



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:00 PM UTC

PDB ID : 6THZ / pdb_00006thz
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 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

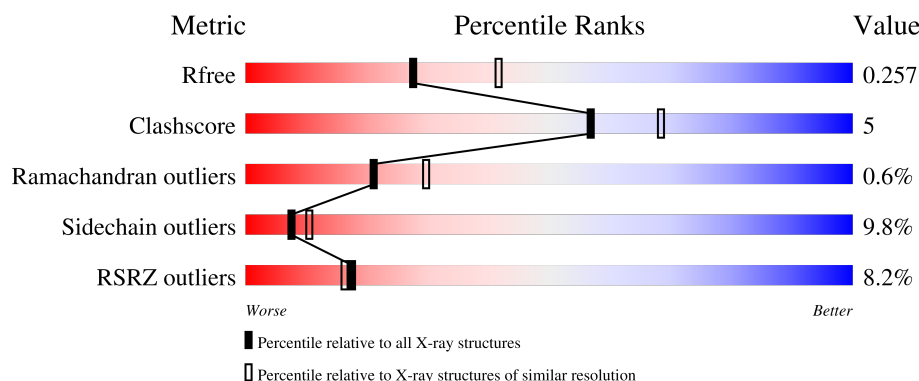
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (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 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	8% 74% 12% • 13%
1	B	308	6% 75% 16% • 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.

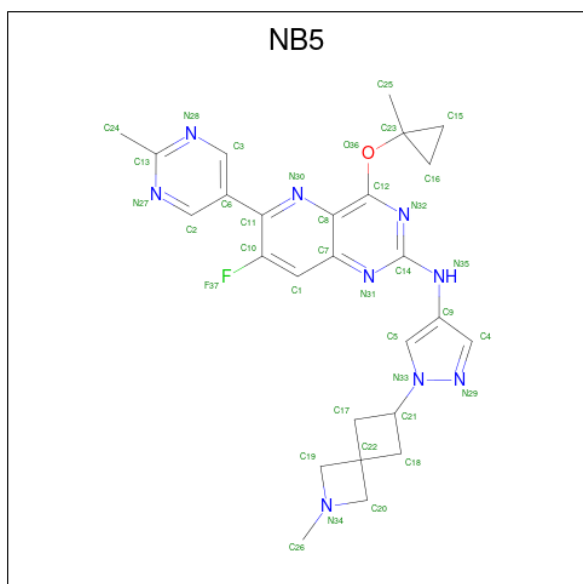
- Molecule 1 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	P	S	0	0	0
			2124	1338	358	412	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 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 (CCD ID: NB5) (formula: C₂₆H₂₈FN₉O) (labeled as "Ligand of Interest" by depositor).



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		

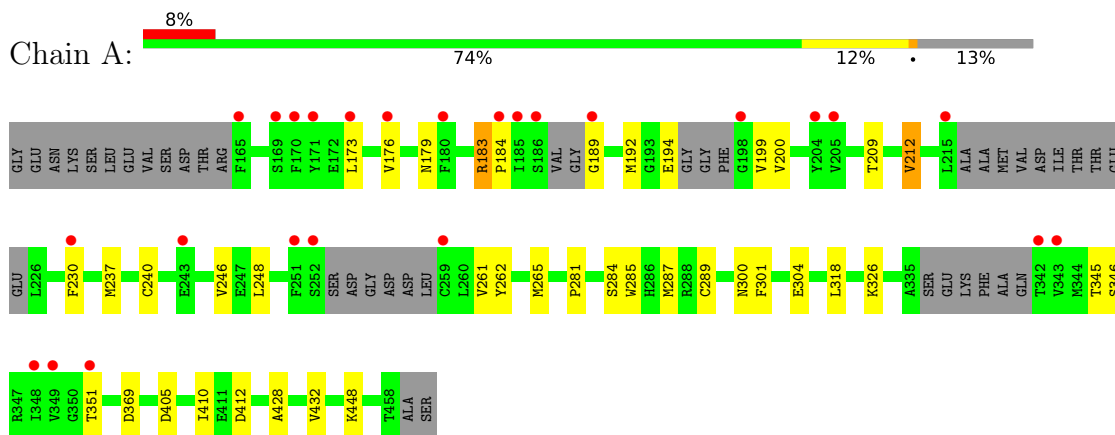
- Molecule 3 is water.

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

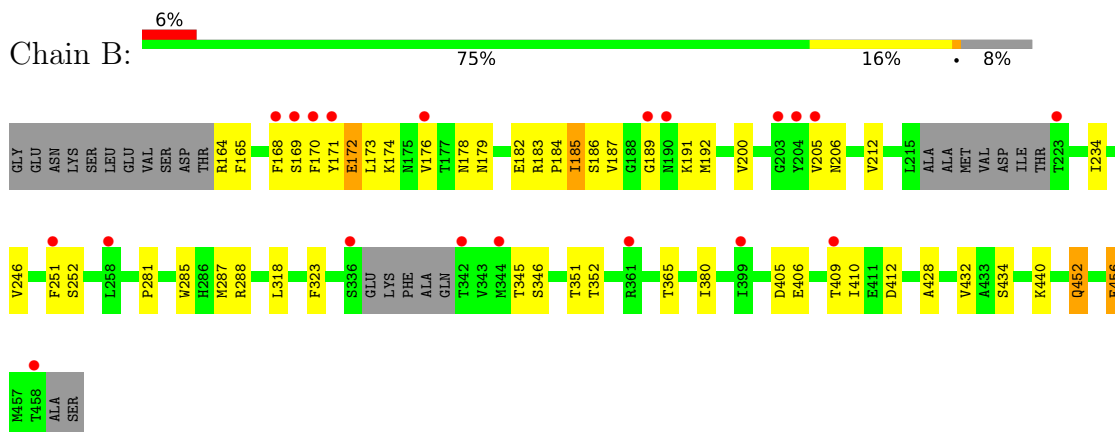
3 Residue-property plots

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 43.67 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.67-2.38) 99.8 (43.67-2.38)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.37Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.231 , 0.274 (Not available) , 0.257	Depositor DCC
R_{free} test set	1370 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 67.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4542	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage'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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, NB5, TPO

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	0/2135	1.36	13/2871 (0.5%)
1	B	0.89	0/2253	1.40	18/3034 (0.6%)
All	All	0.87	0/4388	1.38	31/5905 (0.5%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	GLU	CA-C-N	9.74	133.72	120.38
1	B	172	GLU	C-N-CA	9.74	133.72	120.38
1	B	168	PHE	CA-CB-CG	6.68	120.48	113.80
1	A	351	THR	CA-C-N	6.35	130.35	120.82
1	A	351	THR	C-N-CA	6.35	130.35	120.82
1	B	351	THR	CA-C-N	6.30	130.28	120.82
1	B	351	THR	C-N-CA	6.30	130.28	120.82
1	A	412	ASP	CA-CB-CG	6.24	118.83	112.60
1	B	412	ASP	CA-CB-CG	6.22	118.82	112.60
1	A	230	PHE	CA-CB-CG	6.21	120.01	113.80
1	B	251	PHE	CA-CB-CG	5.63	119.44	113.80
1	A	285	TRP	CA-C-N	5.53	127.69	120.28
1	A	285	TRP	C-N-CA	5.53	127.69	120.28
1	B	169	SER	CA-C-N	5.44	131.93	121.54
1	B	169	SER	C-N-CA	5.44	131.93	121.54
1	B	178	ASN	CA-CB-CG	5.31	117.91	112.60
1	A	369	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	289	CYS	CA-C-N	5.17	127.16	120.44
1	A	289	CYS	C-N-CA	5.17	127.16	120.44
1	A	405	ASP	CA-C-N	5.16	129.66	122.08
1	A	405	ASP	C-N-CA	5.16	129.66	122.08
1	B	285	TRP	CA-C-N	5.13	127.15	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	TRP	C-N-CA	5.13	127.15	120.28
1	B	405	ASP	CA-C-N	5.08	129.54	122.08
1	B	405	ASP	C-N-CA	5.08	129.54	122.08
1	B	410	ILE	CA-C-N	5.04	127.03	120.28
1	B	410	ILE	C-N-CA	5.04	127.03	120.28
1	A	410	ILE	CA-C-N	5.04	127.03	120.28
1	A	410	ILE	C-N-CA	5.04	127.03	120.28
1	B	251	PHE	CA-C-N	5.01	131.10	121.54
1	B	251	PHE	C-N-CA	5.01	131.10	121.54

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	2124	0	2104	16	0
1	B	2238	0	2202	23	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	40	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 5.

All (40) 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:265:MET:HE1	1:A:326:LYS:HD2	1.75	0.69
1:B:287:MET:HE2	1:B:323:PHE:HB2	1.78	0.66
1:A:237:MET:HE3	1:A:262:TYR:HE2	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:GLN:NE2	1:B:456:GLU:OE1	2.32	0.63
1:B:173:LEU:HD12	1:B:173:LEU:H	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:C4	2:B:501:NB5:N32	2.66	0.57
1:A:284:SER:H	1:A:287:MET:HE3	1.69	0.56
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:287:MET:HE2	1:B:323:PHE:CB	2.40	0.51
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:A:192:MET:HE3	1:A:200:VAL:HG12	1.96	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:B:171:TYR:CD1	1:B:171:TYR:N	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:A:265:MET:CE	1:A:326:LYS:HD2	2.46	0.42
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:HD3	1:A:448:LYS:HA	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:B:192:MET:HE3	1:B:200:VAL:HG12	2.03	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

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	253/308 (82%)	236 (93%)	16 (6%)	1 (0%)	30	40
1	B	275/308 (89%)	257 (94%)	16 (6%)	2 (1%)	18	26
All	All	528/616 (86%)	493 (93%)	32 (6%)	3 (1%)	21	30

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

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	33/266 (12%)	29 (88%)	4 (12%)	5	6
1	B	130/266 (49%)	118 (91%)	12 (9%)	8	12
All	All	163/532 (31%)	147 (90%)	16 (10%)	7	10

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	183	ARG
1	A	209	THR

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Mol	Chain	Res	Type
1	A	212	VAL
1	B	185	ILE
1	B	186	SER
1	B	206	ASN
1	B	234	ILE
1	B	352	THR
1	B	365	THR
1	B	406	GLU
1	B	409	THR
1	B	434	SER
1	B	440	LYS
1	B	452	GLN
1	B	456	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	206	ASN
1	B	435	GLN
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	SEP	B	346	1	8,9,10	0.85	0	7,12,14	2.06	2 (28%)
1	SEP	A	346	1	8,9,10	0.84	0	7,12,14	2.13	2 (28%)

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	1.20	0	10,14,16	1.42	1 (10%)
1	TPO	B	345	1	8,10,11	0.97	0	10,14,16	1.48	2 (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
1	SEP	B	346	1	-	0/6/8/10	-
1	SEP	A	346	1	-	0/6/8/10	-
1	TPO	A	345	1	-	3/9/11/13	-
1	TPO	B	345	1	-	3/9/11/13	-

There are no bond length outliers.

All (7) 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	3.05	117.72	105.85
1	A	345	TPO	O2P-P-OG1	2.97	117.43	105.85
1	A	346	SEP	O3P-P-OG	2.30	112.66	106.67
1	B	346	SEP	O3P-P-OG	2.21	112.44	106.67
1	B	345	TPO	P-OG1-CB	-2.10	117.63	123.33

There are no chirality outliers.

All (6) torsion outliers are listed below:

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	N-CA-CB-OG1
1	B	345	TPO	O-C-CA-CB
1	A	345	TPO	CA-CB-OG1-P
1	B	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 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	NB5	A	501	-	36,43,43	1.38	4 (11%)	39,67,67	1.71	7 (17%)
2	NB5	B	501	-	36,43,43	1.47	7 (19%)	39,67,67	2.05	9 (23%)

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	A	501	-	-	2/15/41/41	0/7/7/7
2	NB5	B	501	-	-	6/15/41/41	0/7/7/7

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NB5	C6-C11	-3.76	1.45	1.49
2	B	501	NB5	C20-C22	-3.44	1.51	1.54
2	A	501	NB5	O36-C12	2.88	1.40	1.36
2	B	501	NB5	O36-C12	2.70	1.40	1.36
2	B	501	NB5	C20-N34	-2.51	1.46	1.49
2	B	501	NB5	C19-C22	-2.50	1.52	1.54
2	A	501	NB5	C1-C7	-2.44	1.38	1.41
2	B	501	NB5	C17-C21	-2.42	1.53	1.55
2	A	501	NB5	C8-C7	-2.25	1.38	1.42
2	B	501	NB5	C1-C7	-2.11	1.38	1.41
2	B	501	NB5	C14-N35	2.00	1.41	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NB5	C17-C21-N33	-6.27	113.62	118.18
2	A	501	NB5	C23-O36-C12	-4.87	118.16	123.24
2	B	501	NB5	C23-O36-C12	-4.87	118.16	123.24
2	B	501	NB5	C18-C22-C17	4.81	93.31	88.14
2	A	501	NB5	C18-C22-C17	3.90	92.34	88.14
2	A	501	NB5	C1-C7-C8	-3.06	116.59	119.63
2	B	501	NB5	C1-C7-C8	-2.99	116.66	119.63
2	B	501	NB5	F37-C10-C1	-2.84	116.26	120.21
2	A	501	NB5	C7-C8-N30	2.83	124.44	121.41
2	B	501	NB5	C7-C8-N30	2.70	124.30	121.41
2	A	501	NB5	C17-C21-N33	-2.65	116.25	118.18
2	A	501	NB5	C5-N33-N29	2.35	114.04	112.45
2	B	501	NB5	C14-N35-C9	-2.32	123.11	127.69
2	A	501	NB5	N31-C14-N32	-2.26	122.55	126.25
2	B	501	NB5	N31-C14-N32	-2.15	122.73	126.25
2	B	501	NB5	C14-N32-C12	2.15	119.03	115.38

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NB5	C5-C9-N35-C14
2	A	501	NB5	C17-C21-N33-N29
2	B	501	NB5	C5-C9-N35-C14
2	B	501	NB5	C17-C21-N33-N29
2	B	501	NB5	C18-C21-N33-N29
2	B	501	NB5	C15-C23-O36-C12
2	B	501	NB5	C16-C23-O36-C12
2	B	501	NB5	C18-C21-N33-C5

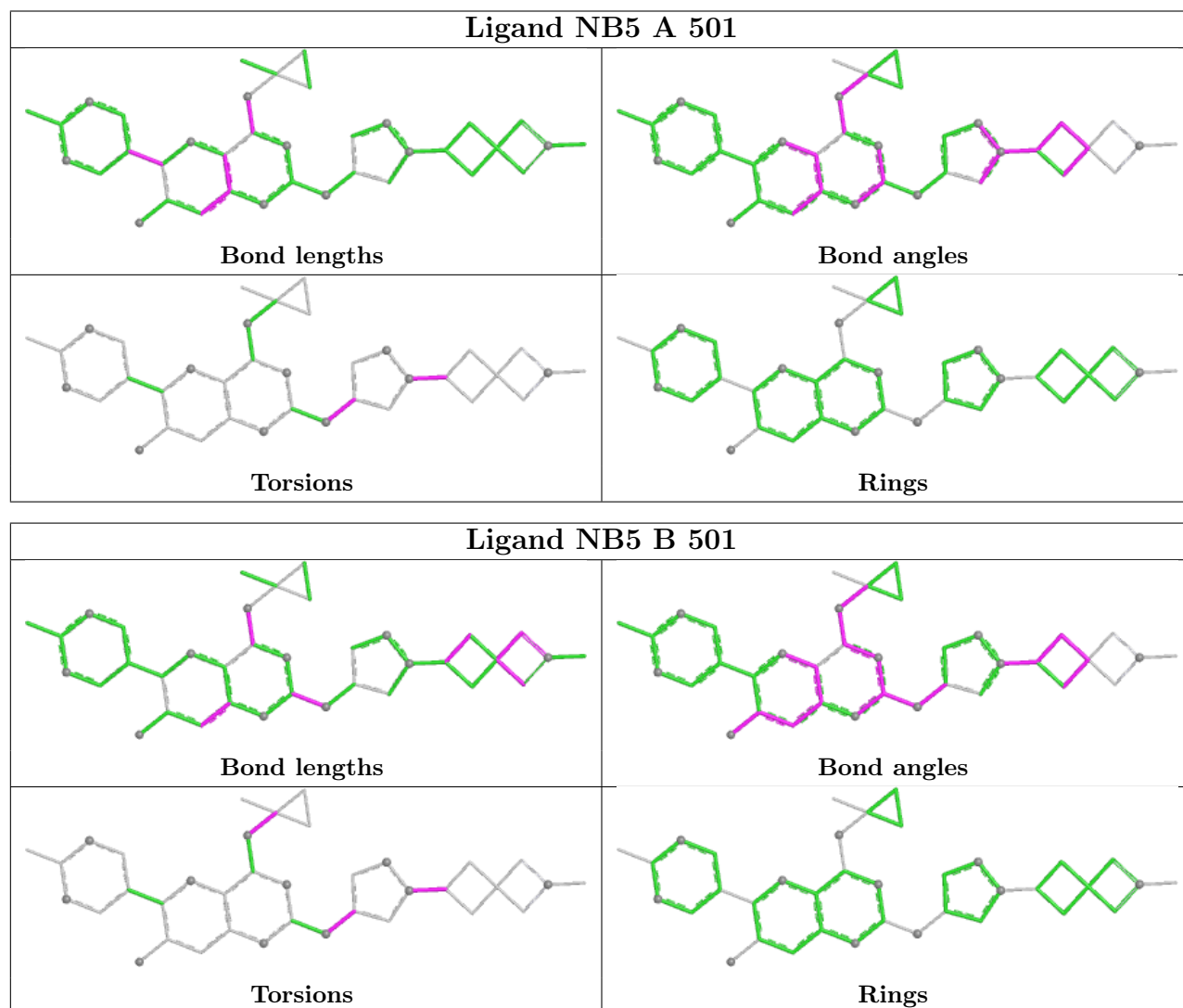
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NB5	1	0
2	B	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.43	25 (9%) 14 13	34, 69, 150, 197	0
1	B	281/308 (91%)	0.51	20 (7%) 22 20	38, 71, 118, 164	0
All	All	546/616 (88%)	0.47	45 (8%) 17 16	34, 70, 141, 197	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	171	TYR	5.0
1	B	170	PHE	4.4
1	B	176	VAL	4.0
1	A	185	ILE	4.0
1	A	252	SER	3.9
1	B	251	PHE	3.6
1	B	258	LEU	3.6
1	A	251	PHE	3.5
1	B	458	THR	3.3
1	A	176	VAL	3.3
1	A	230	PHE	3.0
1	A	165	PHE	2.9
1	B	336	SER	2.9
1	A	343	VAL	2.9
1	B	190	ASN	2.9
1	A	348	ILE	2.9
1	A	351	THR	2.9
1	A	170	PHE	2.8
1	A	259	CYS	2.8
1	B	169	SER	2.7
1	A	342	THR	2.6
1	B	344	MET	2.6
1	B	204	TYR	2.6
1	A	173	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	189	GLY	2.5
1	A	171	TYR	2.5
1	B	409	THR	2.4
1	B	168	PHE	2.3
1	B	203	GLY	2.3
1	B	205	VAL	2.3
1	A	189	GLY	2.2
1	A	198	GLY	2.2
1	A	169	SER	2.2
1	B	361	ARG	2.2
1	B	223	THR	2.2
1	A	215	LEU	2.2
1	B	399	ILE	2.2
1	B	342	THR	2.1
1	A	184	PRO	2.1
1	A	205	VAL	2.1
1	A	349	VAL	2.1
1	A	204	TYR	2.0
1	A	180	PHE	2.0
1	A	186	SER	2.0
1	A	243	GLU	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($\text{\AA}^2$)	Q<0.9
1	SEP	A	346	10/11	0.23	0.14	145,149,159,160	0
1	SEP	B	346	10/11	0.30	0.12	146,156,164,167	0
1	TPO	B	345	11/12	0.69	0.12	145,151,154,158	0
1	TPO	A	345	11/12	0.70	0.13	137,143,146,148	0

6.3 Carbohydrates [i](#)

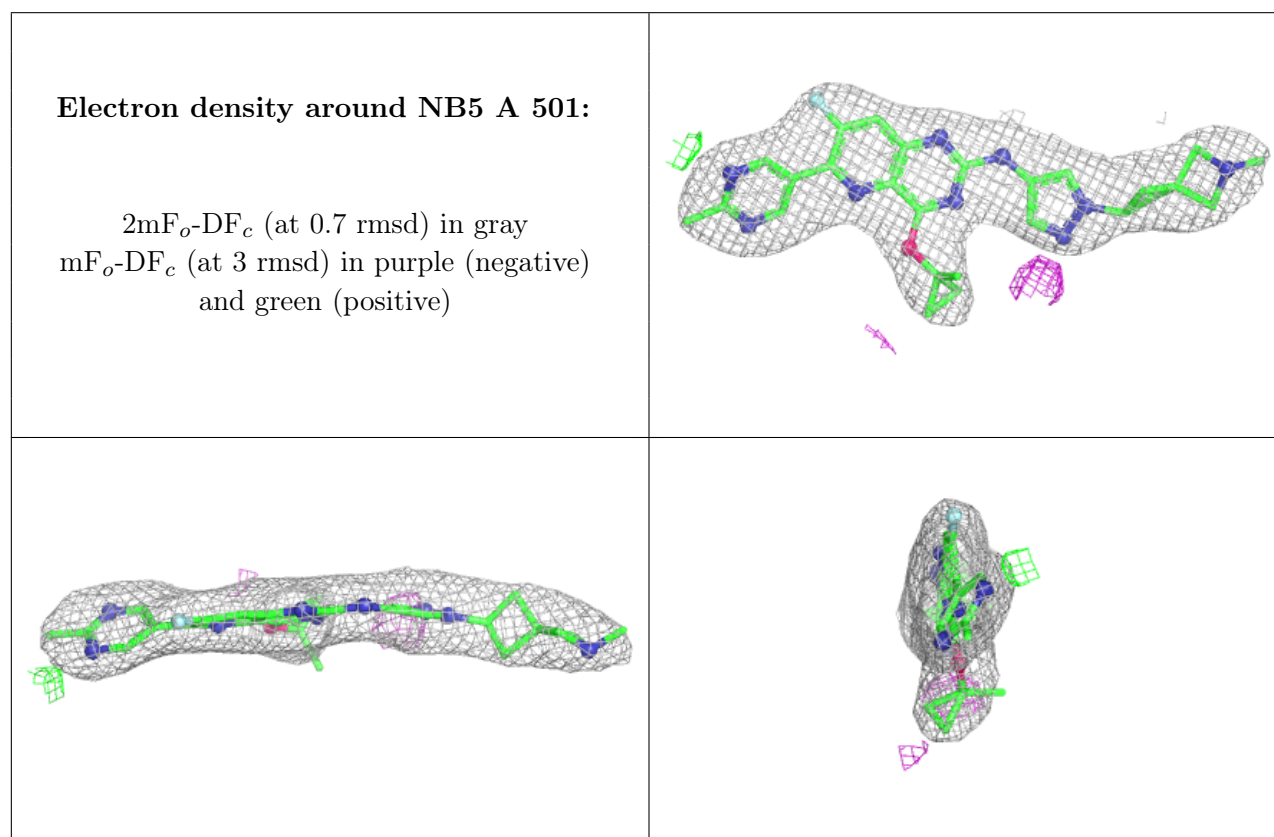
There are no oligosaccharides in this entry.

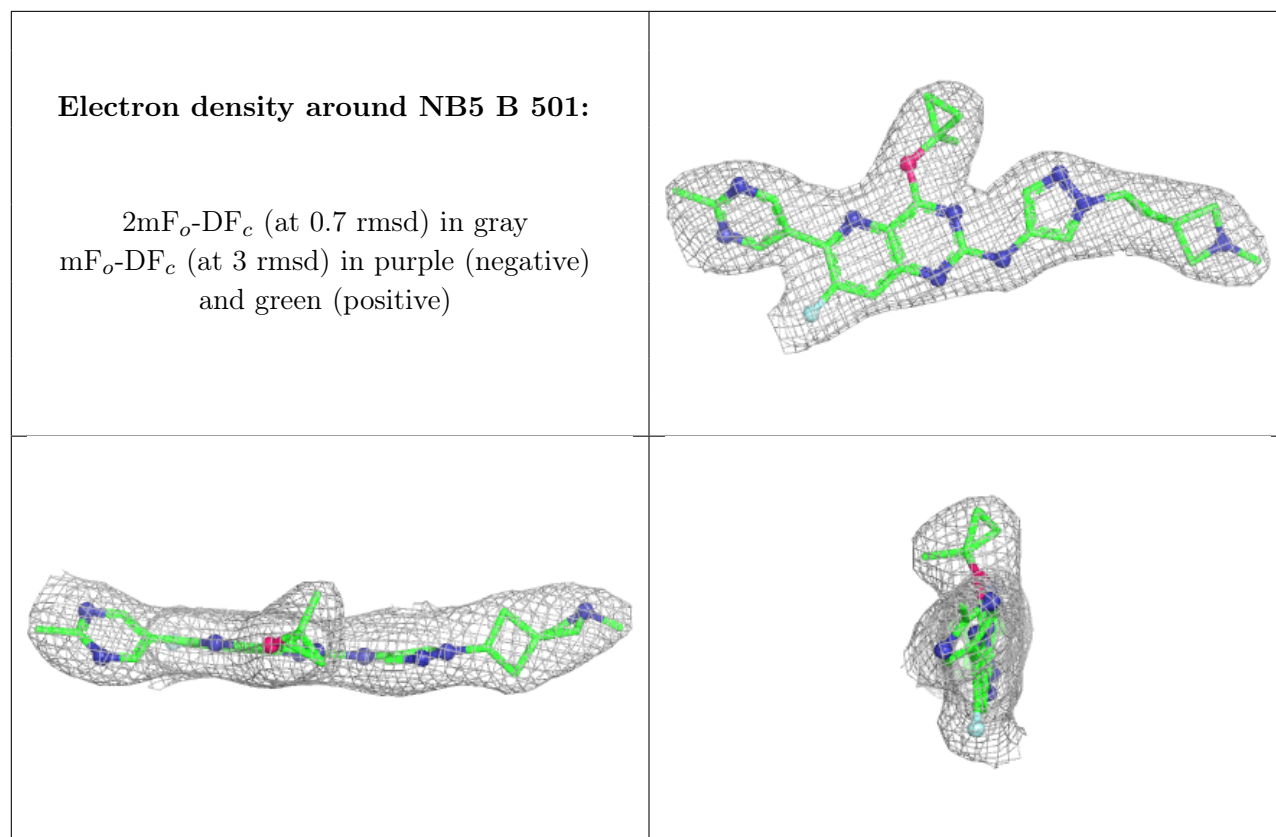
6.4 Ligands ⓘ

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	NB5	A	501	37/37	0.93	0.08	46,52,73,74	0
2	NB5	B	501	37/37	0.93	0.08	34,42,52,55	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.