



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 2O4Q / pdb_00002o4q
Title : Structure of Phosphotriesterase mutant G60A
Authors : Kim, J.; Ramagopal, U.A.; Tsai, P.C.; Raushel, F.M.; Almo, S.C.
Deposited on : 2006-12-04
Resolution : 1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

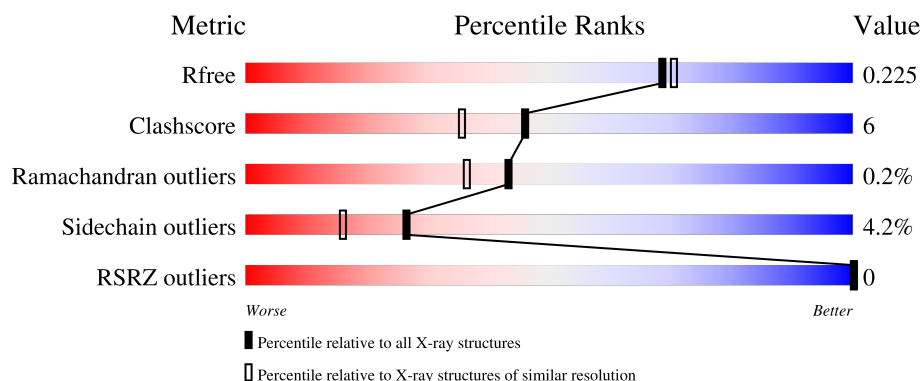
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	331	86% 12% .
1	B	331	87% 11% .
1	K	331	87% 12% .
1	P	331	85% 12% .

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
3	CAC	A	1	-	X	-	-
3	CAC	B	2	-	X	-	-
3	CAC	K	3	-	X	-	-
3	CAC	P	4	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11215 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 Parathion hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	3	0
			2548	1609	454	478	7			
1	B	330	Total	C	N	O	S	0	3	0
			2546	1608	453	478	7			
1	K	331	Total	C	N	O	S	0	2	0
			2542	1606	453	476	7			
1	P	330	Total	C	N	O	S	0	0	0
			2525	1597	450	471	7			

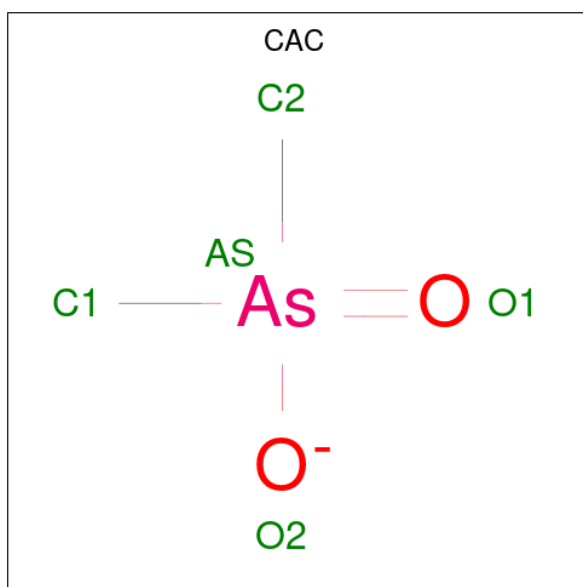
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ALA	GLY	engineered mutation	UNP P0A434
B	60	ALA	GLY	engineered mutation	UNP P0A434
K	60	ALA	GLY	engineered mutation	UNP P0A434
P	60	ALA	GLY	engineered mutation	UNP P0A434

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	K	2	Total	Zn	0	0
			2	2		
2	P	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CACODYLATE ION (CCD ID: CAC) (formula: C₂H₆AsO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	As	C	O	0	0
			5	1	2	2		
3	B	1	Total	As	C	O	0	0
			5	1	2	2		
3	K	1	Total	As	C	O	0	0
			5	1	2	2		
3	P	1	Total	As	C	O	0	0
			5	1	2	2		

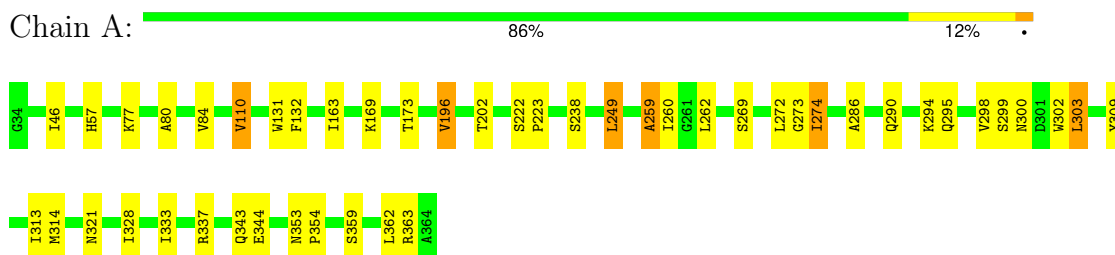
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	278	Total	O	0	0
			278	278		
4	B	246	Total	O	0	0
			246	246		
4	K	268	Total	O	0	0
			268	268		
4	P	234	Total	O	0	0
			234	234		

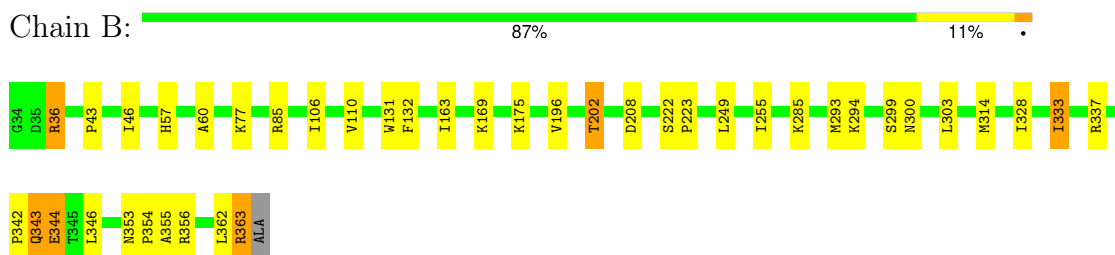
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

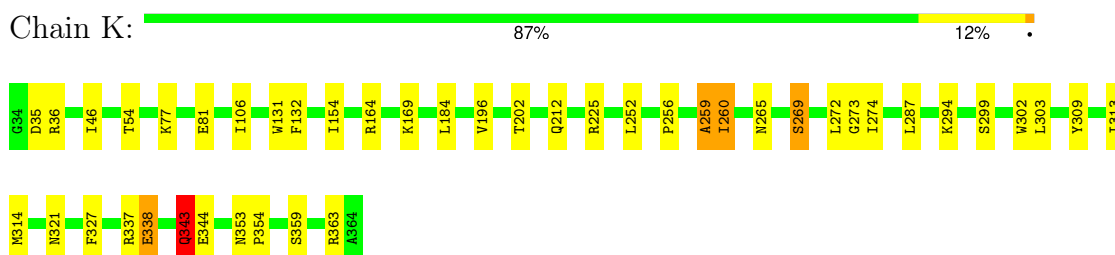
- Molecule 1: Parathion hydrolase



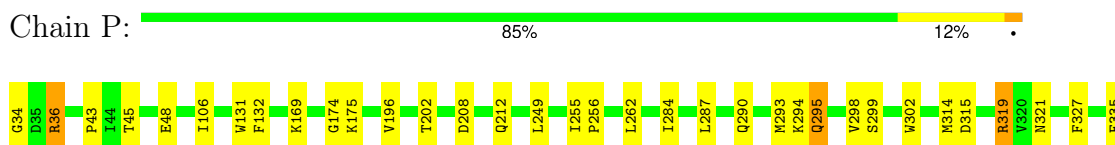
- Molecule 1: Parathion hydrolase



- Molecule 1: Parathion hydrolase



- Molecule 1: Parathion hydrolase



L336	R337	E338	K339	G340	V341	P342	Q343	E344		N353	P354	A355	R356		P360	T361	L362	R363	ALA
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.30Å 68.30Å 90.03Å 90.05° 100.42° 89.96°	Depositor
Resolution (Å)	31.64 – 1.95 31.64 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.1 (31.64-1.95) 96.9 (31.64-1.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.164 , 0.226 0.166 , 0.225	Depositor DCC
R_{free} test set	4597 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 28.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.467 for -h,k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11215	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.96% 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: CAC, KCX, ZN

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	0.92	1/2583 (0.0%)	0.96	2/3509 (0.1%)
1	B	0.86	1/2581 (0.0%)	0.90	1/3504 (0.0%)
1	K	0.90	0/2577	0.95	0/3500
1	P	0.86	0/2560	0.92	3/3476 (0.1%)
All	All	0.89	2/10301 (0.0%)	0.93	6/13989 (0.0%)

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	1
1	K	0	1
1	P	0	2
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	333	ILE	CA-CB	8.32	1.59	1.53
1	B	60	ALA	CA-CB	5.24	1.59	1.53

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	255	ILE	CA-C-N	-6.79	113.91	120.83
1	P	255	ILE	C-N-CA	-6.79	113.91	120.83
1	P	255	ILE	N-CA-CB	6.25	114.71	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	333	ILE	N-CA-CB	5.68	114.08	110.50
1	B	255	ILE	N-CA-CB	5.39	114.13	110.52

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	THR	Peptide
1	A	363	ARG	Peptide
1	B	202	THR	Peptide
1	K	202	THR	Peptide
1	P	202	THR	Peptide

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	2548	0	2565	32	0
1	B	2546	0	2559	24	0
1	K	2542	0	2560	35	0
1	P	2525	0	2546	27	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	K	2	0	0	0	0
2	P	2	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	K	5	0	0	0	0
3	P	5	0	0	0	0
4	A	278	0	0	6	0
4	B	246	0	0	4	0
4	K	268	0	0	6	0
4	P	234	0	0	2	0
All	All	11215	0	10230	118	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 6.

The worst 5 of 118 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:259:ALA:HB2	1:A:272:LEU:HB2	1.29	1.12
1:B:337:ARG:HH21	1:B:343:GLN:HG2	0.92	1.06
1:B:337:ARG:NH2	1:B:343:GLN:HG2	1.70	1.05
1:K:259:ALA:HB2	1:K:272:LEU:HB2	1.39	1.03
1:K:225:ARG:HD3	4:K:2451:HOH:O	1.61	0.98

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	331/331 (100%)	314 (95%)	16 (5%)	1 (0%)	36	28
1	B	330/331 (100%)	317 (96%)	13 (4%)	0	100	100
1	K	330/331 (100%)	318 (96%)	10 (3%)	2 (1%)	21	12
1	P	327/331 (99%)	315 (96%)	12 (4%)	0	100	100
All	All	1318/1324 (100%)	1264 (96%)	51 (4%)	3 (0%)	43	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	259	ALA
1	A	259	ALA
1	K	343	GLN

5.3.2 Protein sidechains [i](#)

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	267/264 (101%)	257 (96%)	10 (4%)	30	20
1	B	267/264 (101%)	256 (96%)	11 (4%)	27	17
1	K	266/264 (101%)	256 (96%)	10 (4%)	29	19
1	P	264/264 (100%)	250 (95%)	14 (5%)	20	9
All	All	1064/1056 (101%)	1019 (96%)	45 (4%)	26	16

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	338	GLU
1	P	293	MET
1	K	343	GLN
1	P	196	VAL
1	P	299	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	212	GLN
1	K	312	ASN
1	P	343	GLN
1	K	343	GLN
1	B	312	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	KCX	B	169	2,1	10,11,12	0.92	1 (10%)	6,12,14	1.79	1 (16%)
1	KCX	A	169	2,1	10,11,12	0.96	1 (10%)	6,12,14	1.59	1 (16%)
1	KCX	P	169	2,1	10,11,12	0.91	1 (10%)	6,12,14	1.89	1 (16%)
1	KCX	K	169	2,1	10,11,12	0.94	0	6,12,14	1.10	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	B	169	2,1	-	0/9/10/12	-
1	KCX	A	169	2,1	-	0/9/10/12	-
1	KCX	P	169	2,1	-	0/9/10/12	-
1	KCX	K	169	2,1	-	0/9/10/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	169	KCX	OQ1-CX	2.22	1.25	1.21
1	P	169	KCX	OQ1-CX	2.16	1.25	1.21
1	A	169	KCX	OQ1-CX	2.15	1.25	1.21

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	169	KCX	OQ1-CX-NZ	-4.40	118.23	124.92
1	B	169	KCX	OQ1-CX-NZ	-4.04	118.78	124.92
1	A	169	KCX	OQ1-CX-NZ	-3.68	119.32	124.92
1	K	169	KCX	OQ1-CX-NZ	-2.38	121.30	124.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\# Z > 2$
3	CAC	P	4	2	2,4,4	2.82	2 (100%)	4,6,6	2.56	2 (50%)
3	CAC	B	2	2	2,4,4	2.67	2 (100%)	4,6,6	3.31	2 (50%)
3	CAC	K	3	2	2,4,4	3.17	2 (100%)	4,6,6	4.08	3 (75%)
3	CAC	A	1	2	2,4,4	3.35	2 (100%)	4,6,6	1.93	2 (50%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	CAC	AS-C1	3.44	1.98	1.90
3	A	1	CAC	AS-C2	3.27	1.98	1.90
3	K	3	CAC	AS-C1	3.22	1.97	1.90
3	K	3	CAC	AS-C2	3.12	1.97	1.90
3	P	4	CAC	AS-C1	3.00	1.97	1.90

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	3	CAC	O1-AS-C2	-6.29	103.67	111.50
3	B	2	CAC	O1-AS-C2	-5.57	104.58	111.50
3	K	3	CAC	O2-AS-C2	3.70	114.80	105.84
3	K	3	CAC	O2-AS-C1	3.50	114.31	105.84
3	P	4	CAC	O2-AS-C1	3.49	114.29	105.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	330/331 (99%)	-1.37	0 100 100	5, 16, 42, 76	3 (0%)
1	B	329/331 (99%)	-1.34	0 100 100	8, 20, 38, 51	5 (1%)
1	K	330/331 (99%)	-1.36	0 100 100	6, 16, 41, 78	2 (0%)
1	P	329/331 (99%)	-1.35	0 100 100	11, 20, 38, 53	3 (0%)
All	All	1318/1324 (99%)	-1.35	0 100 100	5, 18, 41, 78	13 (0%)

There are no RSRZ outliers to report.

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	KCX	A	169	12/13	0.99	0.03	8,12,16,17	0
1	KCX	B	169	12/13	0.99	0.04	9,14,18,18	0
1	KCX	K	169	12/13	0.99	0.03	7,13,14,16	0
1	KCX	P	169	12/13	0.99	0.03	10,14,16,17	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CAC	A	1	5/5	0.99	0.04	12,16,22,24	5
3	CAC	P	4	5/5	0.99	0.05	10,16,20,21	5
2	ZN	B	2403	1/1	1.00	0.01	18,18,18,18	0
2	ZN	B	2404	1/1	1.00	0.01	22,22,22,22	0
2	ZN	K	2405	1/1	1.00	0.01	14,14,14,14	0
2	ZN	K	2406	1/1	1.00	0.01	18,18,18,18	0
2	ZN	P	2407	1/1	1.00	0.01	14,14,14,14	1
2	ZN	P	2408	1/1	1.00	0.01	19,19,19,19	0
2	ZN	A	2401	1/1	1.00	0.01	16,16,16,16	0
3	CAC	B	2	5/5	1.00	0.04	13,13,21,22	5
3	CAC	K	3	5/5	1.00	0.03	12,12,22,25	5
2	ZN	A	2402	1/1	1.00	0.01	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.