



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 12, 2024 – 04:11 AM EST

PDB ID : 2OTD
Title : The crystal structure of the glycerophosphodiester phosphodiesterase from *Shigella flexneri* 2a
Authors : Zhang, R.; Wu, R.; Clancy, S.; Jiang, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2007-02-07
Resolution : 2.60 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)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

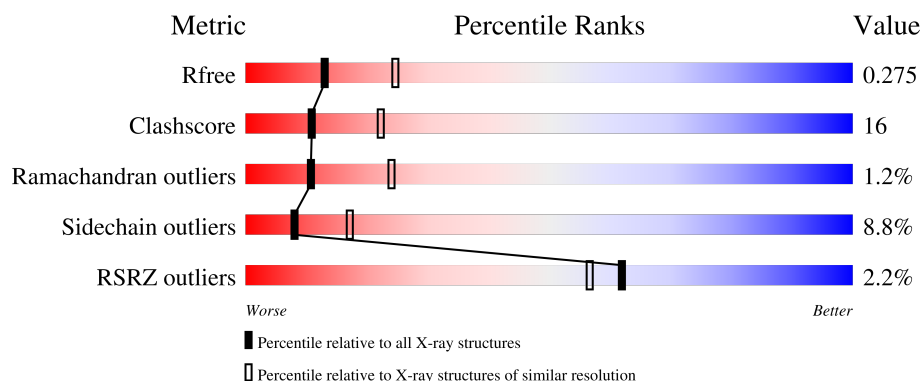
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.60 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	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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	247	 73% 25% ..
1	B	247	 7% 62% 30% 7% .
1	C	247	 72% 24% ..
1	D	247	 72% 24% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7764 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 Glycerophosphodiester phosphodiesterase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	Se	0	0	0
			1903	1208	338	347	4	6			
1	B	245	Total	C	N	O	S	Se	0	0	0
			1903	1208	338	347	4	6			
1	C	245	Total	C	N	O	S	Se	0	0	0
			1903	1208	338	347	4	6			
1	D	245	Total	C	N	O	S	Se	0	0	0
			1903	1208	338	347	4	6			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q83PU8
A	37	MSE	MET	modified residue	UNP Q83PU8
A	109	MSE	MET	modified residue	UNP Q83PU8
A	110	MSE	MET	modified residue	UNP Q83PU8
A	128	MSE	MET	modified residue	UNP Q83PU8
A	140	MSE	MET	modified residue	UNP Q83PU8
A	201	MSE	MET	modified residue	UNP Q83PU8
B	1	MSE	MET	modified residue	UNP Q83PU8
B	37	MSE	MET	modified residue	UNP Q83PU8
B	109	MSE	MET	modified residue	UNP Q83PU8
B	110	MSE	MET	modified residue	UNP Q83PU8
B	128	MSE	MET	modified residue	UNP Q83PU8
B	140	MSE	MET	modified residue	UNP Q83PU8
B	201	MSE	MET	modified residue	UNP Q83PU8
C	1	MSE	MET	modified residue	UNP Q83PU8
C	37	MSE	MET	modified residue	UNP Q83PU8
C	109	MSE	MET	modified residue	UNP Q83PU8
C	110	MSE	MET	modified residue	UNP Q83PU8
C	128	MSE	MET	modified residue	UNP Q83PU8
C	140	MSE	MET	modified residue	UNP Q83PU8
C	201	MSE	MET	modified residue	UNP Q83PU8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MSE	MET	modified residue	UNP Q83PU8
D	37	MSE	MET	modified residue	UNP Q83PU8
D	109	MSE	MET	modified residue	UNP Q83PU8
D	110	MSE	MET	modified residue	UNP Q83PU8
D	128	MSE	MET	modified residue	UNP Q83PU8
D	140	MSE	MET	modified residue	UNP Q83PU8
D	201	MSE	MET	modified residue	UNP Q83PU8

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	41	Total	O	0	0
			41	41		
3	B	21	Total	O	0	0
			21	21		

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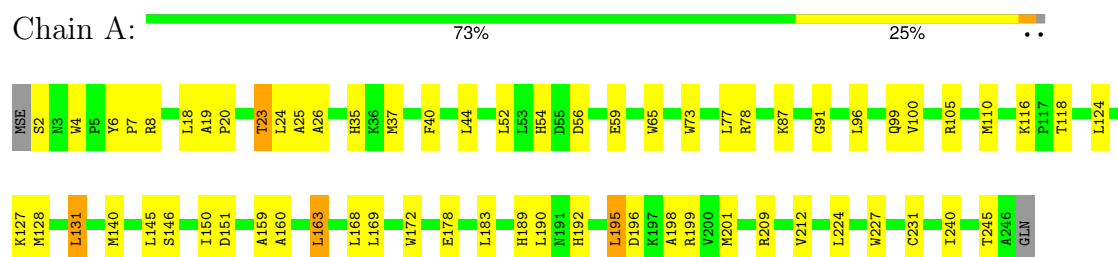
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	43	Total 43	O 43	0	0
3	D	27	Total 27	O 27	0	0

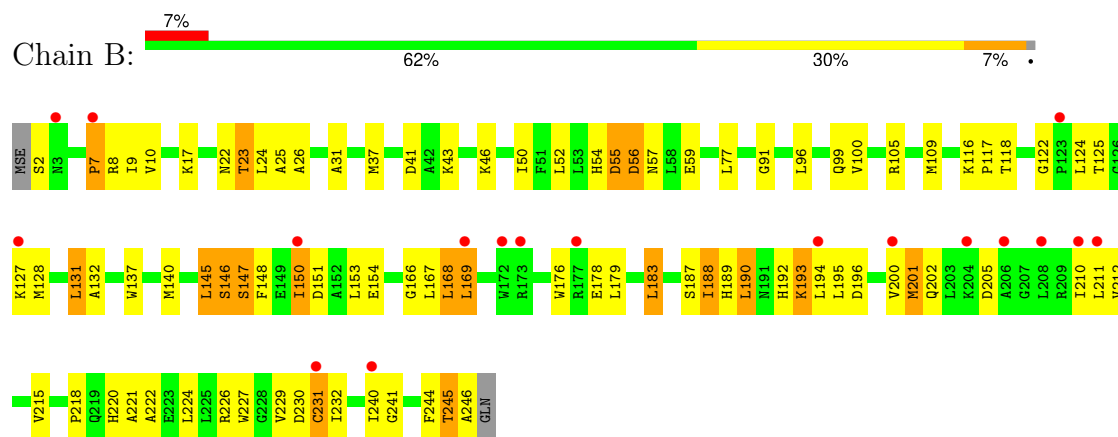
3 Residue-property plots [i](#)

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.

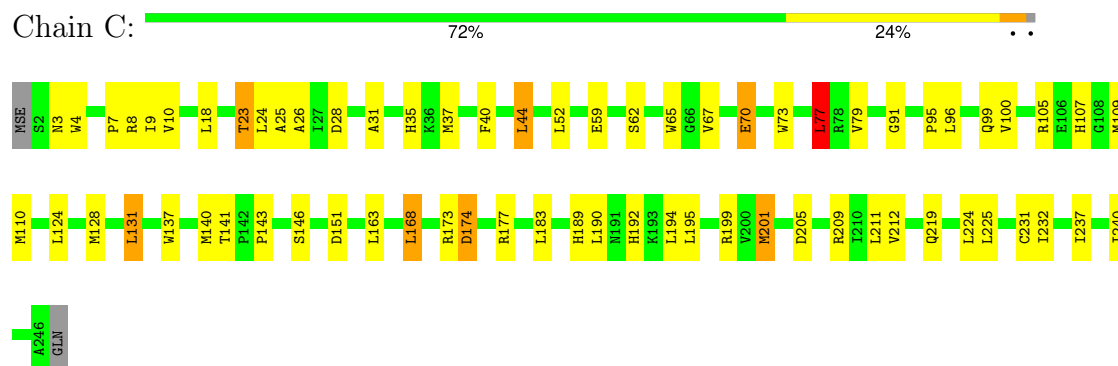
- Molecule 1: Glycerophosphodiester phosphodiesterase



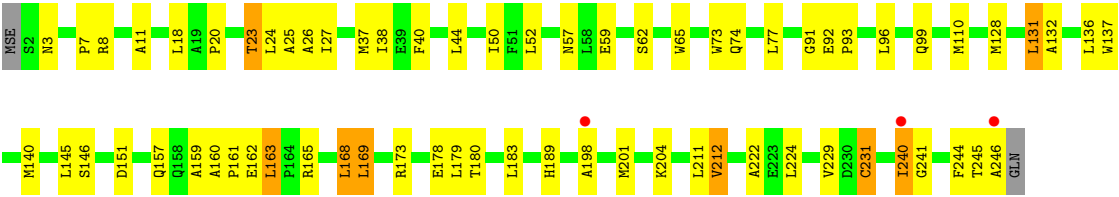
- Molecule 1: Glycerophosphodiester phosphodiesterase



- Molecule 1: Glycerophosphodiester phosphodiesterase



- Molecule 1: Glycerophosphodiester phosphodiesterase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.62Å 82.19Å 223.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.06 – 2.60 40.06 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.06-2.60) 99.7 (40.06-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.221 , 0.276 0.224 , 0.275	Depositor DCC
R_{free} test set	2366 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7764	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: 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	0.66	0/1941	0.79	0/2626
1	B	0.60	0/1941	0.69	1/2626 (0.0%)
1	C	0.77	2/1941 (0.1%)	0.81	1/2626 (0.0%)
1	D	0.64	1/1941 (0.1%)	0.72	0/2626
All	All	0.67	3/7764 (0.0%)	0.75	2/10504 (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	1
1	B	0	1
1	C	0	1
1	D	0	2
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	70	GLU	CG-CD	6.04	1.61	1.51
1	D	231	CYS	CB-SG	-5.60	1.72	1.81
1	C	231	CYS	CB-SG	-5.17	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	LEU	CA-CB-CG	5.24	127.34	115.30
1	C	131	LEU	CA-CB-CG	5.13	127.09	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	91	GLY	Peptide
1	B	91	GLY	Peptide
1	C	91	GLY	Peptide
1	D	240	ILE	Peptide
1	D	91	GLY	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	1903	0	1901	46	0
1	B	1903	0	1901	94	0
1	C	1903	0	1901	65	0
1	D	1903	0	1901	56	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	41	0	0	2	0
3	B	21	0	0	4	0
3	C	43	0	0	5	0
3	D	27	0	0	4	0
All	All	7764	0	7604	248	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 16.

The worst 5 of 248 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:124:LEU:HD11	1:D:128:MSE:CE	1.74	1.16
1:C:110:MSE:CE	1:C:141:THR:HG21	1.82	1.09
1:B:188:ILE:HG23	1:B:190:LEU:HD11	1.36	1.08
1:C:124:LEU:HD11	1:D:128:MSE:HE1	1.37	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ILE:HD12	1:B:150:ILE:H	1.24	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	Percentiles	
1	A	243/247 (98%)	234 (96%)	7 (3%)	2 (1%)	16	34
1	B	243/247 (98%)	220 (90%)	17 (7%)	6 (2%)	4	8
1	C	243/247 (98%)	231 (95%)	8 (3%)	4 (2%)	8	17
1	D	243/247 (98%)	233 (96%)	10 (4%)	0	100	100
All	All	972/988 (98%)	918 (94%)	42 (4%)	12 (1%)	11	24

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	7	PRO
1	B	55	ASP
1	C	240	ILE
1	C	77	LEU
1	A	151	ASP

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	197/192 (103%)	183 (93%)	14 (7%)	12	26
1	B	197/192 (103%)	175 (89%)	22 (11%)	5	9
1	C	197/192 (103%)	183 (93%)	14 (7%)	12	26
1	D	197/192 (103%)	178 (90%)	19 (10%)	7	14
All	All	788/768 (103%)	719 (91%)	69 (9%)	8	17

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	151	ASP
1	D	168	LEU
1	D	212	VAL
1	B	168	LEU
1	B	150	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	220	HIS
1	D	99	GLN
1	D	135	GLN
1	D	35	HIS
1	B	99	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](#)

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](#)

4 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	$\# Z > 2$
2	PO4	D	301	-	4,4,4	0.61	0	6,6,6	1.32	0
2	PO4	C	301	-	4,4,4	1.01	0	6,6,6	0.31	0
2	PO4	A	301	-	4,4,4	0.93	0	6,6,6	0.76	0
2	PO4	B	301	-	4,4,4	0.85	0	6,6,6	0.41	0

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, 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	239/247 (96%)	-0.50	0 100 100	15, 23, 37, 45	0
1	B	239/247 (96%)	0.67	18 (7%) 22 17	9, 46, 72, 79	0
1	C	239/247 (96%)	-0.76	0 100 100	8, 17, 27, 33	0
1	D	239/247 (96%)	-0.22	3 (1%) 74 70	18, 36, 54, 58	0
All	All	956/988 (96%)	-0.20	21 (2%) 62 57	8, 25, 61, 79	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	208	LEU	3.8
1	B	200	VAL	3.8
1	B	240	ILE	3.5
1	D	246	ALA	2.9
1	B	172	TRP	2.8

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	PO4	B	301	5/5	0.66	0.20	109,109,110,111	0
2	PO4	A	301	5/5	0.69	0.29	101,101,101,102	0
2	PO4	D	301	5/5	0.79	0.23	75,79,81,82	0
2	PO4	C	301	5/5	0.80	0.26	94,97,97,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.