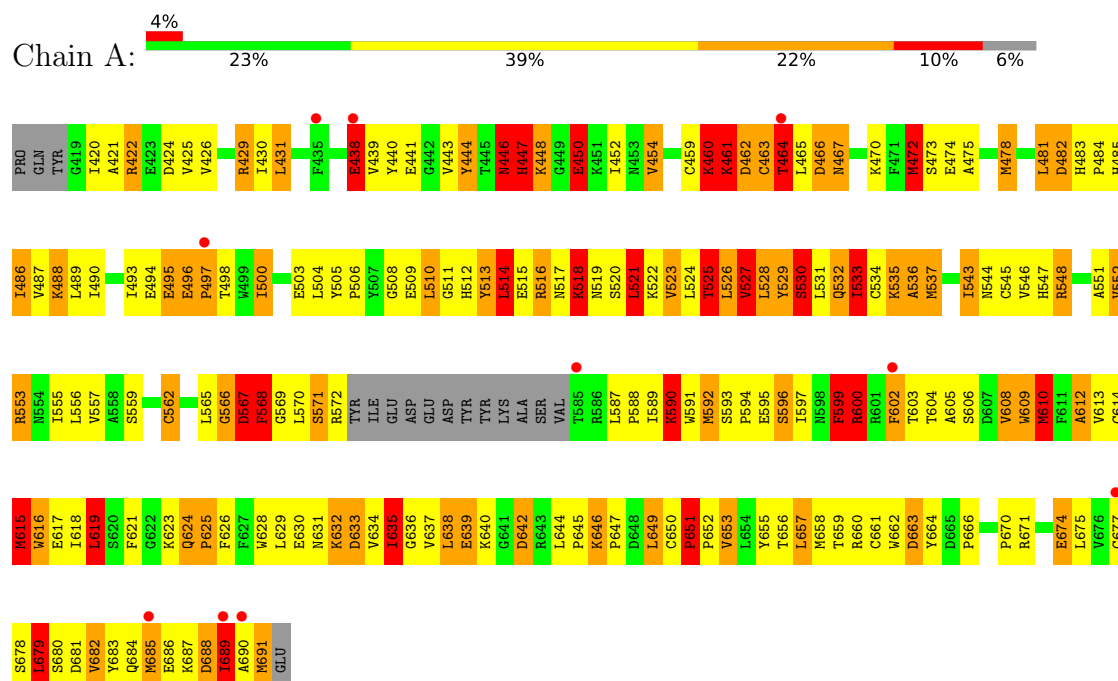
- Molecule 4 is water.

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 30.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.9 (30.00-2.70) 97.7 (30.00-2.70)	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 (4.71%)	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)	0.34 , 45.0	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

5.1 Standard geometry

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	1.79	38/2163 (1.8%)	1.83	56/2926 (1.9%)

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 (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	685	MET	SD-CE	12.19	2.10	1.79
1	A	537	MET	SD-CE	-10.80	1.52	1.79
1	A	545	CYS	CA-C	-8.43	1.42	1.52
1	A	527	VAL	CA-CB	8.04	1.65	1.54
1	A	658	MET	CG-SD	7.85	2.00	1.80
1	A	568	PHE	CA-C	-7.20	1.43	1.52
1	A	605	ALA	CA-CB	7.15	1.65	1.53
1	A	557	VAL	CA-CB	-7.04	1.45	1.54
1	A	528	LEU	CA-C	7.01	1.61	1.52
1	A	635	ILE	CA-CB	6.93	1.62	1.54
1	A	547	HIS	CA-C	-6.63	1.44	1.52
1	A	464	THR	CA-CB	6.60	1.64	1.53
1	A	525	THR	CA-CB	6.55	1.61	1.53
1	A	533	ILE	CA-CB	-6.32	1.47	1.54
1	A	680	SER	N-CA	-6.22	1.37	1.46
1	A	473	SER	N-CA	-6.21	1.39	1.46
1	A	472	MET	SD-CE	6.20	1.95	1.79
1	A	536	ALA	CA-CB	-6.16	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	670	PRO	C-O	-5.78	1.17	1.23
1	A	510	LEU	C-O	-5.60	1.16	1.24
1	A	618	ILE	CA-CB	-5.57	1.47	1.54
1	A	616	TRP	N-CA	-5.56	1.39	1.46
1	A	658	MET	SD-CE	-5.55	1.65	1.79
1	A	567	ASP	N-CA	5.53	1.53	1.46
1	A	553	ARG	NE-CZ	5.53	1.39	1.33
1	A	618	ILE	N-CA	-5.49	1.40	1.46
1	A	425	VAL	C-O	-5.40	1.18	1.24
1	A	609	TRP	CA-CB	-5.38	1.45	1.53
1	A	547	HIS	C-O	-5.32	1.18	1.24
1	A	546	VAL	N-CA	-5.28	1.39	1.46
1	A	603	THR	CA-C	-5.26	1.46	1.53
1	A	447	HIS	CA-C	5.25	1.59	1.52
1	A	500	ILE	CA-CB	5.24	1.60	1.54
1	A	478	MET	SD-CE	5.22	1.92	1.79
1	A	610	MET	C-O	-5.17	1.17	1.24
1	A	529	TYR	C-O	5.04	1.30	1.24
1	A	486	ILE	CA-C	-5.03	1.46	1.52
1	A	552	VAL	CA-C	5.02	1.60	1.53

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	606	SER	N-CA-C	-10.76	100.28	113.41
1	A	568	PHE	N-CA-C	-10.31	88.85	110.80
1	A	552	VAL	CB-CA-C	9.59	125.17	111.65
1	A	590	LYS	N-CA-C	-9.00	101.40	112.38
1	A	559	SER	N-CA-C	-8.96	100.07	108.13
1	A	653	VAL	CB-CA-C	-8.81	96.85	111.29
1	A	608	VAL	N-CA-C	-8.77	101.44	111.00
1	A	521	LEU	N-CA-C	8.12	122.94	109.46
1	A	628	TRP	N-CA-C	7.91	120.99	111.82
1	A	568	PHE	N-CA-CB	7.18	122.63	110.49
1	A	450	GLU	N-CA-C	7.05	120.92	110.48
1	A	534	CYS	CA-C-N	-6.85	109.90	120.31
1	A	534	CYS	C-N-CA	-6.85	109.90	120.31
1	A	658	MET	N-CA-C	-6.80	104.80	113.23
1	A	679	LEU	N-CA-C	-6.68	104.14	112.90
1	A	530	SER	CA-C-N	-6.67	111.76	120.44
1	A	530	SER	C-N-CA	-6.67	111.76	120.44
1	A	615	MET	N-CA-C	-6.63	104.13	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	656	THR	N-CA-C	-6.62	104.85	113.12
1	A	543	ILE	N-CA-C	-6.48	105.03	111.77
1	A	439	VAL	N-CA-C	-6.48	99.14	108.53
1	A	592	MET	N-CA-C	6.34	119.57	109.24
1	A	462	ASP	N-CA-C	6.18	119.02	109.07
1	A	553	ARG	CB-CA-C	-6.15	98.52	110.46
1	A	599	PHE	N-CA-C	6.14	120.80	112.88
1	A	617	GLU	N-CA-C	-6.09	104.72	111.36
1	A	651	PRO	N-CA-C	6.07	118.11	110.70
1	A	552	VAL	CA-C-N	5.95	129.07	120.38
1	A	552	VAL	C-N-CA	5.95	129.07	120.38
1	A	484	PRO	CA-C-N	-5.89	113.23	122.49
1	A	484	PRO	C-N-CA	-5.89	113.23	122.49
1	A	454	VAL	N-CA-C	5.83	117.47	108.44
1	A	614	CYS	N-CA-C	-5.79	104.94	112.23
1	A	446	ASN	N-CA-C	5.75	118.81	110.42
1	A	431	LEU	N-CA-C	5.72	117.20	110.97
1	A	421	ALA	N-CA-C	5.59	118.68	109.85
1	A	612	ALA	N-CA-C	-5.58	105.10	111.07
1	A	619	LEU	N-CA-C	-5.52	106.53	113.20
1	A	426	VAL	CB-CA-C	5.45	118.67	111.21
1	A	444	TYR	N-CA-C	-5.42	103.75	110.41
1	A	556	LEU	CA-CB-CG	-5.40	97.39	116.30
1	A	511	GLY	N-CA-C	-5.38	106.26	112.50
1	A	625	PRO	CA-C-O	-5.38	115.40	121.43
1	A	551	ALA	CA-C-N	-5.37	112.50	120.82
1	A	551	ALA	C-N-CA	-5.37	112.50	120.82
1	A	642	ASP	N-CA-C	5.35	117.47	108.96
1	A	568	PHE	CB-CA-C	-5.24	99.99	110.42
1	A	652	PRO	CA-C-O	-5.20	111.13	120.60
1	A	508	GLY	N-CA-C	5.17	123.33	112.17
1	A	424	ASP	N-CA-C	5.15	119.19	113.01
1	A	571	SER	N-CA-C	5.12	116.07	108.60
1	A	459	CYS	N-CA-C	5.11	117.25	107.75
1	A	431	LEU	CA-CB-CG	-5.07	98.55	116.30
1	A	680	SER	CB-CA-C	5.04	120.05	110.27
1	A	674	GLU	N-CA-C	5.01	117.40	111.33
1	A	569	GLY	N-CA-C	-5.01	108.73	114.69

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	167	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	169	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 39.

All (169) 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: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:523:VAL:C	2.25	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:567:ASP:HA	1:A:570:LEU:HD12	1.72	0.72
1:A:448:LYS:HG2	1:A:448:LYS:O	1.87	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
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:548:ARG:O	1:A:610:MET:HE1	1.90	0.70
1:A:619:LEU:HD23	1:A:619:LEU:N	2.06	0.69
1:A:524:LEU:O	1:A:524:LEU:HG	1.89	0.69
1:A:523:VAL:HG22	1:A:649:LEU:HB3	1.74	0.69
1:A:567:ASP:O	1:A:567:ASP:CG	2.35	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:HD21	1.74	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: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:517:ASN:C	1:A:519:ASN:H	2.06	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:537:MET:CE	1:A:565:LEU:HD21	2.30	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:LYS:HB2	1:A:505:TYR:OH	2.03	0.58
1:A:485:HIS:CE1	1:A:532:GLN:HE21	2.17	0.57
1:A:681:ASP:C	1:A:683:TYR:H	2.12	0.57
1:A:465:LEU:O	1:A:466:ASP:C	2.47	0.57
1:A:587:LEU:O	1:A:589:ILE:N	2.36	0.57
1:A:688:ASP:C	1:A:690:ALA:H	2.13	0.57
1:A:430:ILE:HG12	1:A:440:TYR:HE2	1.70	0.57
1:A:537:MET:HE3	1:A:565:LEU:CD2	2.35	0.56
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:513:TYR:CD2	1:A:513:TYR:C	2.84	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
1:A:509:GLU:HG2	1:A:553:ARG:O	2.09	0.53
1:A:463:CYS:O	1:A:464:THR:C	2.51	0.53
1:A:537:MET:HA	1:A:537:MET:HE2	1.90	0.53
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:530:SER:O	1:A:531:LEU:C	2.51	0.52
1:A:609:TRP:C	1:A:609:TRP:CD1	2.88	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:493:ILE:O	1:A:498:THR:HA	2.10	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:537:MET:HE3	1:A:565:LEU:HD22	1.94	0.49
1:A:533:ILE:O	1:A:536:ALA:N	2.46	0.49
1:A:592:MET:HE2	1:A:597:ILE:HG12	1.95	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:537:MET:HE2	1:A:537:MET:CA	2.43	0.48
1:A:429:ARG:HD3	1:A:441:GLU:HB3	1.95	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:516:ARG:O	1:A:517:ASN:CG	2.56	0.48
1:A:567:ASP:OD1	1:A:567:ASP:C	2.53	0.48
1:A:510:LEU:HB3	1:A:552:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:517:ASN:C	1:A:519:ASN:N	2.69	0.47
1:A:609:TRP:CE3	1:A:662:TRP:HA	2.49	0.47
1:A:537:MET:HE2	1:A:537:MET:N	2.30	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: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:537:MET:HE1	1:A:565:LEU:CD2	2.39	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:465:LEU:C	1:A:467:ASN:N	2.73	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:688:ASP:O	1:A:689:ILE:C	2.56	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
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:681:ASP:C	1:A:683:TYR:N	2.74	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:589:ILE:C	1:A:591:TRP:N	2.71	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:523:VAL:O	1:A:524:LEU:C	2.60	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:523:VAL:C	1:A:525:THR:N	2.75	0.43
1:A:688:ASP:C	1:A:690:ALA:N	2.66	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:522:LYS:C	1:A:524:LEU:N	2.78	0.42
1:A:523:VAL:C	1:A:525:THR:H	2.27	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:474:GLU:CD	1:A:567:ASP:OD1	2.63	0.42
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:615:MET:O	1:A:616:TRP:C	2.63	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: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
1:A:512:HIS:O	1:A:516:ARG:HG2	2.21	0.40
1:A:593:SER:O	1:A:594:PRO:C	2.63	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 ⓘ

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	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
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 [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	237/252 (94%)	164 (69%)	73 (31%)	0 1

All (73) 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	450	GLU
1	A	452	ILE
1	A	454	VAL
1	A	461	LYS
1	A	463	CYS
1	A	464	THR
1	A	467	ASN
1	A	470	LYS
1	A	472	MET
1	A	478	MET
1	A	481	LEU
1	A	488	LYS
1	A	489	LEU
1	A	494	GLU
1	A	495	GLU
1	A	500	ILE
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	527	VAL
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	555	ILE
1	A	567	ASP
1	A	572	ARG

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Mol	Chain	Res	Type
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	604	THR
1	A	608	VAL
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	646	LYS
1	A	649	LEU
1	A	653	VAL
1	A	657	LEU
1	A	659	THR
1	A	663	ASP
1	A	666	PRO
1	A	671	ARG
1	A	677	CYS
1	A	679	LEU
1	A	684	GLN
1	A	687	LYS
1	A	689	ILE
1	A	691	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	447	HIS
1	A	467	ASN
1	A	485	HIS

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Mol	Chain	Res	Type
1	A	512	HIS
1	A	517	ASN
1	A	532	GLN
1	A	544	ASN
1	A	554	ASN
1	A	598	ASN
1	A	624	GLN

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 ⓘ

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	$\# Z > 2$
2	349	A	999	-	38,41,41	1.89	9 (23%)	51,61,61	2.76	22 (43%)
3	PO4	A	1001	-	4,4,4	0.93	0	6,6,6	2.25	2 (33%)

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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	-3.34	1.36	1.40
2	A	999	349	C11-C10	-2.33	1.35	1.39
2	A	999	349	C13-C18	-2.24	1.39	1.43
2	A	999	349	F3-C2	2.24	1.41	1.33
2	A	999	349	C35-C34	2.08	1.58	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	C11-C12-C13	6.05	128.04	120.80
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	F1-C2-C5	-4.39	104.86	112.65
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
2	A	999	349	C10-N9-C8	-3.84	119.02	129.38
2	A	999	349	C12-C11-C10	-3.67	116.07	120.30
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	999	349	C26-C25-C24	-2.25	117.58	120.88

There are no chirality outliers.

All (10) torsion outliers are listed below:

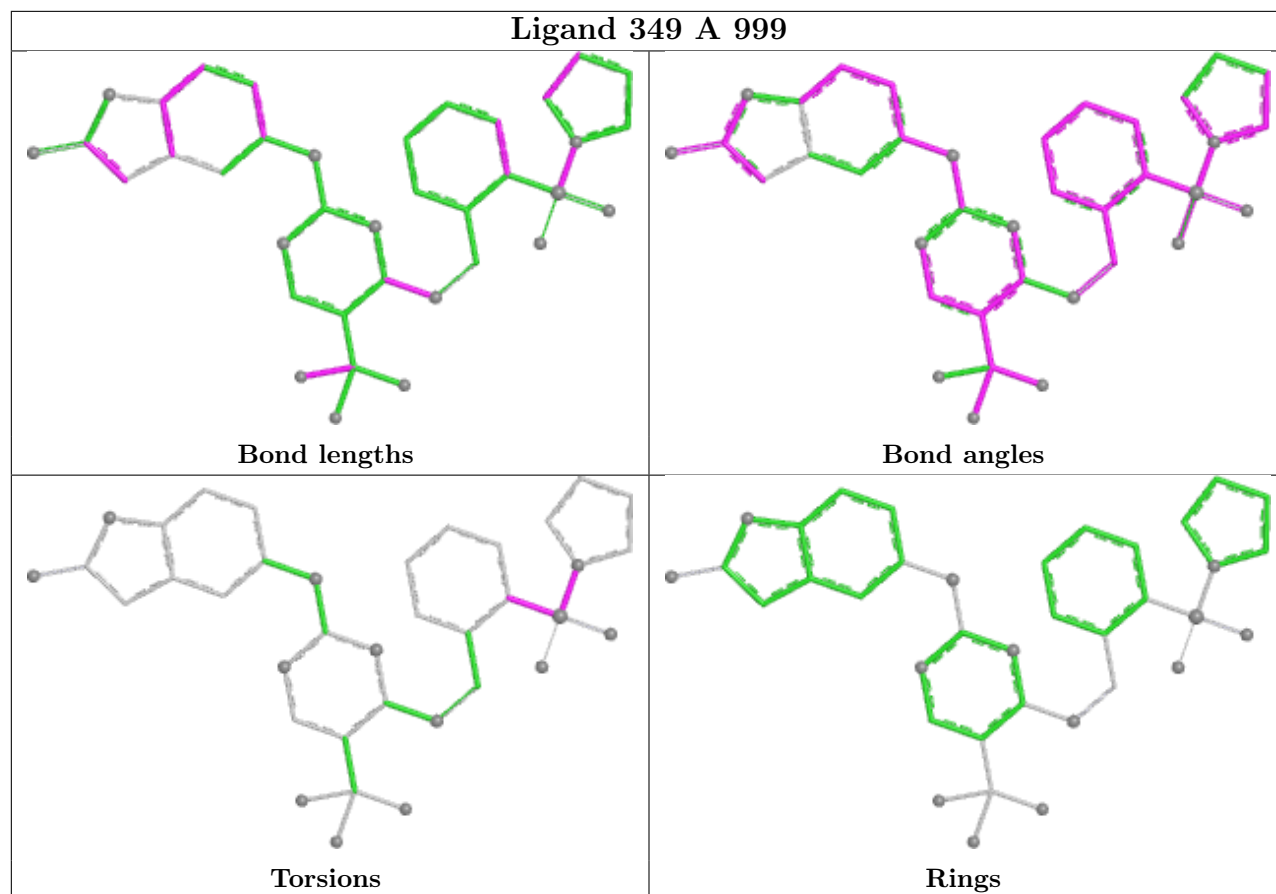
Mol	Chain	Res	Type	Atoms
2	A	999	349	C28-C29-S30-N33
2	A	999	349	C24-C29-S30-N33
2	A	999	349	C37-N33-S30-O31
2	A	999	349	C37-N33-S30-C29
2	A	999	349	C37-N33-S30-O32
2	A	999	349	C24-C29-S30-O32
2	A	999	349	C24-C29-S30-O31
2	A	999	349	C34-N33-S30-O32
2	A	999	349	C28-C29-S30-O32
2	A	999	349	C28-C29-S30-O31

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%)	0.41	10 (3%) 44 40	35, 60, 88, 97	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	464	THR	5.1
1	A	435	PHE	2.9
1	A	677	CYS	2.7
1	A	689	ILE	2.6
1	A	497	PRO	2.4
1	A	602	PHE	2.3
1	A	438	GLU	2.3
1	A	585	THR	2.2
1	A	690	ALA	2.1
1	A	685	MET	2.1

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](#)

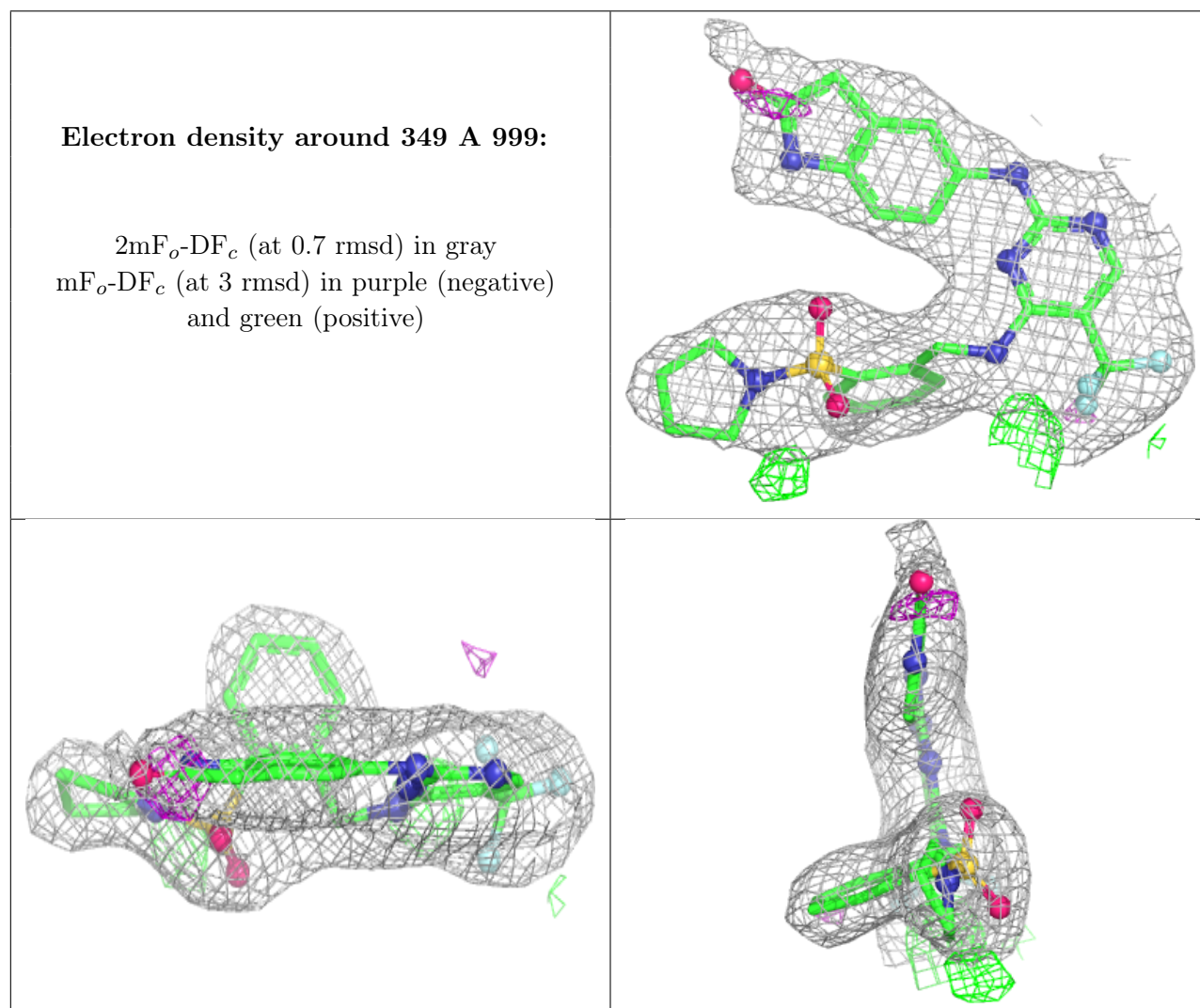
There are no oligosaccharides in this entry.

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
3	PO4	A	1001	5/5	0.89	0.12	73,78,80,80	0
2	349	A	999	37/37	0.93	0.10	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.