Full wwPDB X-ray Structure Validation Report ⓘ

Oct 19, 2020 – 10:10 AM BST

PDB ID	:	6THX
Title	:	IRAK4 in complex with inhibitor
Authors	:	Xue, Y.; Aagaard, A.; Degorce, S.L.
Deposited on	:	2019-11-21
Resolution	:	1.99 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 following versions of software and data (see references ⓘ) were used in the production of this report:

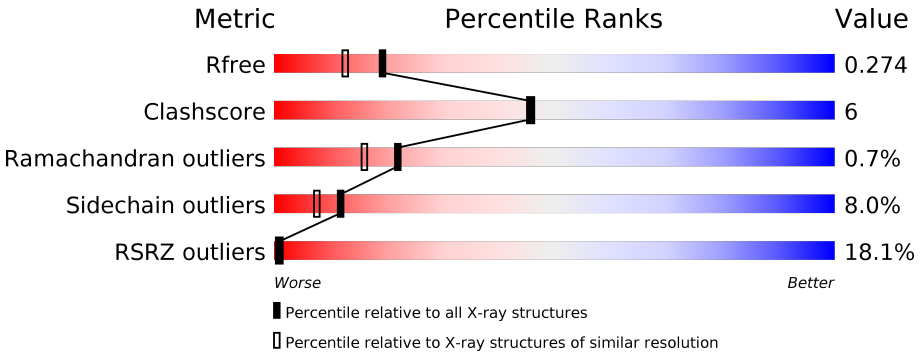
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 1.99 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on 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	308	20% 71% 17% • 9%
1	B	308	13% 79% 12% • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4699 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.

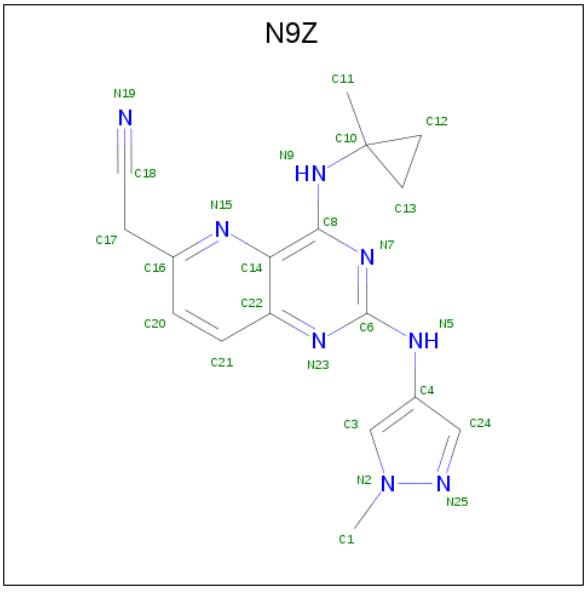
- Molecule 1 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	P	S	0	0	0
			2207	1387	373	431	2	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 2-[4-[(1-methylcyclopropyl)amino]-2-[(1-methylpyrazol-4-yl)amino]pyrido[3,2-d]pyrimidin-6-yl]ethanenitrile (three-letter code: N9Z) (formula: $C_{17}H_{18}N_8$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N 25 17 8	0	0
2	B	1	Total C N 25 17 8	0	0

- Molecule 3 is water.

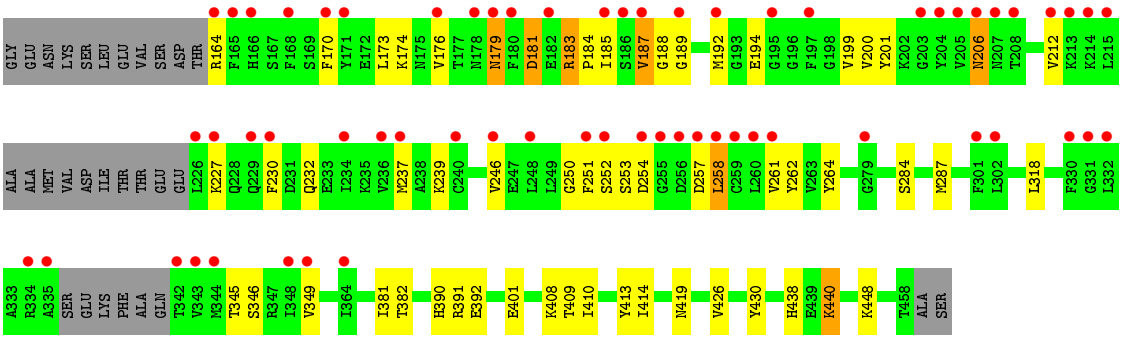
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	93	Total O 93 93	0	0
3	B	111	Total O 111 111	0	0

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.

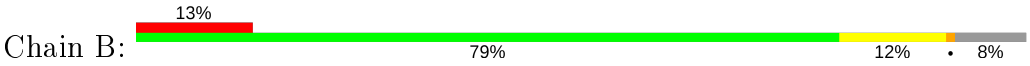
- Molecule 1: Interleukin-1 receptor-associated kinase 4

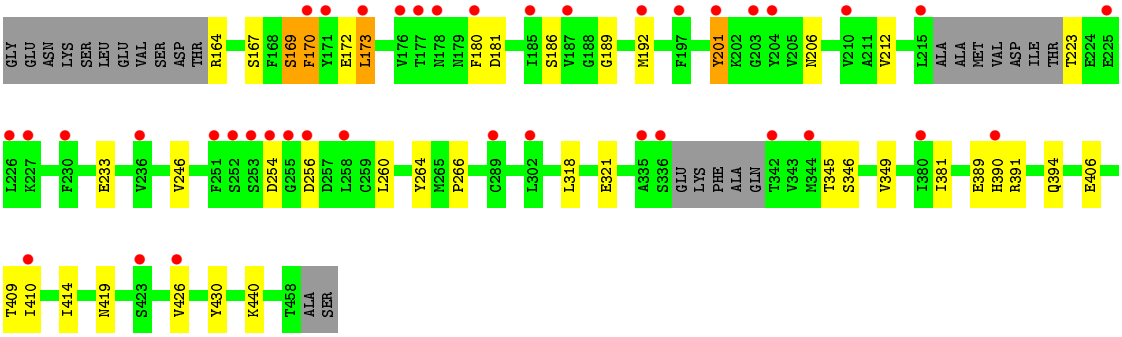
Chain A:



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

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	87.88Å 109.23Å 142.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.09 – 1.99 71.09 – 1.99	Depositor EDS
% Data completeness (in resolution range)	100.0 (71.09-1.99) 100.0 (71.09-1.99)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 2.00Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.231 , 0.254 0.233 , 0.274	Depositor DCC
R_{free} test set	2360 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	41.9	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 63.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4699	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.25% 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: N9Z, TPO, 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	0.61	0/2222	0.68	0/2992
1	B	0.57	0/2253	0.69	0/3034
All	All	0.59	0/4475	0.69	0/6026

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	2207	0	2178	37	0
1	B	2238	0	2202	25	0
2	A	25	0	0	1	0
2	B	25	0	0	1	0
3	A	93	0	0	1	0
3	B	111	0	0	0	0
All	All	4699	0	4380	57	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 (57) 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:390:HIS:HB3	1:B:391:ARG:HA	1.30	1.14
1:A:284:SER:H	1:A:287:MET:HE3	1.28	0.97
1:B:192:MET:SD	1:B:264:TYR:HE1	1.94	0.90
1:A:170:PHE:HE2	1:A:174:LYS:HZ2	0.93	0.89
1:B:266:PRO:HG2	1:B:321:GLU:HG3	1.55	0.87
1:A:390:HIS:O	1:B:390:HIS:HB3	1.77	0.85
1:A:391:ARG:HA	1:B:390:HIS:HB3	1.72	0.71
1:A:173:LEU:HA	1:A:176:VAL:HG22	1.72	0.71
1:A:192:MET:SD	1:A:264:TYR:HE1	2.14	0.70
1:A:183:ARG:HG2	1:A:189:GLY:HA3	1.74	0.70
1:A:246:VAL:HG11	1:A:318:LEU:HD12	1.74	0.68
1:B:246:VAL:HG11	1:B:318:LEU:HD12	1.77	0.65
1:B:192:MET:SD	1:B:264:TYR:CE1	2.85	0.65
1:B:180:PHE:HD1	1:B:201:TYR:CE1	2.18	0.61
1:A:381:ILE:HG21	1:A:410:ILE:HD11	1.82	0.61
1:A:410:ILE:HD13	1:A:430:TYR:CD1	2.36	0.60
1:A:179:ASN:O	1:A:179:ASN:ND2	2.31	0.60
1:A:230:PHE:CD2	1:A:258:LEU:HD22	2.37	0.59
1:A:181:ASP:OD2	1:A:183:ARG:NH1	2.34	0.59
1:A:390:HIS:O	1:B:390:HIS:CB	2.52	0.57
1:B:201:TYR:N	1:B:201:TYR:CD1	2.73	0.57
1:A:250:GLY:O	1:A:261:VAL:N	2.35	0.56
1:A:230:PHE:CG	1:A:258:LEU:HD22	2.41	0.56
1:A:170:PHE:HE2	1:A:174:LYS:NZ	1.81	0.55
1:B:381:ILE:HG21	1:B:410:ILE:HD11	1.88	0.55
1:A:392:GLU:H	1:B:390:HIS:CD2	2.26	0.54
1:B:173:LEU:HG	1:B:212:VAL:HG11	1.89	0.53
1:A:392:GLU:H	1:B:390:HIS:HD2	1.56	0.53
1:B:389:GLU:HA	1:B:394:GLN:HG2	1.89	0.53
1:B:172:GLU:H	1:B:172:GLU:CD	2.12	0.52
1:A:438:HIS:CE1	1:A:440:LYS:HD3	2.45	0.51
1:B:233:GLU:HG2	1:B:260:LEU:HD13	1.93	0.51
1:B:321:GLU:CD	1:B:321:GLU:H	2.13	0.51
1:A:192:MET:SD	1:A:264:TYR:CE1	3.00	0.50
1:A:391:ARG:HD3	3:A:641:HOH:O	2.10	0.50
1:A:251:PHE:C	1:A:251:PHE:CD1	2.85	0.49
1:A:184:PRO:HB2	1:A:187:VAL:HG23	1.96	0.47
1:A:230:PHE:CE2	1:A:258:LEU:CD2	2.98	0.47
1:A:414:ILE:HG12	1:A:426:VAL:HG11	1.97	0.46
1:B:414:ILE:HG12	1:B:426:VAL:HG11	1.97	0.46
1:A:237:MET:HE3	1:A:262:TYR:HE2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:PHE:CZ	1:A:258:LEU:HD23	2.51	0.45
1:B:180:PHE:HD1	1:B:201:TYR:CZ	2.34	0.45
1:A:391:ARG:HA	1:B:390:HIS:CD2	2.52	0.44
1:A:174:LYS:O	1:A:179:ASN:N	2.48	0.43
1:A:200:VAL:HA	1:A:212:VAL:O	2.18	0.43
1:A:230:PHE:CZ	1:A:258:LEU:CD2	3.01	0.43
1:A:438:HIS:HE1	1:A:440:LYS:HD3	1.82	0.43
1:B:410:ILE:HD13	1:B:430:TYR:CD1	2.54	0.43
1:B:169:SER:O	1:B:170:PHE:HB2	2.20	0.42
2:B:501:N9Z:C24	2:B:501:N9Z:N7	2.82	0.42
1:A:230:PHE:CE2	1:A:258:LEU:HD22	2.55	0.42
2:A:501:N9Z:N7	2:A:501:N9Z:C24	2.83	0.42
1:B:181:ASP:CG	1:B:189:GLY:HA2	2.40	0.41
1:A:230:PHE:CD1	1:A:258:LEU:HD22	2.56	0.41
1:B:181:ASP:OD2	1:B:189:GLY:HA2	2.21	0.41
1:A:382:THR:HG22	1:A:413:TYR:HB3	2.02	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	271/308 (88%)	258 (95%)	10 (4%)	3 (1%)	14 8
1	B	275/308 (89%)	264 (96%)	10 (4%)	1 (0%)	34 30
All	All	546/616 (89%)	522 (96%)	20 (4%)	4 (1%)	22 16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	170	PHE
1	A	181	ASP

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Mol	Chain	Res	Type
1	A	206	ASN
1	A	188	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	242/266 (91%)	218 (90%)	24 (10%)	8 4
1	B	246/266 (92%)	231 (94%)	15 (6%)	18 14
All	All	488/532 (92%)	449 (92%)	39 (8%)	12 7

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	ARG
1	A	179	ASN
1	A	183	ARG
1	A	185	ILE
1	A	187	VAL
1	A	194	GLU
1	A	199	VAL
1	A	201	TYR
1	A	206	ASN
1	A	227	LYS
1	A	232	GLN
1	A	239	LYS
1	A	252	SER
1	A	253	SER
1	A	254	ASP
1	A	257	ASP
1	A	258	LEU
1	A	349	VAL
1	A	401	GLU
1	A	408	LYS
1	A	409	THR

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Mol	Chain	Res	Type
1	A	419	ASN
1	A	440	LYS
1	A	448	LYS
1	B	164	ARG
1	B	167	SER
1	B	169	SER
1	B	173	LEU
1	B	186	SER
1	B	201	TYR
1	B	206	ASN
1	B	223	THR
1	B	254	ASP
1	B	256	ASP
1	B	349	VAL
1	B	406	GLU
1	B	409	THR
1	B	419	ASN
1	B	440	LYS

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

Mol	Chain	Res	Type
1	A	232	GLN
1	A	390	HIS
1	A	419	ASN
1	B	390	HIS
1	B	419	ASN
1	B	452	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 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	B	345	1	8,10,11	1.11	0	10,14,16	1.14	1 (10%)
1	TPO	A	345	1	8,10,11	1.13	0	10,14,16	1.15	1 (10%)
1	SEP	B	346	1	8,9,10	0.74	0	8,12,14	2.48	4 (50%)
1	SEP	A	346	1	8,9,10	0.71	0	8,12,14	2.26	3 (37%)

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	B	345	1	-	4/9/11/13	-
1	TPO	A	345	1	-	4/9/11/13	-
1	SEP	B	346	1	-	0/5/8/10	-
1	SEP	A	346	1	-	0/5/8/10	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	346	SEP	OG-CB-CA	5.65	113.64	108.14
1	A	346	SEP	OG-CB-CA	5.40	113.40	108.14
1	B	346	SEP	O3P-P-OG	2.57	113.57	106.73
1	B	346	SEP	OG-P-O1P	2.28	112.87	106.47
1	A	345	TPO	O2P-P-OG1	2.15	115.63	105.99
1	A	346	SEP	OG-P-O1P	2.14	112.48	106.47
1	B	345	TPO	O2P-P-OG1	2.13	115.54	105.99
1	B	346	SEP	P-OG-CB	-2.13	112.43	118.30
1	A	346	SEP	O3P-P-OG	2.11	112.36	106.73

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	O-C-CA-CB

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

There are no ring outliers.

No monomer is involved in short contacts.

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	$\#\|Z\| > 2$
2	N9Z	A	501	-	25,28,28	1.51	4 (16%)	30,41,41	1.38	4 (13%)
2	N9Z	B	501	-	25,28,28	1.51	4 (16%)	30,41,41	1.52	6 (20%)

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	N9Z	A	501	-	-	0/8/16/16	0/4/4/4
2	N9Z	B	501	-	-	0/8/16/16	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	N9Z	C8-N9	4.06	1.41	1.35
2	B	501	N9Z	C8-N9	3.45	1.40	1.35
2	B	501	N9Z	C24-C4	3.22	1.41	1.38
2	A	501	N9Z	C24-C4	2.87	1.41	1.38
2	B	501	N9Z	C11-C10	-2.77	1.48	1.53
2	B	501	N9Z	C4-N5	-2.47	1.35	1.40
2	A	501	N9Z	C4-N5	-2.13	1.36	1.40
2	A	501	N9Z	C8-N7	2.11	1.35	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	N9Z	C13-C10-N9	3.69	120.66	115.64
2	B	501	N9Z	C13-C10-N9	3.31	120.14	115.64
2	B	501	N9Z	C3-N2-N25	3.29	114.42	111.56
2	B	501	N9Z	C12-C10-N9	3.04	119.78	115.64
2	A	501	N9Z	C3-N2-N25	2.86	114.05	111.56
2	B	501	N9Z	C21-C22-C14	-2.64	116.47	119.40
2	A	501	N9Z	C21-C22-C14	-2.48	116.65	119.40
2	B	501	N9Z	C4-C3-N2	-2.34	104.81	107.58
2	B	501	N9Z	N23-C6-N7	-2.24	122.68	126.23
2	A	501	N9Z	C4-C3-N2	-2.06	105.15	107.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

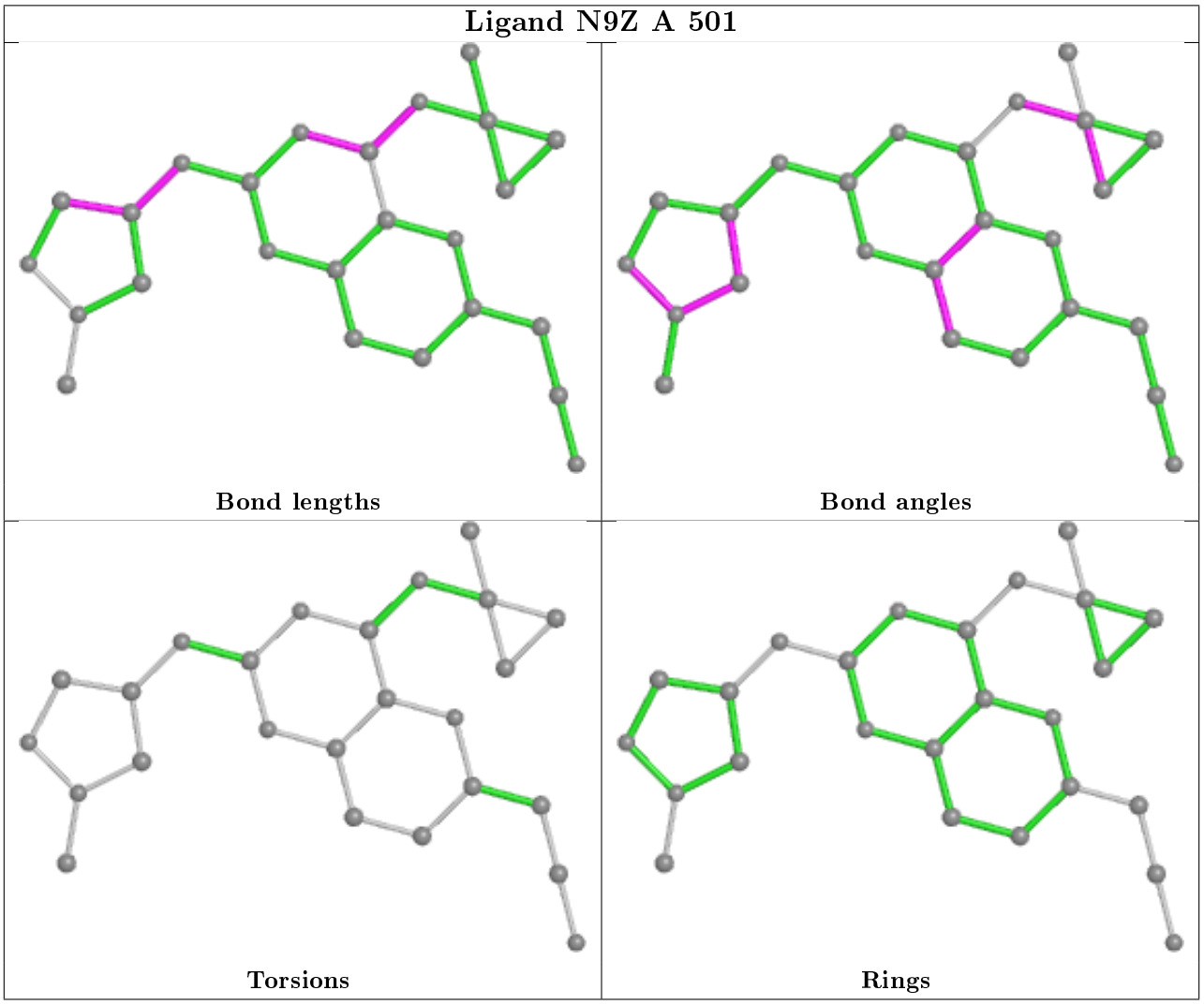
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	N9Z	1	0
2	B	501	N9Z	1	0

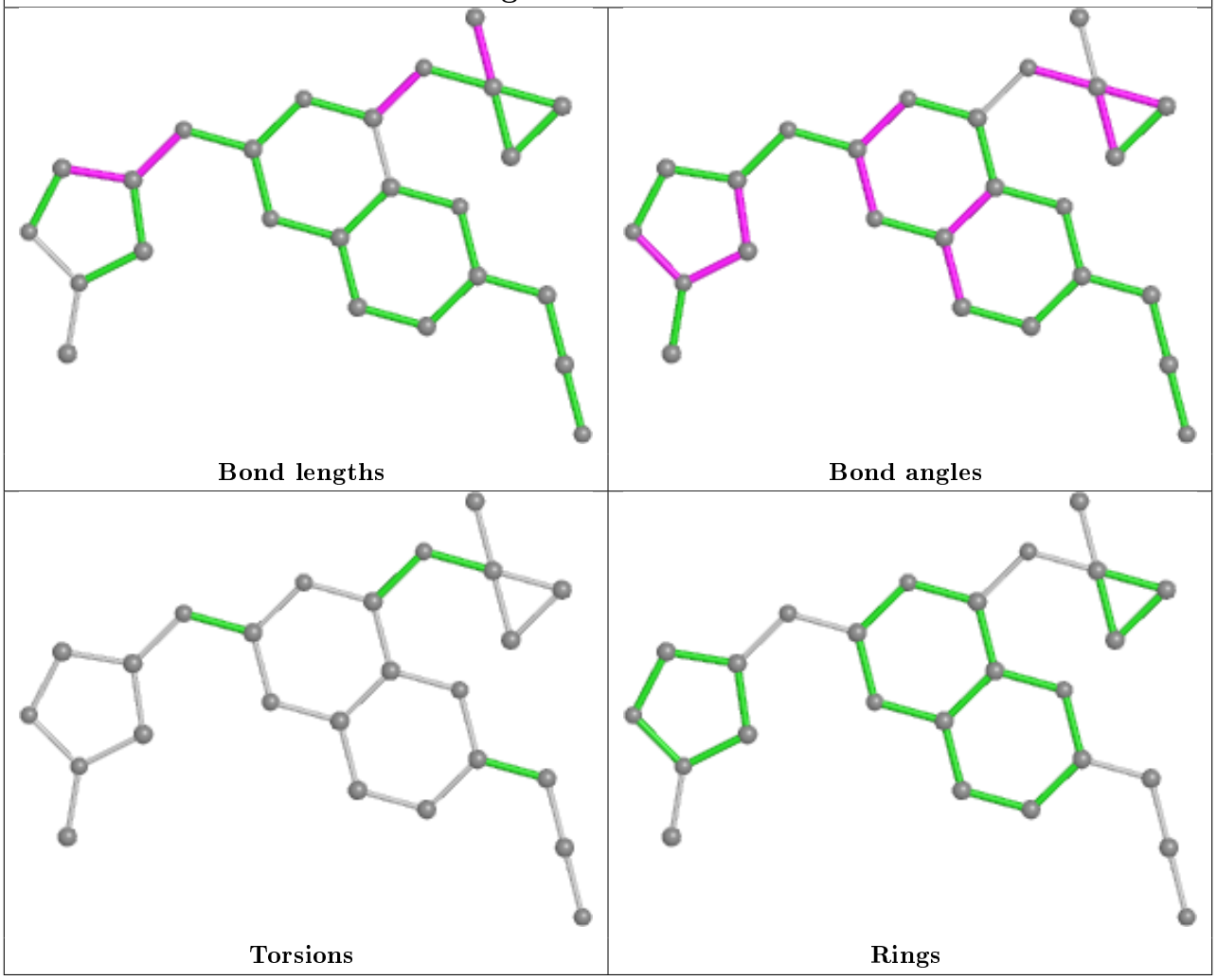
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 N9Z A 501



Ligand N9Z B 501



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, 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	277/308 (89%)	1.31	62 (22%)	0	0	35, 59, 123, 150	0
1	B	281/308 (91%)	0.98	39 (13%)	2	2	37, 59, 97, 132	0
All	All	558/616 (90%)	1.15	101 (18%)	1	1	35, 59, 118, 150	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	PHE	13.7
1	A	343	VAL	9.0
1	A	170	PHE	8.9
1	B	342	THR	7.2
1	A	171	TYR	6.8
1	A	234	ILE	6.3
1	A	168	PHE	6.0
1	A	195	GLY	5.9
1	A	207	ASN	5.7
1	A	251	PHE	5.6
1	A	203	GLY	5.3
1	A	226	LEU	5.3
1	A	258	LEU	5.2
1	B	255	GLY	5.2
1	B	170	PHE	5.1
1	A	240	CYS	5.0
1	A	342	THR	4.9
1	A	236	VAL	4.5
1	A	256	ASP	4.4
1	B	176	VAL	4.4
1	A	364	ILE	4.3
1	A	260	LEU	4.3
1	A	252	SER	4.1
1	A	261	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	186	SER	4.0
1	A	248	LEU	4.0
1	A	164	ARG	4.0
1	B	203	GLY	3.9
1	A	255	GLY	3.9
1	B	173	LEU	3.8
1	A	212	VAL	3.8
1	B	192	MET	3.7
1	B	227	LYS	3.7
1	A	259	CYS	3.6
1	A	176	VAL	3.6
1	A	227	LYS	3.6
1	B	335	ALA	3.5
1	A	205	VAL	3.5
1	A	332	LEU	3.5
1	B	252	SER	3.5
1	A	349	VAL	3.4
1	B	254	ASP	3.4
1	A	208	THR	3.4
1	A	204	TYR	3.3
1	A	254	ASP	3.2
1	B	258	LEU	3.2
1	A	178	ASN	3.1
1	A	165	PHE	3.0
1	A	229	GLN	3.0
1	B	426	VAL	3.0
1	A	335	ALA	3.0
1	A	179	ASN	2.9
1	A	330	PHE	2.9
1	A	348	ILE	2.9
1	B	251	PHE	2.9
1	A	214	LYS	2.9
1	B	225	GLU	2.9
1	B	230	PHE	2.9
1	A	215	LEU	2.8
1	B	410	ILE	2.8
1	A	197	PHE	2.8
1	A	182	GLU	2.7
1	B	215	LEU	2.7
1	B	236	VAL	2.6
1	B	344	MET	2.6
1	B	253	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	302	LEU	2.5
1	A	166	HIS	2.5
1	A	344	MET	2.5
1	A	257	ASP	2.5
1	B	256	ASP	2.5
1	A	237	MET	2.4
1	B	210	VAL	2.4
1	A	185	ILE	2.4
1	A	246	VAL	2.4
1	B	187	VAL	2.4
1	A	334	ARG	2.4
1	B	201	TYR	2.3
1	A	301	PHE	2.3
1	B	180	PHE	2.3
1	A	187	VAL	2.3
1	B	204	TYR	2.2
1	A	279	GLY	2.2
1	B	423	SER	2.2
1	B	390	HIS	2.2
1	B	289	CYS	2.2
1	A	192	MET	2.2
1	A	180	PHE	2.2
1	B	178	ASN	2.2
1	B	380	ILE	2.2
1	B	185	ILE	2.1
1	A	189	GLY	2.1
1	A	331	GLY	2.1
1	B	336	SER	2.1
1	B	197	PHE	2.1
1	B	171	TYR	2.0
1	A	206	ASN	2.0
1	B	226	LEU	2.0
1	B	177	THR	2.0
1	B	302	LEU	2.0
1	A	213	LYS	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, 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
1	SEP	B	346	10/11	0.71	0.18	113,116,121,121	0
1	TPO	B	345	11/12	0.80	0.14	118,119,121,121	0
1	TPO	A	345	11/12	0.82	0.22	117,118,120,120	0
1	SEP	A	346	10/11	0.84	0.27	116,118,121,121	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

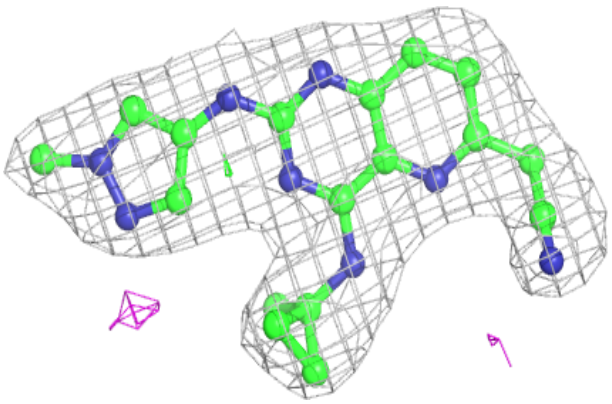
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

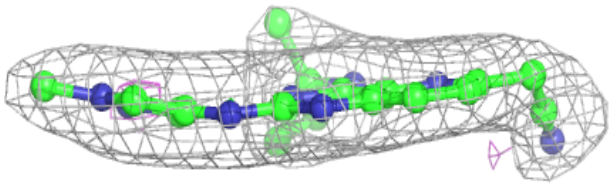
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	N9Z	A	501	25/25	0.97	0.13	48,52,56,59	0
2	N9Z	B	501	25/25	0.97	0.14	42,45,51,54	0

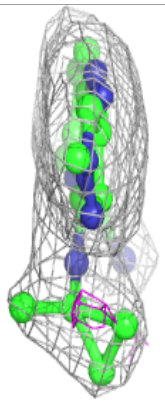
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around N9Z 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)

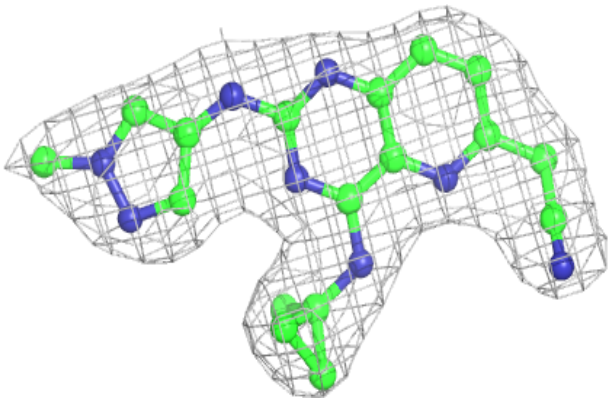


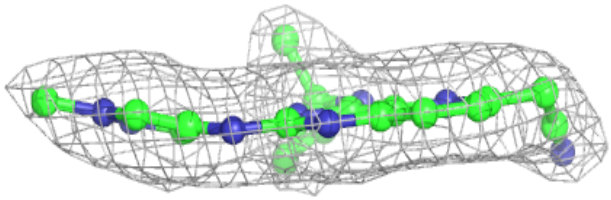


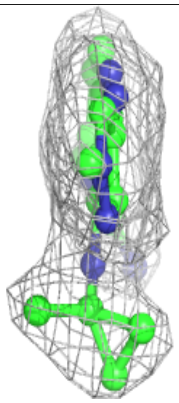


Electron density around N9Z B 501:

$2mF_o$-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.