



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 01:10 AM UTC

PDB ID : 4RMZ / pdb_00004rmz
Title : Crystal Structure of IRAK-4
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Deposited on : 2014-10-22
Resolution : 2.20 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

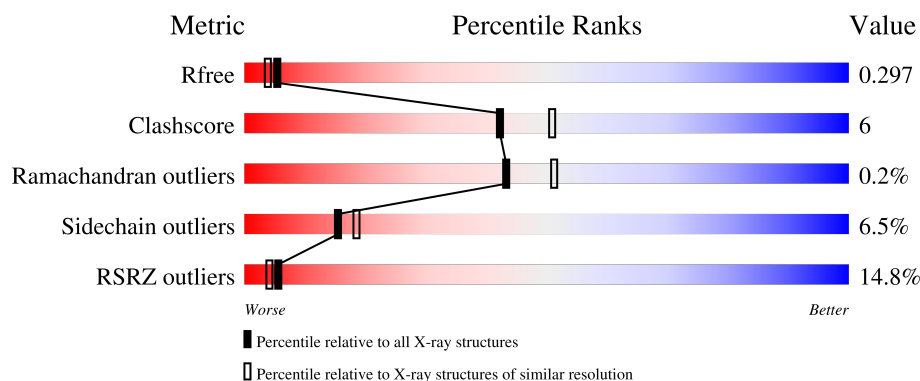
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	307	
1	B	307	

2 Entry composition [i](#)

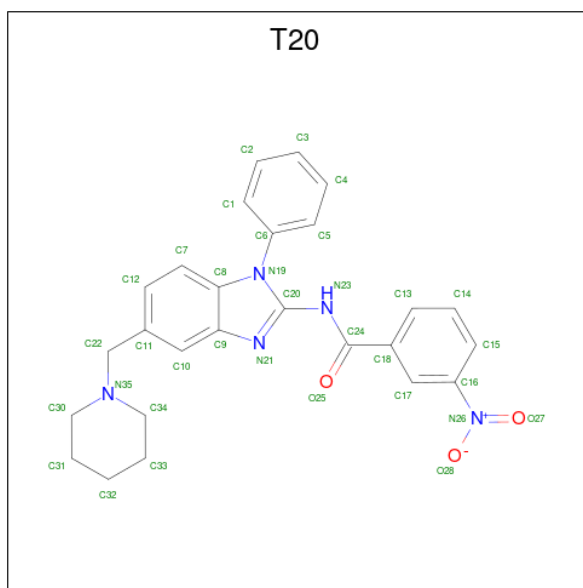
There are 3 unique types of molecules in this entry. The entry contains 4726 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	287	Total	C	N	O	P	S	0	1	0
			2268	1421	379	451	3	14			
1	B	284	Total	C	N	O	P	S	0	0	0
			2240	1407	375	442	2	14			

- Molecule 2 is 3-nitro-N-{1-phenyl-5-[(piperidin-1-yl)methyl]-1H-1,3-benzimidazol-2-yl}benzamide (CCD ID: T20) (formula: C₂₆H₂₅N₅O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			34	26	5	3		
2	B	1	Total	C	N	O	0	0
			34	26	5	3		

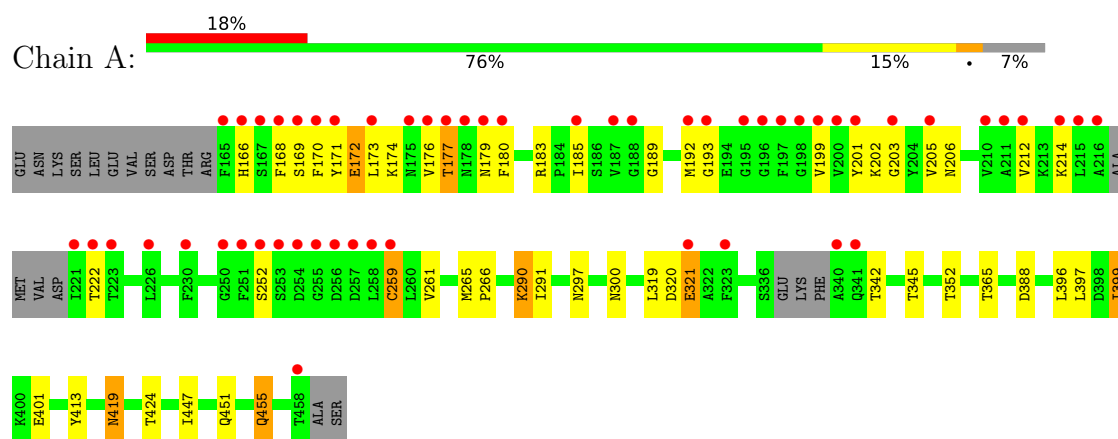
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	72	Total 72	O 72	0	0
3	B	78	Total 78	O 78	0	0

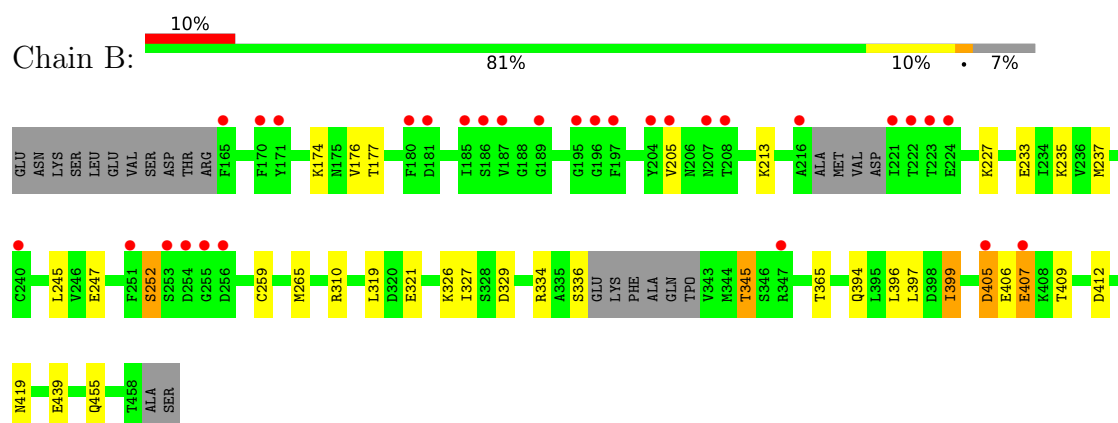
3 Residue-property plots [i](#)

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



- 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	87.73Å 116.81Å 140.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 30.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-2.20) 99.5 (30.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.236 , 0.296 0.240 , 0.297	Depositor DCC
R_{free} test set	1863 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.885	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4726	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.30% 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: T20, SEP, 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	0.80	0/2274	0.95	1/3062 (0.0%)
1	B	0.68	0/2255	0.87	1/3038 (0.0%)
All	All	0.74	0/4529	0.91	2/6100 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	GLY	N-CA-C	5.88	119.58	110.88
1	B	407	GLU	N-CA-C	-5.25	106.38	112.89

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	2268	0	2230	42	0
1	B	2240	0	2205	15	0
2	A	34	0	0	2	0
2	B	34	0	0	1	0
3	A	72	0	0	6	1
3	B	78	0	0	2	0
All	All	4726	0	4435	57	1

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:199:VAL:HG12	3:A:615:HOH:O	1.72	0.89
1:A:174:LYS:HG2	1:A:179:ASN:HA	1.58	0.86
1:A:265:MET:HE1	1:A:320:ASP:HB3	1.63	0.81
1:B:405:ASP:O	1:B:407:GLU:N	2.26	0.68
1:A:265:MET:CE	1:A:320:ASP:HB3	2.24	0.67
1:A:203:GLY:HA3	3:A:622:HOH:O	1.94	0.67
1:A:166:HIS:CD2	1:A:168:PHE:HE1	2.13	0.66
1:A:172:GLU:O	1:A:176:VAL:HG22	1.97	0.64
1:B:237:MET:HA	1:B:237:MET:HE2	1.80	0.62
1:A:419:ASN:HD22	1:A:419:ASN:C	2.11	0.58
1:A:171:TYR:HB2	3:A:619:HOH:O	2.03	0.57
1:A:199:VAL:HG13	1:A:201:TYR:HE1	1.70	0.57
1:A:205:VAL:O	1:A:205:VAL:HG12	2.04	0.55
1:B:334:ARG:NH2	1:B:345:TPO:O1P	2.40	0.55
1:B:245:LEU:HD23	1:B:327:ILE:HB	1.89	0.53
1:A:179:ASN:O	1:A:180:PHE:C	2.53	0.52
1:A:396:LEU:O	1:A:399:ILE:HB	2.09	0.52
1:A:166:HIS:CD2	1:A:168:PHE:CE1	2.96	0.52
1:B:310:ARG:HD2	3:B:633:HOH:O	2.10	0.51
1:A:321:GLU:H	1:A:321:GLU:CD	2.19	0.50
1:A:265:MET:HE3	1:A:319:LEU:C	2.36	0.50
1:B:409:THR:HG22	1:B:412:ASP:OD2	2.12	0.49
1:B:396:LEU:O	1:B:399:ILE:HB	2.12	0.49
1:A:174:LYS:HD2	1:A:179:ASN:HD22	1.79	0.48
1:B:213:LYS:HE3	2:B:501:T20:O28	2.14	0.48
1:A:300:ASN:HA	1:A:447:ILE:HG21	1.96	0.48
1:A:185:ILE:HD11	2:A:501:T20:C22	2.44	0.47
1:B:176:VAL:HG23	1:B:177:THR:HG23	1.96	0.47
1:B:265:MET:HE3	1:B:319:LEU:C	2.40	0.47
1:A:266:PRO:HD2	1:A:320:ASP:HA	1.96	0.46
1:A:419:ASN:C	1:A:419:ASN:ND2	2.73	0.46
1:A:169[A]:SER:OG	1:A:172:GLU:HG2	2.16	0.46
1:B:252:SER:HB3	1:B:259:CYS:HB2	1.97	0.46
1:A:290:LYS:HG3	1:A:291:ILE:N	2.31	0.46
1:A:455:GLN:NE2	3:A:632:HOH:O	2.43	0.45
1:A:174:LYS:HD2	1:A:179:ASN:ND2	2.31	0.45
1:A:203:GLY:CA	3:A:622:HOH:O	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:PHE:CD2	1:A:261:VAL:HG21	2.51	0.45
1:A:169[B]:SER:HB3	3:A:603:HOH:O	2.17	0.44
1:B:176:VAL:HG11	1:B:205:VAL:HG12	1.99	0.44
1:A:252:SER:HB3	1:A:259:CYS:HB2	1.99	0.43
1:A:170:PHE:O	1:A:173:LEU:N	2.49	0.43
1:A:199:VAL:HG13	1:A:201:TYR:CE1	2.52	0.43
1:A:192:MET:HE2	1:A:202:LYS:N	2.34	0.43
1:B:247:GLU:HG3	3:B:654:HOH:O	2.18	0.43
1:A:192:MET:HE2	1:A:201:TYR:C	2.45	0.42
1:A:185:ILE:HD11	2:A:501:T20:C11	2.49	0.42
1:A:388:ASP:OD1	1:A:388:ASP:C	2.62	0.42
1:B:265:MET:CE	1:B:326:LYS:HD2	2.50	0.42
1:B:409:THR:HG22	1:B:412:ASP:CG	2.44	0.42
1:A:265:MET:HE3	1:A:320:ASP:N	2.35	0.41
1:A:297:ASN:ND2	1:A:451:GLN:OE1	2.52	0.41
1:A:399:ILE:HG13	1:A:413:TYR:CZ	2.55	0.41
1:A:173:LEU:O	1:A:177:THR:HB	2.20	0.41
1:A:183:ARG:O	1:A:189:GLY:HA3	2.20	0.41
1:A:205:VAL:O	1:A:206:ASN:HB3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:620:HOH:O	3:A:620:HOH:O[4_585]	2.12	0.08

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	279/307 (91%)	262 (94%)	17 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	276/307 (90%)	264 (96%)	11 (4%)	1 (0%)	30	34
All	All	555/614 (90%)	526 (95%)	28 (5%)	1 (0%)	43	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	406	GLU

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	248/265 (94%)	232 (94%)	16 (6%)	15	18
1	B	246/265 (93%)	230 (94%)	16 (6%)	15	18
All	All	494/530 (93%)	462 (94%)	32 (6%)	15	18

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	GLU
1	A	177	THR
1	A	212	VAL
1	A	214	LYS
1	A	222	THR
1	A	259	CYS
1	A	290	LYS
1	A	321	GLU
1	A	352	THR
1	A	365	THR
1	A	397	LEU
1	A	399	ILE
1	A	401	GLU
1	A	419	ASN
1	A	424	THR

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Mol	Chain	Res	Type
1	A	455	GLN
1	B	174	LYS
1	B	227	LYS
1	B	233	GLU
1	B	235	LYS
1	B	252	SER
1	B	321	GLU
1	B	329	ASP
1	B	336	SER
1	B	365	THR
1	B	394	GLN
1	B	397	LEU
1	B	399	ILE
1	B	405	ASP
1	B	419	ASN
1	B	439	GLU
1	B	455	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	HIS
1	A	179	ASN
1	A	206	ASN
1	A	267	ASN
1	A	293	GLN
1	A	297	ASN
1	A	394	GLN
1	A	419	ASN
1	A	451	GLN
1	A	455	GLN
1	B	178	ASN
1	B	390	HIS
1	B	419	ASN

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	SEP	A	346	1	8,9,10	0.64	0	7,12,14	1.34	0
1	TPO	B	345	1	8,10,11	0.86	0	10,14,16	1.10	1 (10%)
1	SEP	B	346	1	8,9,10	0.64	0	7,12,14	1.19	0
1	TPO	A	345	1	8,10,11	1.03	1 (12%)	10,14,16	1.02	0
1	TPO	A	342	1	8,10,11	0.71	0	10,14,16	1.28	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	-	2/6/8/10	-
1	TPO	B	345	1	-	2/9/11/13	-
1	SEP	B	346	1	-	5/6/8/10	-
1	TPO	A	345	1	-	2/9/11/13	-
1	TPO	A	342	1	-	1/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	TPO	P-OG1	2.04	1.63	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	TPO	O3P-P-O2P	2.25	116.23	107.80
1	B	345	TPO	O3P-P-O2P	2.12	115.75	107.80

There are no chirality outliers.

All (12) 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	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	O-C-CA-CB
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	342	TPO	C-CA-CB-CG2
1	B	346	SEP	CB-OG-P-O1P
1	A	345	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	345	TPO	1	0

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	T20	A	501	-	38,38,38	2.13	11 (28%)	51,53,53	1.98	13 (25%)
2	T20	B	501	-	38,38,38	2.13	11 (28%)	51,53,53	1.84	10 (19%)

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	T20	A	501	-	-	1/18/28/28	0/5/5/5
2	T20	B	501	-	-	2/18/28/28	0/5/5/5

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	T20	O27-N26	6.16	1.33	1.22
2	A	501	T20	O27-N26	5.26	1.31	1.22
2	B	501	T20	C24-N23	4.77	1.45	1.37
2	A	501	T20	C7-C8	4.57	1.46	1.39
2	B	501	T20	C5-C6	4.55	1.47	1.39
2	A	501	T20	C12-C11	4.51	1.47	1.38
2	A	501	T20	C5-C6	4.18	1.47	1.39
2	A	501	T20	C24-N23	4.08	1.44	1.37
2	B	501	T20	C12-C11	3.99	1.46	1.38
2	A	501	T20	C20-N23	3.18	1.48	1.37
2	B	501	T20	C7-C8	2.98	1.44	1.39
2	A	501	T20	C10-C9	2.94	1.44	1.40
2	B	501	T20	C20-N23	2.75	1.46	1.37
2	B	501	T20	C22-C11	2.54	1.56	1.51
2	B	501	T20	C14-C13	2.45	1.43	1.38
2	B	501	T20	C3-C2	2.31	1.43	1.38
2	A	501	T20	O25-C24	2.16	1.28	1.23
2	A	501	T20	C17-C16	2.14	1.42	1.39
2	A	501	T20	C22-C11	2.09	1.55	1.51
2	A	501	T20	C4-C5	-2.09	1.35	1.38
2	B	501	T20	O25-C24	2.03	1.28	1.23
2	B	501	T20	C2-C1	2.02	1.42	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	T20	C22-N35-C34	8.57	129.50	111.07
2	B	501	T20	C22-N35-C34	7.50	127.20	111.07
2	A	501	T20	N19-C20-N21	-4.48	107.81	113.57
2	B	501	T20	C15-C16-N26	3.88	122.73	119.34
2	B	501	T20	C22-N35-C30	-3.81	102.87	111.07
2	A	501	T20	C22-N35-C30	-3.45	103.65	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	T20	C9-N21-C20	3.31	109.22	104.06
2	A	501	T20	C6-N19-C20	-3.31	121.62	126.89
2	B	501	T20	C17-C16-N26	-3.19	115.99	118.74
2	B	501	T20	C31-C30-N35	3.02	115.99	111.30
2	B	501	T20	N19-C20-N21	-2.93	109.81	113.57
2	A	501	T20	C8-C9-N21	-2.80	106.64	110.19
2	A	501	T20	C18-C24-N23	2.74	120.19	116.25
2	B	501	T20	C7-C8-C9	-2.72	119.09	122.23
2	A	501	T20	O25-C24-N23	-2.71	118.32	122.27
2	A	501	T20	C7-C8-C9	-2.64	119.18	122.23
2	A	501	T20	C7-C8-N19	2.48	135.05	130.54
2	A	501	T20	C8-N19-C20	2.30	110.53	107.12
2	B	501	T20	C8-C9-N21	-2.26	107.32	110.19
2	B	501	T20	C9-N21-C20	2.23	107.53	104.06
2	B	501	T20	C9-C8-N19	2.20	106.89	105.25
2	A	501	T20	C6-N19-C8	2.19	127.85	124.24
2	A	501	T20	C10-C9-N21	2.15	133.95	129.31

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	T20	C15-C16-N26-O27
2	B	501	T20	C17-C16-N26-O27
2	A	501	T20	C1-C6-N19-C8

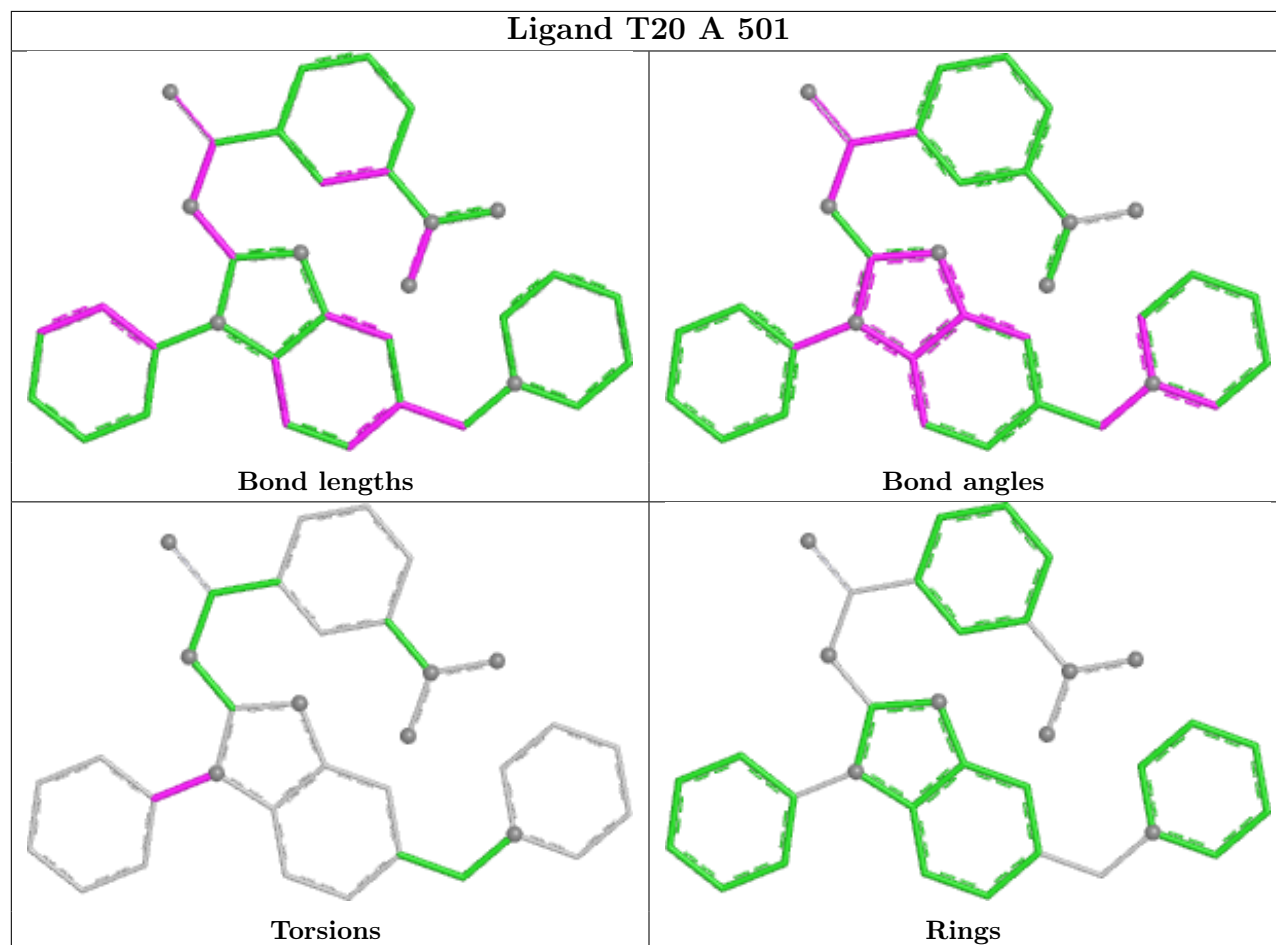
There are no ring outliers.

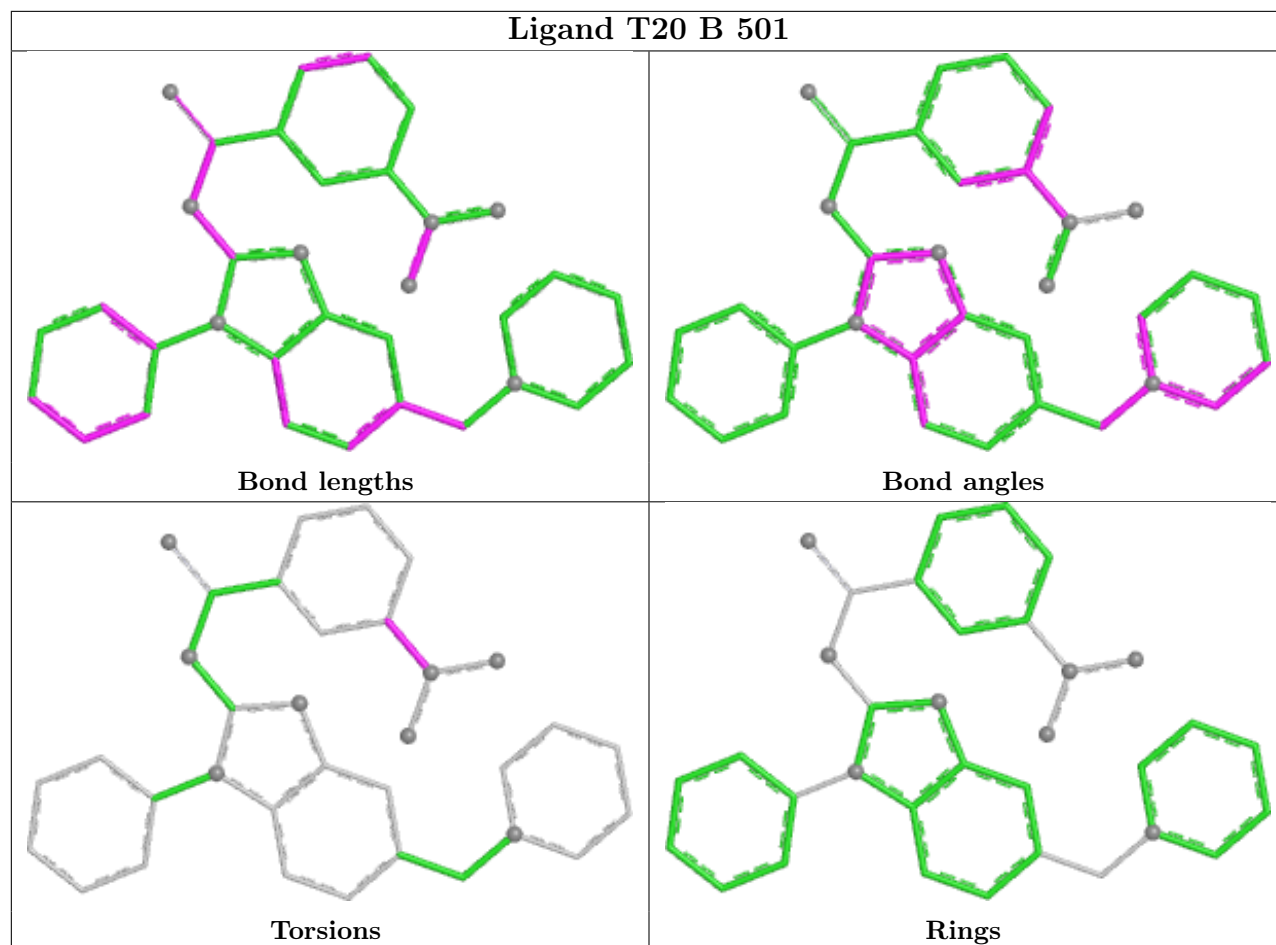
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	T20	2	0
2	B	501	T20	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	284/307 (92%)	0.86	54 (19%) 3 2	21, 37, 72, 96	1 (0%)
1	B	282/307 (91%)	0.50	30 (10%) 11 8	19, 38, 76, 98	0
All	All	566/614 (92%)	0.68	84 (14%) 5 4	19, 38, 75, 98	1 (0%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	221	ILE	6.6
1	A	255	GLY	6.1
1	A	168	PHE	5.7
1	A	257	ASP	5.3
1	B	221	ILE	4.9
1	A	252	SER	4.7
1	B	185	ILE	4.7
1	A	201	TYR	4.6
1	A	258	LEU	4.6
1	A	340	ALA	4.5
1	A	251	PHE	4.3
1	A	205	VAL	4.1
1	A	203	GLY	4.0
1	A	173	LEU	4.0
1	A	195	GLY	4.0
1	A	175	ASN	4.0
1	A	187	VAL	3.9
1	A	167	SER	3.9
1	B	207	ASN	3.7
1	A	212	VAL	3.6
1	A	171	TYR	3.6
1	B	251	PHE	3.5
1	A	259	CYS	3.4
1	A	197	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	200	VAL	3.4
1	A	185	ILE	3.3
1	A	196	GLY	3.3
1	B	170	PHE	3.3
1	B	171	TYR	3.3
1	A	254	ASP	3.2
1	A	223	THR	3.1
1	A	179	ASN	3.1
1	A	215	LEU	3.1
1	A	222	THR	3.1
1	A	210	VAL	3.1
1	B	254	ASP	3.0
1	A	176	VAL	3.0
1	B	216	ALA	3.0
1	B	204	TYR	3.0
1	A	250	GLY	3.0
1	A	199	VAL	2.9
1	B	255	GLY	2.9
1	A	192	MET	2.9
1	A	170	PHE	2.8
1	A	177	THR	2.8
1	B	187	VAL	2.8
1	A	198	GLY	2.8
1	B	405	ASP	2.8
1	A	226	LEU	2.8
1	B	197	PHE	2.8
1	A	458	THR	2.7
1	B	256	ASP	2.7
1	B	208	THR	2.7
1	A	169[A]	SER	2.7
1	A	188	GLY	2.7
1	A	321	GLU	2.6
1	A	216	ALA	2.6
1	A	165	PHE	2.6
1	A	214	LYS	2.6
1	A	193	GLY	2.6
1	B	205	VAL	2.6
1	B	165	PHE	2.5
1	A	341	GLN	2.5
1	A	180	PHE	2.5
1	B	253	SER	2.5
1	A	211	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	222	THR	2.4
1	B	196	GLY	2.4
1	B	180	PHE	2.4
1	B	240	CYS	2.3
1	B	195	GLY	2.3
1	A	178	ASN	2.3
1	B	186	SER	2.3
1	A	253	SER	2.2
1	A	256	ASP	2.2
1	A	323	PHE	2.2
1	B	181	ASP	2.1
1	A	230	PHE	2.1
1	B	223	THR	2.1
1	B	407	GLU	2.1
1	B	189	GLY	2.1
1	B	347	ARG	2.1
1	B	224	GLU	2.0
1	A	166	HIS	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	TPO	A	342	11/12	0.85	0.14	51,69,78,78	0
1	SEP	A	346	10/11	0.87	0.10	43,56,76,78	0
1	SEP	B	346	10/11	0.87	0.10	46,56,69,69	0
1	TPO	B	345	11/12	0.90	0.09	41,44,56,58	0
1	TPO	A	345	11/12	0.94	0.08	38,39,48,48	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,

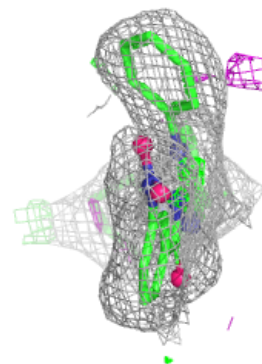
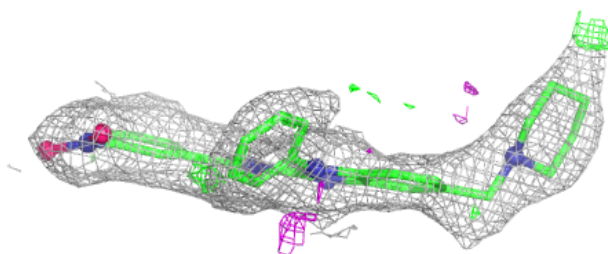
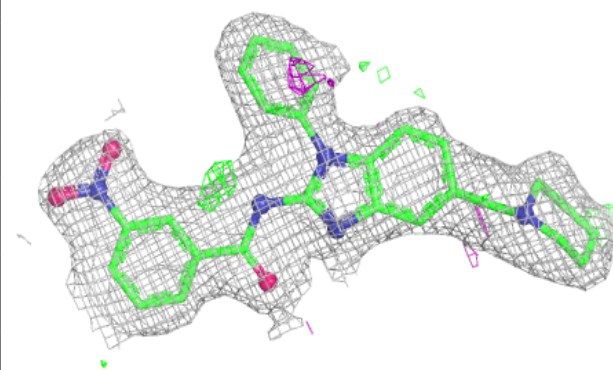
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	T20	A	501	34/34	0.87	0.13	40,43,51,56	0
2	T20	B	501	34/34	0.93	0.10	27,34,46,56	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.

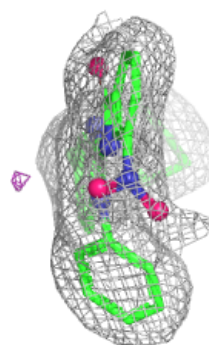
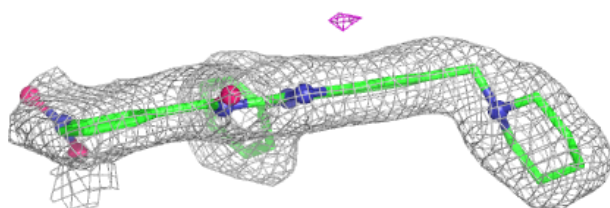
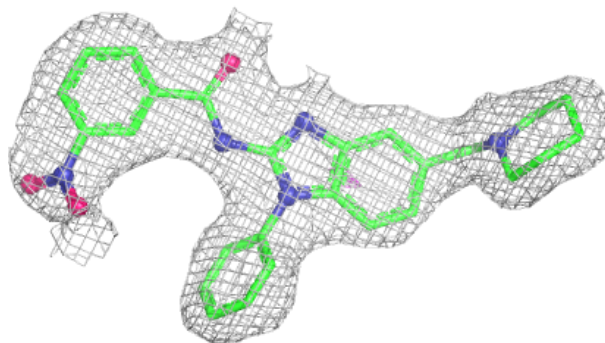
Electron density around T20 A 501:

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 T20 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.