



Full wwPDB X-ray Structure Validation Report

Oct 19, 2020 – 10:08 AM BST

PDB ID : 6THZ
Title : IRAK4 IN COMPLEX WITH inhibitor
Authors : Xue, Y.; Aagaard, A.; Degorce, S.L.
Deposited on : 2019-11-21
Resolution : 2.38 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

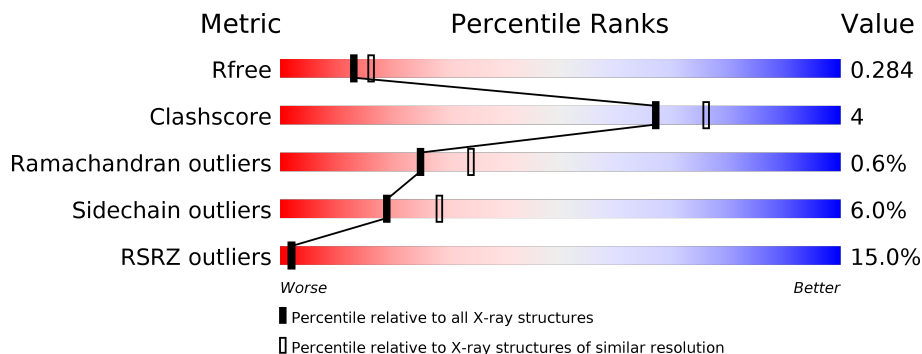
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 $\leq 5\%$. 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	 16% 74% 11% • 13%
1	B	308	 11% 78% 13% • 8%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4542 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.

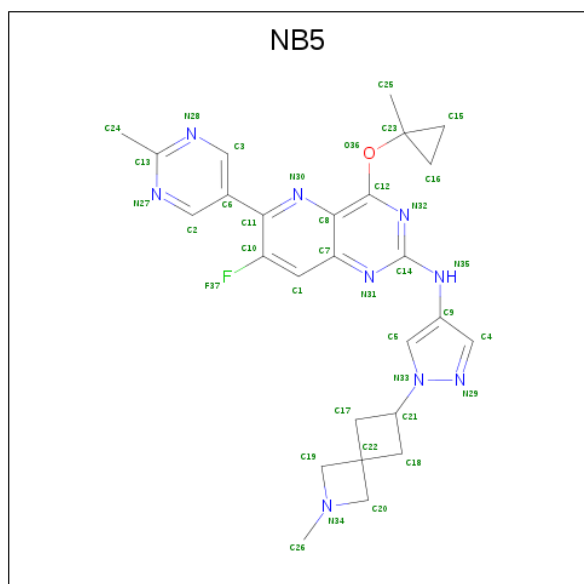
- Molecule 1 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
1	A	267	Total 2124	C 1338	N 358	O 412	P 2	S 14	0	0	0
1	B	283	Total 2238	C 1404	N 377	O 441	P 2	S 14	0	0	0

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 7-fluoranyl- {N}-[1-(2-methyl-2-azaspiro[3.3]heptan-6-yl)pyrazol-4-yl]-4-(1-methylcyclopropyl)oxy-6-(2-methylpyrimidin-5-yl)pyrido[3,2-d]pyrimidin-2-amine (three-letter code: NB5) (formula: C₂₆H₂₈FN₉O) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			37	26	1	9	1		
2	B	1	Total	C	F	N	O	0	0
			37	26	1	9	1		

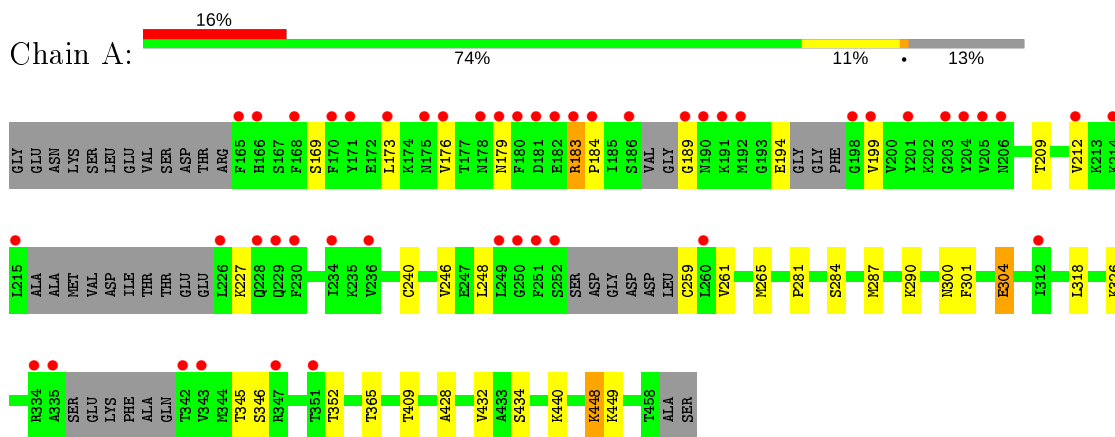
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total	O	0	0
			50	50		
3	B	56	Total	O	0	0
			56	56		

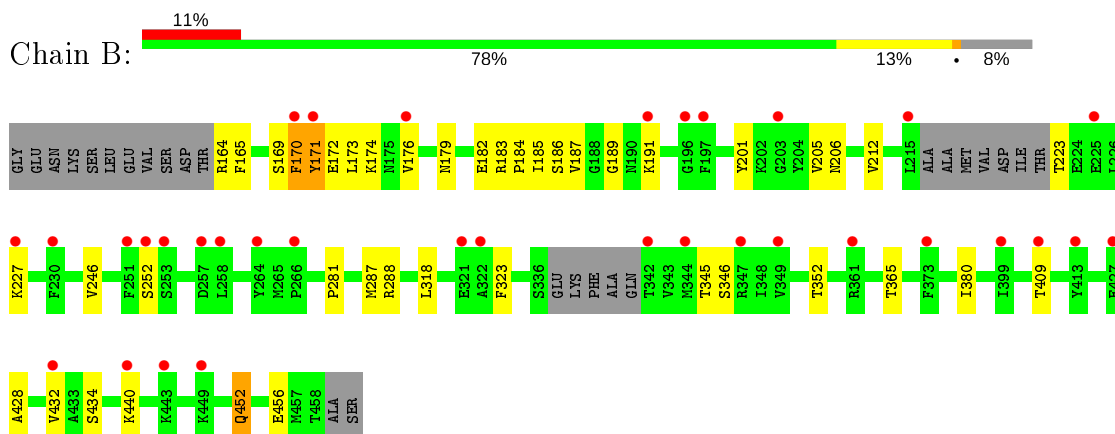
3 Residue-property plots [i](#)

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	85.93Å 108.57Å 142.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.67 – 2.38 43.68 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.67-2.38) 99.9 (43.68-2.38)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.37Å)	Xtrriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.231 , 0.274 0.242 , 0.284	Depositor DCC
R_{free} test set	1370 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtrriage
Anisotropy	0.572	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 65.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4542	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.75% 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: TPO, NB5, 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	0.49	0/2135	0.67	0/2871
1	B	0.52	0/2253	0.70	0/3034
All	All	0.50	0/4388	0.69	0/5905

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 [i](#)

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	2124	0	2104	13	0
1	B	2238	0	2202	20	0
2	A	37	0	0	1	0
2	B	37	0	0	1	0
3	A	50	0	0	0	0
3	B	56	0	0	0	0
All	All	4542	0	4306	34	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 (34) 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:B:183:ARG:HB3	1:B:187:VAL:CG2	2.09	0.82
1:B:183:ARG:HB3	1:B:187:VAL:HG21	1.74	0.70
1:A:284:SER:H	1:A:287:MET:HE3	1.59	0.67
1:B:452:GLN:NE2	1:B:456:GLU:OE1	2.32	0.63
1:B:173:LEU:H	1:B:173:LEU:HD12	1.62	0.62
1:B:184:PRO:O	1:B:187:VAL:HG22	1.99	0.62
1:A:183:ARG:HG2	1:A:189:GLY:HA3	1.85	0.59
2:B:501:NB5:N32	2:B:501:NB5:C4	2.66	0.57
1:A:194:GLU:HB3	1:A:199:VAL:HG13	1.87	0.56
1:B:182:GLU:HA	1:B:191:LYS:HB2	1.88	0.55
1:B:185:ILE:HA	1:B:189:GLY:O	2.07	0.54
1:A:281:PRO:HB3	1:B:281:PRO:HB3	1.91	0.52
1:B:246:VAL:HG11	1:B:318:LEU:HD12	1.94	0.49
1:A:246:VAL:HG11	1:A:318:LEU:HD12	1.95	0.48
1:B:173:LEU:HD23	1:B:212:VAL:HG11	1.95	0.48
1:B:176:VAL:HG11	1:B:205:VAL:HG22	1.95	0.47
1:A:300:ASN:O	1:A:304:GLU:HB2	2.16	0.46
1:A:212:VAL:HG22	1:A:261:VAL:HG13	1.98	0.45
1:A:265:MET:CE	1:A:326:LYS:HD2	2.46	0.45
1:B:171:TYR:N	1:B:171:TYR:CD1	2.82	0.45
1:B:172:GLU:O	1:B:176:VAL:HG13	2.17	0.45
1:A:240:CYS:HB3	1:A:301:PHE:HE2	1.81	0.44
1:B:172:GLU:HB2	1:B:173:LEU:HD12	1.99	0.44
1:A:173:LEU:HA	1:A:176:VAL:HG22	2.00	0.44
1:B:174:LYS:HG3	1:B:179:ASN:HA	2.01	0.42
1:B:288:ARG:HB3	1:B:380:ILE:HG23	2.01	0.42
1:B:164:ARG:HB3	1:B:165:PHE:H	1.73	0.42
2:A:501:NB5:N32	2:A:501:NB5:C4	2.80	0.42
1:B:428:ALA:O	1:B:432:VAL:HG23	2.20	0.42
1:A:428:ALA:O	1:A:432:VAL:HG23	2.19	0.42
1:A:448:LYS:HA	1:A:448:LYS:HD3	1.78	0.42
1:B:287:MET:CE	1:B:323:PHE:HB2	2.49	0.41
1:B:183:ARG:CB	1:B:187:VAL:HG21	2.47	0.40
1:A:248:LEU:HD12	1:A:261:VAL:O	2.22	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	253/308 (82%)	236 (93%)	16 (6%)	1 (0%)	34	46
1	B	275/308 (89%)	257 (94%)	16 (6%)	2 (1%)	22	30
All	All	528/616 (86%)	493 (93%)	32 (6%)	3 (1%)	25	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	PRO
1	B	170	PHE
1	B	252	SER

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	234/266 (88%)	219 (94%)	15 (6%)	17	25
1	B	246/266 (92%)	232 (94%)	14 (6%)	20	30
All	All	480/532 (90%)	451 (94%)	29 (6%)	19	28

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	SER
1	A	179	ASN
1	A	183	ARG

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Mol	Chain	Res	Type
1	A	209	THR
1	A	227	LYS
1	A	259	CYS
1	A	290	LYS
1	A	304	GLU
1	A	352	THR
1	A	365	THR
1	A	409	THR
1	A	434	SER
1	A	440	LYS
1	A	448	LYS
1	A	449	LYS
1	B	169	SER
1	B	170	PHE
1	B	171	TYR
1	B	186	SER
1	B	201	TYR
1	B	206	ASN
1	B	223	THR
1	B	227	LYS
1	B	352	THR
1	B	365	THR
1	B	409	THR
1	B	434	SER
1	B	440	LYS
1	B	452	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	206	ASN
1	B	452	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](#)

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	SEP	A	346	1	8,9,10	0.80	0	8,12,14	2.07	2 (25%)
1	TPO	B	345	1	8,10,11	0.93	0	10,14,16	1.36	1 (10%)
1	SEP	B	346	1	8,9,10	0.81	0	8,12,14	2.01	2 (25%)
1	TPO	A	345	1	8,10,11	1.14	0	10,14,16	1.30	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	SEP	A	346	1	-	0/5/8/10	-
1	TPO	B	345	1	-	3/9/11/13	-
1	SEP	B	346	1	-	0/5/8/10	-
1	TPO	A	345	1	-	3/9/11/13	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	SEP	OG-CB-CA	4.84	112.86	108.14
1	B	346	SEP	OG-CB-CA	4.64	112.67	108.14
1	B	345	TPO	O2P-P-OG1	2.62	117.72	105.99
1	A	345	TPO	O2P-P-OG1	2.55	117.43	105.99
1	A	346	SEP	O3P-P-OG	2.23	112.66	106.73
1	B	346	SEP	O3P-P-OG	2.14	112.44	106.73

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

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

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	NB5	B	501	-	35,43,43	1.69	10 (28%)	45,67,67	1.76	11 (24%)
2	NB5	A	501	-	35,43,43	1.56	7 (20%)	45,67,67	1.73	9 (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	NB5	B	501	-	-	2/9/41/41	0/7/7/7
2	NB5	A	501	-	-	0/9/41/41	0/7/7/7

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NB5	C6-C11	-3.63	1.45	1.49
2	B	501	NB5	C20-C22	-3.32	1.51	1.54
2	B	501	NB5	C17-C22	-3.22	1.51	1.54
2	B	501	NB5	C4-C9	3.17	1.41	1.38
2	B	501	NB5	C18-C22	-3.17	1.51	1.54
2	A	501	NB5	O36-C12	2.86	1.40	1.36
2	A	501	NB5	C4-C9	2.81	1.41	1.38
2	A	501	NB5	C8-C7	-2.72	1.38	1.42
2	B	501	NB5	O36-C12	2.68	1.40	1.36
2	B	501	NB5	C14-N35	2.44	1.41	1.36
2	A	501	NB5	C1-C7	-2.38	1.38	1.41
2	B	501	NB5	C19-C22	-2.36	1.52	1.54
2	B	501	NB5	C1-C10	2.26	1.38	1.35
2	B	501	NB5	C1-C7	-2.06	1.38	1.41
2	A	501	NB5	C14-N35	2.04	1.40	1.36
2	A	501	NB5	C9-N35	-2.04	1.36	1.40
2	B	501	NB5	C8-C7	-2.02	1.39	1.42

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NB5	C23-O36-C12	-5.01	118.16	123.25
2	B	501	NB5	C23-O36-C12	-5.01	118.16	123.25
2	A	501	NB5	C22-C18-C21	-3.51	85.61	88.09
2	B	501	NB5	C22-C18-C21	-3.43	85.67	88.09
2	A	501	NB5	C22-C17-C21	-3.43	85.67	88.09
2	B	501	NB5	F37-C10-C1	-3.18	116.26	120.47
2	A	501	NB5	C1-C7-C8	-3.06	116.59	119.70
2	B	501	NB5	C22-C17-C21	-3.02	85.95	88.09
2	B	501	NB5	C1-C7-C8	-3.00	116.66	119.70
2	A	501	NB5	C7-C8-N30	2.89	124.44	121.31
2	A	501	NB5	C1-C10-C11	-2.87	120.14	124.11
2	B	501	NB5	C7-C8-N30	2.76	124.30	121.31
2	B	501	NB5	C1-C10-C11	-2.64	120.45	124.11
2	A	501	NB5	N31-C14-N32	-2.32	122.55	126.23
2	A	501	NB5	C5-N33-C21	2.25	127.48	125.48
2	B	501	NB5	N31-C14-N32	-2.21	122.73	126.23
2	B	501	NB5	C14-N32-C12	2.18	119.03	115.18
2	B	501	NB5	C9-C5-N33	-2.14	105.01	107.59
2	B	501	NB5	C9-N35-C14	-2.11	123.11	129.23
2	A	501	NB5	C14-N32-C12	2.01	118.72	115.18

There are no chirality outliers.

All (2) torsion outliers are listed below:

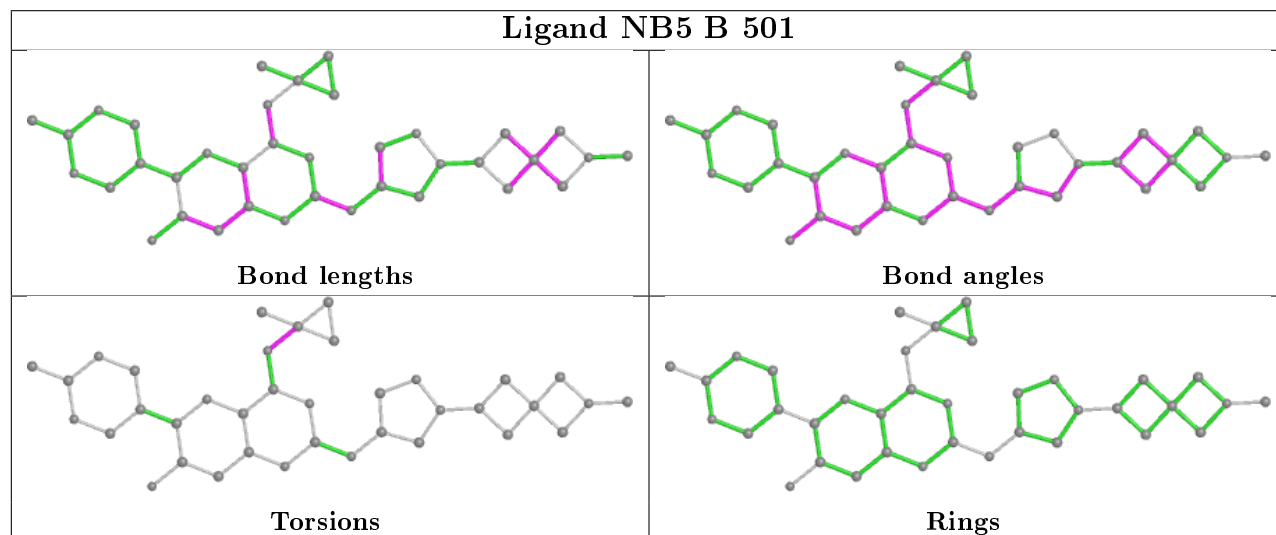
Mol	Chain	Res	Type	Atoms
2	B	501	NB5	C15-C23-O36-C12
2	B	501	NB5	C16-C23-O36-C12

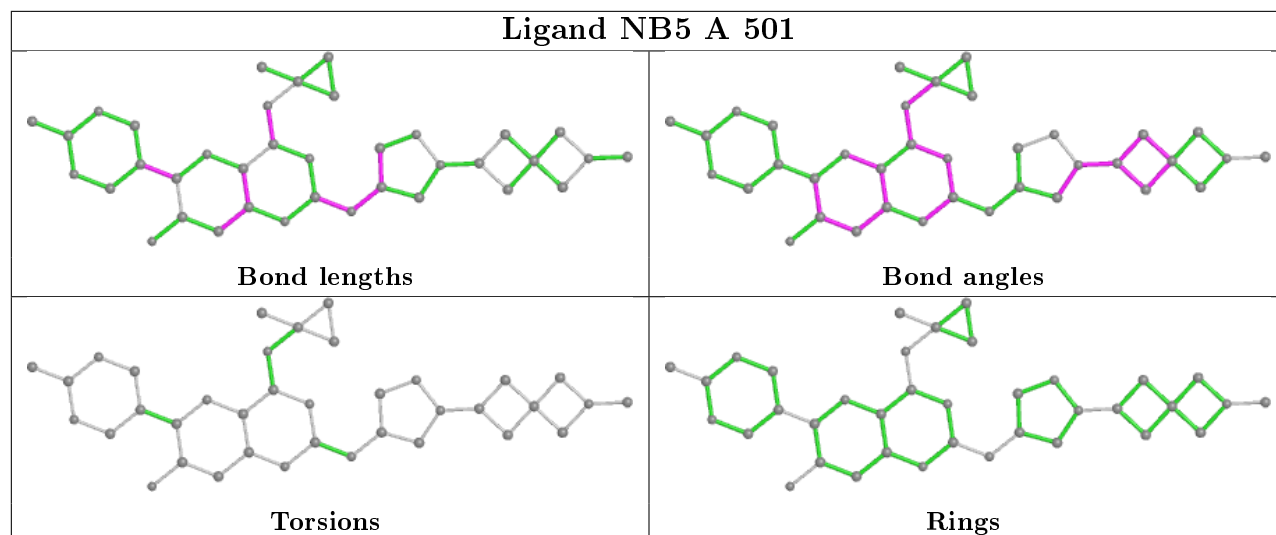
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	NB5	1	0
2	A	501	NB5	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	265/308 (86%)	0.96	48 (18%) 1 1	34, 69, 150, 197	0
1	B	281/308 (91%)	0.78	34 (12%) 4 4	38, 71, 118, 164	0
All	All	546/616 (88%)	0.87	82 (15%) 2 2	34, 70, 141, 197	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	TYR	8.7
1	A	215	LEU	6.9
1	A	203	GLY	6.7
1	A	179	ASN	6.1
1	B	171	TYR	6.0
1	A	343	VAL	5.9
1	A	251	PHE	5.7
1	B	251	PHE	5.6
1	A	342	THR	5.5
1	A	230	PHE	5.2
1	A	186	SER	5.2
1	A	250	GLY	5.1
1	A	170	PHE	5.0
1	A	199	VAL	4.7
1	A	226	LEU	4.6
1	A	165	PHE	4.5
1	A	180	PHE	4.3
1	A	334	ARG	4.2
1	A	347	ARG	3.9
1	A	351	THR	3.9
1	A	190	ASN	3.8
1	B	170	PHE	3.8
1	B	258	LEU	3.8
1	A	212	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	252	SER	3.7
1	B	227	LYS	3.6
1	B	230	PHE	3.6
1	B	176	VAL	3.4
1	A	201	TYR	3.4
1	A	189	GLY	3.4
1	A	183	ARG	3.4
1	B	215	LEU	3.3
1	A	166	HIS	3.2
1	B	344	MET	3.1
1	A	191	LYS	3.0
1	A	229	GLN	3.0
1	B	399	ILE	3.0
1	B	225	GLU	2.9
1	B	347	ARG	2.9
1	B	342	THR	2.9
1	B	440	LYS	2.9
1	A	184	PRO	2.9
1	B	361	ARG	2.9
1	B	449	LYS	2.9
1	A	234	ILE	2.8
1	A	204	TYR	2.8
1	A	236	VAL	2.8
1	A	335	ALA	2.7
1	A	168	PHE	2.7
1	A	205	VAL	2.6
1	B	197	PHE	2.6
1	A	182	GLU	2.6
1	B	203	GLY	2.6
1	B	321	GLU	2.5
1	B	413	TYR	2.5
1	B	257	ASP	2.4
1	B	253	SER	2.4
1	A	206	ASN	2.4
1	A	181	ASP	2.3
1	A	198	GLY	2.3
1	A	214	LYS	2.3
1	A	260	LEU	2.3
1	B	443	LYS	2.3
1	A	178	ASN	2.2
1	B	349	VAL	2.2
1	B	252	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	173	LEU	2.2
1	B	409	THR	2.2
1	A	176	VAL	2.1
1	A	249	LEU	2.1
1	B	266	PRO	2.1
1	B	432	VAL	2.1
1	A	312	ILE	2.1
1	A	228	GLN	2.1
1	B	196	GLY	2.1
1	B	264	TYR	2.1
1	A	192	MET	2.1
1	B	427	GLU	2.0
1	B	322	ALA	2.0
1	B	191	LYS	2.0
1	B	373	PHE	2.0
1	A	175	ASN	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	0.26	0.38	145,149,159,160	0
1	TPO	B	345	11/12	0.71	0.23	145,151,154,158	0
1	TPO	A	345	11/12	0.75	0.28	137,143,146,148	0
1	SEP	B	346	10/11	0.81	0.20	146,156,164,167	0

6.3 Carbohydrates [i](#)

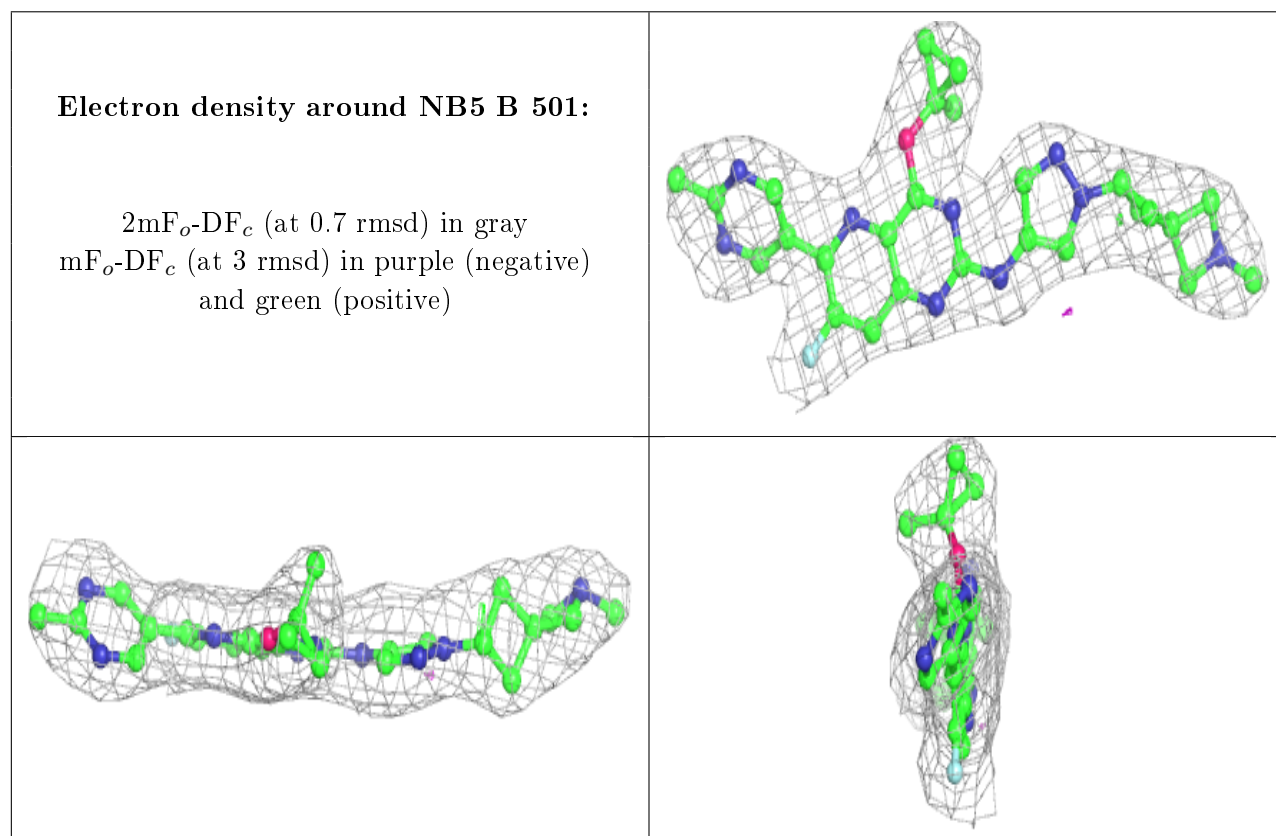
There are no monosaccharides in this entry.

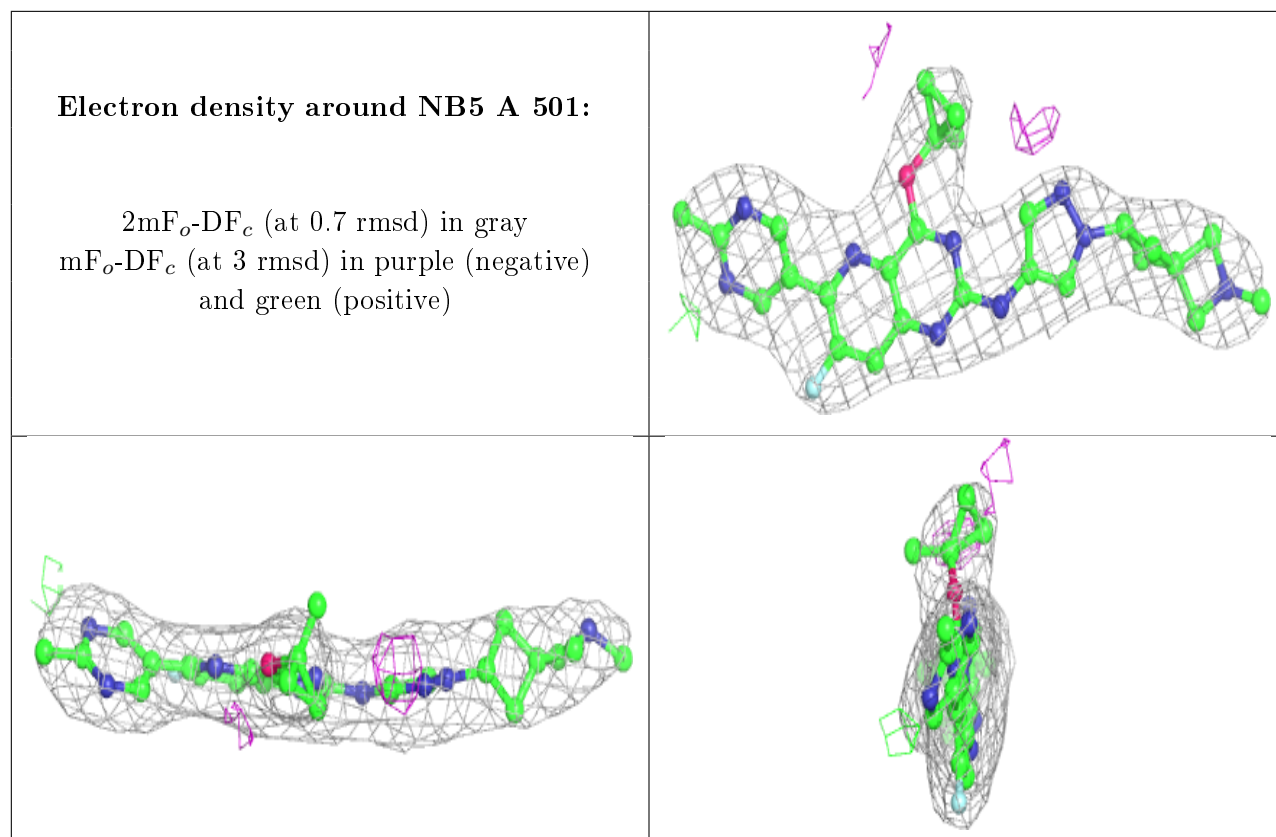
6.4 Ligands [i](#)

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, 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
2	NB5	B	501	37/37	0.93	0.14	34,42,52,55	0
2	NB5	A	501	37/37	0.96	0.13	46,52,73,74	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 [i](#)

There are no such residues in this entry.