

wwPDB X-ray Structure Validation Summary Report (i)

Aug 23, 2023 - 06:13 AM EDT

PDB ID	:	3CS2
Title	:	Crystal structure of PTE G60A mutant
Authors	:	Kim, J.; Almo, S.C.
Deposited on	:	2008-04-08
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 (i) 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 (1)) were used in the production of this report:

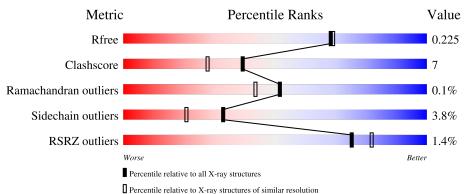
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (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 <=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	А	331	^{2%} 82%	17%	•
1	В	331	86%	12%	•
1	K	331	87%	11%	•
1	Р	331	85%	13%	•



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11352 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	331	Total	С	Ν	Ο	S	0	3	0
1	Л		2548	1609	454	478	7	0	5	0
1	В	330	Total	С	Ν	0	S	0	3	0
1	D	550	2546	1608	453	478	7	0		
1	K	331	Total	С	Ν	0	S	0	2	0
1	Т	991	2542	1606	453	476	7	0	2	0
1	P	330	Total	С	Ν	Ο	S	0	0	0
		330	2525	1597	450	471	$\overline{7}$	0	0	U

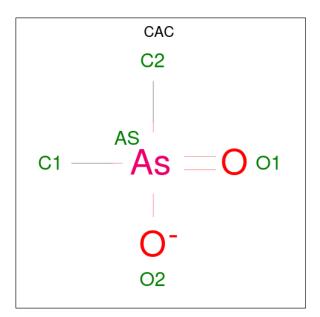
• Molecule 1 is a protein called Parathion hydrolase.

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	60	ALA	GLY	engineered mutation	UNP P0A434
В	60	ALA	GLY	engineered mutation	UNP P0A434
K	60	ALA	GLY	engineered mutation	UNP P0A434
Р	60	ALA	GLY	engineered mutation	UNP P0A434

• Molecule 2 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	А	1	Total 5		С 2	O 2	0	0
2	В	1	Total 5	As 1	C 2	O 2	0	0
2	K	1	Total 5	As 1	С 2	0 2	0	0
2	Р	1	Total 5	As 1	C 2	O 2	0	0

• Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	2	Total Co 2 2	0	0
3	В	2	Total Co 2 2	0	0
3	K	2	Total Co 2 2	0	0
3	Р	2	Total Co 2 2	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	305	Total O 305 305	0	0

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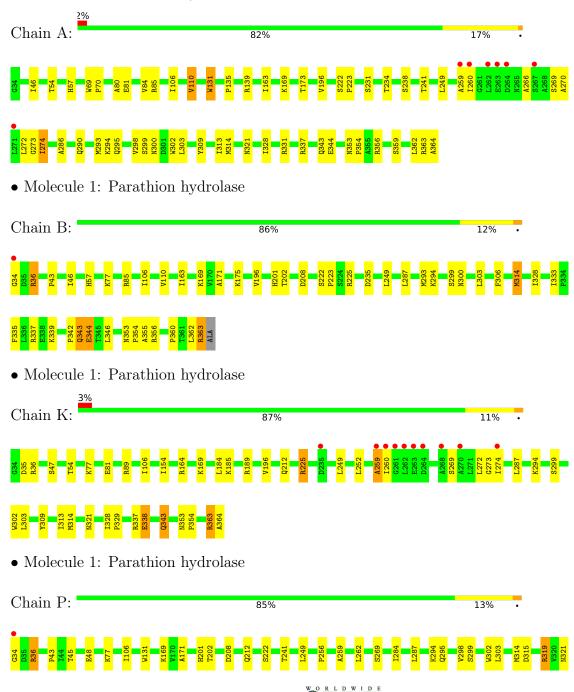
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	276	Total O 276 276	0	0
4	Κ	312	Total O 312 312	0	0
4	Р	270	Total O 270 270	0	0



3 Residue-property plots (i)

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





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Depositor
Resolution (Å)	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	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
$\frac{\mathbf{R}_{sym}}{< I/\sigma(I) > 1}$	(Not available) 2.92 (at 1.95Å)	Depositor Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Depositor DCC
R_{free} test set	4597 reflections (5.02%)	wwPDB-VP
Wilson B-factor $(Å^2)$	19.9	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.35 , 33.8	EDS
L-test for twinning ²	$< L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.467 for -h,k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11352	wwPDB-VP
Average B, all atoms $(Å^2)$	22.0	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.

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.



¹Intensities estimated from amplitudes.

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: CO, CAC, 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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.69	0/2583	0.74	2/3509~(0.1%)	
1	В	0.62	0/2581	0.69	0/3504	
1	Κ	0.68	0/2577	0.77	4/3500~(0.1%)	
1	Р	0.63	0/2560	0.70	1/3476~(0.0%)	
All	All	0.66	0/10301	0.73	7/13989~(0.1%)	

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	K	225	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	K	225	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	K	89	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	А	131	TRP	CA-CB-CG	5.31	123.78	113.70
1	А	356	ARG	NE-CZ-NH2	-5.31	117.65	120.30

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	А	2548	0	2564	46	0
1	В	2546	0	2558	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Κ	2542	0	2559	42	0
1	Р	2525	0	2545	34	0
2	А	5	0	0	0	0
2	В	5	0	0	0	0
2	Κ	5	0	0	0	0
2	Р	5	0	0	0	0
3	А	2	0	0	0	0
3	В	2	0	0	0	0
3	Κ	2	0	0	0	0
3	Р	2	0	0	0	0
4	А	305	0	0	8	0
4	В	276	0	0	4	0
4	Κ	312	0	0	13	0
4	Р	270	0	0	5	0
All	All	11352	0	10226	152	0

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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.

The worst 5 of 152 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:K:259:ALA:HB2	1:K:272:LEU:HB2	1.26	1.11
1:A:259:ALA:HB2	1:A:272:LEU:HB2	1.15	1.10
1:B:337:ARG:NH2	1:B:343:GLN:HG2	1.67	1.08
1:B:337:ARG:HH21	1:B:343:GLN:HG2	0.90	1.05
1:K:225:ARG:HD3	4:K:2451:HOH:O	1.58	1.02

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	Perce	entiles
1	А	331/331~(100%)	317~(96%)	14 (4%)	0	100	100
1	В	330/331~(100%)	316~(96%)	14 (4%)	0	100	100
1	Κ	330/331~(100%)	319~(97%)	10 (3%)	1 (0%)	41	30
1	Р	327/331~(99%)	317~(97%)	10 (3%)	0	100	100
All	All	1318/1324~(100%)	1269~(96%)	48 (4%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Κ	259	ALA

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 Outlier		Percentile		
1	А	267/264~(101%)	260~(97%)	7 (3%)	46	36	
1	В	267/264~(101%)	255~(96%)	12~(4%)	27	15	
1	Κ	266/264~(101%)	258~(97%)	8 (3%)	41	30	
1	Р	264/264~(100%)	250~(95%)	14~(5%)	22	10	
All	All	1064/1056~(101%)	1023~(96%)	41 (4%)	33	19	

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Р	222	SER
1	Р	337	ARG
1	Р	241	THR
1	Р	303	LEU
1	Р	343	GLN

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such side chains are listed below:



Mol	Chain	Res	Type
1	Κ	343	GLN
1	Р	290	GLN
1	Р	343	GLN
1	В	312	ASN
1	Κ	212	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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).

ſ	Mol Type		Mol	Chain Res		Link	B	ond leng	gths	B	Bond ang	gles
	WIOI	туре	Ullaili	Res		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
	1	KCX	Р	169	3,1	9,11,12	0.83	1 (11%)	$5,\!12,\!14$	1.86	1 (20%)	
	1	KCX	K	169	3,1	9,11,12	0.91	0	5,12,14	2.15	1 (20%)	
	1	KCX	В	169	3,1	9,11,12	0.79	0	5,12,14	1.85	1 (20%)	
	1	KCX	А	169	3,1	9,11,12	1.04	1 (11%)	5,12,14	1.72	1 (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	Р	169	3,1	-	0/9/10/12	-
1	KCX	K	169	3,1	-	0/9/10/12	-
1	KCX	В	169	3,1	-	0/9/10/12	-
1	KCX	А	169	3,1	-	0/9/10/12	-

All (2) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
1	А	169	KCX	OQ1-CX	2.40	1.26	1.21
1	Р	169	KCX	OQ1-CX	2.08	1.25	1.21

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	Κ	169	KCX	OQ1-CX-NZ	-4.63	117.78	124.96
1	Р	169	KCX	OQ1-CX-NZ	-3.88	118.94	124.96
1	В	169	KCX	OQ1-CX-NZ	-3.78	119.09	124.96
1	А	169	KCX	OQ1-CX-NZ	-3.10	120.16	124.96

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 monosaccharides 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		
	туре	Chain			Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
2	CAC	А	1	3	0,4,4	-	-	0,6,6	-	-	
2	CAC	K	3	3	0,4,4	-	-	0,6,6	-	-	
2	CAC	В	2	3	0,4,4	-	-	0,6,6	-	-	
2	CAC	Р	4	3	0,4,4	-	-	$0,\!6,\!6$	-	-	

There are no bond length outliers.

There are no bond angle outliers.



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 (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 (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, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	330/331~(99%)	-0.32	7 (2%) 63 72	11, 17, 37, 62	0
1	В	329/331~(99%)	-0.30	1 (0%) 94 96	11, 21, 36, 44	2 (0%)
1	Κ	330/331~(99%)	-0.29	10 (3%) 50 59	11, 17, 37, 64	0
1	Р	329/331~(99%)	-0.33	1 (0%) 94 96	12, 21, 37, 45	3 (0%)
All	All	1318/1324~(99%)	-0.31	19 (1%) 75 82	11, 19, 37, 64	5 (0%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	Κ	260	ILE	6.6
1	Κ	262	LEU	6.0
1	А	263	GLU	5.2
1	А	259	ALA	4.8
1	А	262	LEU	4.4

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, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q < 0.9
1	KCX	В	169	12/13	0.94	0.10	$13,\!16,\!17,\!17$	0
1	KCX	А	169	12/13	0.95	0.08	11,13,16,17	0
1	KCX	Κ	169	12/13	0.97	0.07	12,14,14,15	0
1	KCX	Р	169	12/13	0.98	0.07	13,15,16,16	0



6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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
2	CAC	А	1	5/5	0.99	0.09	17,18,21,23	5
2	CAC	В	2	5/5	0.99	0.08	16,17,21,21	5
2	CAC	K	3	5/5	0.99	0.10	16,17,22,23	5
2	CAC	Р	4	5/5	0.99	0.10	20,22,24,24	5
3	CO	В	4	1/1	0.99	0.05	$17,\!17,\!17,\!17$	0
3	CO	Р	8	1/1	0.99	0.04	$17,\!17,\!17,\!17$	0
3	CO	В	3	1/1	1.00	0.05	14,14,14,14	0
3	CO	А	365	1/1	1.00	0.05	12,12,12,12	0
3	CO	Κ	5	1/1	1.00	0.06	11,11,11,11	0
3	CO	K	6	1/1	1.00	0.07	14,14,14,14	0
3	CO	Р	7	1/1	1.00	0.07	$15,\!15,\!15,\!15$	0
3	CO	А	2	1/1	1.00	0.06	$13,\!13,\!13,\!13$	0

6.5 Other polymers (i)

There are no such residues in this entry.

