



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 07:00 AM UTC

PDB ID : 7QG3 / pdb_00007qg3
Title : IRAK4 in complex with inhibitor
Authors : Xue, Y.; Aagaard, A.; Robb, G.R.; Degorce, S.L.
Deposited on : 2021-12-07
Resolution : 2.11 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

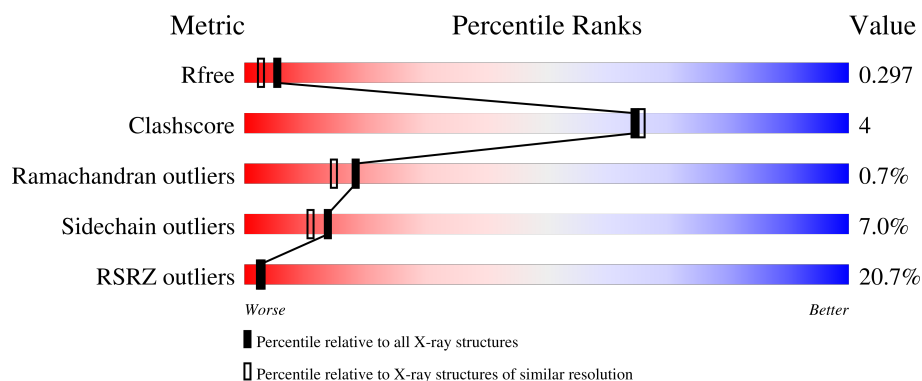
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	308	21% 77% 12% 10%
1	B	308	17% 75% 15% 8%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4548 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.

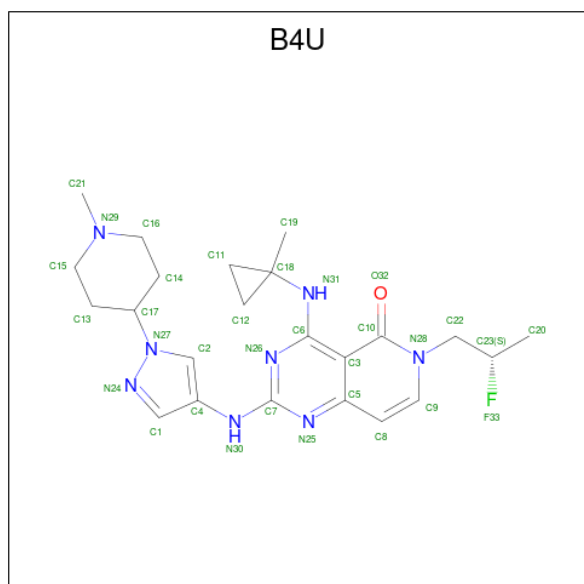
- Molecule 1 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	P	S	0	0	0
			2214	1391	372	434	3	14			
1	B	283	Total	C	N	O	P	S	0	0	0
			2238	1404	377	441	2	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	GLY	-	expression tag	UNP Q9NWZ3
B	153	GLY	-	expression tag	UNP Q9NWZ3

- Molecule 2 is 6-[(2 {S})-2-fluoranylpropyl]-4-[(1-methylcyclopropyl)amino]-2-[[1-(1-methylpiperidin-4-yl)pyrazol-4-yl]amino]pyrido[4,3-d]pyrimidin-5-one (CCD ID: B4U) (formula: C₂₃H₃₁FN₈O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			33	23	1	8	1		
2	B	1	Total	C	F	N	O	0	0
			33	23	1	8	1		

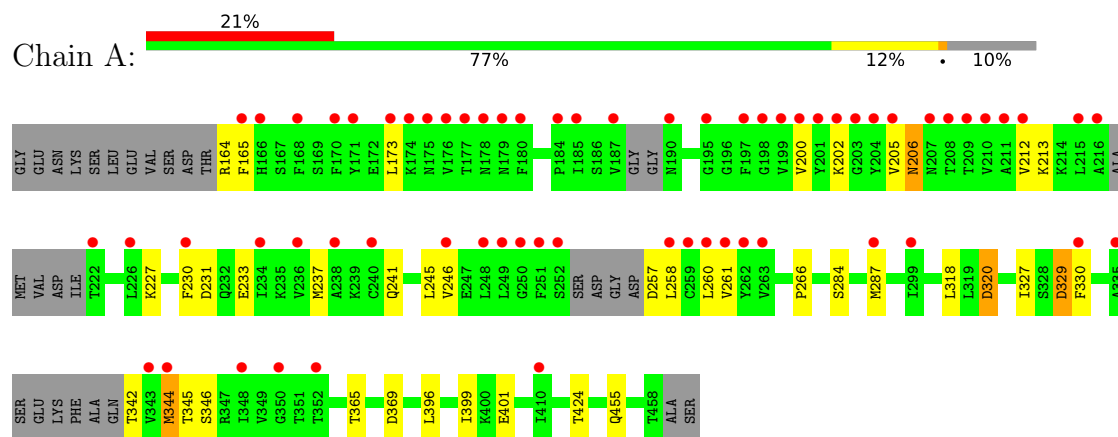
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	14	Total	O	0	0
			14	14		

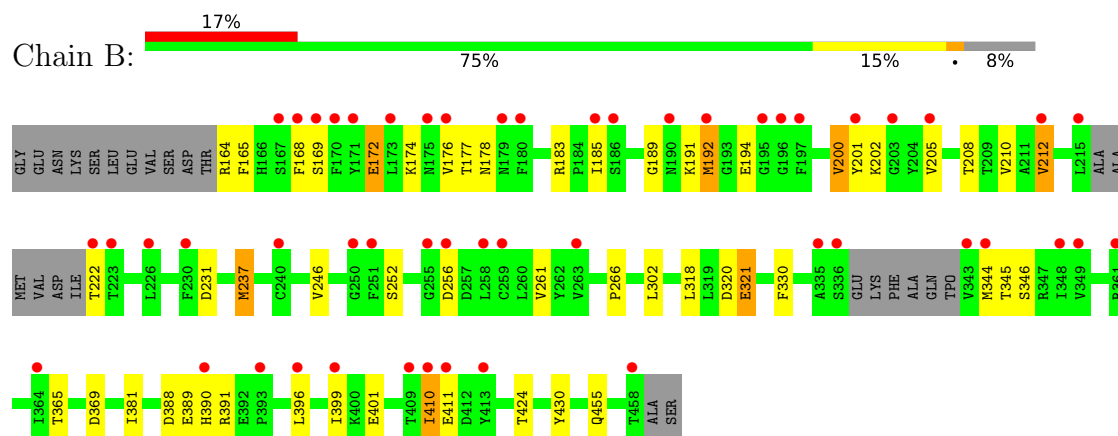
3 Residue-property plots [i](#)

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: Interleukin-1 receptor-associated kinase 4



- Molecule 1: Interleukin-1 receptor-associated kinase 4



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	87.33Å 110.71Å 142.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.42 – 2.11 44.42 – 2.11	Depositor EDS
% Data completeness (in resolution range)	93.3 (44.42-2.11) 93.8 (44.42-2.11)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.12Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.272 , 0.304 0.269 , 0.297	Depositor DCC
R_{free} test set	1886 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	52.3	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4548	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.5767e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: TPO, B4U, SEP

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	0.85	0/2216	1.36	5/2982 (0.2%)
1	B	0.89	1/2253 (0.0%)	1.39	12/3034 (0.4%)
All	All	0.87	1/4469 (0.0%)	1.37	17/6016 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	192	MET	SD-CE	-5.65	1.65	1.79

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	390	HIS	CA-C-N	6.32	132.68	121.75
1	B	390	HIS	C-N-CA	6.32	132.68	121.75
1	B	168	PHE	CA-CB-CG	5.81	119.61	113.80
1	A	320	ASP	CA-C-N	5.65	129.65	120.60
1	A	320	ASP	C-N-CA	5.65	129.65	120.60
1	B	172	GLU	CA-C-N	5.49	130.01	120.68
1	B	172	GLU	C-N-CA	5.49	130.01	120.68
1	A	230	PHE	CA-CB-CG	5.44	119.24	113.80
1	B	212	VAL	N-CA-CB	5.41	117.54	111.21
1	B	410	ILE	CA-C-N	5.29	127.90	120.28
1	B	410	ILE	C-N-CA	5.29	127.90	120.28
1	A	369	ASP	CA-CB-CG	5.26	117.86	112.60
1	B	369	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	401	GLU	CB-CG-CD	5.25	121.52	112.60
1	B	401	GLU	CB-CG-CD	5.20	121.44	112.60
1	B	174	LYS	CA-C-N	5.04	127.53	120.28
1	B	174	LYS	C-N-CA	5.04	127.53	120.28

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	2214	0	2186	11	0
1	B	2238	0	2202	22	0
2	A	33	0	0	1	0
2	B	33	0	0	1	0
3	A	16	0	0	0	0
3	B	14	0	0	0	0
All	All	4548	0	4388	35	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 4.

All (35) 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:284:SER:H	1:A:287:MET:HE3	1.43	0.84
1:B:266:PRO:HG2	1:B:321:GLU:HG3	1.59	0.83
1:B:183:ARG:HG3	1:B:189:GLY:HA3	1.69	0.73
1:B:192:MET:HE2	1:B:201:TYR:C	2.16	0.71
1:B:381:ILE:HG21	1:B:410:ILE:HD11	1.80	0.62
1:B:183:ARG:HG3	1:B:189:GLY:CA	2.31	0.60
1:A:245:LEU:HD23	1:A:327:ILE:HB	1.84	0.59
1:B:246:VAL:HG11	1:B:318:LEU:HD12	1.84	0.57
1:B:302:LEU:HD11	1:B:330:PHE:HE1	1.70	0.57
1:B:321:GLU:H	1:B:321:GLU:CD	2.15	0.55
1:B:176:VAL:HG11	1:B:205:VAL:HG22	1.90	0.52
1:A:165:PHE:HZ	1:A:241:GLN:CD	2.20	0.49
1:B:388:ASP:HB3	1:B:391:ARG:HB3	1.94	0.49
1:B:192:MET:HE3	1:B:200:VAL:HG12	1.95	0.48
1:B:192:MET:CE	1:B:200:VAL:HG12	2.45	0.47
1:B:410:ILE:HD13	1:B:430:TYR:CD1	2.49	0.47
1:B:266:PRO:HD2	1:B:320:ASP:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:B4U:C1	2:B:501:B4U:N26	2.78	0.46
1:A:246:VAL:HG21	1:A:318:LEU:HD12	1.99	0.45
1:B:396:LEU:O	1:B:399:ILE:HG12	2.17	0.45
1:A:396:LEU:O	1:A:399:ILE:HG12	2.16	0.45
1:A:266:PRO:HD2	1:A:320:ASP:HA	1.98	0.45
2:A:501:B4U:N26	2:A:501:B4U:C1	2.80	0.44
1:B:176:VAL:HG11	1:B:205:VAL:CG2	2.48	0.43
1:B:185:ILE:HD13	1:B:192:MET:HG2	2.00	0.43
1:B:169:SER:HB3	1:B:172:GLU:HG3	2.01	0.43
1:A:237:MET:HE2	1:A:330:PHE:HD2	1.84	0.43
1:A:227:LYS:HG2	1:A:258:LEU:HD11	2.00	0.42
1:B:237:MET:HA	1:B:237:MET:CE	2.50	0.42
1:A:344:MET:HE3	1:A:344:MET:HB3	1.94	0.42
1:A:213:LYS:HB3	1:A:260:LEU:HB2	2.01	0.42
1:B:192:MET:HE2	1:B:202:LYS:N	2.35	0.42
1:A:284:SER:OG	1:A:287:MET:HG3	2.21	0.41
1:B:164:ARG:HB3	1:B:165:PHE:H	1.74	0.40
1:B:176:VAL:HG23	1:B:177:THR:HG23	2.02	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	266/308 (86%)	253 (95%)	10 (4%)	3 (1%)	11	7
1	B	275/308 (89%)	260 (94%)	14 (5%)	1 (0%)	30	28
All	All	541/616 (88%)	513 (95%)	24 (4%)	4 (1%)	18	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	ASP
1	A	206	ASN
1	B	252	SER
1	A	205	VAL

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	242/265 (91%)	227 (94%)	15 (6%)	16	14
1	B	246/265 (93%)	227 (92%)	19 (8%)	12	9
All	All	488/530 (92%)	454 (93%)	34 (7%)	14	11

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	ARG
1	A	173	LEU
1	A	200	VAL
1	A	202	LYS
1	A	206	ASN
1	A	212	VAL
1	A	231	ASP
1	A	233	GLU
1	A	257	ASP
1	A	261	VAL
1	A	329	ASP
1	A	344	MET
1	A	365	THR
1	A	424	THR
1	A	455	GLN
1	B	178	ASN
1	B	191	LYS
1	B	194	GLU
1	B	200	VAL
1	B	208	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	210	VAL
1	B	212	VAL
1	B	222	THR
1	B	231	ASP
1	B	237	MET
1	B	256	ASP
1	B	261	VAL
1	B	321	GLU
1	B	344	MET
1	B	365	THR
1	B	389	GLU
1	B	411	GLU
1	B	424	THR
1	B	455	GLN

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	229	GLN
1	A	300	ASN
1	A	394	GLN
1	A	451	GLN
1	B	175	ASN
1	B	229	GLN
1	B	300	ASN
1	B	451	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

5 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPO	A	345	1	8,10,11	1.31	1 (12%)	10,14,16	1.19	1 (10%)
1	SEP	A	346	1	8,9,10	0.87	0	7,12,14	4.49	2 (28%)
1	TPO	A	342	1	8,10,11	1.41	1 (12%)	10,14,16	1.18	1 (10%)
1	SEP	B	346	1	8,9,10	0.77	0	7,12,14	4.81	2 (28%)
1	TPO	B	345	1	8,10,11	1.20	1 (12%)	10,14,16	1.24	1 (10%)

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
1	TPO	A	345	1	-	3/9/11/13	-
1	SEP	A	346	1	-	5/6/8/10	-
1	TPO	A	342	1	-	1/9/11/13	-
1	SEP	B	346	1	-	5/6/8/10	-
1	TPO	B	345	1	-	3/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	342	TPO	P-OG1	-2.59	1.55	1.59
1	A	345	TPO	CB-CA	2.52	1.59	1.53
1	B	345	TPO	CB-CA	2.30	1.58	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	SEP	OG-CB-CA	11.90	119.72	108.14
1	A	346	SEP	OG-CB-CA	11.20	119.04	108.14
1	B	346	SEP	O3P-P-OG	4.36	118.03	106.67
1	A	346	SEP	O3P-P-OG	3.67	116.24	106.67
1	B	345	TPO	O3P-P-OG1	2.98	117.45	105.85
1	A	345	TPO	O3P-P-OG1	2.54	115.76	105.85
1	A	342	TPO	O2P-P-OG1	2.46	115.45	105.85

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	346	SEP	N-CA-CB-OG
1	A	346	SEP	C-CA-CB-OG
1	A	346	SEP	CB-OG-P-O2P
1	A	346	SEP	CB-OG-P-O3P
1	B	345	TPO	N-CA-CB-OG1
1	B	346	SEP	N-CA-CB-OG
1	B	346	SEP	C-CA-CB-OG
1	B	346	SEP	CB-OG-P-O2P
1	B	346	SEP	CB-OG-P-O3P
1	A	346	SEP	CB-OG-P-O1P
1	B	346	SEP	CB-OG-P-O1P
1	A	345	TPO	CB-OG1-P-O1P
1	B	345	TPO	CB-OG1-P-O1P
1	A	345	TPO	O-C-CA-CB
1	B	345	TPO	O-C-CA-CB
1	A	342	TPO	CB-OG1-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
2	B4U	A	501	-	33,37,37	0.93	2 (6%)	33,55,55	1.95	10 (30%)
2	B4U	B	501	-	33,37,37	0.80	2 (6%)	33,55,55	1.61	8 (24%)

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	B4U	A	501	-	-	1/16/31/31	0/5/5/5
2	B4U	B	501	-	-	1/16/31/31	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	B4U	C22-N28	-2.71	1.44	1.47
2	B	501	B4U	C19-C18	-2.15	1.49	1.53
2	A	501	B4U	C19-C18	-2.03	1.49	1.53
2	B	501	B4U	C7-N30	2.01	1.41	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	B4U	C14-C17-N27	5.53	118.53	110.95
2	A	501	B4U	C2-N27-N24	3.91	115.09	112.45
2	B	501	B4U	C13-C17-N27	3.59	115.86	110.95
2	A	501	B4U	C13-C17-N27	3.55	115.82	110.95
2	A	501	B4U	C11-C18-N31	3.30	120.07	115.60
2	A	501	B4U	C17-N27-N24	-3.18	116.07	120.41
2	B	501	B4U	C13-C15-N29	-3.06	107.25	111.20
2	B	501	B4U	C14-C17-N27	3.05	115.13	110.95
2	B	501	B4U	C14-C16-N29	-3.01	107.31	111.20
2	A	501	B4U	C16-N29-C15	2.57	113.63	109.54
2	B	501	B4U	O32-C10-N28	2.55	123.82	120.77
2	B	501	B4U	C17-N27-N24	-2.46	117.04	120.41
2	B	501	B4U	O32-C10-C3	-2.36	119.30	124.19
2	A	501	B4U	C15-C13-C17	-2.34	106.49	110.78
2	A	501	B4U	C21-N29-C16	-2.31	106.24	110.63
2	A	501	B4U	C21-N29-C15	-2.26	106.33	110.63
2	A	501	B4U	C1-N24-N27	-2.20	103.00	104.14
2	B	501	B4U	C2-N27-N24	2.12	113.88	112.45

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	B4U	C2-C4-N30-C7

Continued on next page...

Continued from previous page...

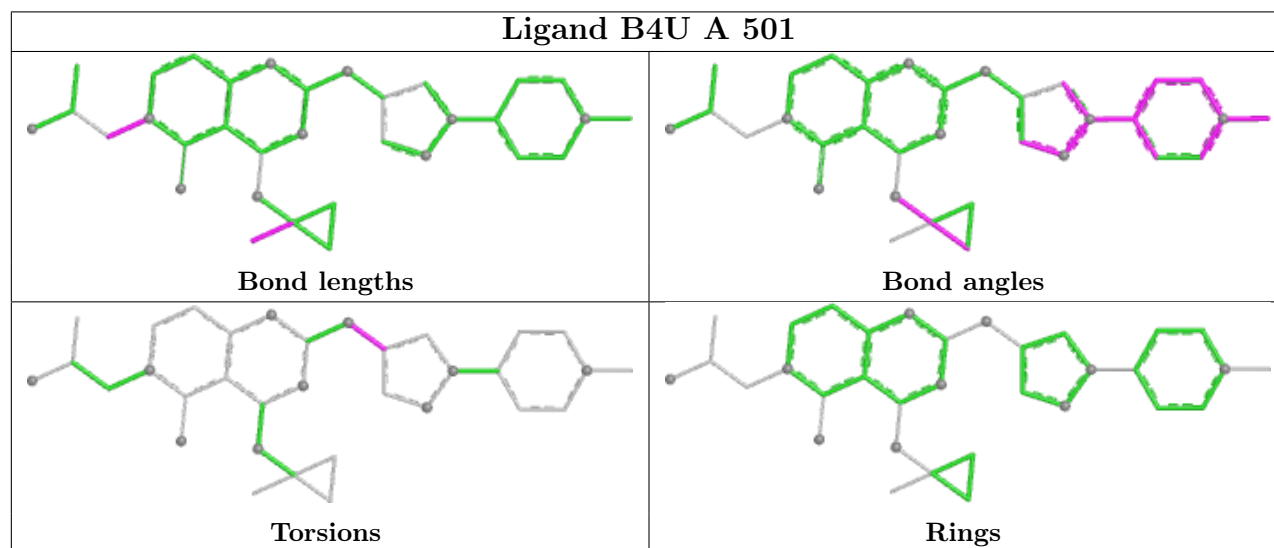
Mol	Chain	Res	Type	Atoms
2	B	501	B4U	C2-C4-N30-C7

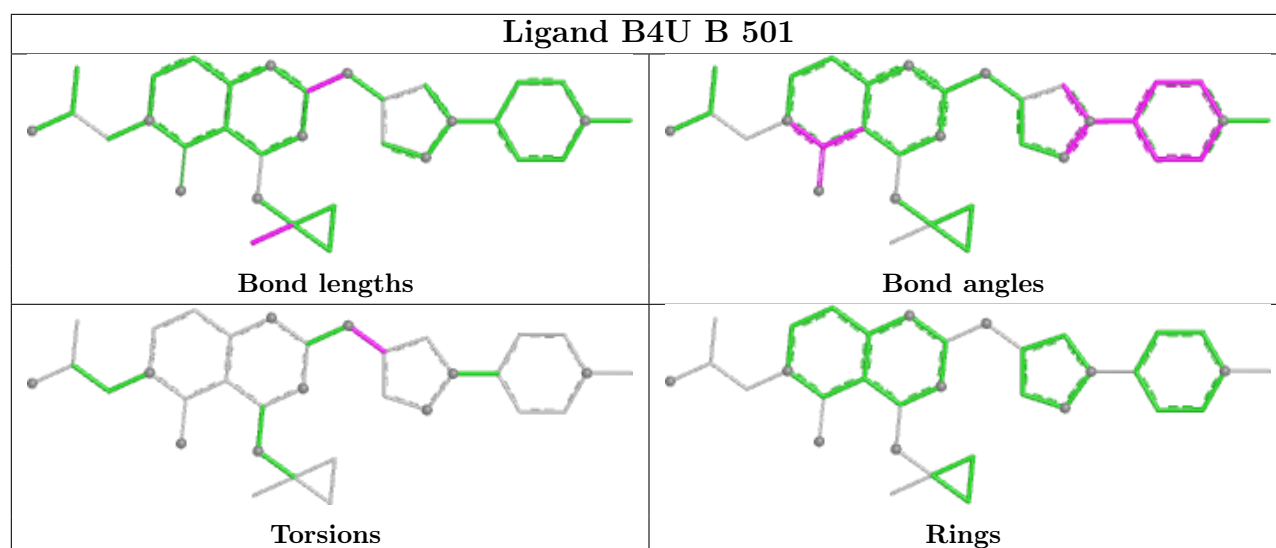
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	B4U	1	0
2	B	501	B4U	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	275/308 (89%)	1.18	64 (23%) 2 2	38, 69, 148, 163	0
1	B	281/308 (91%)	1.06	51 (18%) 3 4	40, 68, 111, 144	0
All	All	556/616 (90%)	1.12	115 (20%) 2 3	38, 69, 143, 163	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	173	LEU	5.9
1	A	252	SER	5.2
1	B	176	VAL	4.9
1	B	343	VAL	4.8
1	A	251	PHE	4.8
1	B	170	PHE	4.6
1	A	260	LEU	4.5
1	B	258	LEU	4.5
1	A	250	GLY	4.4
1	A	200	VAL	4.4
1	B	259	CYS	4.2
1	A	212	VAL	4.2
1	A	230	PHE	4.1
1	A	261	VAL	4.1
1	B	226	LEU	4.0
1	A	165	PHE	3.9
1	A	180	PHE	3.9
1	A	238	ALA	3.9
1	A	168	PHE	3.8
1	A	185	ILE	3.8
1	B	201	TYR	3.8
1	A	171	TYR	3.7
1	A	170	PHE	3.7
1	A	249	LEU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	251	PHE	3.7
1	B	256	ASP	3.7
1	B	168	PHE	3.6
1	A	236	VAL	3.6
1	A	187	VAL	3.5
1	A	211	ALA	3.4
1	A	216	ALA	3.4
1	A	215	LEU	3.4
1	A	246	VAL	3.4
1	A	343	VAL	3.3
1	A	175	ASN	3.3
1	A	179	ASN	3.3
1	A	199	VAL	3.3
1	B	399	ILE	3.2
1	B	185	ILE	3.2
1	A	335	ALA	3.1
1	A	410	ILE	3.1
1	A	174	LYS	3.1
1	A	240	CYS	3.1
1	A	205	VAL	3.1
1	B	205	VAL	3.1
1	B	336	SER	3.0
1	B	458	THR	3.0
1	B	230	PHE	3.0
1	A	176	VAL	3.0
1	A	248	LEU	3.0
1	A	207	ASN	3.0
1	A	226	LEU	2.9
1	A	210	VAL	2.9
1	B	250	GLY	2.9
1	B	255	GLY	2.9
1	B	192	MET	2.8
1	A	178	ASN	2.8
1	B	173	LEU	2.8
1	B	196	GLY	2.8
1	B	167	SER	2.7
1	A	258	LEU	2.7
1	A	197	PHE	2.7
1	A	262	TYR	2.7
1	B	344	MET	2.7
1	B	222	THR	2.6
1	B	169	SER	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	390	HIS	2.6
1	A	177	THR	2.6
1	A	202	LYS	2.6
1	B	195	GLY	2.6
1	A	201	TYR	2.5
1	A	204	TYR	2.5
1	B	393	PRO	2.5
1	A	209	THR	2.5
1	B	197	PHE	2.5
1	B	179	ASN	2.5
1	B	364	ILE	2.4
1	B	171	TYR	2.4
1	B	409	THR	2.4
1	A	344	MET	2.4
1	A	208	THR	2.4
1	A	222	THR	2.4
1	B	175	ASN	2.3
1	A	299	ILE	2.3
1	B	411	GLU	2.3
1	A	234	ILE	2.3
1	B	263	VAL	2.3
1	A	348	ILE	2.2
1	A	259	CYS	2.2
1	B	180	PHE	2.2
1	B	335	ALA	2.2
1	B	413	TYR	2.2
1	B	361	ARG	2.2
1	B	410	ILE	2.2
1	B	349	VAL	2.2
1	A	195	GLY	2.2
1	A	350	GLY	2.2
1	A	166	HIS	2.2
1	B	396	LEU	2.2
1	A	190	ASN	2.2
1	A	287	MET	2.2
1	A	263	VAL	2.1
1	B	212	VAL	2.1
1	B	203	GLY	2.1
1	B	186	SER	2.1
1	B	190	ASN	2.1
1	B	215	LEU	2.1
1	B	240	CYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	352	THR	2.1
1	B	348	ILE	2.1
1	A	184	PRO	2.0
1	A	198	GLY	2.0
1	A	203	GLY	2.0
1	A	330	PHE	2.0
1	B	223	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	SEP	A	346	10/11	0.20	0.20	134,135,137,137	0
1	SEP	B	346	10/11	0.36	0.14	130,132,136,136	0
1	TPO	A	342	11/12	0.37	0.17	142,143,144,144	4
1	TPO	B	345	11/12	0.68	0.15	130,133,136,136	0
1	TPO	A	345	11/12	0.74	0.14	134,135,138,139	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

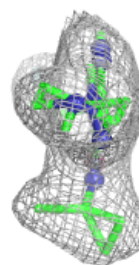
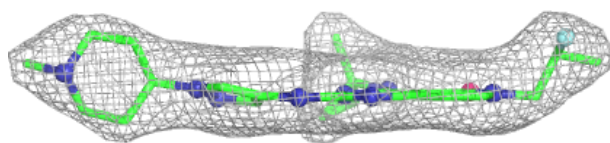
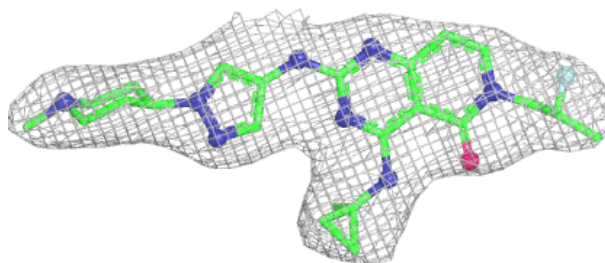
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	B4U	A	501	33/33	0.90	0.11	58,62,69,71	0
2	B4U	B	501	33/33	0.93	0.10	33,48,68,69	0

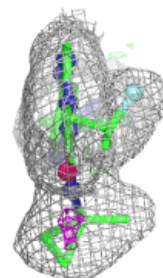
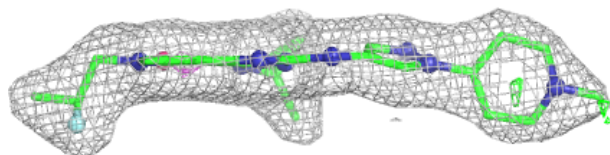
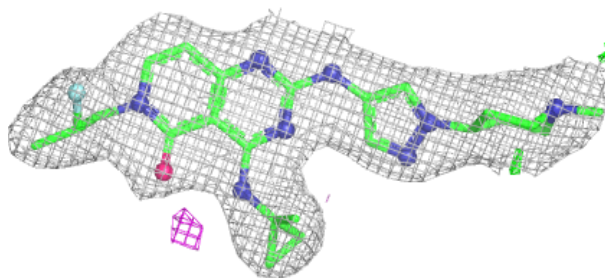
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around B4U A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around B4U B 501:**

$2mF_o-DF_c$ (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.