



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:21 PM EDT

PDB ID : 5CSH / pdb_00005csh
Title : Crystal Structure of CK2alpha with Compound 4 bound
Authors : Brear, P.; De Fusco, C.; Georgiou, K.H.; Spring, D.; Hyvonen, M.
Deposited on : 2015-07-23
Resolution : 1.59 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

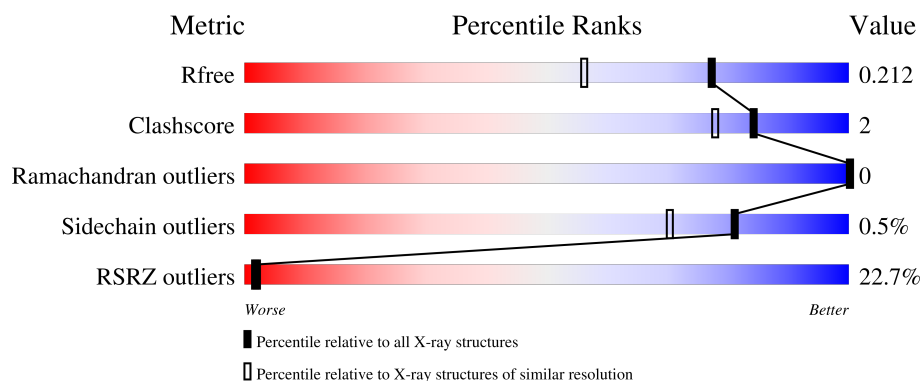
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.59 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	352	35% 86% 7% 8%
1	B	352	7% 85% 7% 8%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6050 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 Casein kinase II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	3	0
			2763	1772	483	497	11			
1	B	323	Total	C	N	O	S	0	7	0
			2772	1773	486	502	11			

There are 50 discrepancies between the modelled and reference sequences:

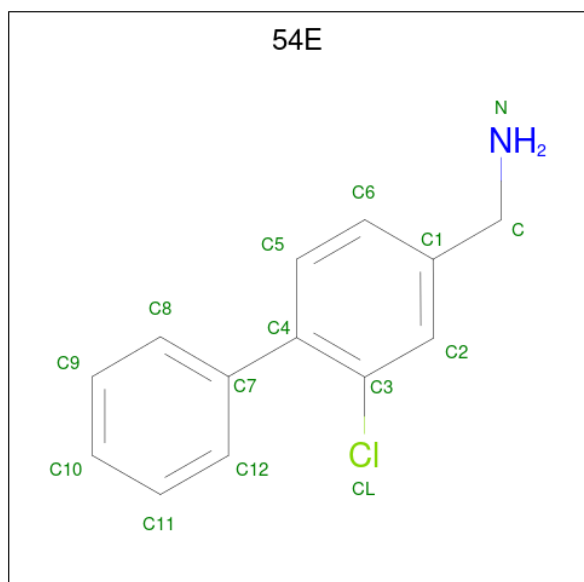
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	GLY	-	expression tag	UNP P68400
A	-21	SER	-	expression tag	UNP P68400
A	-20	MET	-	expression tag	UNP P68400
A	-19	ASP	-	expression tag	UNP P68400
A	-18	ILE	-	expression tag	UNP P68400
A	-17	GLU	-	expression tag	UNP P68400
A	-16	PHE	-	expression tag	UNP P68400
A	-15	ASP	-	expression tag	UNP P68400
A	-14	ASP	-	expression tag	UNP P68400
A	-13	ASP	-	expression tag	UNP P68400
A	-12	ALA	-	expression tag	UNP P68400
A	-11	ASP	-	expression tag	UNP P68400
A	-10	ASP	-	expression tag	UNP P68400
A	-9	ASP	-	expression tag	UNP P68400
A	-8	GLY	-	expression tag	UNP P68400
A	-7	SER	-	expression tag	UNP P68400
A	-6	GLY	-	expression tag	UNP P68400
A	-5	SER	-	expression tag	UNP P68400
A	-4	GLY	-	expression tag	UNP P68400
A	-3	SER	-	expression tag	UNP P68400
A	-2	GLY	-	expression tag	UNP P68400
A	-1	SER	-	expression tag	UNP P68400
A	0	GLY	-	expression tag	UNP P68400
A	1	SER	-	expression tag	UNP P68400
A	21	SER	ARG	engineered mutation	UNP P68400

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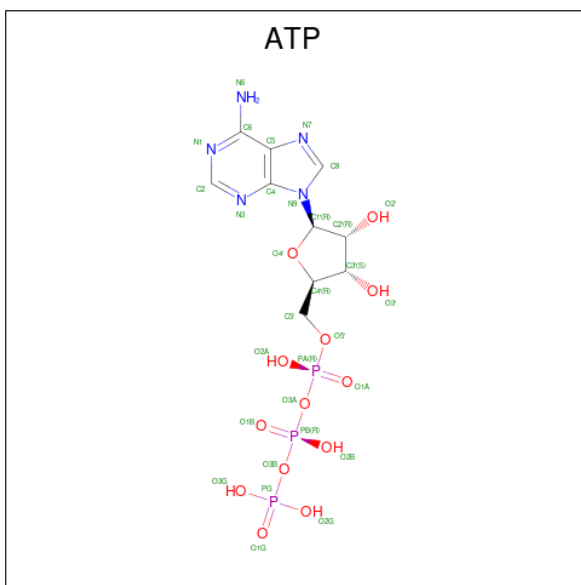
Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	GLY	-	expression tag	UNP P68400
B	-21	SER	-	expression tag	UNP P68400
B	-20	MET	-	expression tag	UNP P68400
B	-19	ASP	-	expression tag	UNP P68400
B	-18	ILE	-	expression tag	UNP P68400
B	-17	GLU	-	expression tag	UNP P68400
B	-16	PHE	-	expression tag	UNP P68400
B	-15	ASP	-	expression tag	UNP P68400
B	-14	ASP	-	expression tag	UNP P68400
B	-13	ASP	-	expression tag	UNP P68400
B	-12	ALA	-	expression tag	UNP P68400
B	-11	ASP	-	expression tag	UNP P68400
B	-10	ASP	-	expression tag	UNP P68400
B	-9	ASP	-	expression tag	UNP P68400
B	-8	GLY	-	expression tag	UNP P68400
B	-7	SER	-	expression tag	UNP P68400
B	-6	GLY	-	expression tag	UNP P68400
B	-5	SER	-	expression tag	UNP P68400
B	-4	GLY	-	expression tag	UNP P68400
B	-3	SER	-	expression tag	UNP P68400
B	-2	GLY	-	expression tag	UNP P68400
B	-1	SER	-	expression tag	UNP P68400
B	0	GLY	-	expression tag	UNP P68400
B	1	SER	-	expression tag	UNP P68400
B	21	SER	ARG	engineered mutation	UNP P68400

- Molecule 2 is 1-(2-chlorobiphenyl-4-yl)methanamine (CCD ID: 54E) (formula: C₁₃H₁₂ClN).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 15	C 13	Cl 1	N 1	0	0
2	A	1	Total 15	C 13	Cl 1	N 1	0	0
2	B	1	Total 30	C 26	Cl 2	N 2	0	1
2	B	1	Total 15	C 13	Cl 1	N 1	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 19	C 10	N 5	O 4	0	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

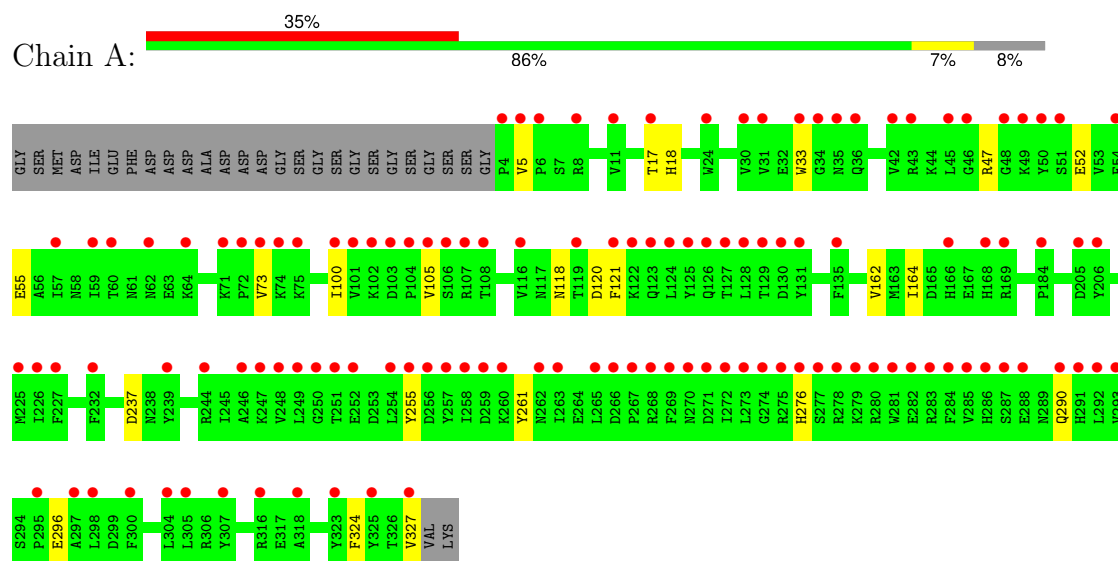
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	98	Total	O	0	0
			98	98		
5	B	284	Total	O	0	0
			284	284		

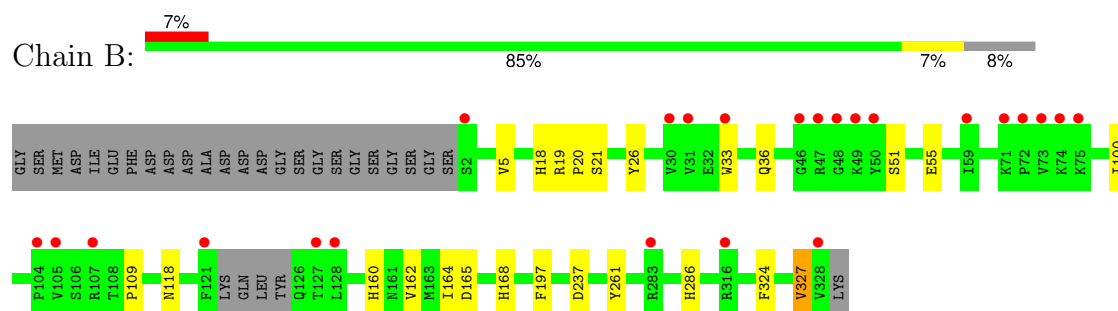
3 Residue-property plots [i](#)

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: Casein kinase II subunit alpha



• Molecule 1: Casein kinase II subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	64.30Å 69.15Å 334.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.50 – 1.59 83.50 – 1.59	Depositor EDS
% Data completeness (in resolution range)	98.7 (83.50-1.59) 99.4 (83.50-1.59)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 1.59Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.193 , 0.207 0.198 , 0.212	Depositor DCC
R_{free} test set	5042 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6050	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.30% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, 54E, ATP

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	0.82	0/2838	1.07	5/3839 (0.1%)
1	B	0.92	1/2845 (0.0%)	1.01	8/3848 (0.2%)
All	All	0.87	1/5683 (0.0%)	1.04	13/7687 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	26	TYR	C-O	-5.26	1.17	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	327	VAL	CA-C-N	7.40	135.02	121.70
1	B	327	VAL	C-N-CA	7.40	135.02	121.70
1	A	121	PHE	CA-CB-CG	7.34	121.14	113.80
1	B	19	ARG	CA-C-N	-5.65	114.43	120.03
1	B	19	ARG	C-N-CA	-5.65	114.43	120.03
1	B	51	SER	N-CA-C	5.43	116.40	108.14
1	B	55	GLU	N-CA-C	-5.25	101.90	110.20
1	A	120	ASP	CA-C-N	5.24	127.25	120.44
1	A	120	ASP	C-N-CA	5.24	127.25	120.44
1	A	55	GLU	N-CA-C	-5.21	101.21	109.96
1	B	237	ASP	CA-CB-CG	5.11	117.71	112.60
1	B	197	PHE	CA-CB-CG	-5.10	108.70	113.80
1	A	237	ASP	CA-CB-CG	5.08	117.68	112.60

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	2763	0	2702	11	9
1	B	2772	0	2702	13	0
2	A	30	0	0	3	0
2	B	45	0	0	2	0
3	A	19	0	12	0	0
3	B	31	0	12	1	0
4	B	8	0	6	0	0
5	A	98	0	0	3	0
5	B	284	0	0	4	1
All	All	6050	0	5434	25	10

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 (25) 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:276:HIS:ND1	5:A:502:HOH:O	2.12	0.83
1:A:18:HIS:ND1	5:A:501:HOH:O	2.11	0.82
2:A:401:54E:N	5:A:503:HOH:O	2.18	0.77
1:B:21:SER:OG	5:B:501:HOH:O	2.07	0.72
1:A:162:VAL:HG11	2:A:401:54E:CL	2.35	0.63
1:A:105:VAL:HG21	1:B:20:PRO:HG2	1.83	0.59
1:B:162:VAL:HG11	2:B:403[A]:54E:CL	2.40	0.57
1:B:286:HIS:HE1	5:B:754:HOH:O	1.87	0.57
1:B:33:TRP:CE3	1:B:100:ILE:HG22	2.40	0.57
2:B:403[A]:54E:CL	2:B:403[A]:54E:C12	2.91	0.55
1:B:18:HIS:HE1	5:B:577:HOH:O	1.91	0.54
1:A:33:TRP:CE3	1:A:100:ILE:HG22	2.46	0.50
1:B:165:ASP:OD2	1:B:168:HIS:HD2	1.95	0.50
1:A:33:TRP:CZ3	1:A:100:ILE:HG22	2.47	0.50
1:B:324:PHE:O	1:B:327:VAL:HG22	2.15	0.47
1:B:33:TRP:CH2	1:B:109:PRO:HB3	2.50	0.47
1:A:47:ARG:HG2	1:A:52:GLU:HG2	1.98	0.46
1:B:36:GLN:CD	5:B:506:HOH:O	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:PHE:O	1:A:327:VAL:HG22	2.16	0.45
1:A:5:VAL:HB	1:A:261:TYR:HA	1.98	0.45
1:B:5:VAL:HB	1:B:261:TYR:HA	1.99	0.44
1:B:160:HIS:HD2	3:B:405:ATP:O3B	2.02	0.42
1:A:118:ASN:HD22	1:A:164:ILE:H	1.67	0.42
1:B:118:ASN:HD22	1:B:164:ILE:H	1.67	0.41
1:A:162:VAL:CG1	2:A:401:54E:CL	3.05	0.40

All (10) 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)
5:B:755:HOH:O	5:B:755:HOH:O[4_597]	0.70	1.50
1:A:255:TYR:CE2	1:A:290:GLN:OE1[7_447]	1.04	1.16
1:A:255:TYR:CZ	1:A:290:GLN:OE1[7_447]	1.54	0.66
1:A:255:TYR:CD2	1:A:290:GLN:OE1[7_447]	1.61	0.59
1:A:255:TYR:CE2	1:A:290:GLN:CD[7_447]	1.66	0.54
1:A:255:TYR:OH	1:A:290:GLN:NE2[7_447]	1.67	0.53
1:A:255:TYR:CZ	1:A:290:GLN:CD[7_447]	1.83	0.37
1:A:255:TYR:CE2	1:A:290:GLN:NE2[7_447]	1.98	0.22
1:A:255:TYR:CZ	1:A:290:GLN:NE2[7_447]	2.05	0.15
1:A:255:TYR:OH	1:A:290:GLN:CD[7_447]	2.10	0.10

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	325/352 (92%)	314 (97%)	11 (3%)	0	100	100
1	B	326/352 (93%)	320 (98%)	6 (2%)	0	100	100
All	All	651/704 (92%)	634 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	302/319 (95%)	299 (99%)	3 (1%)	68	50
1	B	304/319 (95%)	304 (100%)	0	100	100
All	All	606/638 (95%)	603 (100%)	3 (0%)	81	70

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	73	VAL
1	A	296	GLU

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	118	ASN
1	A	123	GLN
1	A	168	HIS
1	A	207	GLN
1	A	262	ASN
1	B	118	ASN
1	B	160	HIS
1	B	168	HIS
1	B	186	GLN
1	B	207	GLN
1	B	234	HIS
1	B	262	ASN
1	B	286	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	ATP	A	403	-	21,21,33	0.16	0	31,31,52	0.28	0
2	54E	A	401	-	16,16,16	0.19	0	21,21,21	0.43	0
2	54E	B	404	-	16,16,16	0.21	0	21,21,21	0.23	0
2	54E	B	403[B]	-	16,16,16	0.31	0	21,21,21	0.31	0
3	ATP	B	405	-	32,33,33	0.49	0	48,52,52	0.56	0
2	54E	B	403[A]	-	16,16,16	0.22	0	21,21,21	0.28	0
2	54E	A	402	-	16,16,16	0.29	0	21,21,21	0.24	0
4	ACT	B	401	-	3,3,3	1.10	0	3,3,3	1.48	0
4	ACT	B	402	-	3,3,3	1.29	0	3,3,3	0.93	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
3	ATP	A	403	-	-	0/6/22/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	54E	A	401	-	-	0/6/6/6	0/2/2/2
2	54E	B	404	-	-	0/6/6/6	0/2/2/2
2	54E	B	403[B]	-	-	0/6/6/6	0/2/2/2
3	ATP	B	405	-	-	11/22/38/38	0/3/3/3
2	54E	B	403[A]	-	-	0/6/6/6	0/2/2/2
2	54E	A	402	-	-	0/6/6/6	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	405	ATP	PB-O3B-PG-O2G
3	B	405	ATP	C5'-O5'-PA-O1A
3	B	405	ATP	C5'-O5'-PA-O2A
3	B	405	ATP	C5'-O5'-PA-O3A
3	B	405	ATP	C4'-C5'-O5'-PA
3	B	405	ATP	PA-O3A-PB-O1B
3	B	405	ATP	PB-O3B-PG-O1G
3	B	405	ATP	PB-O3B-PG-O3G
3	B	405	ATP	PA-O3A-PB-O2B
3	B	405	ATP	PB-O3A-PA-O1A
3	B	405	ATP	PB-O3A-PA-O2A

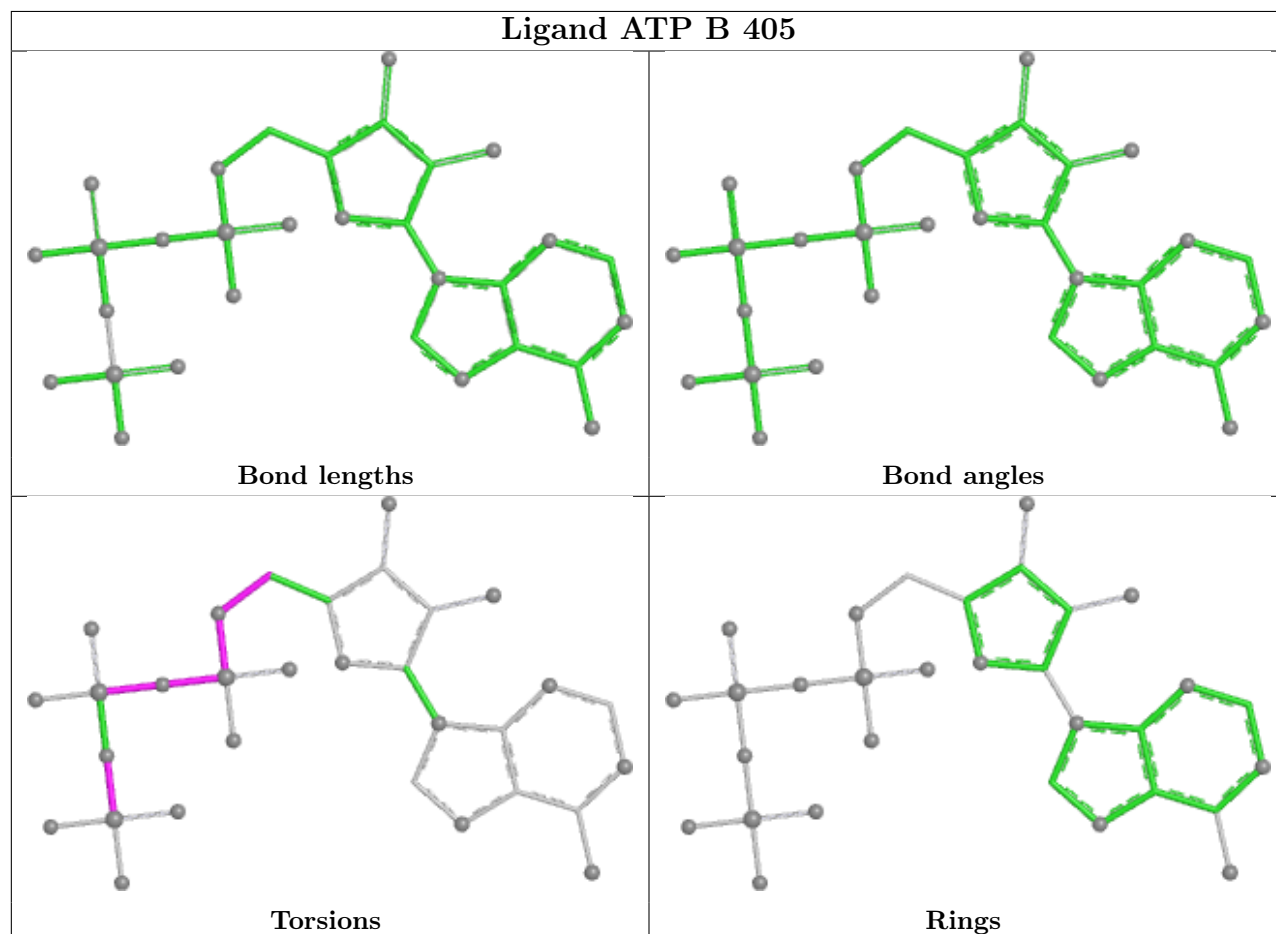
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	54E	3	0
3	B	405	ATP	1	0
2	B	403[A]	54E	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	324/352 (92%)	1.59	123 (37%) 1 0	24, 58, 109, 155	3 (0%)
1	B	323/352 (91%)	0.21	24 (7%) 20 21	8, 23, 52, 87	7 (2%)
All	All	647/704 (91%)	0.90	147 (22%) 2 2	8, 36, 96, 155	10 (1%)

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	328	VAL	7.3
1	A	50	TYR	6.7
1	B	121	PHE	6.1
1	A	327	VAL	6.1
1	A	125	TYR	5.9
1	B	72	PRO	5.9
1	A	128	LEU	5.7
1	B	50	TYR	5.7
1	A	124	LEU	5.6
1	A	104	PRO	5.6
1	A	73	VAL	5.2
1	A	121	PHE	5.0
1	A	33	TRP	4.7
1	A	255	TYR	4.5
1	A	105	VAL	4.2
1	B	33	TRP	4.2
1	B	73	VAL	4.2
1	A	290	GLN	4.2
1	A	45	LEU	4.1
1	A	275	ARG	3.9
1	A	254[A]	LEU	3.9
1	A	272	ILE	3.8
1	A	269	PHE	3.8
1	A	292	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	281	TRP	3.7
1	A	42	VAL	3.7
1	A	100	ILE	3.6
1	A	277	SER	3.6
1	A	5	VAL	3.6
1	A	270	ASN	3.5
1	A	259	ASP	3.5
1	A	48	GLY	3.4
1	A	274	GLY	3.4
1	B	2	SER	3.4
1	A	273	LEU	3.4
1	A	268	ARG	3.3
1	A	283	ARG	3.3
1	A	122	LYS	3.3
1	A	297	ALA	3.3
1	A	278	ARG	3.3
1	A	49	LYS	3.3
1	B	47	ARG	3.2
1	A	249	LEU	3.2
1	A	265	LEU	3.2
1	B	49	LYS	3.2
1	A	127	THR	3.2
1	A	35	ASN	3.2
1	A	263	ILE	3.1
1	B	316	ARG	3.1
1	A	258	ILE	3.1
1	A	30	VAL	3.1
1	B	46	GLY	3.0
1	A	279	LYS	3.0
1	A	43	ARG	2.9
1	A	107	ARG	2.9
1	A	226	ILE	2.9
1	A	74	LYS	2.9
1	A	288	GLU	2.9
1	A	285	VAL	2.9
1	B	283	ARG	2.9
1	B	127	THR	2.9
1	A	71	LYS	2.9
1	A	72	PRO	2.9
1	A	239	TYR	2.9
1	A	260	LYS	2.8
1	A	225	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	34	GLY	2.8
1	A	46	GLY	2.8
1	A	131	TYR	2.8
1	A	75	LYS	2.8
1	A	102	LYS	2.8
1	B	107	ARG	2.7
1	A	267	PRO	2.7
1	A	286	HIS	2.7
1	A	298	LEU	2.7
1	A	257	TYR	2.6
1	B	71	LYS	2.6
1	A	271	ASP	2.6
1	A	57	ILE	2.6
1	A	169	ARG	2.6
1	A	62	ASN	2.6
1	A	184	PRO	2.6
1	A	130	ASP	2.6
1	A	59	ILE	2.6
1	A	318	ALA	2.6
1	B	128	LEU	2.6
1	A	295	PRO	2.6
1	A	287	SER	2.6
1	A	284	PHE	2.5
1	A	293	VAL	2.5
1	A	325	TYR	2.5
1	A	11	VAL	2.5
1	A	251	THR	2.5
1	A	106	SER	2.5
1	A	123	GLN	2.5
1	A	282	GLU	2.4
1	A	64	LYS	2.4
1	A	305	LEU	2.4
1	A	17	THR	2.4
1	A	248	VAL	2.4
1	A	36	GLN	2.4
1	A	250	GLY	2.4
1	B	48	GLY	2.4
1	A	266	ASP	2.4
1	B	59	ILE	2.4
1	A	135	PHE	2.4
1	A	31	VAL	2.4
1	A	4	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	276	HIS	2.4
1	A	168	HIS	2.3
1	A	316	ARG	2.3
1	A	60	THR	2.3
1	A	206	TYR	2.3
1	A	256	ASP	2.3
1	A	232	PHE	2.3
1	A	247	LYS	2.3
1	A	54	PHE	2.3
1	A	300	PHE	2.3
1	B	104	PRO	2.3
1	A	323	TYR	2.3
1	A	246	ALA	2.2
1	A	280	ARG	2.2
1	A	307	TYR	2.2
1	A	166	HIS	2.2
1	B	74	LYS	2.2
1	B	75	LYS	2.2
1	A	116	VAL	2.2
1	A	244	ARG	2.2
1	A	252	GLU	2.2
1	A	51	SER	2.2
1	A	6	PRO	2.1
1	A	108	THR	2.1
1	A	262	ASN	2.1
1	B	105	VAL	2.1
1	A	24	TRP	2.1
1	A	8	ARG	2.1
1	A	126	GLN	2.1
1	B	31	VAL	2.1
1	A	103	ASP	2.1
1	A	205	ASP	2.1
1	A	291	HIS	2.1
1	A	119	THR	2.0
1	A	304	LEU	2.0
1	A	129	THR	2.0
1	A	101	VAL	2.0
1	A	227	PHE	2.0
1	B	30	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

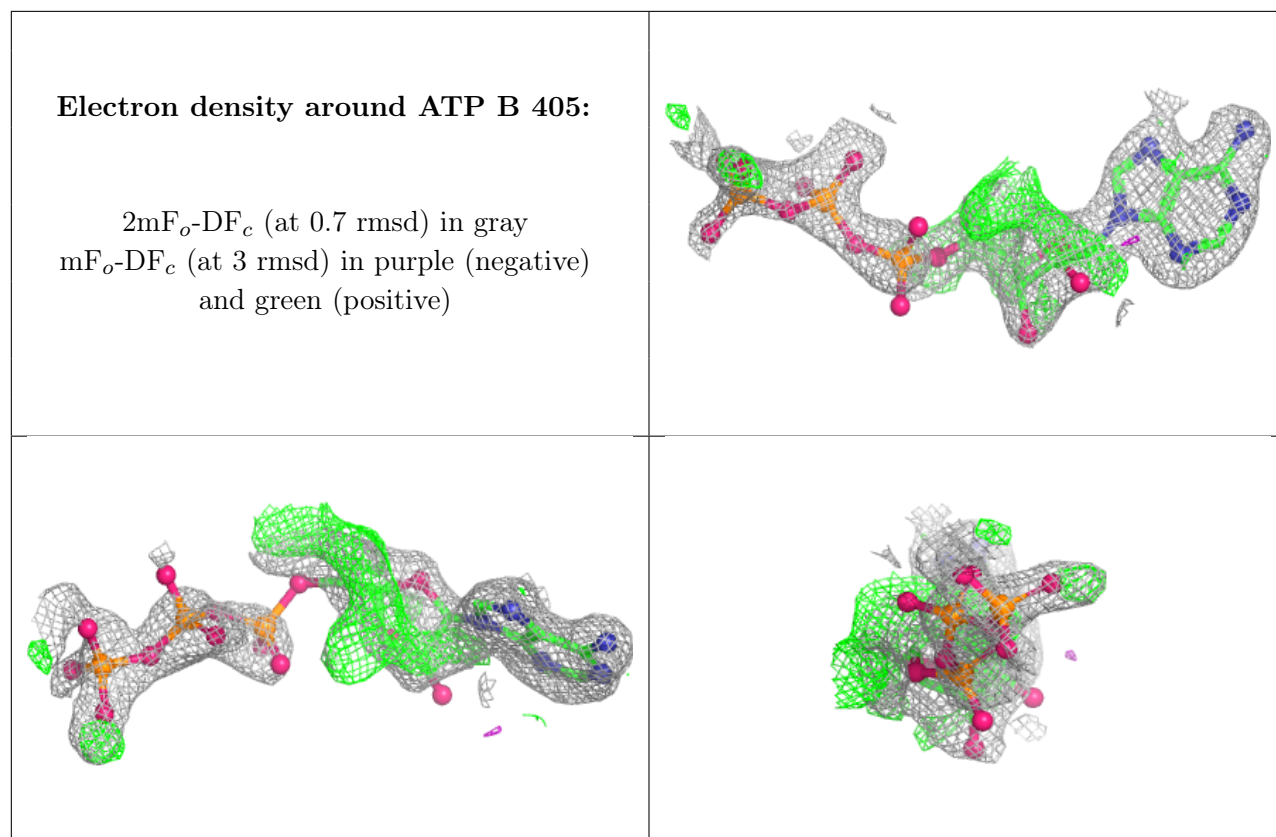
There are no oligosaccharides in this entry.

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	54E	A	401	15/15	0.70	0.22	48,63,74,74	0
3	ATP	B	405	31/31	0.70	0.23	19,47,63,64	31
3	ATP	A	403	19/31	0.73	0.17	43,52,72,72	0
2	54E	B	404	15/15	0.82	0.15	45,49,53,55	0
2	54E	B	403[B]	15/15	0.86	0.11	45,47,54,55	15
2	54E	B	403[A]	15/15	0.86	0.11	14,20,24,33	15
2	54E	A	402	15/15	0.88	0.14	41,45,48,48	0
4	ACT	B	402	4/4	0.91	0.11	34,38,40,42	0
4	ACT	B	401	4/4	0.95	0.08	26,32,33,33	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.