



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 14, 2024 – 11:03 PM EST

PDB ID : 2B7P
Title : Crystal structure of quinolinic acid phosphoribosyltransferase from *Helicobacter pylori* with phthalic acid
Authors : Kim, M.K.; Im, Y.J.; Lee, J.H.; Eom, S.H.
Deposited on : 2005-10-05
Resolution : 2.51 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

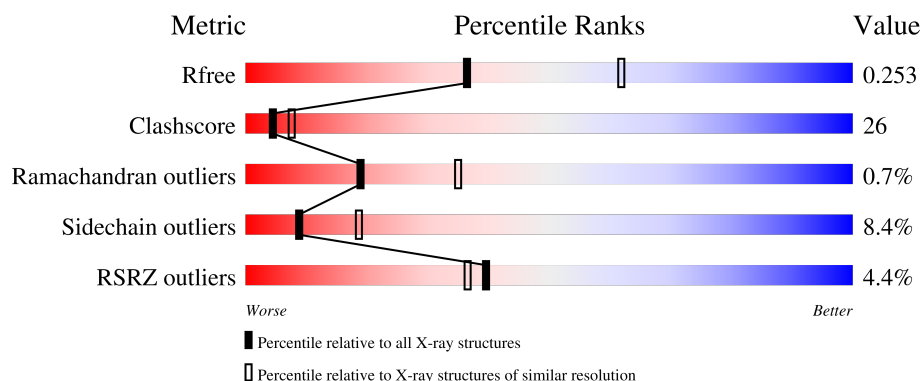
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	273	<div> <div>10%</div> <div>67%</div> <div>29%</div> <div>.</div> </div>
1	B	273	<div> <div>62%</div> <div>33%</div> <div>5%</div> </div>
1	C	273	<div> <div>10%</div> <div>53%</div> <div>38%</div> <div>7%</div> <div>.</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6624 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 Probable nicotinate-nucleotide pyrophosphorylase.

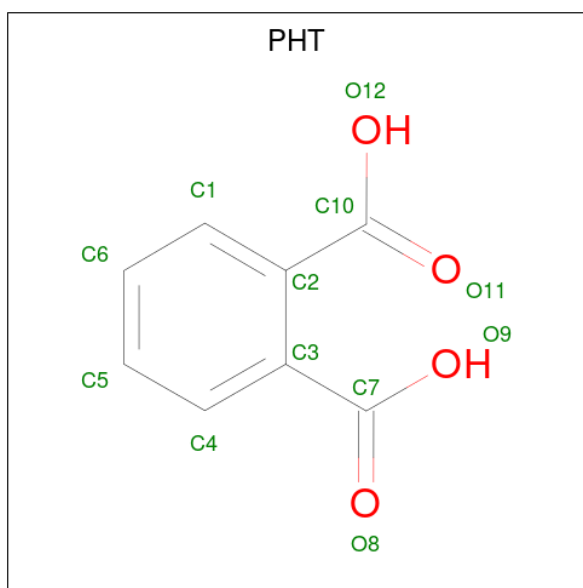
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2161	1368	377	403	13			
1	B	273	Total	C	N	O	S	0	0	0
			2161	1368	377	403	13			
1	C	273	Total	C	N	O	S	0	0	0
			2161	1368	377	403	13			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PHTHALIC ACID (three-letter code: PHT) (formula: $C_8H_6O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	8	4		
3	B	1	Total	C	O	0	0
			12	8	4		
3	C	1	Total	C	O	0	0
			12	8	4		

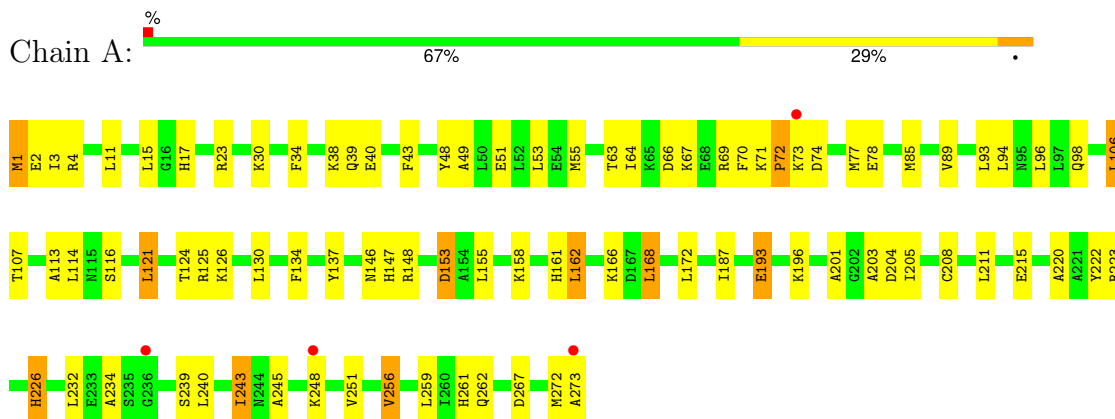
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	0
			43	43		
4	B	30	Total	O	0	0
			30	30		
4	C	17	Total	O	0	0
			17	17		

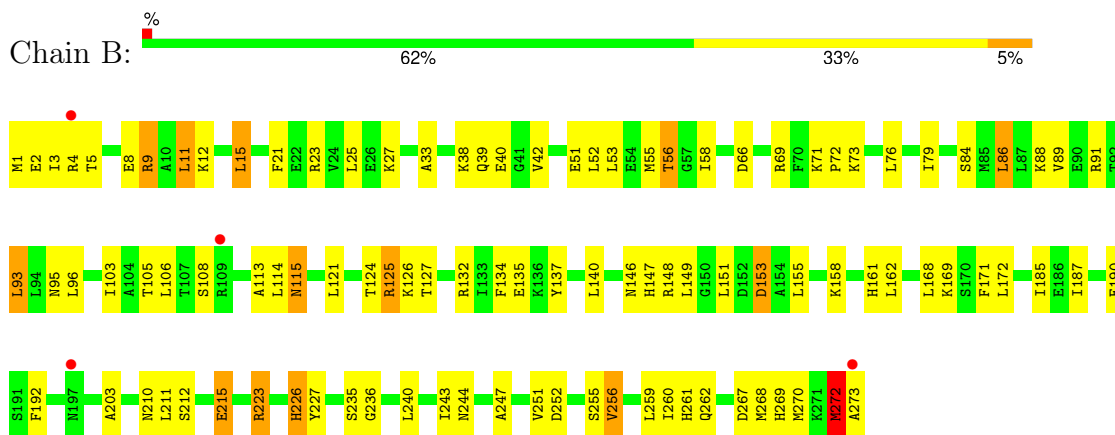
3 Residue-property plots [i](#)

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.

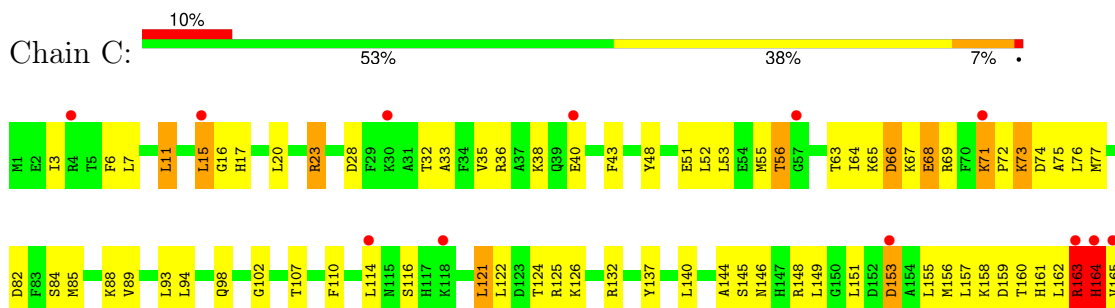
- Molecule 1: Probable nicotinate-nucleotide pyrophosphorylase

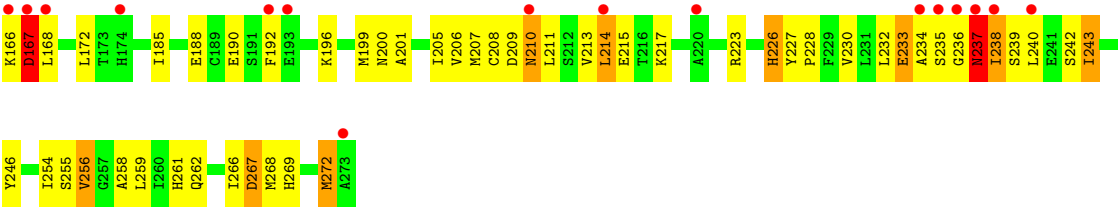


- Molecule 1: Probable nicotinate-nucleotide pyrophosphorylase



- Molecule 1: Probable nicotinate-nucleotide pyrophosphorylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	149.59Å 149.59Å 146.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.51 20.00 – 2.51	Depositor EDS
% Data completeness (in resolution range)	88.4 (20.00-2.51) 93.2 (20.00-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.09 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.260 0.223 , 0.253	Depositor DCC
R_{free} test set	4938 reflections (9.28%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for -h,-l,-k 0.013 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6624	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: PHT, SO4

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	0.45	1/2193 (0.0%)	0.68	1/2942 (0.0%)
1	B	0.40	0/2193	0.68	1/2942 (0.0%)
1	C	1.18	12/2193 (0.5%)	1.25	17/2942 (0.6%)
All	All	0.77	13/6579 (0.2%)	0.91	19/8826 (0.2%)

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	B	0	1
1	C	2	4
All	All	2	5

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	164	HIS	CB-CG	-31.53	0.93	1.50
1	C	237	ASN	C-N	-21.44	0.84	1.34
1	C	237	ASN	C-O	18.05	1.57	1.23
1	C	237	ASN	CB-CG	-12.08	1.23	1.51
1	C	68	GLU	CB-CG	-11.62	1.30	1.52

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	237	ASN	O-C-N	-39.55	59.41	122.70
1	C	237	ASN	CA-C-N	17.44	155.58	117.20
1	C	164	HIS	CB-CA-C	-14.93	80.54	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	164	HIS	CA-CB-CG	13.23	136.09	113.60
1	C	238	ILE	CA-CB-CG1	10.99	131.88	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	237	ASN	CA
1	C	238	ILE	CB

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	272	MET	Mainchain
1	C	163	ARG	Peptide
1	C	167	ASP	Mainchain,Peptide
1	C	237	ASN	Mainchain

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	2161	0	2207	77	0
1	B	2161	0	2207	106	0
1	C	2161	0	2202	170	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
3	A	12	0	4	0	0
3	B	12	0	4	0	0
3	C	12	0	4	0	0
4	A	43	0	0	3	0
4	B	30	0	0	2	0
4	C	17	0	0	1	0
All	All	6624	0	6628	340	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 26.

The worst 5 of 340 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:C:235:SER:CB	1:C:238:ILE:CD1	1.76	1.58
1:C:235:SER:CB	1:C:238:ILE:HD11	1.20	1.55
1:C:235:SER:HB3	1:C:238:ILE:CD1	1.29	1.47
1:C:164:HIS:CB	1:C:164:HIS:CD2	2.02	1.42
1:C:235:SER:OG	1:C:255:SER:O	1.54	1.25

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	271/273 (99%)	256 (94%)	15 (6%)	0	100	100
1	B	271/273 (99%)	249 (92%)	20 (7%)	2 (1%)	19	35
1	C	271/273 (99%)	248 (92%)	19 (7%)	4 (2%)	8	16
All	All	813/819 (99%)	753 (93%)	54 (7%)	6 (1%)	19	35

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	66	ASP
1	C	163	ARG
1	C	272	MET
1	C	73	LYS
1	C	237	ASN

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	233/233 (100%)	215 (92%)	18 (8%)	10	22
1	B	233/233 (100%)	211 (91%)	22 (9%)	7	15
1	C	233/233 (100%)	214 (92%)	19 (8%)	9	19
All	All	699/699 (100%)	640 (92%)	59 (8%)	9	19

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	137	TYR
1	C	237	ASN
1	B	226	HIS
1	C	226	HIS
1	C	164	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	99	HIS
1	C	161	HIS
1	C	146	ASN
1	C	197	ASN
1	B	98	GLN

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

6 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	PHT	B	1002	-	12,12,12	1.80	2 (16%)	16,16,16	1.15	0
3	PHT	A	1001	-	12,12,12	1.82	4 (33%)	16,16,16	1.14	1 (6%)
2	SO4	A	2001	-	4,4,4	0.52	0	6,6,6	1.14	0
3	PHT	C	1003	-	12,12,12	1.78	3 (25%)	16,16,16	1.09	0
2	SO4	B	2002	-	4,4,4	0.43	0	6,6,6	1.13	0
2	SO4	C	2003	-	4,4,4	0.49	0	6,6,6	1.07	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	PHT	B	1002	-	-	4/8/8/8	0/1/1/1
3	PHT	A	1001	-	-	4/8/8/8	0/1/1/1
3	PHT	C	1003	-	-	4/8/8/8	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	PHT	C4-C3	3.65	1.45	1.39
3	C	1003	PHT	C4-C3	3.52	1.45	1.39
3	B	1002	PHT	C4-C3	3.28	1.44	1.39
3	B	1002	PHT	O8-C7	2.93	1.31	1.22
3	C	1003	PHT	O8-C7	2.84	1.31	1.22

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	PHT	C4-C3-C2	-2.00	117.01	119.26

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1003	PHT	O12-C10-C2-C1
3	C	1003	PHT	O11-C10-C2-C1
3	B	1002	PHT	O11-C10-C2-C1
3	B	1002	PHT	O12-C10-C2-C1
3	C	1003	PHT	O11-C10-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2003	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	16:GLY	C	17:HIS	N	1.18
1	C	233:GLU	C	234:ALA	N	1.17
1	C	163:ARG	C	164:HIS	N	1.16
1	C	237:ASN	C	238:ILE	N	0.84

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	273/273 (100%)	-0.16	4 (1%) 71 68	23, 35, 51, 62	0
1	B	273/273 (100%)	-0.00	4 (1%) 71 68	23, 39, 55, 66	0
1	C	273/273 (100%)	0.76	28 (10%) 13 12	33, 51, 77, 93	0
All	All	819/819 (100%)	0.20	36 (4%) 39 36	23, 41, 70, 93	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	235	SER	9.2
1	C	236	GLY	7.7
1	C	234	ALA	7.6
1	B	273	ALA	6.6
1	C	237	ASN	5.4

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 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, 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(\AA^2)	Q<0.9
2	SO4	C	2003	5/5	0.87	0.14	58,60,61,61	0
3	PHT	C	1003	12/12	0.90	0.13	56,62,63,64	0
3	PHT	A	1001	12/12	0.93	0.09	33,34,41,43	0
3	PHT	B	1002	12/12	0.94	0.10	38,39,44,47	0
2	SO4	A	2001	5/5	0.94	0.10	54,55,57,57	0
2	SO4	B	2002	5/5	0.96	0.07	44,46,46,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.