wwPDB X-ray Structure Validation Summary Report (i)

Jan 27, 2024 – 11:51 AM EST

PDB ID	:	1BRL
Title	:	THREE-DIMENSIONAL STRUCTURE OF BACTERIAL LUCIFERASE FROM VIBRIO HARVEYI AT 2.4 ANGSTROMS RESOLUTION
Authors	:	Fisher, A.J.; Rayment, I.
Deposited on	:	1995-03-20
Resolution	:	2.40 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 (i)) were used in the production of this report:

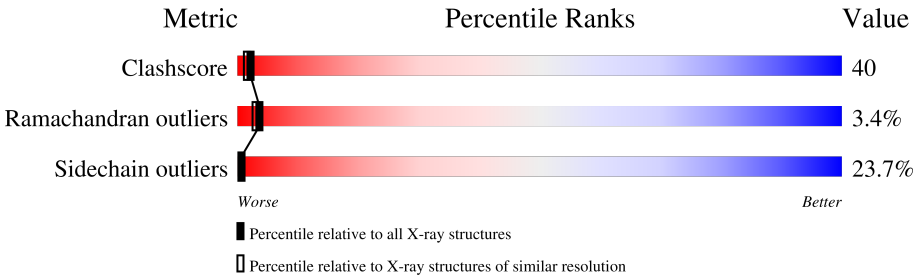
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	355	28% 43% 21%
1	C	355	29% 42% 21%
2	B	324	37% 43% 16%
2	D	324	38% 41% 17%

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	PO4	A	356	-	X	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10432 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.

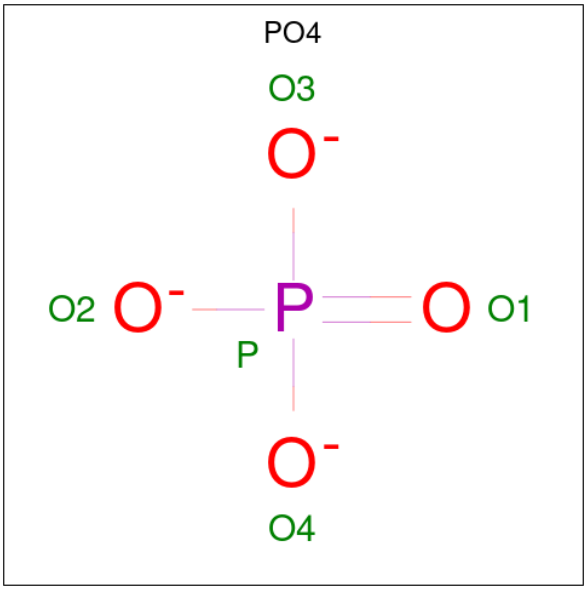
- Molecule 1 is a protein called BACTERIAL LUCIFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2679	1694	447	521	17			
1	C	340	Total	C	N	O	S	0	0	0
			2679	1694	447	521	17			

- Molecule 2 is a protein called BACTERIAL LUCIFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	319	Total	C	N	O	S	0	0	0
			2498	1572	427	484	15			
2	D	319	Total	C	N	O	S	0	0	0
			2498	1572	427	484	15			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	28	Total O 28 28	0	0
4	B	45	Total O 45 45	0	0

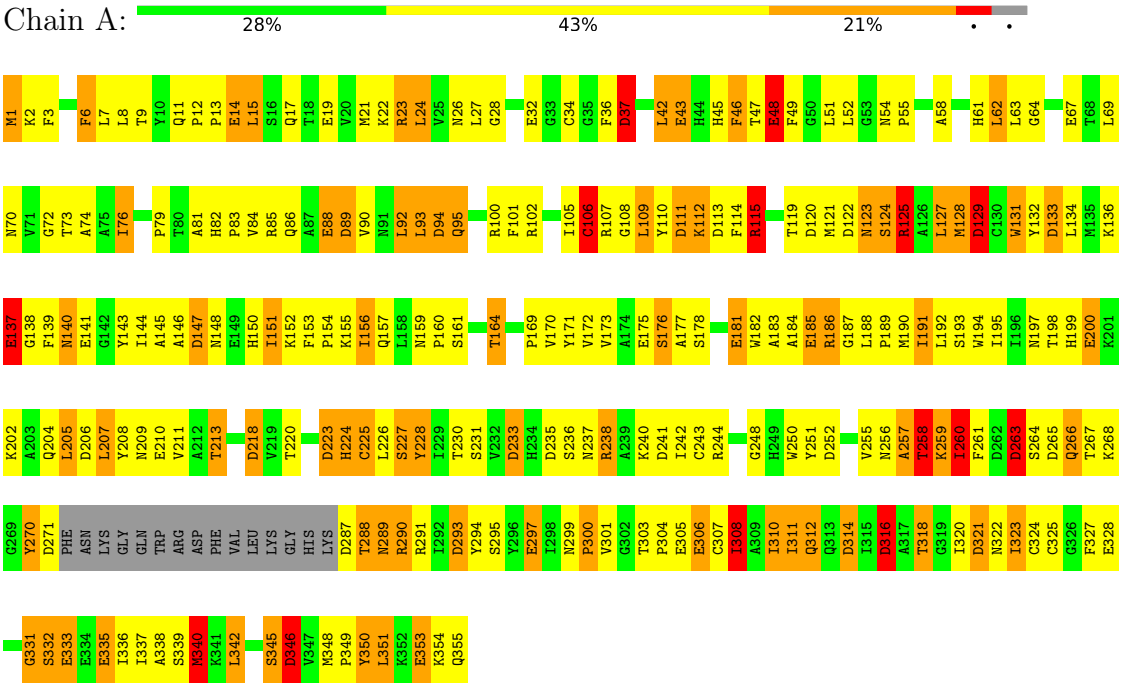
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

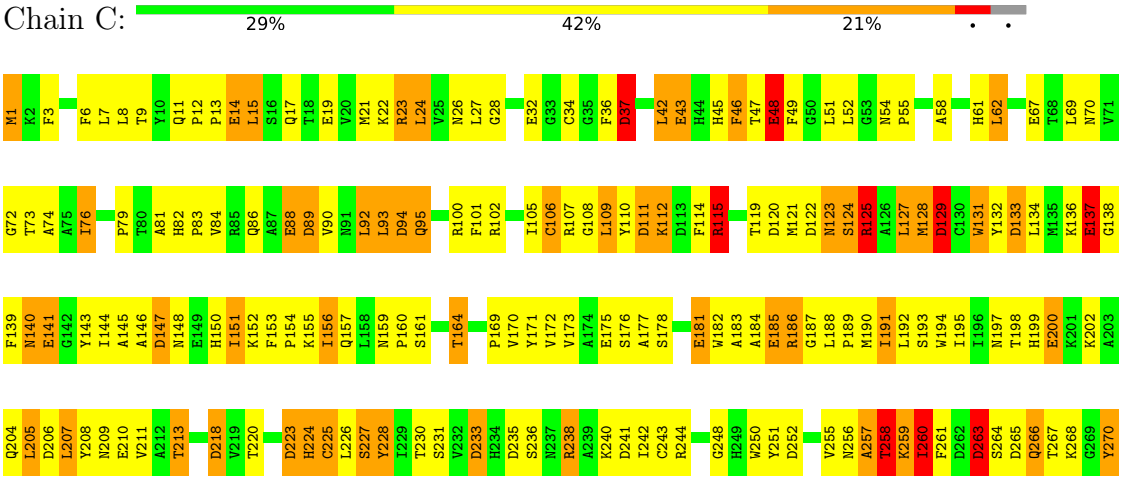
• Molecule 1: BACTERIAL LUCIFERASE

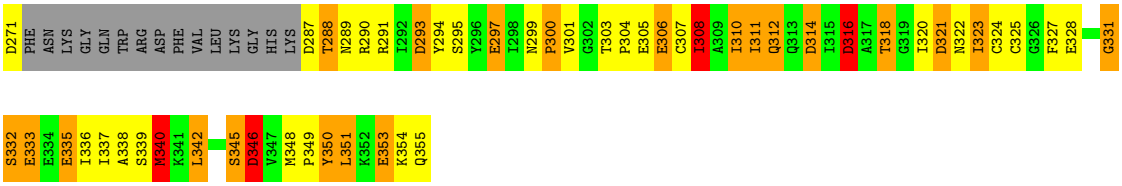
Chain A:



• Molecule 1: BACTERIAL LUCIFERASE

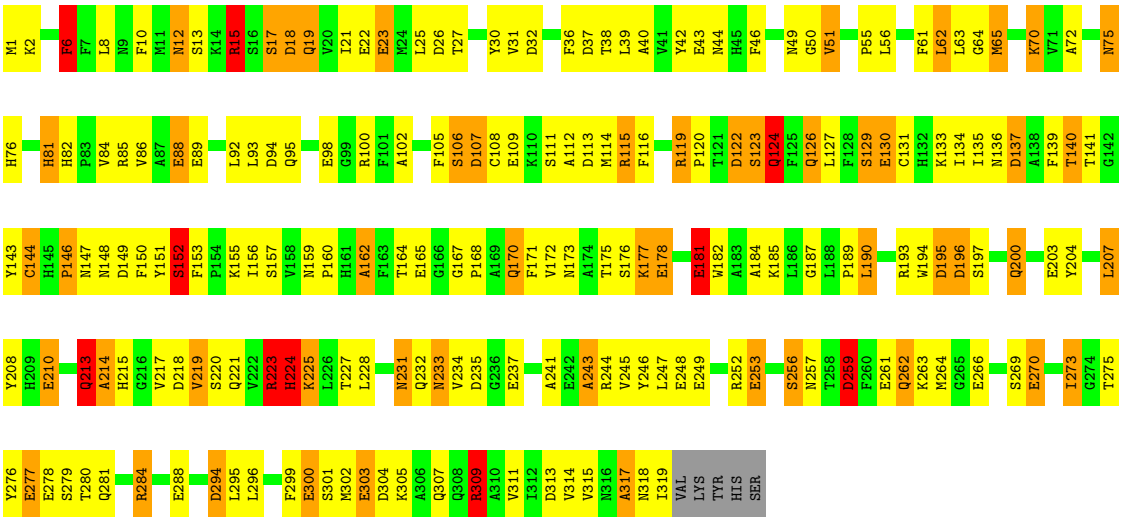
Chain C:





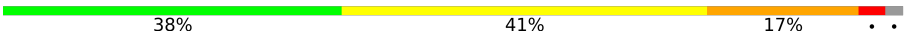
• Molecule 2: BACTERIAL LUCIFERASE

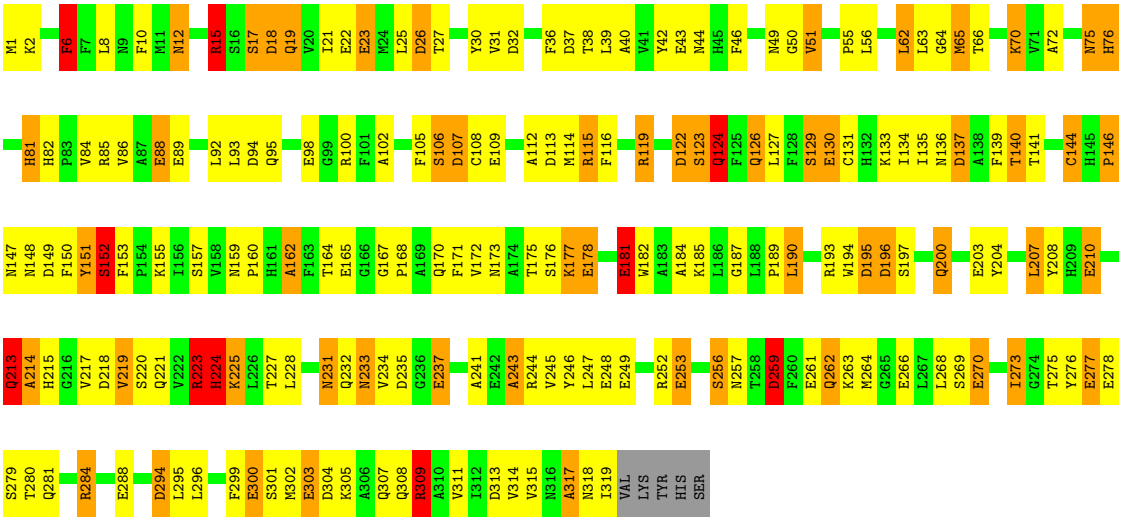
Chain B:



• Molecule 2: BACTERIAL LUCIFERASE

Chain D:





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.90Å 112.70Å 301.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.40)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.208 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10432	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.12	22/2740 (0.8%)	1.63	52/3716 (1.4%)
1	C	1.12	22/2740 (0.8%)	1.63	51/3716 (1.4%)
2	B	1.12	22/2552 (0.9%)	1.62	44/3457 (1.3%)
2	D	1.12	22/2552 (0.9%)	1.62	45/3457 (1.3%)
All	All	1.12	88/10584 (0.8%)	1.62	192/14346 (1.3%)

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
2	B	2	0
2	D	2	0
All	All	4	0

The worst 5 of 88 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	200	GLU	CD-OE1	7.93	1.34	1.25
1	A	200	GLU	CD-OE1	7.90	1.34	1.25
1	C	48	GLU	CD-OE1	7.78	1.34	1.25
1	A	48	GLU	CD-OE1	7.76	1.34	1.25
1	A	32	GLU	CD-OE2	7.39	1.33	1.25

The worst 5 of 192 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	294	ASP	CB-CG-OD1	-10.15	109.16	118.30
2	D	294	ASP	CB-CG-OD1	-10.13	109.18	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	252	ASP	CB-CG-OD1	-8.74	110.43	118.30
1	C	252	ASP	CB-CG-OD1	-8.72	110.45	118.30
2	B	313	ASP	CB-CG-OD1	-8.54	110.61	118.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	284	ARG	CA
2	B	317	ALA	CA
2	D	284	ARG	CA
2	D	317	ALA	CA

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	A	2679	0	2552	252	2
1	C	2679	0	2552	244	15
2	B	2498	0	2362	165	0
2	D	2498	0	2362	161	11
3	A	5	0	0	2	0
4	A	28	0	0	3	0
4	B	45	0	0	1	2
All	All	10432	0	9828	799	15

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 40.

The worst 5 of 799 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:266:GLN:HG3	1:A:268:LYS:HB3	1.50	0.94
1:C:266:GLN:HG3	1:C:268:LYS:HB3	1.50	0.94
2:D:181:GLU:HG3	2:D:182:TRP:H	1.33	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:CYS:HB2	1:A:173:VAL:HG22	1.51	0.92
1:C:106:CYS:HB2	1:C:173:VAL:HG22	1.51	0.91

The worst 5 of 15 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:SER:O	2:D:237:GLU:CD[4_467]	0.67	1.53
1:C:345:SER:O	2:D:237:GLU:OE2[4_467]	0.78	1.42
1:C:141:GLU:OE2	2:D:26:ASP:OD2[4_567]	1.08	1.12
1:A:237:ASN:ND2	1:C:291:ARG:CB[2_464]	1.10	1.10
1:C:345:SER:C	2:D:237:GLU:OE2[4_467]	1.38	0.82

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	336/355 (95%)	288 (86%)	36 (11%)	12 (4%)	3	3
1	C	336/355 (95%)	288 (86%)	36 (11%)	12 (4%)	3	3
2	B	317/324 (98%)	265 (84%)	42 (13%)	10 (3%)	4	3
2	D	317/324 (98%)	265 (84%)	42 (13%)	10 (3%)	4	3
All	All	1306/1358 (96%)	1106 (85%)	156 (12%)	44 (3%)	3	3

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	ASP
1	A	257	ALA
1	A	260	ILE
1	A	263	ASP
1	A	270	TYR

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	286/303 (94%)	214 (75%)	72 (25%)	0	0
1	C	286/303 (94%)	215 (75%)	71 (25%)	0	0
2	B	265/274 (97%)	206 (78%)	59 (22%)	1	1
2	D	265/274 (97%)	206 (78%)	59 (22%)	1	1
All	All	1102/1154 (96%)	841 (76%)	261 (24%)	1	1

5 of 261 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	181	GLU
2	D	224	HIS
2	D	319	ILE
2	B	157	SER
2	B	144	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	308	GLN
2	D	233	ASN
1	C	95	GLN
2	D	232	GLN
2	D	145	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	PO4	A	356	-	4,4,4	2.71	4 (100%)	6,6,6	0.61	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	356	PO4	P-O2	-3.00	1.45	1.54
3	A	356	PO4	P-O4	-2.99	1.45	1.54
3	A	356	PO4	P-O3	-2.65	1.46	1.54
3	A	356	PO4	P-O1	-2.11	1.45	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	356	PO4	2	0

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.