



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:27 AM UTC

PDB ID : 5OY4 / pdb_00005oy4
Title : GSK3beta complex with N-(6-(3,4-dihydroxyphenyl)-1H-pyrazolo[3,4-b]pyridin-3-yl)acetamide
Authors : Bax, B.D.; Convery, M.A.
Deposited on : 2017-09-07
Resolution : 3.20 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

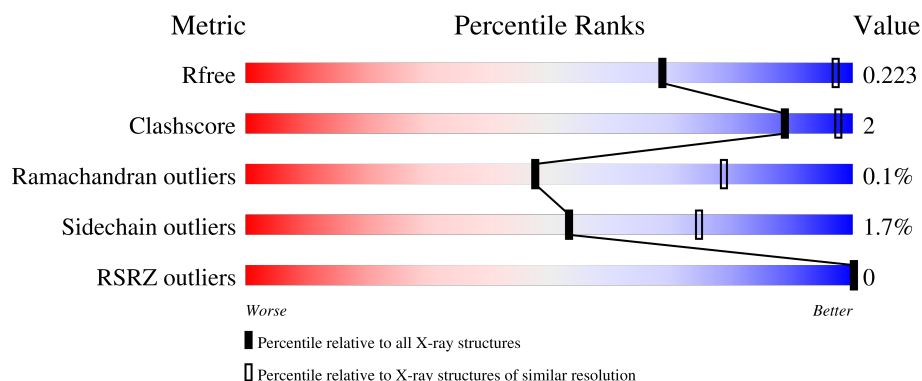
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	420	 78% 5% 17%
1	B	420	 78% 6% 16%
2	X	279	 8% 91%
2	Y	279	 8% 91%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5988 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.

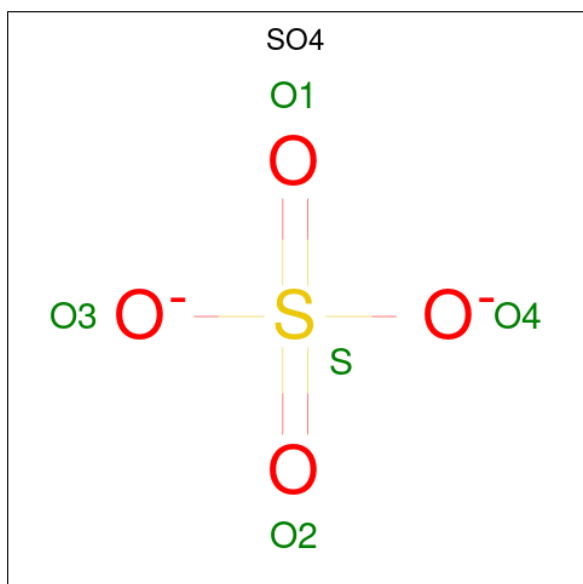
- Molecule 1 is a protein called Glycogen synthase kinase-3 beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	P	S	0	0	0
			2752	1772	464	504	1	11			
1	B	354	Total	C	N	O	P	S	0	0	0
			2790	1789	474	515	1	11			

- Molecule 2 is a protein called Proto-oncogene FRAT1.

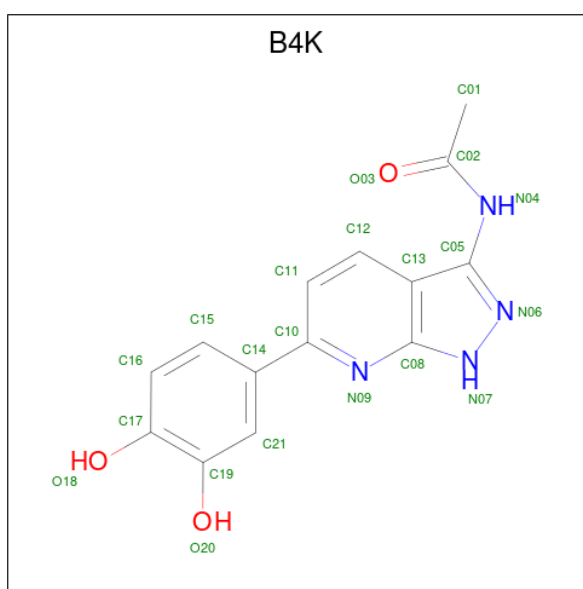
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	X	25	Total	C	N	O	0	0	0
			194	123	39	32			
2	Y	24	Total	C	N	O	0	0	0
			184	117	36	31			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is {N}-[6-[3,4-bis(oxidanyl)phenyl]-1 {H}-pyrazolo[3,4-b]pyridin-3-yl]ethanamide (CCD ID: B4K) (formula: C₁₄H₁₂N₄O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 21 14 4 3	0	0
4	B	1	Total C N O 21 14 4 3	0	0

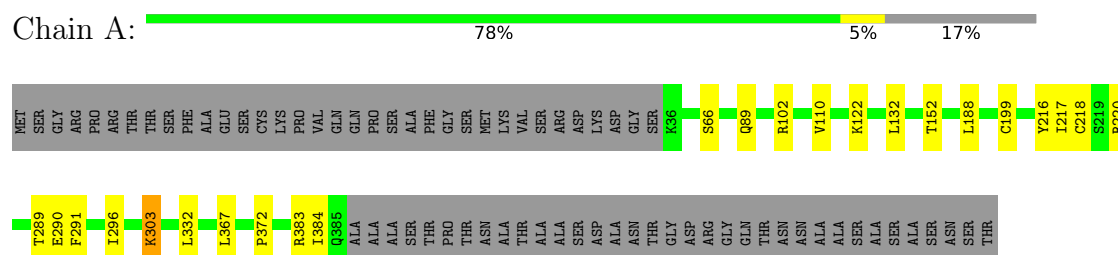
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total O 4 4	0	0
5	B	2	Total O 2 2	0	0

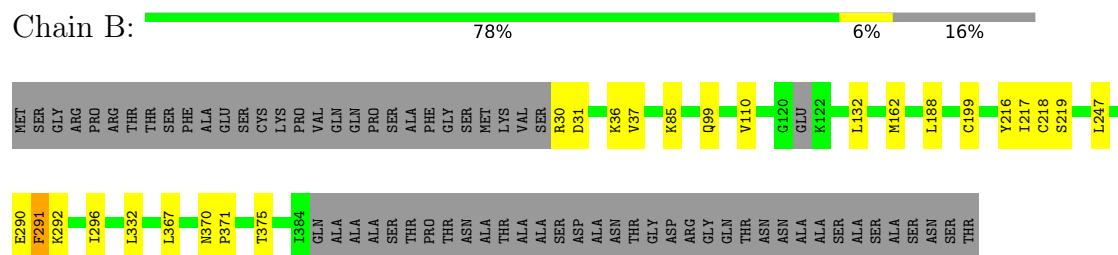
3 Residue-property plots

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.

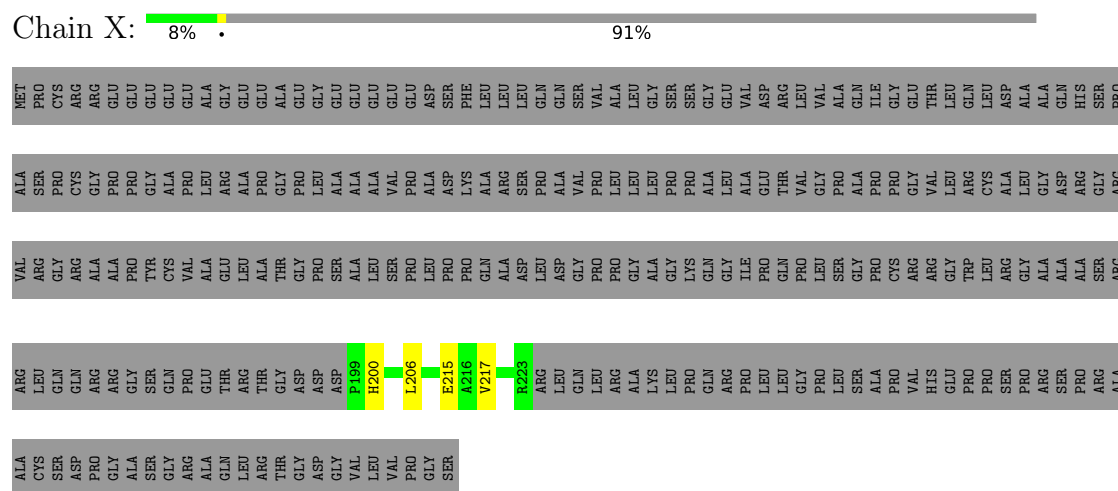
- Molecule 1: Glycogen synthase kinase-3 beta



- Molecule 1: Glycogen synthase kinase-3 beta



- Molecule 2: Proto-oncogene FRAT1



- Molecule 2: Proto-oncogene FRAT1

Chain Y: 8% 91%

CYS	ARG	VAL	ALA	MET
SER	LEU	ARG	SER	
ASP	GLN	GLY	PRO	
PRO	GLN	ARG	CYS	
GLY	ARG	ALA	ARG	
ALA	ARG	ALA	PRO	
SER	GLY	PRO	PRO	
GLY	SER	TYR	GLY	
ARG	GLN	CYS	ALA	
ALA	PRO	VAL	PRO	
GLN	GLU	ALA	LEU	
LEU	THR	GLU	ARG	
ARG	ARG	LEU	ALA	
THR	GLY	THR	PRO	
GLY	GLY	THR	GLY	
ASP	ASP	PRO	PRO	
GLY	ASP	SER	LEU	
VAL	ASP	SER	ALA	
LEU	P199	ALA	ALA	
VAL	H200	LEU	ALA	
PRO	V217	SER	VAL	
GLY		PRO	PRO	
SER	L220	LEU	ALA	
	H221	PRO	ASP	
	S222	GLN	LYS	
	ARG	ALA	ARG	
	LEU	ASP	SER	
	ARG	LEU	PRO	
	GLN	LEU	ALA	
	ARG	GLY	LEU	
	ALA	LYS	LEU	
	LEU	LEU	LEU	
	PRO	GLY	LEU	
	GLN	LYS	PRO	
	ARG	GLN	ALA	
	PRO	PRO	LEU	
	LEU	ILE	ALA	
	GLY	PRO	GLU	
	LEU	GLN	THR	
	PRO	LEU	VAL	
	LEU	SER	GLY	
	ALA	GLY	ALA	
	PRO	PRO	PRO	
	VAL	CYS	PRO	
	HIS	ARG	GLY	
	GLU	ARG	VAL	
	PRO	GLY	LEU	
	PRO	THR	ARG	
	SER	LEU	CYS	
	PRO	ARG	ALA	
	ARG	GLY	LEU	
	PRO	ALA	GLY	
	ARG	ALA	ASP	
	PRO	ALA	GLN	
	ALA	SER	ARG	

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	152.69Å 152.69Å 212.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 3.20 19.97 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.97-3.20) 97.6 (19.97-3.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.57 (at 3.22Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.194 , 0.229 0.193 , 0.223	Depositor DCC
R_{free} test set	778 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	89.9	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 61.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5988	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.87% 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: B4K, SO4, PTR

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	0.77	0/2805	1.15	8/3827 (0.2%)
1	B	0.78	1/2842 (0.0%)	1.15	7/3873 (0.2%)
2	X	0.78	0/196	1.51	3/263 (1.1%)
2	Y	0.78	0/185	1.46	1/248 (0.4%)
All	All	0.78	1/6028 (0.0%)	1.17	19/8211 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	371	PRO	CA-C	5.95	1.57	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	370	ASN	CA-CB-CG	5.86	118.46	112.60
2	X	200	HIS	N-CA-C	-5.68	105.07	112.23
1	A	290	GLU	CA-C-N	5.51	132.06	121.54
1	A	290	GLU	C-N-CA	5.51	132.06	121.54
1	A	383	ARG	CA-C-N	5.45	127.80	120.50
1	A	383	ARG	C-N-CA	5.45	127.80	120.50
1	B	371	PRO	N-CA-C	5.41	117.29	110.70
1	B	290	GLU	CA-C-N	5.39	131.83	121.54
1	B	290	GLU	C-N-CA	5.39	131.83	121.54
2	Y	200	HIS	N-CA-C	-5.37	105.08	111.69
1	B	31	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	122	LYS	CA-C-N	5.35	128.84	120.82
1	A	122	LYS	C-N-CA	5.35	128.84	120.82
1	A	66	SER	CA-C-N	5.16	127.19	120.28
1	A	66	SER	C-N-CA	5.16	127.19	120.28
1	B	31	ASP	CA-C-N	5.08	127.33	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	ASP	C-N-CA	5.08	127.33	120.38
2	X	200	HIS	CA-C-N	5.07	127.08	120.28
2	X	200	HIS	C-N-CA	5.07	127.08	120.28

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	2752	0	2719	9	0
1	B	2790	0	2749	14	0
2	X	194	0	205	2	0
2	Y	184	0	198	1	0
3	A	15	0	0	0	0
3	B	5	0	0	0	0
4	A	21	0	0	2	0
4	B	21	0	0	4	0
5	A	4	0	0	0	0
5	B	2	0	0	0	0
All	All	5988	0	5871	23	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 2.

All (23) 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:291:PHE:HD1	1:B:292:LYS:H	1.42	0.65
1:B:132:LEU:HD13	4:B:502:B4K:C21	2.32	0.60
1:A:132:LEU:HD13	4:A:504:B4K:C21	2.34	0.56
1:A:296:ILE:HD11	2:X:217:VAL:HG13	1.89	0.54
1:A:332:LEU:HD11	1:A:367:LEU:HA	1.90	0.54
1:A:217:ILE:O	1:A:218:CYS:HB2	2.08	0.53
1:B:132:LEU:HD13	4:B:502:B4K:C14	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ILE:O	1:B:218:CYS:HB2	2.11	0.51
1:A:110:VAL:HG21	1:A:188:LEU:HD12	1.92	0.51
1:B:110:VAL:HG21	1:B:188:LEU:HD12	1.91	0.50
1:B:30:ARG:HB2	1:B:37:VAL:H	1.76	0.50
1:B:199:CYS:HB2	4:B:502:B4K:C21	2.42	0.50
1:B:296:ILE:HD11	2:Y:217:VAL:HG13	1.94	0.48
2:X:206:LEU:HD11	2:X:215:GLU:HG2	1.96	0.48
1:B:332:LEU:HD11	1:B:367:LEU:HA	1.96	0.47
1:A:199:CYS:HB2	4:A:504:B4K:C21	2.47	0.44
1:B:162:MET:HE2	1:B:247:LEU:HB2	2.00	0.43
1:A:110:VAL:CG2	1:A:188:LEU:HD12	2.49	0.42
1:B:110:VAL:CG2	1:B:188:LEU:HD12	2.49	0.42
1:A:372:PRO:HB2	1:B:375:THR:HG23	2.01	0.42
1:A:303:LYS:HA	1:A:303:LYS:HD3	1.85	0.42
1:B:85:LYS:HD2	4:B:502:B4K:C16	2.51	0.41
1:B:30:ARG:HB2	1:B:36:LYS:HA	2.03	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	347/420 (83%)	337 (97%)	9 (3%)	1 (0%)	36	68
1	B	349/420 (83%)	340 (97%)	9 (3%)	0	100	100
2	X	23/279 (8%)	23 (100%)	0	0	100	100
2	Y	22/279 (8%)	22 (100%)	0	0	100	100
All	All	741/1398 (53%)	722 (97%)	18 (2%)	1 (0%)	48	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	ARG

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	298/363 (82%)	291 (98%)	7 (2%)	44	70
1	B	303/363 (84%)	300 (99%)	3 (1%)	68	80
2	X	21/213 (10%)	21 (100%)	0	100	100
2	Y	20/213 (9%)	19 (95%)	1 (5%)	22	55
All	All	642/1152 (56%)	631 (98%)	11 (2%)	53	75

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	102	ARG
1	A	152	THR
1	A	289	THR
1	A	291	PHE
1	A	303	LYS
1	A	384	ILE
1	B	99	GLN
1	B	219	SER
1	B	291	PHE
2	Y	220	LEU

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	46	GLN
1	A	89	GLN
1	A	151	GLN
1	A	287	ASN
1	A	299	HIS

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Mol	Chain	Res	Type
1	B	299	HIS

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	216	1	15,16,17	2.10	6 (40%)	17,22,24	0.88	0
1	PTR	A	216	1	15,16,17	1.98	4 (26%)	17,22,24	1.42	2 (11%)

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	216	1	-	1/10/11/13	0/1/1/1
1	PTR	A	216	1	-	1/10/11/13	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	PTR	CE2-CZ	3.53	1.45	1.38
1	B	216	PTR	CE2-CZ	3.44	1.45	1.38
1	A	216	PTR	CE1-CZ	3.43	1.45	1.38
1	A	216	PTR	P-OH	-3.42	1.53	1.59
1	B	216	PTR	CE1-CZ	3.28	1.44	1.38
1	B	216	PTR	P-OH	-3.27	1.53	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	216	PTR	CD2-CG	3.05	1.44	1.38
1	B	216	PTR	CD1-CG	2.95	1.44	1.38
1	A	216	PTR	CD1-CG	2.73	1.44	1.38
1	B	216	PTR	CE2-CD2	2.28	1.42	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	PTR	O3P-P-OH	3.26	114.95	105.32
1	A	216	PTR	OH-P-O1P	-2.90	99.81	109.48

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	216	PTR	O-C-CA-CB
1	B	216	PTR	O-C-CA-CB

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](#)

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	$\# Z > 2$
3	SO4	A	503	-	4,4,4	0.20	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	B4K	B	502	-	23,23,23	0.57	0	27,33,33	1.26	3 (11%)
3	SO4	A	502	-	4,4,4	0.23	0	6,6,6	0.16	0
4	B4K	A	504	-	23,23,23	0.70	0	27,33,33	1.12	4 (14%)
3	SO4	A	501	-	4,4,4	0.20	0	6,6,6	0.26	0
3	SO4	B	501	-	4,4,4	0.28	0	6,6,6	0.22	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	B4K	B	502	-	-	0/8/8/8	0/3/3/3
4	B4K	A	504	-	-	0/8/8/8	0/3/3/3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	502	B4K	C12-C13-C05	3.29	137.17	131.38
4	A	504	B4K	C12-C13-C05	2.93	136.53	131.38
4	B	502	B4K	C08-N07-N06	2.57	112.60	111.18
4	A	504	B4K	C08-N07-N06	2.53	112.58	111.18
4	A	504	B4K	N07-C08-N09	2.13	127.39	125.64
4	A	504	B4K	C11-C12-C13	-2.13	117.35	120.86
4	B	502	B4K	C11-C12-C13	-2.03	117.52	120.86

There are no chirality outliers.

There are no torsion outliers.

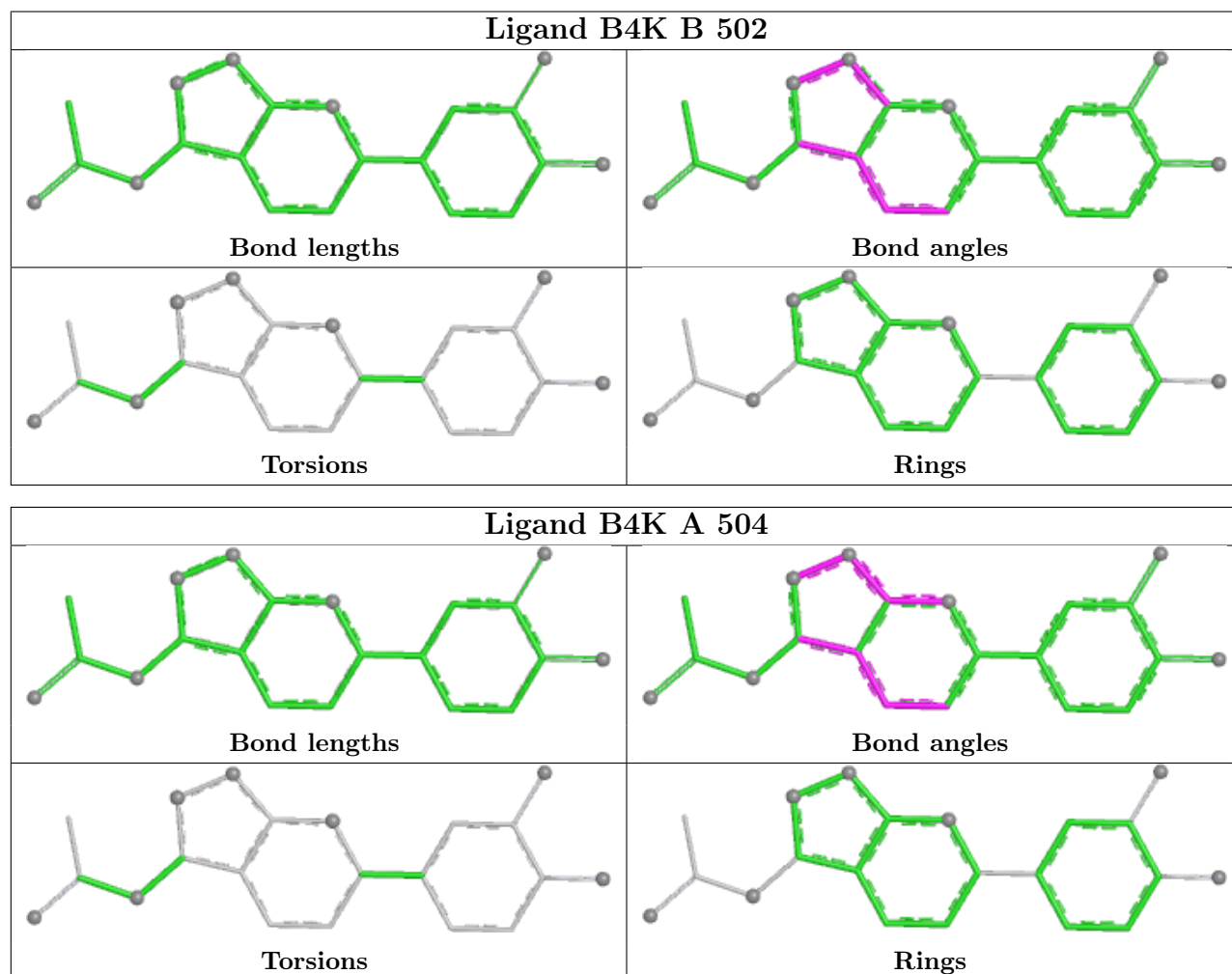
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	502	B4K	4	0
4	A	504	B4K	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	349/420 (83%)	-0.55	0 100 100	56, 90, 154, 176	0
1	B	353/420 (84%)	-0.51	0 100 100	56, 90, 140, 166	0
2	X	25/279 (8%)	-0.47	0 100 100	76, 86, 115, 120	0
2	Y	24/279 (8%)	-0.47	0 100 100	85, 96, 121, 144	0
All	All	751/1398 (53%)	-0.53	0 100 100	56, 91, 148, 176	0

There are no RSRZ outliers to report.

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	PTR	A	216	16/17	0.89	0.12	101,109,113,113	0
1	PTR	B	216	16/17	0.89	0.09	117,124,125,126	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

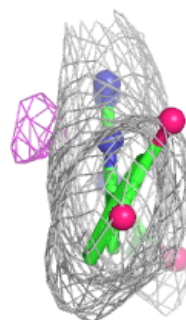
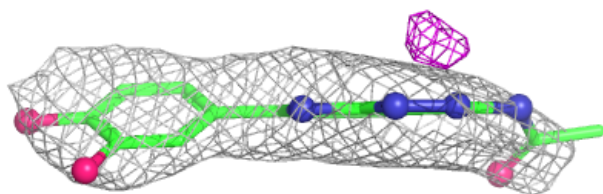
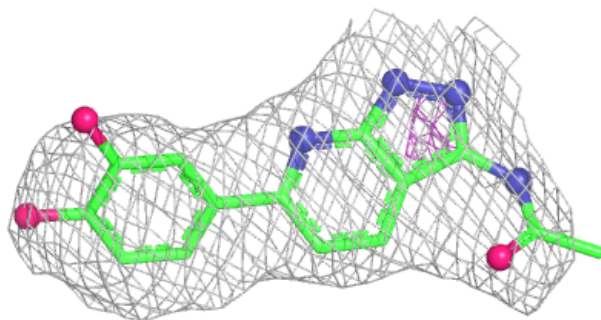
labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	503	5/5	0.68	0.19	160,162,162,164	0
3	SO4	A	502	5/5	0.72	0.16	189,191,194,194	0
4	B4K	A	504	21/21	0.91	0.09	85,90,105,107	0
3	SO4	A	501	5/5	0.93	0.09	88,88,94,95	0
4	B4K	B	502	21/21	0.93	0.07	76,81,89,95	0
3	SO4	B	501	5/5	0.96	0.06	90,91,96,98	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.

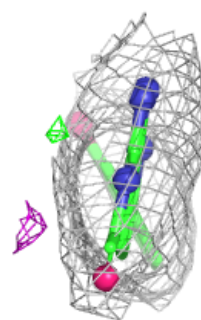
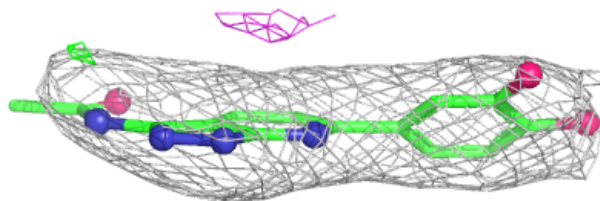
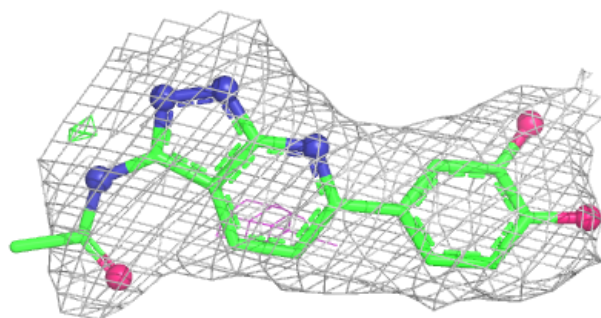
Electron density around B4K A 504:

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 B4K B 502:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.