



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:46 AM UTC

PDB ID : 5CLP / pdb_00005clp
Title : Crystal Structure of CK2alpha with 3,4-dichlorophenethylamine bound
Authors : Brear, P.; De Fusco, C.; Georgiou, K.H.; Spring, D.; Hyvonen, M.
Deposited on : 2015-07-16
Resolution : 1.68 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
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

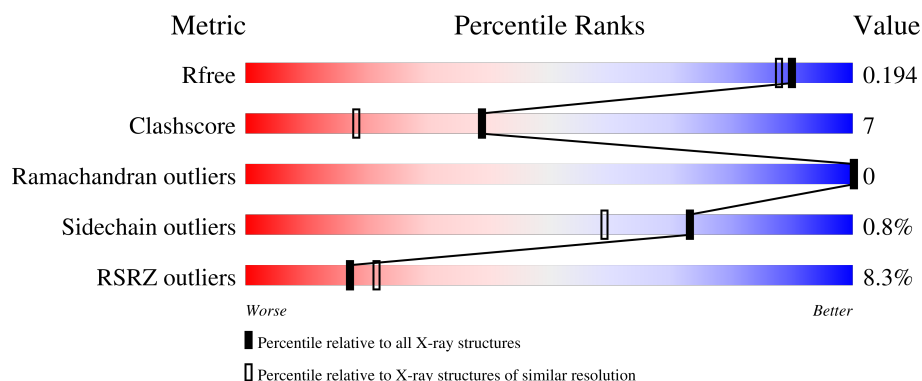
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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	9% 84% 8% 9%
1	B	352	6% 86% 7% 7%

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
2	42J	A	401[A]	-	-	X	-
2	42J	A	401[B]	-	-	X	-
2	42J	B	401[A]	-	-	X	-
2	42J	B	401[B]	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6220 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	322	Total	C	N	O	S	0	9	0
			2777	1778	486	501	12			
1	B	327	Total	C	N	O	S	0	7	0
			2807	1800	489	506	12			

There are 50 discrepancies between the modelled and reference sequences:

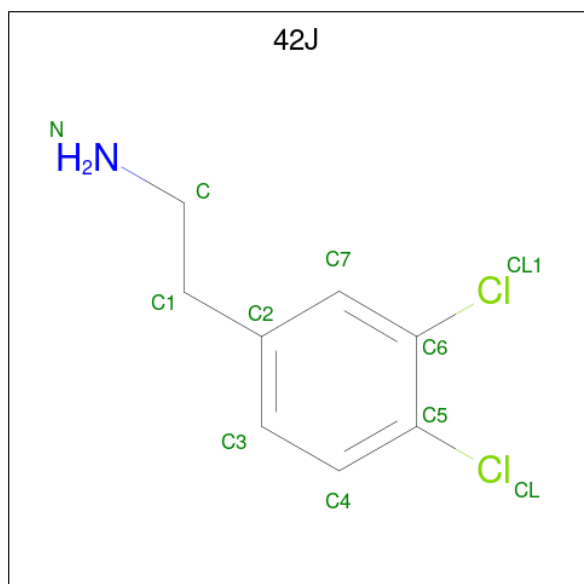
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	GLY	-	expression tag	UNP P68400
A	-21	SER	-	expression tag	UNP P68400
A	-20	MET	-	expression tag	UNP P68400
A	-19	ASP	-	expression tag	UNP P68400
A	-18	ILE	-	expression tag	UNP P68400
A	-17	GLU	-	expression tag	UNP P68400
A	-16	PHE	-	expression tag	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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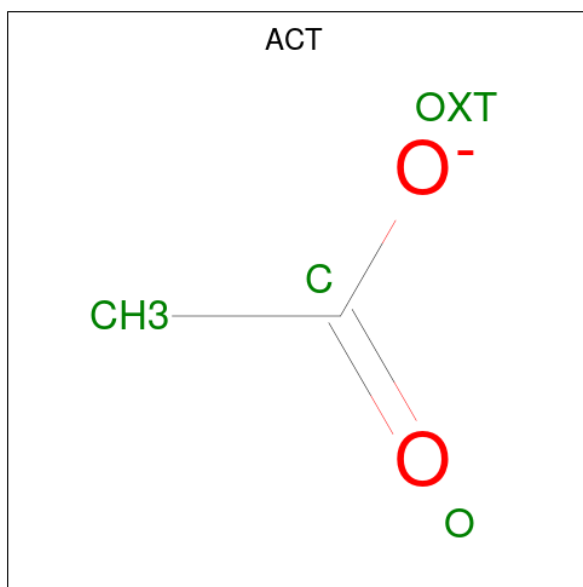
Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	GLY	-	expression tag	UNP P68400
B	-21	SER	-	expression tag	UNP P68400
B	-20	MET	-	expression tag	UNP P68400
B	-19	ASP	-	expression tag	UNP P68400
B	-18	ILE	-	expression tag	UNP P68400
B	-17	GLU	-	expression tag	UNP P68400
B	-16	PHE	-	expression tag	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 2-(3,4-dichlorophenyl)ethanamine (CCD ID: 42J) (formula: $C_8H_9Cl_2N$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	0	1
			22	16	4	2		
2	A	1	Total	C	Cl	N	0	0
			11	8	2	1		
2	A	1	Total	C	Cl	N	0	0
			11	8	2	1		
2	A	1	Total	C	Cl	N	0	1
			22	16	4	2		
2	A	1	Total	C	Cl	N	0	0
			11	8	2	1		
2	A	1	Total	C	Cl	N	0	0
			11	8	2	1		
2	B	1	Total	C	Cl	N	0	1
			22	16	4	2		
2	B	1	Total	C	Cl	N	0	1
			22	16	4	2		
2	B	1	Total	C	Cl	N	0	0
			11	8	2	1		
2	B	1	Total	C	Cl	N	0	1
			22	16	4	2		
2	B	1	Total	C	Cl	N	0	0
			11	8	2	1		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

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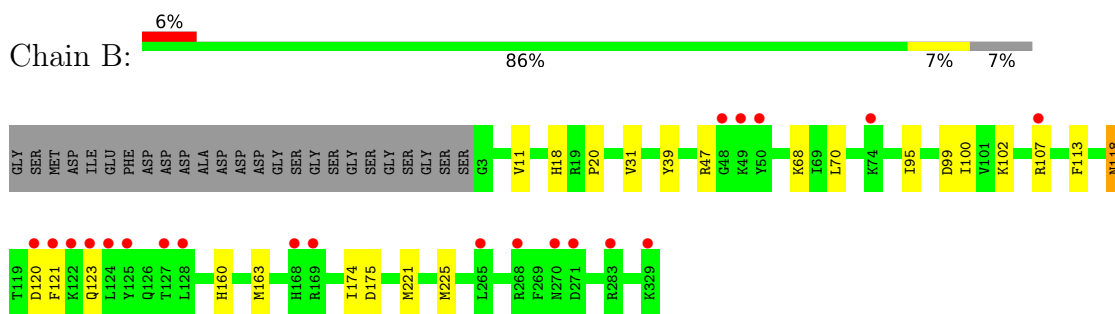
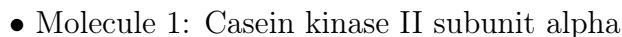
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	178	Total	O	0	0
			178	178		
4	B	270	Total	O	0	0
			270	270		

- 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	65.04Å 69.03Å 334.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	167.17 – 1.68 167.17 – 1.68	Depositor EDS
% Data completeness (in resolution range)	98.4 (167.17-1.68) 99.9 (167.17-1.68)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 1.68Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.178 , 0.193 0.177 , 0.194	Depositor DCC
R_{free} test set	4331 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.1	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	6220	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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: ACT, 42J

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.80	0/2849	0.99	1/3853 (0.0%)
1	B	0.87	0/2885	0.99	7/3902 (0.2%)
All	All	0.84	0/5734	0.99	8/7755 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	ARG	CA-C-N	5.63	127.18	122.17
1	B	47	ARG	C-N-CA	5.63	127.18	122.17
1	B	99	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	117	ASN	CA-CB-CG	5.23	117.83	112.60
1	B	123	GLN	CA-C-N	5.22	127.28	120.28
1	B	123	GLN	C-N-CA	5.22	127.28	120.28
1	B	120	ASP	CA-C-N	5.15	127.90	120.38
1	B	120	ASP	C-N-CA	5.15	127.90	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2777	0	2719	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2807	0	2749	31	0
2	A	88	0	72	32	0
2	B	88	0	72	27	0
3	A	8	0	6	0	0
3	B	4	0	3	0	0
4	A	178	0	0	2	0
4	B	270	0	0	5	1
All	All	6220	0	5621	78	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (78) 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:174:ILE:HB	2:A:401[B]:42J:H8	1.14	1.06
1:B:68:LYS:HD3	2:B:401[A]:42J:N	1.73	1.04
1:B:174:ILE:HB	2:B:401[B]:42J:H8	1.20	1.02
2:A:401[A]:42J:H2	2:A:401[A]:42J:N	1.91	0.84
2:A:401[B]:42J:H6	4:A:543:HOH:O	1.80	0.81
1:B:174:ILE:HB	2:B:401[B]:42J:N	1.96	0.80
1:A:174:ILE:HB	2:A:401[B]:42J:N	1.97	0.78
1:B:68:LYS:HD3	2:B:401[A]:42J:H8	1.48	0.78
2:A:401[A]:42J:H2	2:A:401[A]:42J:H8	1.50	0.76
1:B:68:LYS:CD	2:B:401[A]:42J:N	2.52	0.73
1:A:283:ARG:C	2:A:406:42J:H9	1.97	0.71
2:B:401[A]:42J:N	4:B:501:HOH:O	2.21	0.71
2:B:401[B]:42J:H6	4:B:557:HOH:O	1.89	0.71
1:B:121:PHE:CZ	1:B:225:MET:HE1	2.25	0.71
1:B:68:LYS:HZ3	2:B:401[A]:42J:H6	1.55	0.71
1:B:31:VAL:HG13	1:B:100[B]:ILE:HD12	1.73	0.70
1:A:68:LYS:HD3	2:A:401[A]:42J:H6	1.76	0.67
1:A:175:ASP:H	2:A:401[A]:42J:H5	1.59	0.67
1:B:68:LYS:NZ	2:B:401[A]:42J:H6	2.12	0.65
1:A:113:PHE:CZ	2:A:401[B]:42J:H7	2.32	0.64
2:B:401[A]:42J:N	2:B:401[A]:42J:H2	2.12	0.64
1:B:11[B]:VAL:HG11	4:B:729:HOH:O	1.99	0.62
1:B:102:LYS:HE2	1:B:107:ARG:HB3	1.81	0.62
1:B:175:ASP:H	2:B:401[A]:42J:H5	1.64	0.62
1:B:95:ILE:HG21	2:B:401[B]:42J:H9	1.65	0.61
1:A:140:ILE:HD11	2:A:404[B]:42J:CL1	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ILE:CB	2:A:401[B]:42J:H8	2.03	0.59
1:A:95:ILE:HG21	2:A:401[B]:42J:H9	1.69	0.57
1:A:236:HIS:HE1	4:A:581:HOH:O	1.87	0.57
1:A:107:ARG:HG3	1:A:107:ARG:HH11	1.70	0.57
1:A:8:ARG:HH11	1:A:184:PRO:HB2	1.70	0.56
1:A:251:THR:HB	1:A:255:TYR:CE2	2.41	0.55
1:B:113:PHE:CZ	2:B:401[B]:42J:H7	2.42	0.54
1:B:174:ILE:CB	2:B:401[B]:42J:H8	2.07	0.54
1:A:285:VAL:HG21	2:A:405:42J:CL1	2.45	0.54
1:B:18:HIS:HE1	4:B:696:HOH:O	1.92	0.53
2:B:401[B]:42J:N	2:B:401[B]:42J:H3	2.22	0.53
2:A:401[A]:42J:N	2:A:401[A]:42J:C3	2.69	0.53
1:B:175:ASP:H	2:B:401[B]:42J:C	2.21	0.53
2:B:401[A]:42J:N	2:B:401[A]:42J:C3	2.73	0.51
1:A:68:LYS:NZ	2:A:401[A]:42J:C	2.73	0.51
1:B:39:TYR:O	2:B:404[A]:42J:H5	2.11	0.50
2:B:401[B]:42J:N	2:B:401[B]:42J:C7	2.73	0.50
1:A:31:VAL:HG13	1:A:100[B]:ILE:HD12	1.93	0.50
1:A:68:LYS:NZ	2:A:401[A]:42J:H6	2.27	0.49
1:A:175:ASP:H	2:A:401[B]:42J:C	2.25	0.49
1:A:175:ASP:HA	2:A:401[A]:42J:H7	1.95	0.49
1:B:118:ASN:HB2	1:B:163[B]:MET:HE1	1.94	0.49
2:B:402[A]:42J:H6	4:B:501:HOH:O	2.12	0.48
1:B:121:PHE:HZ	1:B:225:MET:HE1	1.74	0.48
1:A:283:ARG:C	2:A:406:42J:N	2.70	0.47
1:A:68:LYS:CD	2:A:401[A]:42J:H6	2.42	0.47
1:A:221:MET:CE	2:A:404[A]:42J:H2	2.45	0.46
1:B:102:LYS:HD3	1:B:107:ARG:HE	1.81	0.46
1:A:67:VAL:HG12	1:A:69[B]:ILE:HD13	1.96	0.46
1:B:163[B]:MET:SD	2:B:402[B]:42J:H1	2.56	0.46
1:B:175:ASP:HA	2:B:401[A]:42J:C	2.45	0.46
1:A:163[B]:MET:SD	2:A:402:42J:H1	2.56	0.46
1:A:269:PHE:HB3	1:A:273:LEU:HD22	1.98	0.45
2:A:401[B]:42J:N	2:A:401[B]:42J:H3	2.31	0.45
1:A:290:GLN:HB2	2:A:405:42J:H4	1.98	0.45
1:B:175:ASP:HB2	2:B:401[A]:42J:H7	1.99	0.44
1:A:140:ILE:CD1	2:A:404[B]:42J:CL1	3.03	0.44
1:B:175:ASP:CB	2:B:401[A]:42J:H7	2.47	0.44
1:A:68:LYS:NZ	2:A:401[A]:42J:H7	2.33	0.44
1:A:283:ARG:HA	2:A:406:42J:N	2.33	0.43
1:A:68:LYS:HZ3	2:A:401[A]:42J:H7	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:MET:CE	2:B:403:42J:H2	2.48	0.43
1:A:68:LYS:HE3	1:A:70:LEU:HD21	2.00	0.42
1:B:221:MET:HE1	2:B:403:42J:H2	2.01	0.42
2:A:401[A]:42J:H8	2:A:401[A]:42J:C3	2.27	0.41
1:B:68:LYS:HE3	1:B:70:LEU:HD21	2.02	0.41
1:A:68:LYS:CE	2:A:401[A]:42J:H6	2.50	0.41
1:A:105:VAL:HG11	1:B:20:PRO:HG2	2.02	0.41
1:A:163[B]:MET:HE2	2:A:401[B]:42J:CL	2.58	0.41
1:A:175:ASP:N	2:A:401[A]:42J:H5	2.32	0.41
1:B:175:ASP:HA	2:B:401[A]:42J:H6	2.02	0.41
1:B:221:MET:HE2	1:B:221:MET:HB3	1.89	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:502:HOH:O	4:B:502:HOH:O[4_597]	0.97	1.23

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	327/352 (93%)	320 (98%)	7 (2%)	0	100	100
1	B	332/352 (94%)	325 (98%)	7 (2%)	0	100	100
All	All	659/704 (94%)	645 (98%)	14 (2%)	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	305/319 (96%)	302 (99%)	3 (1%)	68	52
1	B	308/319 (97%)	306 (99%)	2 (1%)	78	67
All	All	613/638 (96%)	608 (99%)	5 (1%)	73	59

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	HIS
1	A	273	LEU
1	A	296	GLU
1	B	118	ASN
1	B	160	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	118	ASN
1	A	160	HIS
1	A	168	HIS
1	A	207	GLN
1	A	236	HIS
1	A	262	ASN
1	A	270	ASN
1	B	18	HIS
1	B	29	HIS
1	B	118	ASN
1	B	126	GLN
1	B	168	HIS
1	B	186	GLN
1	B	207	GLN
1	B	262	ASN
1	B	270	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

19 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	42J	B	401[A]	-	11,11,11	0.28	0	14,14,14	0.19	0
2	42J	A	403	-	11,11,11	0.31	0	14,14,14	0.16	0
3	ACT	A	408	-	3,3,3	1.14	0	3,3,3	0.92	0
2	42J	B	404[A]	-	11,11,11	0.30	0	14,14,14	0.16	0
3	ACT	A	407	-	3,3,3	1.28	0	3,3,3	0.92	0
2	42J	A	404[A]	-	11,11,11	0.30	0	14,14,14	0.16	0
2	42J	B	402[A]	-	11,11,11	0.29	0	14,14,14	0.16	0
2	42J	A	401[A]	-	11,11,11	0.17	0	14,14,14	0.79	1 (7%)
2	42J	B	401[B]	-	11,11,11	0.27	0	14,14,14	0.17	0
2	42J	B	404[B]	-	11,11,11	0.33	0	14,14,14	0.17	0
2	42J	B	402[B]	-	11,11,11	0.30	0	14,14,14	0.18	0
2	42J	A	404[B]	-	11,11,11	0.29	0	14,14,14	0.23	0
2	42J	A	401[B]	-	11,11,11	0.30	0	14,14,14	0.18	0
2	42J	A	402	-	11,11,11	0.29	0	14,14,14	0.16	0
3	ACT	B	406	-	3,3,3	1.13	0	3,3,3	1.01	0
2	42J	A	405	-	11,11,11	0.30	0	14,14,14	0.16	0
2	42J	B	403	-	11,11,11	0.29	0	14,14,14	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	42J	B	405	-	11,11,11	0.29	0	14,14,14	0.17	0
2	42J	A	406	-	11,11,11	0.30	0	14,14,14	0.16	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	42J	B	401[A]	-	-	3/3/3/3	0/1/1/1
2	42J	A	403	-	-	0/3/3/3	0/1/1/1
2	42J	A	401[B]	-	-	2/3/3/3	0/1/1/1
2	42J	A	402	-	-	0/3/3/3	0/1/1/1
2	42J	B	401[B]	-	-	3/3/3/3	0/1/1/1
2	42J	B	404[A]	-	-	1/3/3/3	0/1/1/1
2	42J	B	404[B]	-	-	3/3/3/3	0/1/1/1
2	42J	B	405	-	-	0/3/3/3	0/1/1/1
2	42J	A	404[A]	-	-	0/3/3/3	0/1/1/1
2	42J	B	402[A]	-	-	0/3/3/3	0/1/1/1
2	42J	A	405	-	-	3/3/3/3	0/1/1/1
2	42J	A	404[B]	-	-	0/3/3/3	0/1/1/1
2	42J	B	402[B]	-	-	0/3/3/3	0/1/1/1
2	42J	B	403	-	-	0/3/3/3	0/1/1/1
2	42J	A	406	-	-	0/3/3/3	0/1/1/1
2	42J	A	401[A]	-	-	2/3/3/3	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401[A]	42J	C1-C-N	2.85	120.52	112.71

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	405	42J	N-C-C1-C2
2	B	404[A]	42J	N-C-C1-C2
2	B	404[B]	42J	N-C-C1-C2
2	B	401[A]	42J	C-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	B	401[A]	42J	C-C1-C2-C7
2	B	401[B]	42J	N-C-C1-C2
2	A	401[A]	42J	C-C1-C2-C3
2	B	401[B]	42J	C-C1-C2-C7
2	A	401[A]	42J	C-C1-C2-C7
2	B	404[B]	42J	C-C1-C2-C7
2	B	404[B]	42J	C-C1-C2-C3
2	A	401[B]	42J	C-C1-C2-C7
2	B	401[B]	42J	C-C1-C2-C3
2	A	401[B]	42J	C-C1-C2-C3
2	A	405	42J	C-C1-C2-C7
2	A	405	42J	C-C1-C2-C3
2	B	401[A]	42J	N-C-C1-C2

There are no ring outliers.

13 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401[A]	42J	13	0
2	B	404[A]	42J	1	0
2	A	404[A]	42J	1	0
2	B	402[A]	42J	1	0
2	A	401[A]	42J	14	0
2	B	401[B]	42J	9	0
2	B	402[B]	42J	1	0
2	A	404[B]	42J	2	0
2	A	401[B]	42J	9	0
2	A	402	42J	1	0
2	A	405	42J	2	0
2	B	403	42J	2	0
2	A	406	42J	3	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	322/352 (91%)	0.53	33 (10%) 12 15	11, 31, 61, 87	9 (2%)
1	B	327/352 (92%)	0.08	21 (6%) 25 32	8, 21, 52, 80	7 (2%)
All	All	649/704 (92%)	0.30	54 (8%) 17 21	8, 26, 59, 87	16 (2%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	124	LEU	9.7
1	B	125	TYR	6.4
1	B	121	PHE	5.2
1	A	50	TYR	4.1
1	B	271	ASP	3.9
1	A	127	THR	3.9
1	B	107	ARG	3.6
1	A	73	VAL	3.5
1	A	271	ASP	3.4
1	B	49	LYS	3.4
1	B	50	TYR	3.4
1	A	128	LEU	3.4
1	A	105	VAL	3.3
1	A	267	PRO	3.1
1	A	169	ARG	3.0
1	A	120	ASP	2.9
1	A	107	ARG	2.9
1	A	49	LYS	2.9
1	A	74	LYS	2.9
1	A	33	TRP	2.8
1	A	268	ARG	2.8
1	B	120	ASP	2.7
1	B	122	LYS	2.6
1	B	265	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	169	ARG	2.6
1	A	278	ARG	2.6
1	B	127	THR	2.6
1	B	270	ASN	2.5
1	A	284	PHE	2.5
1	B	128	LEU	2.5
1	A	274	GLY	2.5
1	A	329	LYS	2.5
1	B	329	LYS	2.5
1	A	230	GLU	2.5
1	B	74	LYS	2.4
1	A	62	ASN	2.4
1	A	239	TYR	2.4
1	B	268	ARG	2.4
1	A	272	ILE	2.4
1	A	328	VAL	2.4
1	A	280	ARG	2.3
1	A	248	VAL	2.3
1	B	283	ARG	2.3
1	A	252	GLU	2.3
1	A	8	ARG	2.2
1	B	48	GLY	2.2
1	B	123	GLN	2.2
1	A	72	PRO	2.2
1	A	116	VAL	2.1
1	A	275	ARG	2.1
1	A	126	GLN	2.1
1	A	131	TYR	2.1
1	A	48	GLY	2.0
1	B	168	HIS	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 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
3	ACT	A	408	4/4	0.69	0.28	72,73,74,74	0
2	42J	B	404[B]	11/11	0.73	0.27	30,46,53,55	11
2	42J	B	404[A]	11/11	0.73	0.27	38,40,45,46	11
2	42J	A	405	11/11	0.78	0.27	90,94,95,96	0
2	42J	B	403	11/11	0.79	0.18	26,40,53,61	0
2	42J	B	405	11/11	0.81	0.17	40,44,50,56	0
2	42J	A	402	11/11	0.82	0.18	37,47,56,62	0
2	42J	A	404[B]	11/11	0.87	0.16	54,59,62,65	11
2	42J	A	404[A]	11/11	0.87	0.16	32,44,49,58	11
2	42J	A	406	11/11	0.87	0.17	52,54,55,55	0
2	42J	B	402[A]	11/11	0.87	0.19	31,41,56,57	11
2	42J	B	402[B]	11/11	0.87	0.19	31,42,56,58	11
2	42J	A	403	11/11	0.89	0.15	37,47,58,59	0
3	ACT	A	407	4/4	0.92	0.10	34,37,37,37	0
2	42J	A	401[A]	11/11	0.93	0.10	11,19,28,29	11
2	42J	A	401[B]	11/11	0.93	0.10	12,35,42,49	11
2	42J	B	401[A]	11/11	0.94	0.08	7,13,21,21	11
2	42J	B	401[B]	11/11	0.94	0.08	8,26,32,41	11
3	ACT	B	406	4/4	0.95	0.09	29,30,31,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.