



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2017 – 09:43 AM EDT

PDB ID : 5MOE
Title : Crystal Structure of CK2alpha with N-(3-(((2-chloro-[1,1'-biphenyl]-4-yl)methyl)amino)propyl)methanesulfonamide bound
Authors : Brear, P.; De Fusco, C.; Georgiou, K.; Iegre, J.; Sore, H.; Hyvonen, M.; Spring, D.
Deposited on : unknown
Resolution : 1.89 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

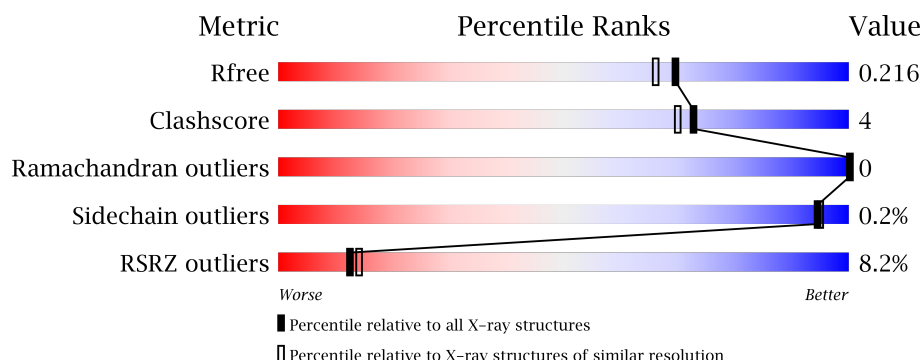
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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}	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>4%</div> <div>87%</div> <div>6%</div> <div>8%</div> </div>
1	B	352	<div> <div>11%</div> <div>87%</div> <div>•</div> <div>8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ACT	A	405	-	-	-	X
5	ACT	B	405	-	-	-	X
6	OQC	A	409	-	-	-	X
6	OQC	A	411	-	-	-	X
6	OQC	B	408	-	-	-	X
6	OQC	B	409	-	-	X	X
7	PO4	A	412	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6006 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	325	Total	C	N	O	S	0	7	0
			2796	1788	492	505	11			
1	B	323	Total	C	N	O	S	0	4	0
			2761	1768	483	498	12			

There are 50 discrepancies between the modelled and reference sequences:

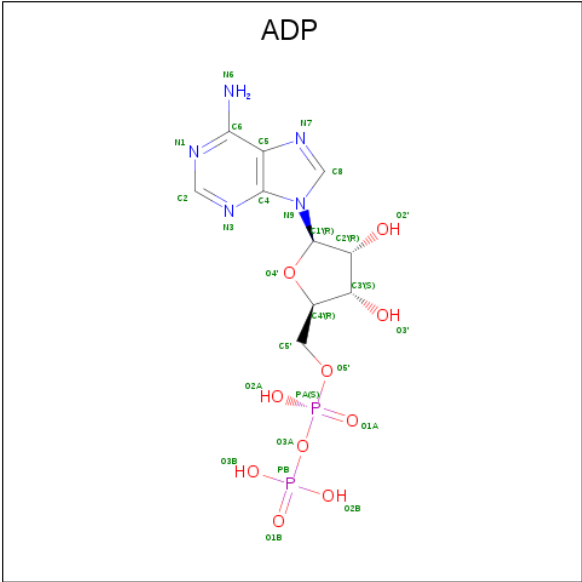
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	GLY	-	expression tag	UNP P68400
A	-21	SER	-	expression tag	UNP P68400
A	-20	MET	-	expression tag	UNP P68400
A	-19	ASP	-	expression tag	UNP P68400
A	-18	ILE	-	expression tag	UNP P68400
A	-17	GLU	-	expression tag	UNP P68400
A	-16	PHE	-	expression tag	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 ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

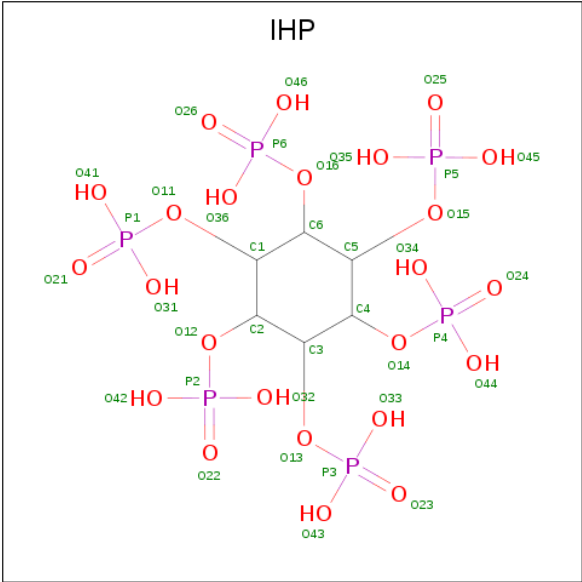


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

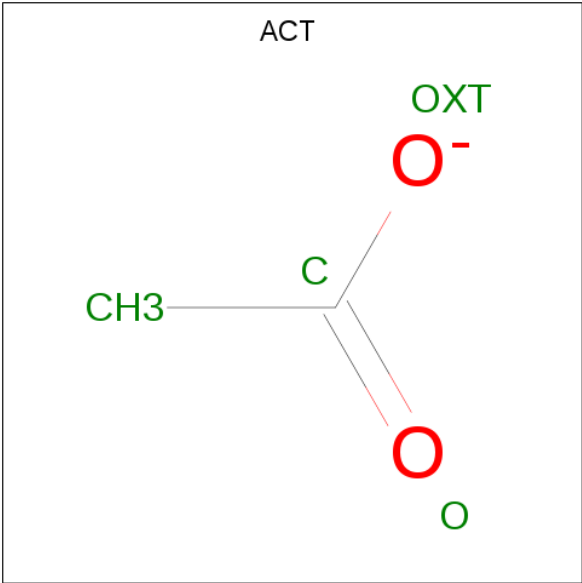
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mg	0	0
			2	2		
3	A	2	Total	Mg	0	0
			2	2		

- Molecule 4 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: C₆H₁₈O₂₄P₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 36	C 6	O 24	P 6	0	0
4	B	1	Total 36	C 6	O 24	P 6	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



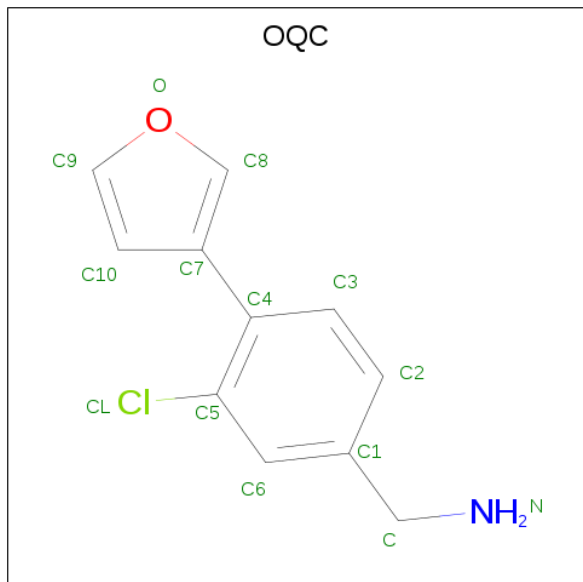
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

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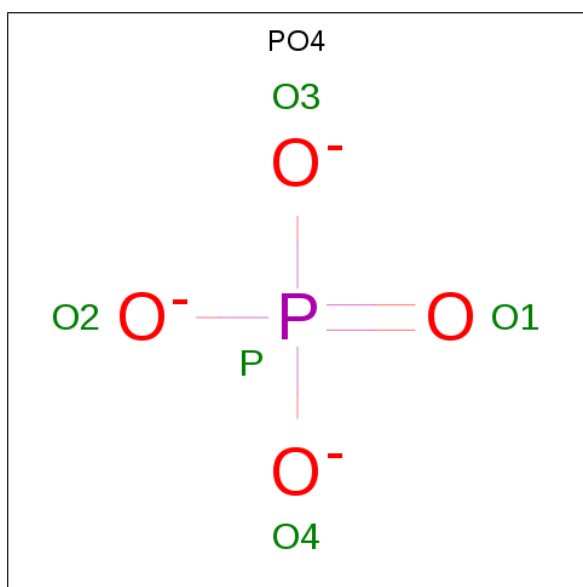
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is [3-chloranyl-4-(furan-3-yl)phenyl]methanamine (three-letter code: OQC) (formula: C₁₁H₁₀ClNO).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Cl	N	O	0	0
			14	11	1	1	1		
6	A	1	Total	C	Cl	N	O	0	0
			14	11	1	1	1		
6	A	1	Total	C	Cl	N	O	0	0
			14	11	1	1	1		
6	B	1	Total	C	Cl	N	O	0	0
			14	11	1	1	1		
6	B	1	Total	C	Cl	N	O	0	0
			14	11	1	1	1		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

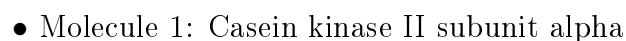


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	151	Total	O	0	0
			151	151		
8	B	65	Total	O	0	0
			65	65		

- 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	64.61Å 68.23Å 333.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	166.74 – 1.89 166.74 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.5 (166.74-1.89) 99.9 (166.74-1.89)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 1.88Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.197 , 0.208 0.202 , 0.216	Depositor DCC
R_{free} test set	3009 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6006	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% 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: MG, ADP, IHP, OQC, ACT, PO4

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	0.58	0/2871	0.61	0/3884
1	B	0.52	0/2836	0.59	0/3835
All	All	0.55	0/5707	0.60	0/7719

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	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35[A]	ASN	Mainchain
1	A	35[B]	ASN	Mainchain
1	B	35[A]	ASN	Mainchain
1	B	35[B]	ASN	Mainchain

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	2796	0	2725	15	0
1	B	2761	0	2693	25	0
2	A	27	0	12	1	0
2	B	27	0	12	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	36	0	6	0	0
4	B	36	0	6	0	0
5	A	16	0	12	0	0
5	B	12	0	9	0	0
6	A	42	0	0	6	0
6	B	28	0	0	19	0
7	A	5	0	0	0	0
8	A	151	0	0	0	0
8	B	65	0	0	1	0
All	All	6006	0	5475	44	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 4.

All (44) 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:225[A]:MET:SD	6:B:409:OQC:C9	2.37	1.12
1:B:225[A]:MET:SD	6:B:409:OQC:O	2.14	1.06
1:B:225[A]:MET:HE1	6:B:409:OQC:C10	1.99	0.91
1:B:225[A]:MET:CE	6:B:409:OQC:C7	2.50	0.89
1:B:225[A]:MET:HE1	6:B:409:OQC:C7	2.04	0.87
1:B:225[A]:MET:SD	6:B:409:OQC:C8	2.63	0.86
1:B:225[B]:MET:SD	6:B:409:OQC:C8	2.73	0.77
1:B:221:MET:HE1	6:B:409:OQC:CL	2.24	0.74
1:B:225[A]:MET:CE	6:B:409:OQC:C10	2.70	0.70
1:B:225[A]:MET:CE	6:B:409:OQC:C8	2.71	0.69
1:B:162:VAL:HG11	6:B:409:OQC:CL	2.36	0.62
1:A:221:MET:HE1	6:A:410:OQC:CL	2.38	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ASP:HB2	6:A:411:OQC:C8	2.31	0.60
6:B:409:OQC:C10	6:B:409:OQC:CL	2.88	0.59
1:B:128:LEU:HD13	1:B:225[B]:MET:HE1	1.84	0.58
6:B:408:OQC:CL	6:B:408:OQC:C10	2.89	0.58
6:A:411:OQC:CL	6:A:411:OQC:C10	2.89	0.58
6:A:410:OQC:C8	6:A:410:OQC:CL	2.90	0.56
1:B:221:MET:CE	6:B:409:OQC:CL	2.92	0.54
1:A:15[B]:VAL:CG1	1:A:19:ARG:NH1	2.71	0.54
1:B:225[A]:MET:SD	6:B:409:OQC:C10	2.94	0.52
1:A:128:LEU:HD13	1:A:225:MET:HE1	1.92	0.51
1:A:68:LYS:HE3	2:A:401:ADP:O1A	2.11	0.50
1:B:103:ASP:HB2	6:B:408:OQC:C8	2.43	0.49
1:B:225[A]:MET:HE2	6:B:409:OQC:C7	2.39	0.48
1:B:225[B]:MET:CA	1:B:225[B]:MET:HE3	2.44	0.47
1:B:303:LYS:HB3	1:B:313:LEU:HG	1.96	0.47
1:A:221:MET:CE	6:A:410:OQC:CL	3.01	0.46
1:B:118:ASN:HD22	1:B:164:ILE:H	1.62	0.46
1:B:128:LEU:HD23	1:B:132:ASP:HB3	1.97	0.46
1:A:110:ALA:HB2	6:A:411:OQC:C9	2.46	0.46
1:B:225[A]:MET:HE2	6:B:409:OQC:C8	2.46	0.46
1:B:225[B]:MET:HG3	6:B:409:OQC:O	2.16	0.45
1:B:5:VAL:HB	1:B:261:TYR:HA	2.00	0.44
1:B:17:THR:HG22	8:B:521:HOH:O	2.18	0.43
1:A:128:LEU:HD13	1:A:225:MET:CE	2.49	0.43
1:A:118:ASN:HD22	1:A:164:ILE:H	1.67	0.42
1:A:5:VAL:HB	1:A:261:TYR:HA	2.01	0.42
1:A:128:LEU:HD23	1:A:132:ASP:HB3	2.02	0.41
1:A:15[B]:VAL:HG13	1:A:19:ARG:NH1	2.35	0.41
1:A:33:TRP:CE3	1:A:100:ILE:HG22	2.56	0.41
1:A:134:ARG:HG2	1:A:323:TYR:CZ	2.55	0.41
1:A:73:VAL:HG11	1:A:77:LYS:CE	2.51	0.41
1:B:120:ASP:HB3	1:B:123:GLN:HB2	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	330/352 (94%)	319 (97%)	11 (3%)	0	100	100
1	B	325/352 (92%)	315 (97%)	10 (3%)	0	100	100
All	All	655/704 (93%)	634 (97%)	21 (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	306/319 (96%)	306 (100%)	0	100	100
1	B	302/319 (95%)	301 (100%)	1 (0%)	94	94
All	All	608/638 (95%)	607 (100%)	1 (0%)	94	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	128	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	186	GLN
1	A	262	ASN
1	B	118	ASN
1	B	186	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 for Mogul analysis.

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	ADP	A	401	3	25,29,29	0.66	0	24,45,45	0.93	2 (8%)
4	IHP	A	404	-	36,36,36	0.68	0	54,60,60	1.02	1 (1%)
5	ACT	A	405	-	1,3,3	4.87	1 (100%)	0,3,3	0.00	-
5	ACT	A	406	-	1,3,3	3.95	1 (100%)	0,3,3	0.00	-
5	ACT	A	407	-	1,3,3	5.91	1 (100%)	0,3,3	0.00	-
5	ACT	A	408	-	1,3,3	5.65	1 (100%)	0,3,3	0.00	-
6	OQC	A	409	-	12,15,15	0.98	1 (8%)	14,20,20	0.90	1 (7%)
6	OQC	A	410	-	12,15,15	0.98	1 (8%)	14,20,20	0.88	1 (7%)
6	OQC	A	411	-	12,15,15	0.96	1 (8%)	14,20,20	0.43	0
7	PO4	A	412	-	4,4,4	2.62	1 (25%)	6,6,6	0.51	0
2	ADP	B	401	3	25,29,29	0.66	0	24,45,45	0.67	0
4	IHP	B	404	-	36,36,36	0.75	0	54,60,60	1.27	5 (9%)
5	ACT	B	405	-	1,3,3	5.21	1 (100%)	0,3,3	0.00	-
5	ACT	B	406	-	1,3,3	5.29	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACT	B	407	-	1,3,3	4.81	1 (100%)	0,3,3	0.00	-
6	OQC	B	408	-	12,15,15	0.98	1 (8%)	14,20,20	0.42	0
6	OQC	B	409	-	12,15,15	0.98	1 (8%)	14,20,20	0.39	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
2	ADP	A	401	3	-	0/12/32/32	0/3/3/3
4	IHP	A	404	-	-	0/30/54/54	0/1/1/1
5	ACT	A	405	-	-	0/0/0/0	0/0/0/0
5	ACT	A	406	-	-	0/0/0/0	0/0/0/0
5	ACT	A	407	-	-	0/0/0/0	0/0/0/0
5	ACT	A	408	-	-	0/0/0/0	0/0/0/0
6	OQC	A	409	-	-	0/4/6/6	0/1/2/2
6	OQC	A	410	-	-	0/4/6/6	0/1/2/2
6	OQC	A	411	-	-	0/4/6/6	0/1/2/2
7	PO4	A	412	-	-	0/0/0/0	0/0/0/0
2	ADP	B	401	3	-	0/12/32/32	0/3/3/3
4	IHP	B	404	-	-	0/30/54/54	0/1/1/1
5	ACT	B	405	-	-	0/0/0/0	0/0/0/0
5	ACT	B	406	-	-	0/0/0/0	0/0/0/0
5	ACT	B	407	-	-	0/0/0/0	0/0/0/0
6	OQC	B	408	-	-	0/4/6/6	0/1/2/2
6	OQC	B	409	-	-	0/4/6/6	0/1/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	408	OQC	C10-C9	-3.01	1.33	1.39
6	B	409	OQC	C10-C9	-2.98	1.33	1.39
6	A	410	OQC	C10-C9	-2.89	1.34	1.39
6	A	411	OQC	C10-C9	-2.88	1.34	1.39
6	A	409	OQC	C10-C9	-2.86	1.34	1.39
5	A	406	ACT	CH3-C	3.95	1.53	1.48
7	A	412	PO4	P-O1	4.57	1.60	1.50
5	B	407	ACT	CH3-C	4.81	1.54	1.48
5	A	405	ACT	CH3-C	4.87	1.55	1.48
5	B	405	ACT	CH3-C	5.21	1.55	1.48
5	B	406	ACT	CH3-C	5.29	1.55	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	408	ACT	CH3-C	5.65	1.56	1.48
5	A	407	ACT	CH3-C	5.91	1.56	1.48

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	ADP	O3A-PB-O1B	-2.12	98.38	111.44
2	A	401	ADP	O5'-PA-O1A	-2.10	100.77	109.25
4	B	404	IHP	C6-C1-C2	-2.01	106.00	110.46
4	B	404	IHP	O14-C4-C3	2.14	113.74	108.68
4	A	404	IHP	C3-C2-C1	2.24	115.42	110.46
4	B	404	IHP	C4-C3-C2	2.30	115.55	110.46
4	B	404	IHP	C6-C5-C4	2.79	116.65	110.46
6	A	410	OQC	C8-C7-C4	3.09	131.85	127.46
6	A	409	OQC	C8-C7-C4	3.19	132.00	127.46
4	B	404	IHP	C5-C4-C3	3.61	118.45	110.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	ADP	1	0
6	A	410	OQC	3	0
6	A	411	OQC	3	0
6	B	408	OQC	2	0
6	B	409	OQC	17	0

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	325/352 (92%)	0.34	13 (4%) 39 43	19, 35, 72, 118	0
1	B	323/352 (91%)	0.74	40 (12%) 4 5	31, 64, 102, 131	0
All	All	648/704 (92%)	0.54	53 (8%) 12 14	19, 49, 96, 131	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	124	LEU	12.8
1	A	121	PHE	11.1
1	B	50	TYR	10.1
1	A	125	TYR	8.8
1	B	125	TYR	8.0
1	B	124	LEU	7.7
1	A	72	PRO	5.8
1	B	126	GLN	5.6
1	B	127	THR	5.3
1	B	48	GLY	5.0
1	B	49	LYS	4.9
1	A	50	TYR	4.7
1	A	123	GLN	4.3
1	A	33	TRP	4.1
1	B	123	GLN	3.8
1	B	288	GLU	3.5
1	B	292	LEU	3.4
1	B	33	TRP	3.3
1	B	166	HIS	3.1
1	A	128	LEU	3.0
1	B	278	ARG	3.0
1	B	167	GLU	2.9
1	A	104	PRO	2.9
1	B	128	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	239	TYR	2.9
1	B	72	PRO	2.8
1	B	270	ASN	2.6
1	B	255	TYR	2.5
1	A	122	LYS	2.5
1	B	47	ARG	2.5
1	B	121	PHE	2.5
1	B	45	LEU	2.5
1	B	105	VAL	2.5
1	B	122	LYS	2.4
1	A	126	GLN	2.4
1	B	256	ASP	2.4
1	A	264	GLU	2.4
1	B	104	PRO	2.3
1	B	62	ASN	2.3
1	B	107	ARG	2.3
1	A	105	VAL	2.2
1	B	46	GLY	2.2
1	B	316	ARG	2.2
1	B	264	GLU	2.1
1	B	286	HIS	2.1
1	B	135	PHE	2.1
1	B	15	VAL	2.1
1	B	119	THR	2.1
1	B	257	TYR	2.1
1	B	251	THR	2.0
1	B	291	HIS	2.0
1	B	22	GLU	2.0
1	B	51	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
5	ACT	B	405	4/4	0.81	0.27	5.36	69,70,70,72	0
6	OQC	A	411	14/14	0.74	0.25	4.15	54,58,62,62	0
5	ACT	A	405	4/4	0.91	0.15	3.66	55,62,64,67	0
6	OQC	B	409	14/14	0.26	0.43	3.08	20,20,20,20	14
6	OQC	A	409	14/14	0.85	0.19	2.83	66,67,71,71	0
6	OQC	B	408	14/14	0.81	0.25	2.58	62,66,72,74	0
7	PO4	A	412	5/5	0.84	0.14	2.21	72,75,76,78	0
3	MG	B	402	1/1	0.93	0.12	1.33	47,47,47,47	0
5	ACT	B	407	4/4	0.86	0.15	1.26	72,74,75,78	0
5	ACT	B	406	4/4	0.69	0.22	0.94	66,69,70,70	0
2	ADP	A	401	27/27	0.86	0.18	0.81	36,50,69,70	0
6	OQC	A	410	14/14	0.63	0.30	0.69	43,58,60,74	0
2	ADP	B	401	27/27	0.80	0.28	0.63	57,78,94,95	0
5	ACT	A	408	4/4	0.90	0.18	0.32	65,67,67,70	0
3	MG	A	403	1/1	0.98	0.10	-0.20	42,42,42,42	0
4	IHP	A	404	36/36	0.73	0.22	-	78,88,93,94	36
5	ACT	A	407	4/4	0.71	0.19	-	58,58,59,62	0
5	ACT	A	406	4/4	0.89	0.16	-	47,52,55,55	0
3	MG	A	402	1/1	0.93	0.14	-	33,33,33,33	0
4	IHP	B	404	36/36	0.59	0.21	-	216,217,218,218	36
3	MG	B	403	1/1	0.86	0.08	-	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.