



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 08:26 PM GMT

PDB ID : 2O4Q  
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 full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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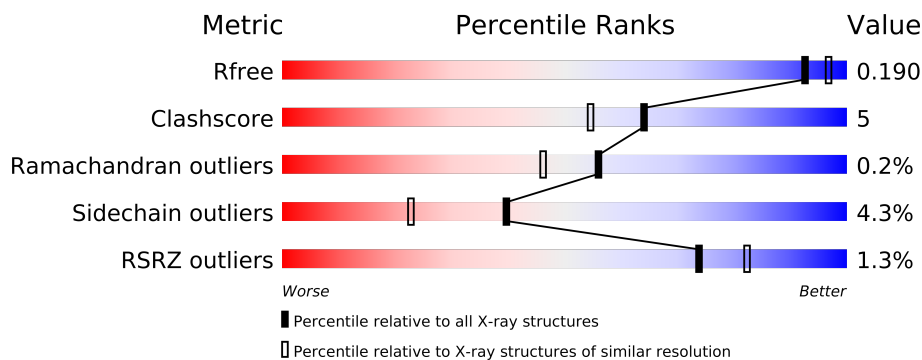
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1321 (1.96-1.96)
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	331	
1	B	331	
1	K	331	
1	P	331	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ZN	P	2407	-	X
3	CAC	A	1	X	-
3	CAC	B	2	X	-
3	CAC	K	3	X	X
3	CAC	P	4	X	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11215 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

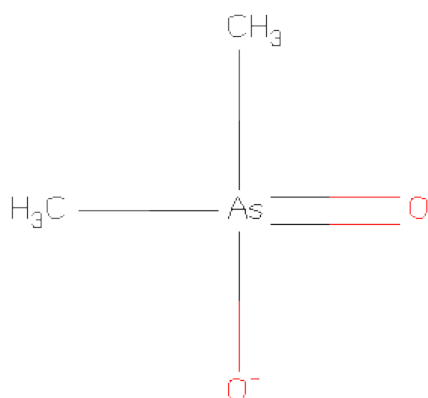
There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is CACODYLATE ION (three-letter code: CAC) (formula: C<sub>2</sub>H<sub>6</sub>AsO<sub>2</sub>).



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		

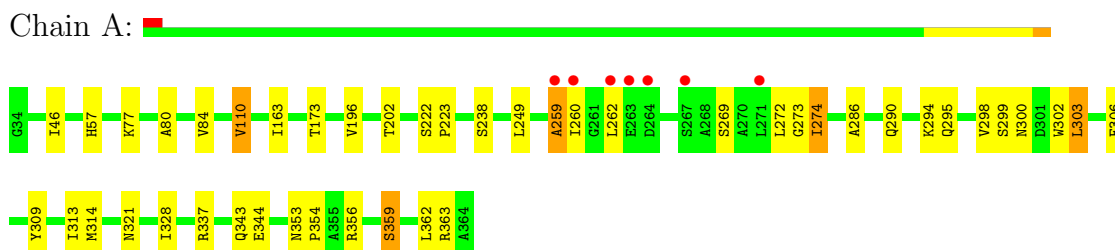
- Molecule 4 is water.

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		

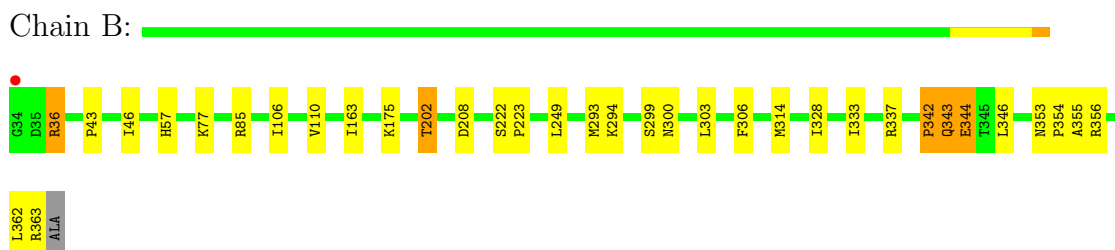
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

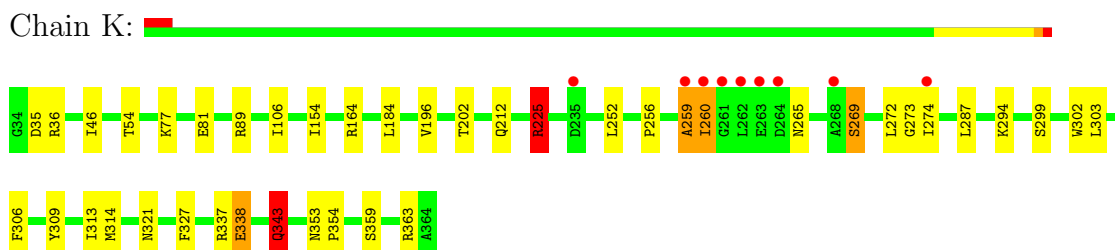
- Molecule 1: Parathion hydrolase



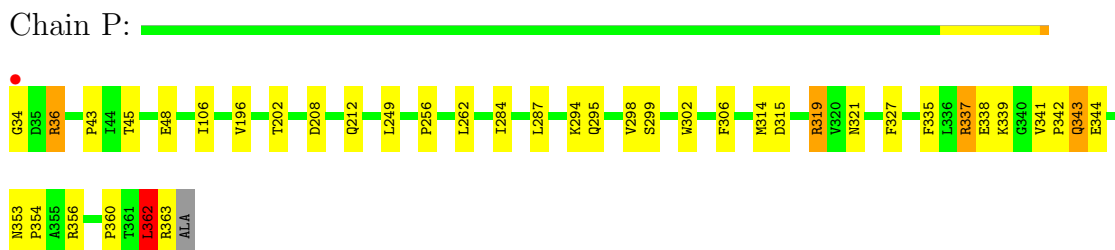
- Molecule 1: Parathion hydrolase



- Molecule 1: Parathion hydrolase



- Molecule 1: Parathion hydrolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.30Å 68.30Å 90.03Å 90.05° 100.42° 89.96°	Depositor
Resolution (Å)	31.64 – 1.95 31.65 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.1 (31.64-1.95) 96.9 (31.65-1.95)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.92 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.164 , 0.226 0.163 , 0.190	Depositor DCC
$R_{free}$ test set	4597 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.9	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 29.2	EDS
Estimated twinning fraction	0.467 for -h,k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 91514 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11215	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, ZN, KCX

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	0.72	0/2583	0.74	1/3509 (0.0%)
1	B	0.65	0/2581	0.68	0/3504
1	K	0.72	0/2577	0.77	3/3500 (0.1%)
1	P	0.66	0/2560	0.69	0/3476
All	All	0.69	0/10301	0.72	4/13989 (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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	225	ARG	NE-CZ-NH2	-9.95	115.33	120.30
1	K	225	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	K	89	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	356	ARG	NE-CZ-NH2	-6.47	117.07	120.30

There are no chirality outliers.

All (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
1	P	362	LEU	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2548	0	2564	31	0
1	B	2546	0	2558	21	0
1	K	2542	0	2559	34	0
1	P	2525	0	2545	25	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	3	0
4	K	268	0	0	6	0
4	P	234	0	0	2	0
All	All	11215	0	10226	111	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (111) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:B:337:ARG:HH21	1:B:343:GLN:CG	1.75	0.98
1:P:337:ARG:HH12	1:P:343:GLN:CG	1.96	0.79
1:P:337:ARG:HH12	1:P:343:GLN:HG3	1.46	0.79
1:P:315:ASP:O	1:P:319:ARG:HD3	1.82	0.78
1:K:337:ARG:HH12	1:K:343:GLN:CG	1.98	0.77
1:A:337:ARG:HH12	1:A:343:GLN:HG2	1.54	0.72
1:B:344[A]:GLU:CD	1:B:344[A]:GLU:H	1.93	0.72
1:A:238:SER:HB3	4:A:2657:HOH:O	1.89	0.71
1:P:362:LEU:O	1:P:363:ARG:HB2	1.90	0.70
1:A:259:ALA:CB	1:A:269:SER:HA	2.22	0.69
1:K:337:ARG:HH22	1:K:343:GLN:HG2	1.58	0.69
1:A:259:ALA:CB	1:A:272:LEU:HB2	2.17	0.69
1:K:337:ARG:HH12	1:K:343:GLN:HG3	1.58	0.68
1:P:36:ARG:HG2	1:P:43:PRO:HB2	1.78	0.65
1:K:77:LYS:HE2	1:K:81:GLU:OE2	1.95	0.65
1:B:77:LYS:HD3	4:B:2624:HOH:O	1.96	0.64
1:B:293:MET:HG2	4:B:2446:HOH:O	1.96	0.64
1:P:337:ARG:HH12	1:P:343:GLN:CB	2.10	0.63
1:A:259:ALA:HB1	1:A:269:SER:HA	1.81	0.62
1:K:259:ALA:N	1:K:273:GLY:O	2.34	0.60
1:B:342:PRO:HB2	1:B:344[A]:GLU:HG2	1.85	0.59
1:B:294:LYS:O	1:B:356:ARG:NH2	2.36	0.59
1:P:337:ARG:NH1	1:P:343:GLN:HG3	2.19	0.58
1:P:295:GLN:NE2	4:P:2533:HOH:O	2.38	0.57
1:B:353:ASN:HB2	1:B:354:PRO:HD3	1.88	0.55
1:K:54:THR:HG23	4:K:2569:HOH:O	2.06	0.54
1:A:46:ILE:HD12	1:A:359[A]:SER:HB2	1.88	0.54
1:K:106:ILE:HG22	1:K:106:ILE:O	2.08	0.53
1:B:36:ARG:HG2	1:B:43:PRO:HB2	1.89	0.53
1:K:302:TRP:CH2	1:K:321:ASN:HB3	2.44	0.53
1:P:106:ILE:O	1:P:106:ILE:HG22	2.09	0.52
1:K:225:ARG:CD	4:K:2451:HOH:O	2.38	0.52
1:B:249:LEU:HD12	1:B:249:LEU:N	2.25	0.52
1:P:294:LYS:O	1:P:356:ARG:NH2	2.43	0.52
1:P:335:PHE:CZ	1:P:339:LYS:HE2	2.46	0.51
1:P:208:ASP:O	1:P:212:GLN:HG3	2.10	0.51
1:B:106:ILE:HG22	1:B:106:ILE:O	2.10	0.51
1:P:362:LEU:O	1:P:363:ARG:CB	2.58	0.51
1:A:290:GLN:NE2	4:A:2647:HOH:O	2.44	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:260:ILE:HG13	1:A:274:ILE:CD1	2.42	0.50
1:A:110:VAL:HG13	1:A:163:ILE:HD12	1.93	0.50
1:K:259:ALA:HB1	1:K:269:SER:HA	1.94	0.49
1:B:202:THR:HB	1:B:208:ASP:HB2	1.95	0.49
1:A:259:ALA:N	1:A:273:GLY:O	2.46	0.48
1:B:333:ILE:HG23	1:B:346:LEU:HD13	1.93	0.48
1:A:353:ASN:HB2	1:A:354:PRO:HD3	1.95	0.48
1:K:309:TYR:HD2	1:K:313:ILE:HG12	1.79	0.48
1:A:286:ALA:O	1:A:290:GLN:HG2	2.13	0.48
1:K:309:TYR:CD2	1:K:313:ILE:HG12	2.49	0.48
1:A:80:ALA:O	1:A:84:VAL:HG23	2.14	0.48
1:K:353:ASN:HB2	1:K:354:PRO:HD3	1.95	0.48
1:K:252:LEU:HD11	1:K:287:LEU:HD12	1.95	0.48
1:A:337:ARG:HH22	1:A:343:GLN:HB2	1.79	0.47
1:A:337:ARG:NH1	4:A:2680:HOH:O	2.47	0.47
1:A:302:TRP:CH2	1:A:321:ASN:HB3	2.50	0.47
1:A:300:ASN:OD1	1:A:328:ILE:HG12	2.14	0.47
1:K:259:ALA:CB	1:K:272:LEU:HB2	2.27	0.47
1:P:256:PRO:HB3	1:P:327:PHE:CD2	2.50	0.47
1:A:337:ARG:HH12	1:A:343:GLN:CG	2.25	0.46
1:A:337:ARG:HH22	1:A:343:GLN:CG	2.29	0.45
1:P:302:TRP:CH2	1:P:321:ASN:HB3	2.51	0.45
1:B:46:ILE:CG2	1:B:355:ALA:HB1	2.46	0.45
1:K:338:GLU:HB3	4:K:2636:HOH:O	2.16	0.45
1:P:343:GLN:HB3	1:P:343:GLN:HE21	1.54	0.45
1:K:343:GLN:HB3	1:K:343:GLN:HE21	1.42	0.45
1:P:45:THR:OG1	1:P:48:GLU:HG3	2.17	0.45
1:K:294:LYS:NZ	4:K:2555:HOH:O	2.50	0.44
1:K:259:ALA:CB	1:K:269:SER:HA	2.48	0.44
1:K:259:ALA:HB3	1:K:273:GLY:H	1.82	0.44
1:A:337:ARG:HH22	1:A:343:GLN:CB	2.31	0.44
1:K:338:GLU:HB3	4:K:2553:HOH:O	2.17	0.44
1:B:300:ASN:OD1	1:B:328:ILE:HG12	2.17	0.44
1:K:184:LEU:HD21	1:K:212:GLN:HG2	1.99	0.44
1:K:225:ARG:HD2	1:K:225:ARG:N	2.32	0.44
1:P:353:ASN:HB2	1:P:354:PRO:HD3	2.00	0.44
1:P:341:VAL:HA	1:P:342:PRO:HD3	1.90	0.44
1:K:259:ALA:CB	1:K:273:GLY:H	2.31	0.44
1:B:85:ARG:NH1	4:B:2473:HOH:O	2.35	0.43
1:A:344:GLU:H	1:A:344:GLU:CD	2.21	0.43
1:K:265:ASN:O	1:K:269:SER:HB2	2.18	0.43
1:K:337:ARG:HH12	1:K:343:GLN:CB	2.30	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:46:ILE:HD12	1:K:359[A]:SER:HB2	2.01	0.43
1:A:222[A]:SER:HA	1:A:223:PRO:HD3	1.92	0.43
1:A:77:LYS:HE3	4:A:2598:HOH:O	2.18	0.43
1:K:256:PRO:HB3	1:K:327:PHE:CD1	2.53	0.43
1:A:309:TYR:HD2	1:A:313:ILE:HG12	1.84	0.43
1:A:249:LEU:HD13	1:A:295:GLN:HA	2.01	0.42
1:A:337:ARG:HH22	1:A:343:GLN:HG3	1.83	0.42
1:P:36:ARG:CG	1:P:43:PRO:HB2	2.49	0.42
1:P:363:ARG:NH2	4:P:2623:HOH:O	2.52	0.42
1:B:57:HIS:O	1:B:303:LEU:HA	2.19	0.42
1:B:344[A]:GLU:CD	1:B:344[A]:GLU:N	2.69	0.42
1:A:309:TYR:CD2	1:A:313:ILE:HG12	2.55	0.42
1:B:110:VAL:CG2	1:B:163:ILE:HG21	2.49	0.42
1:A:294:LYS:HE3	4:A:2612:HOH:O	2.21	0.41
1:K:154:ILE:O	1:K:164:ARG:HB3	2.20	0.41
1:P:249:LEU:HD13	1:P:295:GLN:HA	2.02	0.41
1:K:35:ASP:O	1:K:36:ARG:HD3	2.21	0.41
1:K:260:ILE:O	1:K:260:ILE:HG22	2.19	0.41
1:P:34:GLY:HA3	1:P:360:PRO:O	2.20	0.41
1:A:57:HIS:O	1:A:303:LEU:HA	2.21	0.41
1:B:222:SER:HA	1:B:223:PRO:HD3	1.96	0.40
1:P:287:LEU:HD23	1:P:287:LEU:HA	1.88	0.40
1:K:260:ILE:O	1:K:260:ILE:CG2	2.70	0.40
1:P:284:ILE:HD13	1:P:298:VAL:HG11	2.03	0.40
1:A:173:THR:HG22	4:A:2457:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 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	331/331 (100%)	314 (95%)	16 (5%)	1 (0%)	50	38
1	B	330/331 (100%)	317 (96%)	13 (4%)	0	100	100
1	K	330/331 (100%)	318 (96%)	10 (3%)	2 (1%)	33	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	327/331 (99%)	315 (96%)	12 (4%)	0	100	100
All	All	1318/1324 (100%)	1264 (96%)	51 (4%)	3 (0%)	56	46

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 ⓘ

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%)	255 (96%)	12 (4%)	38	21
1	B	267/264 (101%)	256 (96%)	11 (4%)	41	25
1	K	266/264 (101%)	254 (96%)	12 (4%)	38	21
1	P	264/264 (100%)	252 (96%)	12 (4%)	38	21
All	All	1064/1056 (101%)	1017 (96%)	47 (4%)	40	22

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	VAL
1	A	196	VAL
1	A	262	LEU
1	A	274	ILE
1	A	298	VAL
1	A	299	SER
1	A	303	LEU
1	A	306	PHE
1	A	314	MET
1	A	359[A]	SER
1	A	359[B]	SER
1	A	362	LEU

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Mol	Chain	Res	Type
1	B	36	ARG
1	B	175	LYS
1	B	299	SER
1	B	306	PHE
1	B	314	MET
1	B	342	PRO
1	B	343	GLN
1	B	344[A]	GLU
1	B	344[B]	GLU
1	B	362	LEU
1	B	363	ARG
1	K	196	VAL
1	K	225	ARG
1	K	260	ILE
1	K	269	SER
1	K	274	ILE
1	K	299	SER
1	K	303	LEU
1	K	306	PHE
1	K	314	MET
1	K	338	GLU
1	K	343	GLN
1	K	363	ARG
1	P	36	ARG
1	P	196	VAL
1	P	262	LEU
1	P	299	SER
1	P	306	PHE
1	P	314	MET
1	P	319	ARG
1	P	337	ARG
1	P	338	GLU
1	P	343	GLN
1	P	344	GLU
1	P	362	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	GLN
1	A	290	GLN
1	B	312	ASN

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Mol	Chain	Res	Type
1	K	212	GLN
1	K	295	GLN
1	K	343	GLN
1	P	343	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	A	169	1,2	11,11,12	5.33	4 (36%)	10,12,14	2.36	3 (30%)
1	KCX	B	169	1,2	11,11,12	4.97	3 (27%)	10,12,14	1.87	3 (30%)
1	KCX	K	169	1,2	11,11,12	5.78	2 (18%)	10,12,14	1.79	2 (20%)
1	KCX	P	169	1,2	11,11,12	5.14	2 (18%)	10,12,14	1.94	2 (20%)

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	A	169	1,2	-	0/8/10/12	0/0/0/0
1	KCX	B	169	1,2	-	0/8/10/12	0/0/0/0
1	KCX	K	169	1,2	-	0/8/10/12	0/0/0/0
1	KCX	P	169	1,2	-	0/8/10/12	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	169	KCX	O-C	18.81	1.24	1.11
1	A	169	KCX	O-C	17.16	1.23	1.11
1	P	169	KCX	O-C	16.79	1.22	1.11
1	B	169	KCX	O-C	16.04	1.22	1.11
1	K	169	KCX	CB-CA	2.50	1.55	1.53
1	A	169	KCX	CB-CA	2.45	1.55	1.53
1	A	169	KCX	CX-NZ	2.31	1.35	1.32
1	B	169	KCX	CB-CA	2.28	1.55	1.53
1	B	169	KCX	OQ1-CX	2.15	1.25	1.21
1	P	169	KCX	OQ1-CX	2.09	1.25	1.21
1	A	169	KCX	OQ1-CX	2.08	1.25	1.21

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	KCX	C-CA-N	-5.55	108.29	113.83
1	K	169	KCX	C-CA-N	-4.89	108.94	113.83
1	P	169	KCX	OQ1-CX-NZ	-4.03	118.23	124.94
1	P	169	KCX	C-CA-N	-3.90	109.93	113.83
1	B	169	KCX	OQ1-CX-NZ	-3.70	118.78	124.94
1	B	169	KCX	C-CA-N	-3.48	110.36	113.83
1	A	169	KCX	OQ1-CX-NZ	-3.38	119.32	124.94
1	A	169	KCX	OQ2-CX-NZ	2.99	120.05	116.33
1	B	169	KCX	OQ2-CX-NZ	2.22	119.10	116.33
1	K	169	KCX	OQ1-CX-NZ	-2.19	121.30	124.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	A	1	2	4,4,4	5.09	4 (100%)	6,6,6	6.47	3 (50%)
3	CAC	B	2	2	4,4,4	3.89	4 (100%)	6,6,6	2.73	3 (50%)
3	CAC	K	3	2	4,4,4	4.58	4 (100%)	6,6,6	8.19	4 (66%)
3	CAC	P	4	2	4,4,4	4.18	4 (100%)	6,6,6	6.63	3 (50%)

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	CAC	A	1	2	-	0/0/0/0	0/0/0/0
3	CAC	B	2	2	-	0/0/0/0	0/0/0/0
3	CAC	K	3	2	-	0/0/0/0	0/0/0/0
3	CAC	P	4	2	-	0/0/0/0	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	CAC	O2-AS	7.55	1.76	1.68
3	K	3	CAC	O2-AS	6.14	1.75	1.68
3	P	4	CAC	O2-AS	5.92	1.75	1.68
3	B	2	CAC	O2-AS	5.41	1.74	1.68
3	A	1	CAC	AS-C1	4.65	1.98	1.90
3	A	1	CAC	AS-C2	4.40	1.98	1.90
3	K	3	CAC	AS-C1	4.34	1.97	1.90
3	K	3	CAC	AS-C2	4.19	1.97	1.90
3	P	4	CAC	AS-C1	4.03	1.97	1.90
3	B	2	CAC	AS-C1	3.57	1.96	1.90
3	B	2	CAC	AS-C2	3.52	1.96	1.90
3	P	4	CAC	AS-C2	3.48	1.96	1.90
3	K	3	CAC	O1-AS	3.12	1.77	1.66
3	P	4	CAC	O1-AS	2.58	1.75	1.66
3	B	2	CAC	O1-AS	2.45	1.74	1.66
3	A	1	CAC	O1-AS	2.40	1.74	1.66

All (13) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	3	CAC	O2-AS-O1	-17.55	108.75	112.54
3	P	4	CAC	O2-AS-O1	-14.72	109.36	112.54
3	A	1	CAC	O2-AS-O1	-11.33	110.09	112.54
3	A	1	CAC	O2-AS-C1	-10.28	100.74	109.15
3	K	3	CAC	O2-AS-C2	6.90	114.80	109.15
3	K	3	CAC	O2-AS-C1	6.30	114.31	109.15
3	P	4	CAC	O2-AS-C1	6.28	114.29	109.15
3	B	2	CAC	O2-AS-C1	5.43	113.60	109.15
3	A	1	CAC	O2-AS-C2	3.64	112.14	109.15
3	B	2	CAC	O2-AS-O1	-2.68	111.96	112.54
3	P	4	CAC	C2-AS-C1	-2.44	103.85	109.43
3	B	2	CAC	C2-AS-C1	-2.27	104.25	109.43
3	K	3	CAC	C2-AS-C1	-2.18	104.46	109.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	331/331 (100%)	-0.32	7 (2%) 60 69	10, 16, 42, 76	0
1	B	330/331 (99%)	-0.30	1 (0%) 91 95	10, 20, 38, 51	2 (0%)
1	K	331/331 (100%)	-0.29	9 (2%) 52 60	10, 16, 41, 78	0
1	P	330/331 (99%)	-0.32	1 (0%) 91 95	11, 20, 38, 53	3 (0%)
All	All	1322/1324 (99%)	-0.31	18 (1%) 74 80	10, 18, 41, 78	5 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	260	ILE	5.3
1	K	262	LEU	4.9
1	A	259	ALA	4.7
1	A	263	GLU	4.7
1	K	261	GLY	3.6
1	K	263	GLU	3.2
1	A	262	LEU	3.2
1	K	259	ALA	3.1
1	K	264	ASP	3.1
1	A	267	SER	3.0
1	A	260	ILE	2.8
1	A	271	LEU	2.8
1	K	268	ALA	2.8
1	P	34	GLY	2.7
1	B	34	GLY	2.6
1	K	235	ASP	2.5
1	K	274	ILE	2.3
1	A	264	ASP	2.3

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

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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	KCX	B	169	12/13	0.09	0.40	9,14,18,18	0
1	KCX	A	169	12/13	0.08	0.07	8,12,16,17	0
1	KCX	K	169	12/13	0.07	-0.24	7,13,14,16	0
1	KCX	P	169	12/13	0.07	-1.17	10,14,16,17	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	CAC	P	4	5/5	0.13	5.20	10,16,20,21	5
2	ZN	P	2407	1/1	0.10	3.45	14,14,14,14	1
3	CAC	K	3	5/5	0.10	2.27	12,12,22,25	5
3	CAC	A	1	5/5	0.10	1.28	12,16,22,24	5
3	CAC	B	2	5/5	0.09	0.33	13,13,21,22	5
2	ZN	K	2405	1/1	0.09	0.30	14,14,14,14	0
2	ZN	K	2406	1/1	0.07	-0.37	18,18,18,18	0
2	ZN	B	2403	1/1	0.06	-0.73	18,18,18,18	0
2	ZN	A	2402	1/1	0.06	-0.98	18,18,18,18	0
2	ZN	B	2404	1/1	0.06	-1.43	22,22,22,22	0
2	ZN	A	2401	1/1	0.06	-1.62	16,16,16,16	0
2	ZN	P	2408	1/1	0.06	-2.67	19,19,19,19	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.