



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:27 AM UTC

PDB ID : 5CS6 / pdb_00005cs6
Title : Crystal Structure of CK2alpha with Compound 3 bound
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Deposited on : 2015-07-23
Resolution : 1.88 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

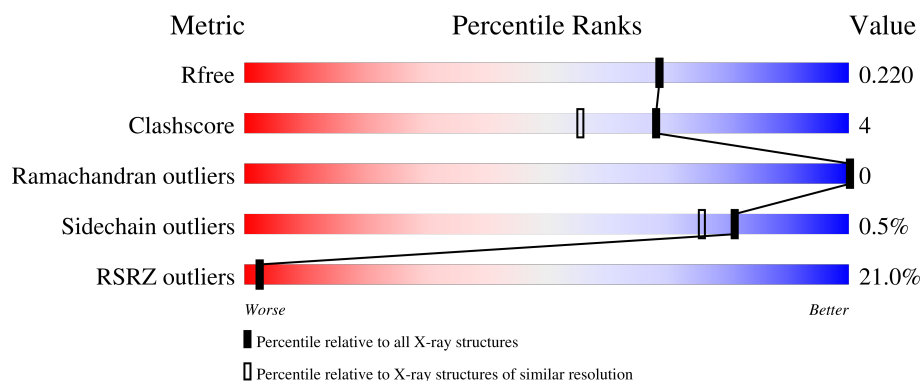
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	4% 85% 8% 7%
1	B	352	34% 80% 9% 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5795 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	327	Total	C	N	O	S	0	7	0
			2813	1801	493	507	12			
1	B	316	Total	C	N	O	S	0	2	0
			2684	1719	473	481	11			

There are 50 discrepancies between the modelled and reference sequences:

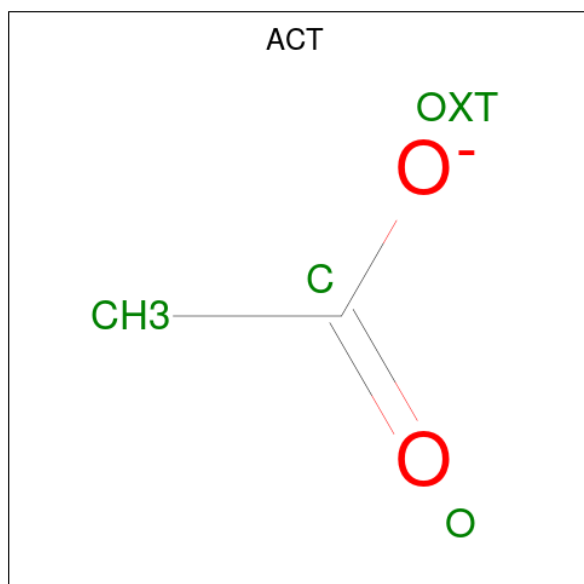
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	GLY	-	expression tag	UNP P68400
A	-21	SER	-	expression tag	UNP P68400
A	-20	MET	-	expression tag	UNP P68400
A	-19	ASP	-	expression tag	UNP P68400
A	-18	ILE	-	expression tag	UNP P68400
A	-17	GLU	-	expression tag	UNP P68400
A	-16	PHE	-	expression tag	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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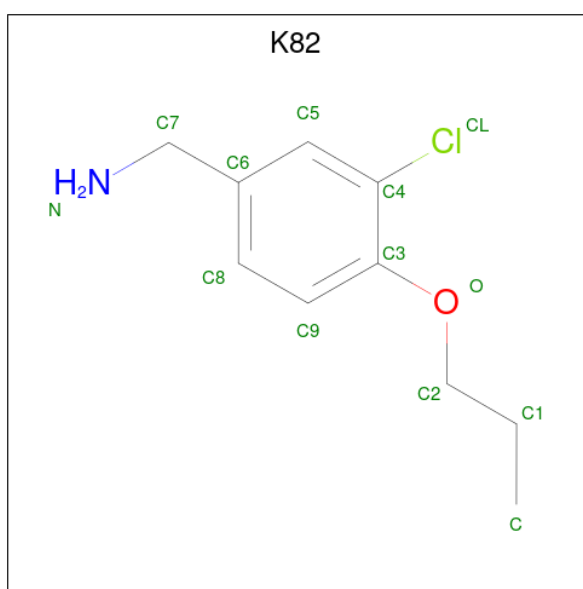
Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	GLY	-	expression tag	UNP P68400
B	-21	SER	-	expression tag	UNP P68400
B	-20	MET	-	expression tag	UNP P68400
B	-19	ASP	-	expression tag	UNP P68400
B	-18	ILE	-	expression tag	UNP P68400
B	-17	GLU	-	expression tag	UNP P68400
B	-16	PHE	-	expression tag	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 ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 3 is 1-(3-chloro-4-propoxyphenyl)methanamine (CCD ID: K82) (formula: $C_{10}H_{14}ClNO$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			13	10	1	1	1		
3	A	1	Total	C	Cl	N	O	0	0
			13	10	1	1	1		
3	A	1	Total	C	Cl	N	O	0	0
			13	10	1	1	1		
3	A	1	Total	C	Cl	N	O	0	0
			13	10	1	1	1		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	198	Total	O	0	0
			198	198		
5	B	27	Total	O	0	0
			27	27		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	64.50Å 68.85Å 335.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	167.94 – 1.88 167.94 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.2 (167.94-1.88) 99.9 (167.94-1.88)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 1.88Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.206 , 0.216 0.209 , 0.220	Depositor DCC
R_{free} test set	3111 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 68.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5795	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.72% 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: K82, 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	0.95	0/2888	1.08	6/3905 (0.2%)
1	B	0.76	0/2756	1.15	2/3726 (0.1%)
All	All	0.87	0/5644	1.12	8/7631 (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	A	237	ASP	CA-CB-CG	6.88	119.48	112.60
1	B	237	ASP	CA-CB-CG	6.63	119.23	112.60
1	A	51	SER	N-CA-C	5.60	116.77	108.60
1	A	314	THR	N-CA-C	-5.45	103.50	110.53
1	A	19	ARG	CA-C-N	-5.23	114.57	119.85
1	A	19	ARG	C-N-CA	-5.23	114.57	119.85
1	B	314	THR	N-CA-C	-5.17	103.86	110.53
1	A	35	ASN	CA-CB-CG	5.15	117.75	112.60

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	2813	0	2751	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2684	0	2627	22	0
2	A	12	0	9	0	0
2	B	4	0	3	0	0
3	A	52	0	0	1	0
4	A	5	0	0	0	0
5	A	198	0	0	4	1
5	B	27	0	0	0	0
All	All	5795	0	5390	39	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 4.

All (39) 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:35:ASN:OD1	1:B:37:ASP:HB2	1.74	0.85
1:B:229:LYS:HZ1	1:B:244[B]:ARG:HH12	1.45	0.65
1:B:229:LYS:HZ1	1:B:244[B]:ARG:NH1	1.94	0.65
1:A:296:GLU:HG3	3:A:407:K82:C2	2.27	0.64
1:B:255:TYR:HA	1:B:258:ILE:HG22	1.80	0.64
1:A:133:ILE:HG23	1:A:225[A]:MET:HE3	1.82	0.61
1:B:84:ILE:HG23	1:B:152:ILE:HD13	1.84	0.59
1:B:229:LYS:NZ	1:B:244[B]:ARG:NH1	2.50	0.59
1:A:236:HIS:HE1	5:A:655:HOH:O	1.87	0.58
1:A:72:PRO:O	1:A:73:VAL:HG23	2.04	0.57
1:A:286:HIS:HE1	5:A:671:HOH:O	1.88	0.56
1:A:50:TYR:HD1	1:A:73:VAL:HG21	1.72	0.55
1:A:222:LEU:HA	1:A:225[A]:MET:HE2	1.91	0.52
1:B:258:ILE:HG13	1:B:263:ILE:HB	1.92	0.52
1:B:8:ARG:HH11	1:B:13:THR:HG21	1.77	0.49
1:A:50:TYR:CD1	1:A:73:VAL:HG21	2.49	0.48
1:A:285:VAL:HG22	1:A:293:VAL:HG11	1.95	0.48
1:A:70:LEU:HD13	1:A:78:ILE:HG12	1.96	0.48
1:B:96:THR:HB	1:B:114:GLU:HG3	1.96	0.48
1:A:118:ASN:HD22	1:A:164:ILE:H	1.61	0.48
1:B:54:PHE:CE2	1:B:69:ILE:HD12	2.49	0.47
1:B:96:THR:HB	1:B:114:GLU:CG	2.45	0.46
1:B:23:TYR:O	1:B:83:LYS:HE3	2.16	0.46
1:B:23:TYR:OH	1:B:150:MET:HE3	2.16	0.45
1:A:73:VAL:CG1	1:A:74:LYS:N	2.80	0.45
1:A:33:TRP:CE3	1:A:100:ILE:HG22	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:HIS:CE1	5:A:655:HOH:O	2.68	0.44
1:A:26:TYR:HE1	1:A:76:LYS:HG2	1.83	0.44
1:B:33:TRP:CZ3	1:B:100:ILE:HG22	2.53	0.43
1:B:165:ASP:HB3	1:B:170:LYS:HB3	2.01	0.43
1:A:90:GLY:HA3	1:B:33:TRP:HD1	1.83	0.43
1:A:118:ASN:ND2	1:A:164:ILE:H	2.17	0.42
1:B:190:VAL:HG11	1:B:205:ASP:HA	2.00	0.42
1:B:100:ILE:HG23	1:B:111:LEU:HD23	2.00	0.42
1:A:183:HIS:HB2	1:A:186:GLN:HE21	1.85	0.42
1:A:23:TYR:CE1	1:B:104:PRO:HB3	2.55	0.41
1:B:183:HIS:HB2	1:B:186:GLN:HE21	1.86	0.41
5:A:539:HOH:O	1:B:107:ARG:HD3	2.20	0.40
1:B:240:ASP:O	1:B:244[A]:ARG:HG2	2.21	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)
5:A:681:HOH:O	5:A:681:HOH:O[4_597]	1.07	1.13

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	332/352 (94%)	320 (96%)	12 (4%)	0	100	100
1	B	314/352 (89%)	301 (96%)	13 (4%)	0	100	100
All	All	646/704 (92%)	621 (96%)	25 (4%)	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	308/319 (97%)	308 (100%)	0	100	100
1	B	293/319 (92%)	290 (99%)	3 (1%)	68	60
All	All	601/638 (94%)	598 (100%)	3 (0%)	81	76

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

Mol	Chain	Res	Type
1	B	40	GLN
1	B	100	ILE
1	B	128	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	186	GLN
1	A	207	GLN
1	A	234	HIS
1	A	262	ASN
1	A	310	GLN
1	B	118	ASN
1	B	168	HIS
1	B	186	GLN
1	B	241	GLN
1	B	262	ASN
1	B	310	GLN

5.3.3 RNA ⓘ

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	K82	A	407	-	13,13,13	0.16	0	16,16,16	0.36	0
2	ACT	B	401	-	3,3,3	1.01	0	3,3,3	1.07	0
3	K82	A	405	-	13,13,13	0.16	0	16,16,16	0.30	0
3	K82	A	406	-	13,13,13	0.14	0	16,16,16	0.36	0
3	K82	A	404	-	13,13,13	0.15	0	16,16,16	0.36	0
4	PO4	A	408	-	4,4,4	2.64	3 (75%)	6,6,6	0.72	0
2	ACT	A	402	-	3,3,3	1.71	1 (33%)	3,3,3	0.86	0
2	ACT	A	403	-	3,3,3	1.10	0	3,3,3	1.05	0
2	ACT	A	401	-	3,3,3	1.26	0	3,3,3	1.24	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	K82	A	405	-	-	1/6/6/6	0/1/1/1
3	K82	A	406	-	-	0/6/6/6	0/1/1/1
3	K82	A	404	-	-	1/6/6/6	0/1/1/1
3	K82	A	407	-	-	0/6/6/6	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	408	PO4	P-O1	4.42	1.60	1.50
2	A	402	ACT	CH3-C	2.62	1.59	1.49
4	A	408	PO4	P-O3	2.04	1.60	1.54
4	A	408	PO4	P-O4	2.00	1.60	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	405	K82	C1-C2-O-C3
3	A	404	K82	C-C1-C2-O

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	407	K82	1	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	327/352 (92%)	0.13	15 (4%)	37 40	14, 38, 75, 105	7 (2%)
1	B	316/352 (89%)	1.84	120 (37%)	1 0	46, 106, 200, 241	2 (0%)
All	All	643/704 (91%)	0.97	135 (20%)	2 2	14, 69, 181, 241	9 (1%)

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	328	VAL	6.1
1	B	33	TRP	5.7
1	B	273	LEU	5.5
1	B	327	VAL	5.1
1	B	257	TYR	5.0
1	B	265	LEU	4.8
1	B	116	VAL	4.8
1	B	251	THR	4.8
1	B	276	HIS	4.7
1	B	5	VAL	4.5
1	B	255	TYR	4.3
1	B	274	GLY	4.3
1	B	258	ILE	4.3
1	B	272	ILE	4.2
1	B	263	ILE	4.1
1	B	254	LEU	4.0
1	B	181	PHE	3.9
1	B	45	LEU	3.9
1	B	298	LEU	3.9
1	A	50	TYR	3.7
1	B	281	TRP	3.7
1	B	285	VAL	3.7
1	A	124	LEU	3.6
1	B	41	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	44[A]	LYS	3.6
1	B	244[A]	ARG	3.6
1	B	20	PRO	3.6
1	B	259	ASP	3.5
1	B	260	LYS	3.5
1	A	33	TRP	3.5
1	B	296	GLU	3.5
1	B	226	ILE	3.4
1	B	250	GLY	3.4
1	B	104	PRO	3.4
1	B	305	LEU	3.3
1	B	50	TYR	3.3
1	B	204	VAL	3.3
1	A	104	PRO	3.3
1	B	6	PRO	3.3
1	B	227	PHE	3.3
1	B	35	ASN	3.3
1	A	72	PRO	3.2
1	B	34	GLY	3.2
1	B	30	VAL	3.2
1	B	105	VAL	3.2
1	B	170	LYS	3.1
1	B	31	VAL	3.1
1	B	57	ILE	3.1
1	B	206	TYR	3.1
1	B	185	GLY	3.1
1	B	19	ARG	3.0
1	B	300	PHE	3.0
1	B	118	ASN	3.0
1	B	256	ASP	3.0
1	B	90	GLY	2.9
1	B	284	PHE	2.9
1	B	54	PHE	2.9
1	B	269	PHE	2.9
1	B	91	GLY	2.8
1	B	190	VAL	2.8
1	B	275	ARG	2.8
1	B	236	HIS	2.8
1	B	65	VAL	2.8
1	B	171	LEU	2.8
1	B	24	TRP	2.8
1	B	4	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	295	PRO	2.7
1	B	42	VAL	2.7
1	B	307	TYR	2.7
1	B	271	ASP	2.7
1	B	277	SER	2.7
1	B	261	TYR	2.7
1	B	253	ASP	2.7
1	A	114[A]	GLU	2.7
1	B	164	ILE	2.7
1	B	229	LYS	2.7
1	B	279	LYS	2.7
1	B	246	ALA	2.6
1	A	121	PHE	2.6
1	B	242	LEU	2.6
1	B	37	ASP	2.6
1	B	182	TYR	2.6
1	B	73	VAL	2.6
1	B	297	ALA	2.6
1	B	12	TYR	2.6
1	B	146	TYR	2.6
1	B	128	LEU	2.6
1	B	247	LYS	2.6
1	A	73	VAL	2.6
1	B	232	PHE	2.5
1	B	106	SER	2.5
1	B	114	GLU	2.5
1	B	107	ARG	2.4
1	B	36	GLN	2.4
1	B	245	ILE	2.4
1	A	105	VAL	2.4
1	B	313	LEU	2.4
1	B	59	ILE	2.4
1	B	299	ASP	2.4
1	B	243	VAL	2.4
1	B	103	ASP	2.4
1	B	46	GLY	2.3
1	B	287	SER	2.3
1	B	202	LEU	2.3
1	B	249	LEU	2.3
1	B	43	ARG	2.3
1	B	15	VAL	2.3
1	B	262	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	125	TYR	2.3
1	B	211	TYR	2.2
1	B	53	VAL	2.2
1	B	101	VAL	2.2
1	B	127	THR	2.2
1	B	290	GLN	2.2
1	A	34	GLY	2.2
1	B	9	ALA	2.2
1	B	326	THR	2.2
1	B	203	LEU	2.2
1	B	23	TYR	2.1
1	B	325	TYR	2.1
1	B	248	VAL	2.1
1	B	21	SER	2.1
1	B	143	ALA	2.1
1	B	293	VAL	2.1
1	B	62	ASN	2.1
1	B	186	GLN	2.1
1	B	69	ILE	2.0
1	B	233	PHE	2.0
1	B	117	ASN	2.0
1	A	116	VAL	2.0
1	B	178	LEU	2.0
1	B	318	ALA	2.0
1	A	57	ILE	2.0
1	B	196	TYR	2.0
1	B	109	PRO	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(Å ²)	Q<0.9
4	PO4	A	408	5/5	0.72	0.16	70,70,75,78	0
2	ACT	B	401	4/4	0.73	0.22	85,86,87,88	0
2	ACT	A	403	4/4	0.74	0.17	76,77,77,77	0
2	ACT	A	402	4/4	0.80	0.17	45,46,46,47	0
3	K82	A	404	13/13	0.82	0.16	43,46,57,59	0
3	K82	A	405	13/13	0.86	0.15	48,58,63,63	0
3	K82	A	406	13/13	0.87	0.13	59,65,72,73	0
3	K82	A	407	13/13	0.88	0.12	63,65,69,70	0
2	ACT	A	401	4/4	0.89	0.11	48,57,57,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.