



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:25 PM UTC

PDB ID : 8T2H / pdb_00008t2h
Title : DYRK1A complex with DYR530
Authors : Montfort, W.R.; Basantes, L.E.
Deposited on : 2023-06-06
Resolution : 1.85 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

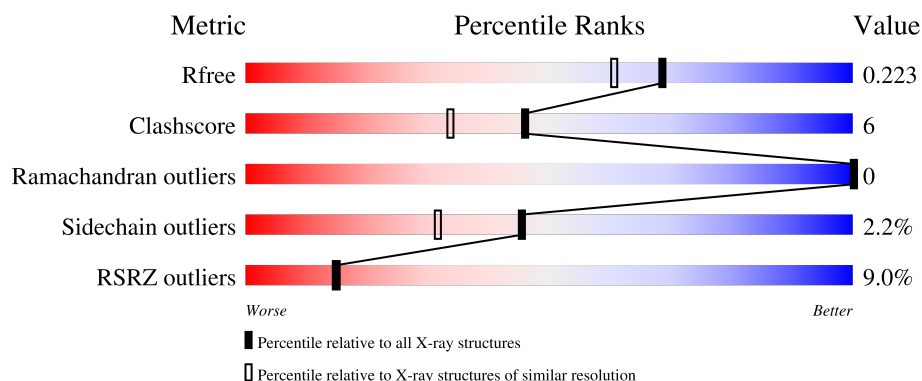
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	365	9% 79% 13% 7%
1	B	365	8% 82% 11% 6%

2 Entry composition [i](#)

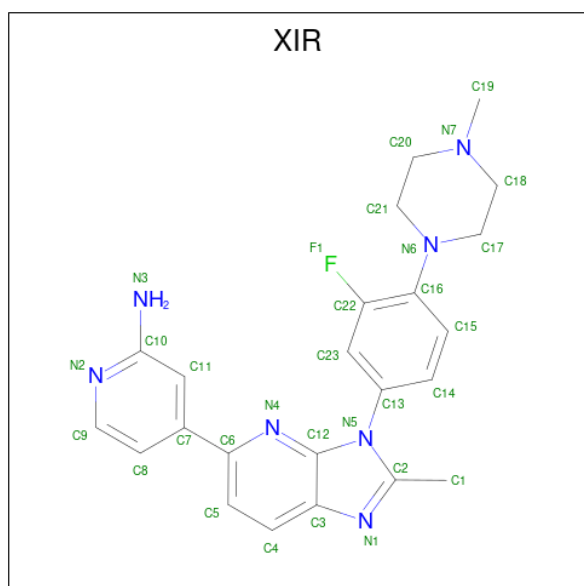
There are 5 unique types of molecules in this entry. The entry contains 6053 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

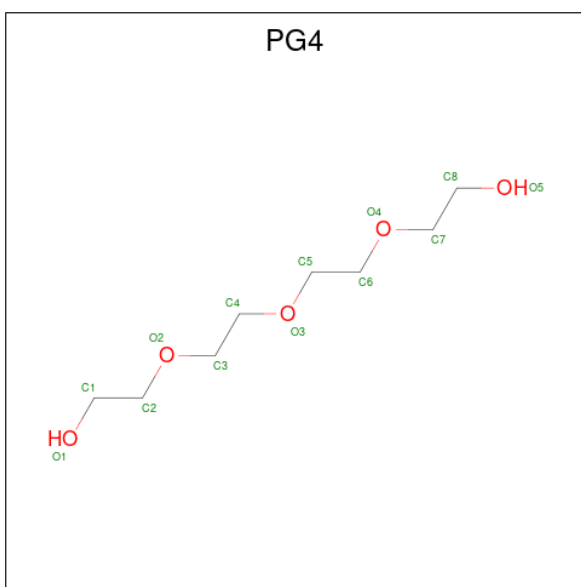
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	P	S	0	0	0
			2779	1789	475	497	1	17			
1	B	342	Total	C	N	O	P	S	0	3	0
			2827	1817	485	507	1	17			

- Molecule 2 is (4P)-4-[(3M)-3-[3-fluoro-4-(4-methylpiperazin-1-yl)phenyl]-2-methyl-3H-imidazo[4,5-b]pyridin-5-yl]pyridin-2-amine (CCD ID: XIR) (formula: C₂₃H₂₄FN₇) (labeled as "Ligand of Interest" by depositor).



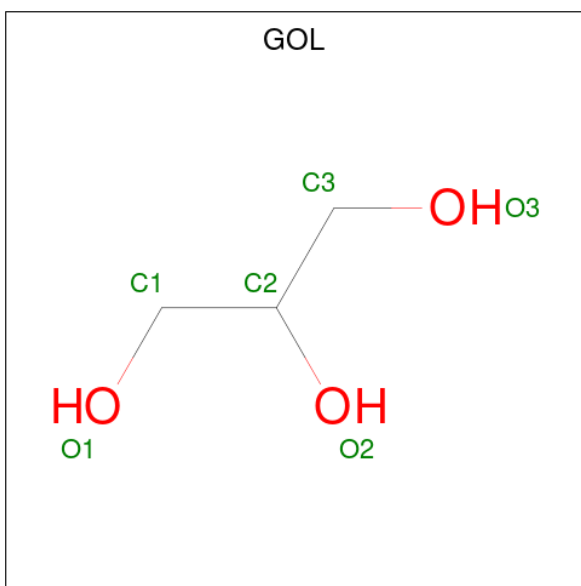
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	F	N	0	0
			31	23	1	7		
2	B	1	Total	C	F	N	0	0
			31	23	1	7		

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

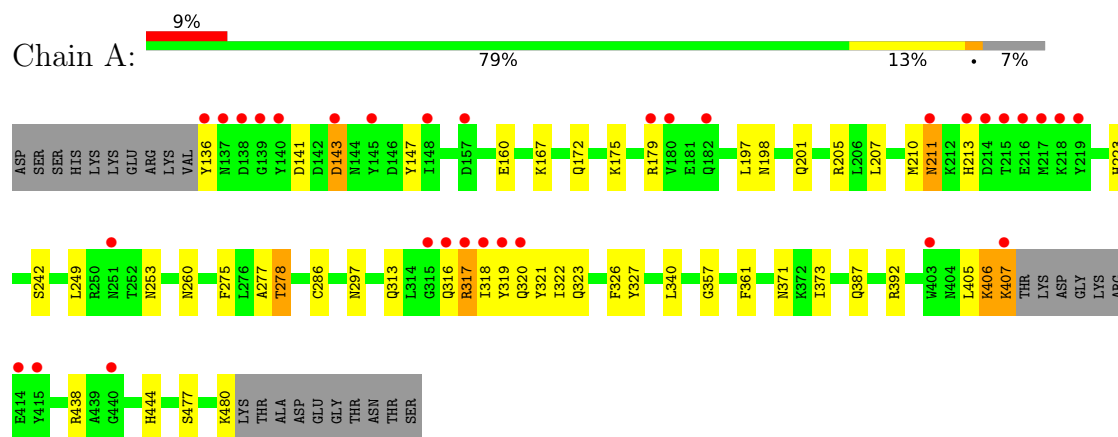
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	175	Total 175	O 175	0	0
5	B	179	Total 179	O 179	0	0

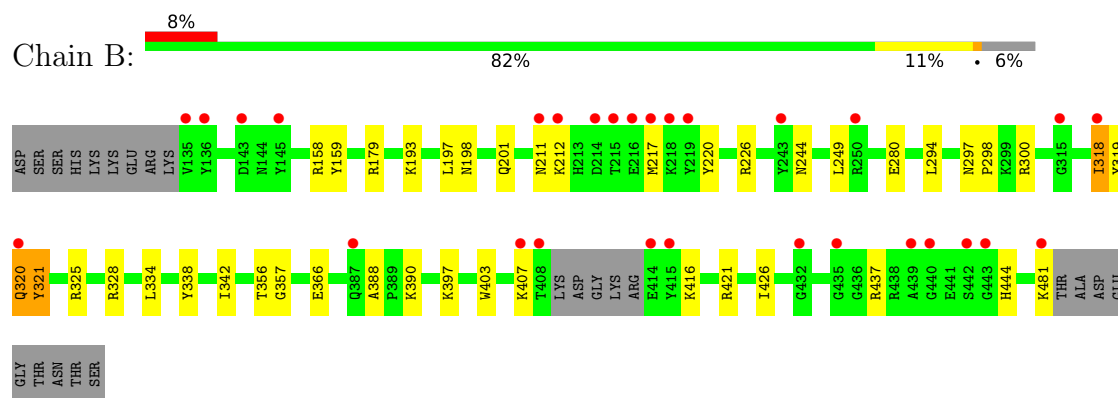
3 Residue-property plots

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: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.47Å 83.21Å 146.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.88 – 1.85 24.88 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (24.88-1.85) 99.9 (24.88-1.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.163 , 0.213 0.198 , 0.223	Depositor DCC
R_{free} test set	3381 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	15.8	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 34.7	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	0.94	EDS
Total number of atoms	6053	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.61% 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: XIR, PTR, GOL, PG4

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	0.65	0/2827	0.99	0/3810
1	B	0.63	0/2875	0.96	2/3876 (0.1%)
All	All	0.64	0/5702	0.97	2/7686 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	ASN	CB-CA-C	5.48	119.88	110.79
1	B	212	LYS	CB-CA-C	-5.22	99.31	110.32

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	438	ARG	Sidechain
1	B	300	ARG	Sidechain
1	B	328	ARG	Sidechain

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	2779	0	2780	43	0
1	B	2827	0	2827	25	0
2	A	31	0	0	0	0
2	B	31	0	0	0	0
3	A	13	0	18	2	0
4	A	12	0	16	1	0
4	B	6	0	8	1	0
5	A	175	0	0	11	0
5	B	179	0	0	8	0
All	All	6053	0	5649	66	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 (66) 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:275:PHE:O	1:A:278:THR:HG23	1.63	0.97
1:A:319:TYR:HB3	1:A:322:ILE:HG21	1.61	0.83
1:A:253:ASN:HB3	4:A:503:GOL:O3	1.82	0.80
1:A:160:GLU:OE1	1:A:179:ARG:NH2	2.19	0.75
1:A:211:ASN:OD1	5:A:601:HOH:O	2.06	0.71
4:B:501:GOL:H11	5:B:655:HOH:O	1.89	0.70
1:A:316:GLN:HA	5:A:615:HOH:O	1.91	0.69
1:A:407:LYS:HE2	1:A:407:LYS:C	2.19	0.68
1:A:313:GLN:H	1:A:316:GLN:HE21	1.41	0.67
1:B:325:ARG:HD3	5:B:616:HOH:O	1.96	0.66
1:B:320:GLN:NE2	1:B:321:PTR:O2P	2.28	0.65
1:A:317:ARG:O	1:A:320:GLN:NE2	2.33	0.62
1:B:244:ASN:HB3	1:B:294:LEU:HD22	1.82	0.61
1:B:197:LEU:O	1:B:201[A]:GLN:HG3	2.03	0.59
1:A:319:TYR:HA	1:B:201[A]:GLN:NE2	2.18	0.58
1:A:444:HIS:CE1	5:A:617:HOH:O	2.55	0.58
1:B:297[B]:ASN:ND2	1:B:298:PRO:HD2	2.18	0.58
1:A:175:LYS:CE	3:A:501:PG4:H71	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ARG:NH1	5:B:604:HOH:O	2.37	0.58
1:B:444:HIS:CE1	5:B:687:HOH:O	2.56	0.57
1:A:211:ASN:CG	5:A:635:HOH:O	2.47	0.57
1:A:319:TYR:HB3	1:A:322:ILE:CG2	2.34	0.57
1:B:249:LEU:HD22	1:B:357:GLY:HA2	1.87	0.57
1:B:280:GLU:HG3	5:B:661:HOH:O	2.05	0.57
1:B:318:ILE:HD13	1:B:318:ILE:O	2.05	0.57
1:A:167:LYS:HD3	1:A:172:GLN:HG2	1.87	0.56
1:B:193:LYS:HD3	5:B:725:HOH:O	2.06	0.55
1:B:366:GLU:OE2	1:B:390:LYS:NZ	2.40	0.55
1:A:477:SER:HA	1:A:480:LYS:HG2	1.90	0.54
1:A:313:GLN:H	1:A:316:GLN:NE2	2.06	0.53
1:B:397:LYS:HE3	1:B:403:TRP:CE2	2.44	0.53
1:A:211:ASN:HD21	1:A:223:HIS:CD2	2.28	0.51
1:A:213:HIS:HD2	5:A:762:HOH:O	1.93	0.50
1:A:275:PHE:O	1:A:278:THR:CG2	2.48	0.50
1:A:392:ARG:O	1:A:406:LYS:HE3	2.12	0.49
1:A:197:LEU:O	1:A:201:GLN:HG3	2.12	0.49
1:B:220:TYR:N	5:B:610:HOH:O	2.44	0.48
1:A:286:CYS:O	1:A:323:GLN:HA	2.14	0.48
1:A:318:ILE:HG12	5:A:615:HOH:O	2.14	0.48
1:A:317:ARG:HB2	1:A:317:ARG:HH21	1.79	0.47
1:B:158:ARG:O	1:B:179:ARG:HG3	2.15	0.47
1:A:320:GLN:OE1	5:A:602:HOH:O	2.20	0.47
1:A:392:ARG:HG3	5:A:642:HOH:O	2.14	0.46
1:A:207:LEU:HA	1:A:210:MET:HE3	1.98	0.46
1:A:143:ASP:OD1	1:A:143:ASP:N	2.49	0.45
1:A:242:SER:HB2	1:A:297:ASN:HA	1.98	0.45
1:A:249:LEU:HD22	1:A:357:GLY:HA2	1.99	0.45
1:A:319:TYR:CE1	1:B:198:ASN:HB3	2.52	0.45
1:A:480:LYS:C	5:A:735:HOH:O	2.60	0.45
1:B:159:TYR:OH	1:B:226:ARG:HD2	2.17	0.45
1:A:136:TYR:HB3	1:A:141:ASP:HB2	1.99	0.44
1:B:356:THR:O	1:B:437:ARG:NH2	2.50	0.44
1:A:326:PHE:HB2	1:A:327:TYR:CE2	2.53	0.43
1:B:244:ASN:CB	1:B:294:LEU:HD22	2.46	0.43
1:A:175:LYS:HE2	3:A:501:PG4:H71	2.00	0.42
1:B:217:MET:HG2	5:B:660:HOH:O	2.19	0.42
1:A:198:ASN:HB3	1:B:319:TYR:CE1	2.55	0.42
1:A:260:ASN:ND2	5:A:617:HOH:O	2.52	0.41
1:A:147:TYR:O	1:A:172:GLN:NE2	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:LEU:HB3	1:B:388:ALA:HB1	2.02	0.41
1:B:421:ARG:HG2	1:B:426:ILE:HD11	2.02	0.41
1:A:260:ASN:CG	5:A:617:HOH:O	2.64	0.41
1:A:361:PHE:CE1	1:A:373:ILE:HA	2.56	0.40
1:B:338:TYR:HB2	1:B:342:ILE:HG21	2.03	0.40
1:A:277:ALA:HA	1:A:340:LEU:CD2	2.52	0.40
1:A:371:ASN:OD1	1:A:405:LEU:HD13	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	334/365 (92%)	320 (96%)	14 (4%)	0	100	100
1	B	340/365 (93%)	326 (96%)	14 (4%)	0	100	100
All	All	674/730 (92%)	646 (96%)	28 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	300/323 (93%)	292 (97%)	8 (3%)	39	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	306/323 (95%)	301 (98%)	5 (2%)	55	44
All	All	606/646 (94%)	593 (98%)	13 (2%)	45	33

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	ASP
1	A	205	ARG
1	A	211	ASN
1	A	278	THR
1	A	317	ARG
1	A	387	GLN
1	A	406	LYS
1	A	407	LYS
1	B	318	ILE
1	B	320	GLN
1	B	407	LYS
1	B	416	LYS
1	B	481	LYS

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

Mol	Chain	Res	Type
1	A	213	HIS
1	A	316	GLN
1	A	371	ASN
1	B	192	ASN
1	B	213	HIS
1	B	475	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	PTR	B	321	1	15,16,17	0.72	0	17,22,24	1.03	1 (5%)
1	PTR	A	321	1	15,16,17	0.68	0	17,22,24	0.93	1 (5%)

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	PTR	B	321	1	-	2/10/11/13	0/1/1/1
1	PTR	A	321	1	-	0/10/11/13	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	PTR	O3P-P-OH	2.34	112.23	105.32
1	B	321	PTR	O3P-P-OH	2.20	111.83	105.32

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	321	PTR	CZ-OH-P-O1P
1	B	321	PTR	CZ-OH-P-O2P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	321	PTR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
4	GOL	A	502	-	5,5,5	0.12	0	5,5,5	0.29	0
2	XIR	B	500	-	34,35,35	0.65	0	47,51,51	1.15	3 (6%)
4	GOL	A	503	-	5,5,5	0.21	0	5,5,5	0.51	0
2	XIR	A	500	-	34,35,35	0.70	0	47,51,51	1.13	1 (2%)
4	GOL	B	501	-	5,5,5	0.13	0	5,5,5	0.47	0
3	PG4	A	501	-	12,12,12	0.23	0	11,11,11	0.21	0

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
4	GOL	A	502	-	-	4/4/4/4	-
2	XIR	B	500	-	-	2/12/22/22	0/5/5/5
4	GOL	A	503	-	-	2/4/4/4	-
2	XIR	A	500	-	-	2/12/22/22	0/5/5/5
4	GOL	B	501	-	-	1/4/4/4	-
3	PG4	A	501	-	-	4/10/10/10	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	XIR	C21-N6-C17	4.87	122.52	111.57
2	B	500	XIR	C21-N6-C17	4.43	121.53	111.57
2	B	500	XIR	C20-C21-N6	2.69	116.44	110.78
2	B	500	XIR	C21-C20-N7	2.40	114.71	110.86

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	502	GOL	O1-C1-C2-C3
4	A	502	GOL	C1-C2-C3-O3
4	A	502	GOL	O2-C2-C3-O3
4	A	503	GOL	C1-C2-C3-O3
2	A	500	XIR	C22-C16-N6-C21
3	A	501	PG4	O4-C7-C8-O5
2	B	500	XIR	C22-C16-N6-C21
4	A	502	GOL	O1-C1-C2-O2
4	A	503	GOL	O2-C2-C3-O3
3	A	501	PG4	C5-C6-O4-C7
3	A	501	PG4	O1-C1-C2-O2
2	A	500	XIR	C15-C16-N6-C21
3	A	501	PG4	O3-C5-C6-O4
4	B	501	GOL	O2-C2-C3-O3
2	B	500	XIR	C15-C16-N6-C21

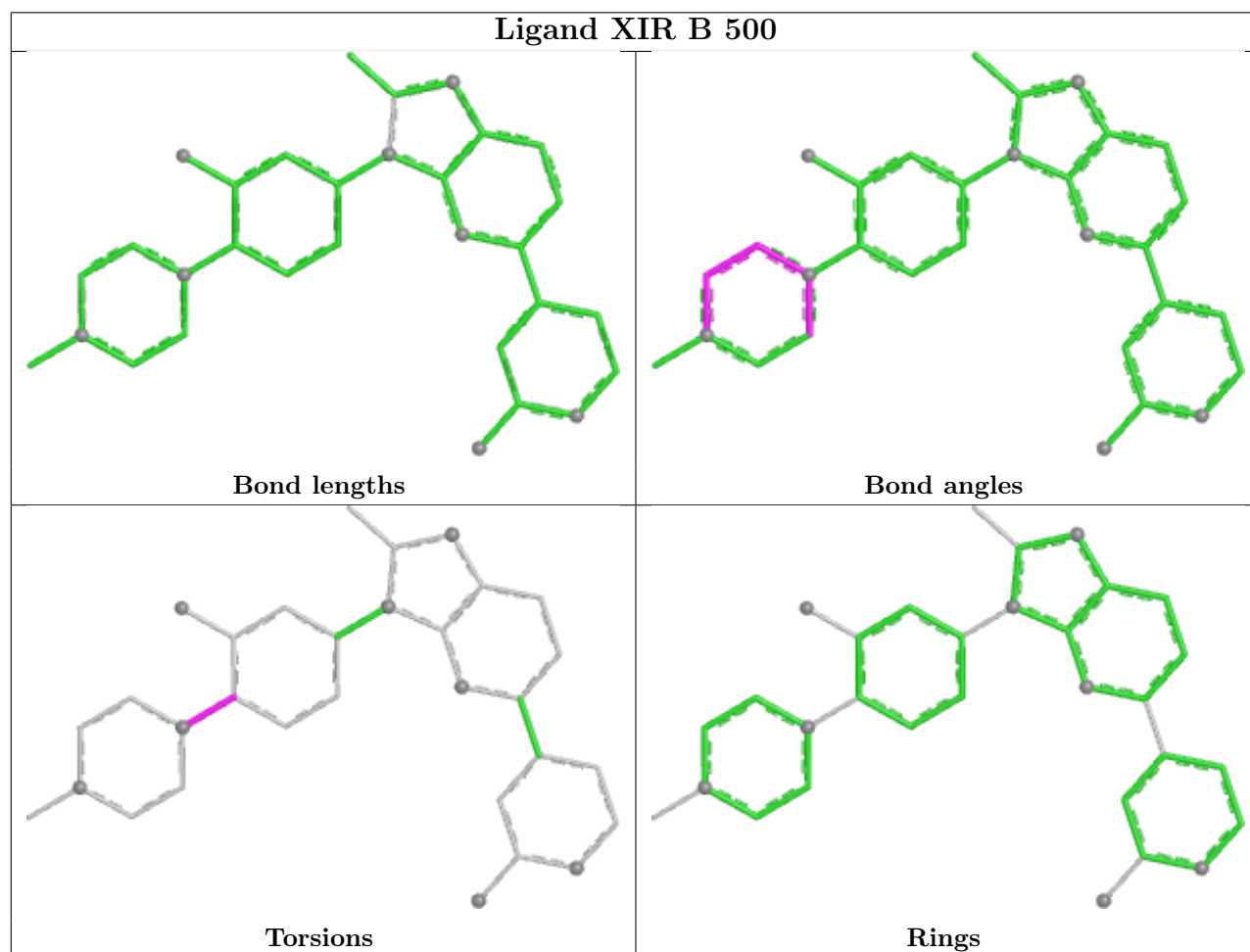
There are no ring outliers.

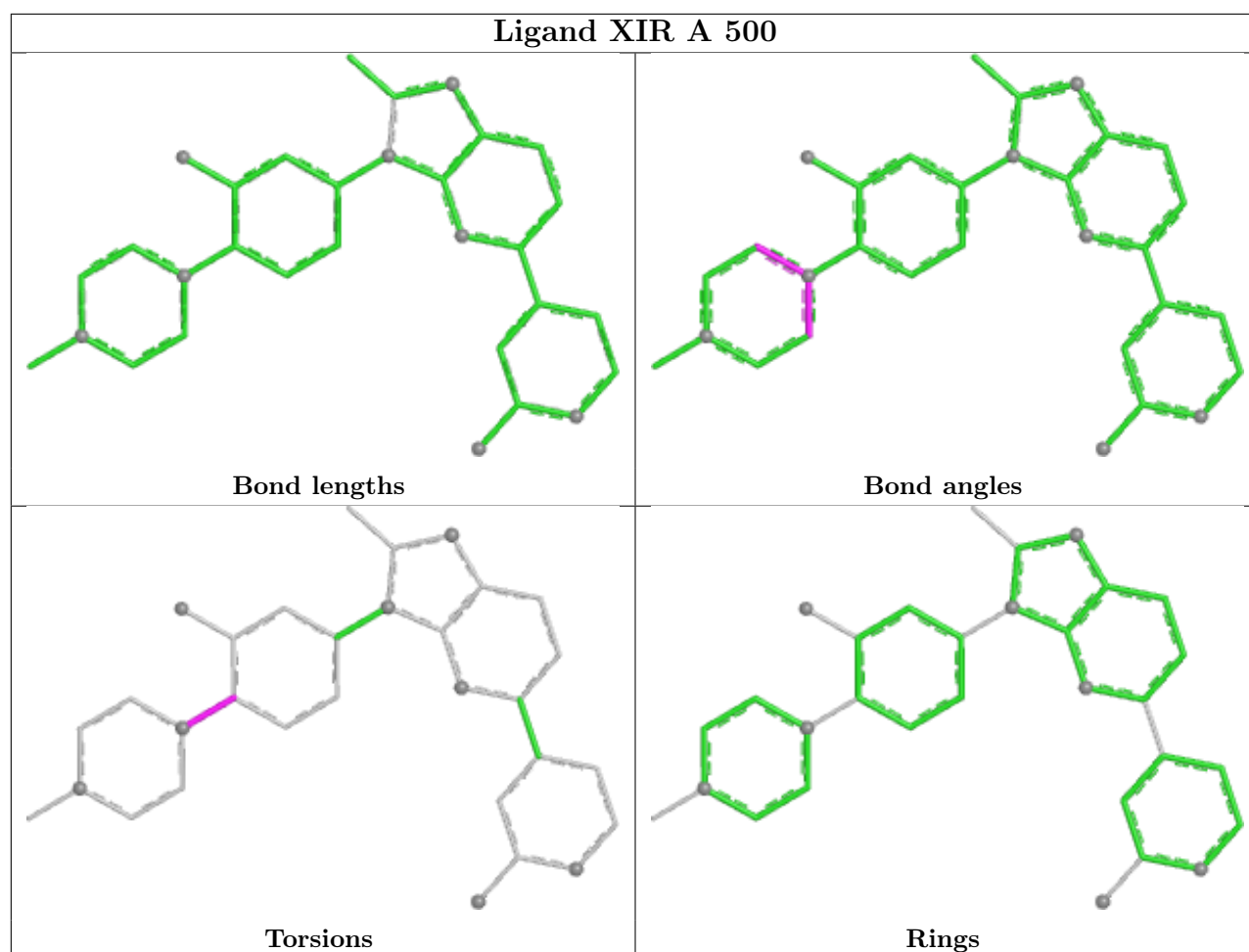
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	GOL	1	0
4	B	501	GOL	1	0
3	A	501	PG4	2	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	338/365 (92%)	0.26	32 (9%) 14 14	9, 18, 45, 77	0
1	B	341/365 (93%)	0.28	29 (8%) 16 17	8, 19, 45, 71	3 (0%)
All	All	679/730 (93%)	0.27	61 (8%) 15 15	8, 19, 45, 77	3 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	ILE	7.2
1	A	407	LYS	7.2
1	A	136	TYR	7.1
1	B	135	VAL	5.8
1	B	408	THR	5.6
1	A	219	TYR	5.2
1	B	219	TYR	5.2
1	B	481	LYS	4.7
1	A	317	ARG	4.3
1	B	136	TYR	4.3
1	A	180	VAL	4.1
1	A	215	THR	4.1
1	B	218	LYS	4.0
1	B	443	GLY	4.0
1	B	318	ILE	4.0
1	B	440	GLY	3.9
1	A	217	MET	3.7
1	A	440	GLY	3.7
1	B	215	THR	3.7
1	A	157	ASP	3.5
1	A	320	GLN	3.5
1	A	139	GLY	3.4
1	B	407	LYS	3.3
1	B	442	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	217	MET	3.3
1	A	140	TYR	3.2
1	A	145	TYR	3.1
1	A	319	TYR	3.1
1	A	138	ASP	3.1
1	B	439	ALA	3.0
1	B	320	GLN	2.9
1	B	214	ASP	2.9
1	A	211	ASN	2.9
1	A	316	GLN	2.8
1	B	435	GLY	2.8
1	A	213	HIS	2.7
1	A	148	ILE	2.7
1	A	414	GLU	2.7
1	A	143	ASP	2.7
1	A	214	ASP	2.7
1	B	414	GLU	2.6
1	B	315	GLY	2.6
1	B	415	TYR	2.5
1	B	143	ASP	2.5
1	A	216	GLU	2.5
1	B	212	LYS	2.5
1	B	145	TYR	2.4
1	A	179	ARG	2.4
1	A	218	LYS	2.4
1	B	243	TYR	2.3
1	A	182	GLN	2.3
1	B	387	GLN	2.3
1	B	432	GLY	2.3
1	A	137	ASN	2.3
1	B	211	ASN	2.2
1	A	315	GLY	2.1
1	A	403	TRP	2.1
1	B	250	ARG	2.1
1	B	216	GLU	2.0
1	A	415	TYR	2.0
1	A	251	ASN	2.0

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

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	PTR	B	321	16/17	0.86	0.14	25,29,49,51	0
1	PTR	A	321	16/17	0.93	0.10	21,23,26,27	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

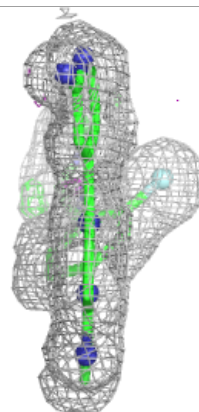
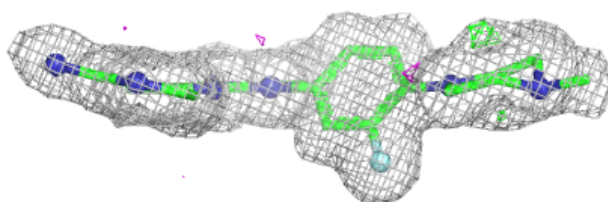
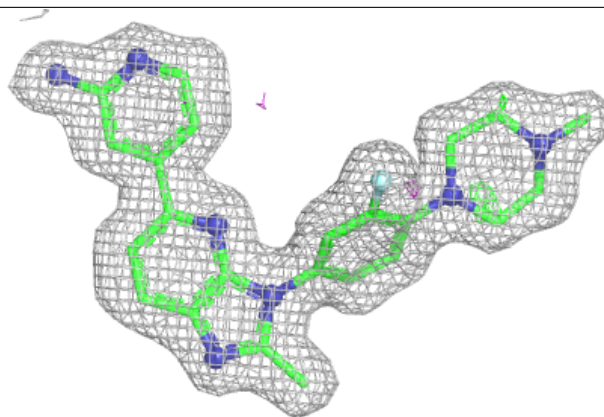
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	503	6/6	0.79	0.17	31,36,39,40	0
4	GOL	B	501	6/6	0.79	0.20	27,35,36,43	0
4	GOL	A	502	6/6	0.84	0.14	37,39,42,43	0
3	PG4	A	501	13/13	0.87	0.16	30,34,51,57	0
2	XIR	A	500	31/31	0.96	0.06	9,11,20,22	0
2	XIR	B	500	31/31	0.96	0.06	11,13,26,28	0

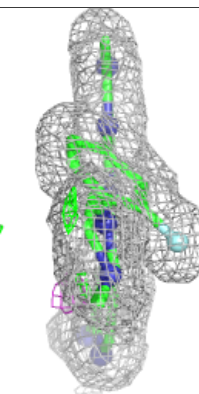
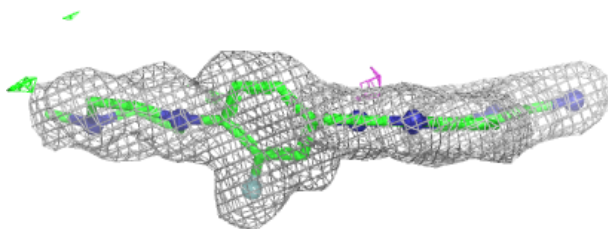
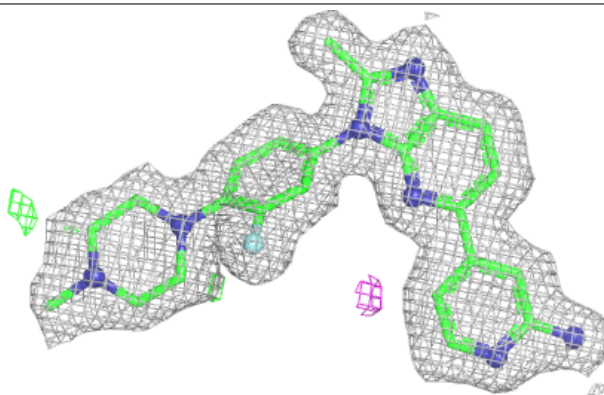
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around XIR A 500:

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

**Electron density around XIR B 500:**

$2mF_o-DF_c$ (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.