



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:07 PM GMT

PDB ID : 1KYV  
Title : Lumazine Synthase from *S.pombe* bound to riboflavin  
Authors : Gerhardt, S.; Haase, I.; Steinbacher, S.; Kaiser, J.T.; Cushman, M.; Bacher, A.; Huber, R.; Fischer, M.  
Deposited on : 2002-02-06  
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

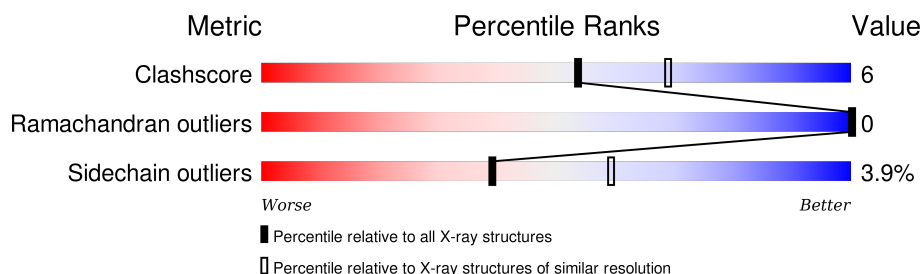
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	159	
1	B	159	
1	C	159	
1	D	159	
1	E	159	

## 2 Entry composition [i](#)

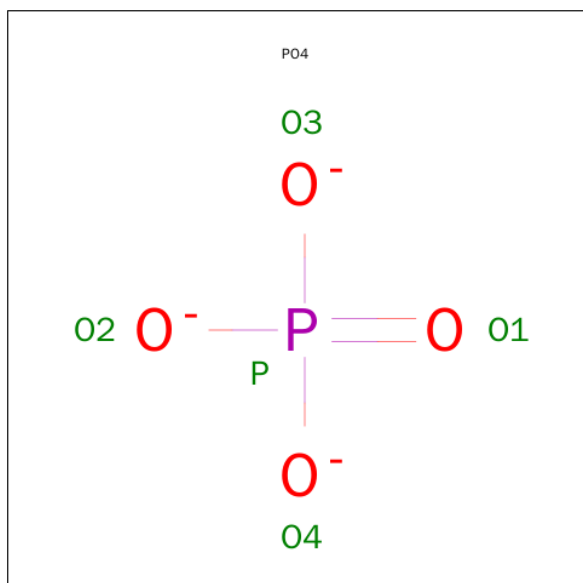
There are 4 unique types of molecules in this entry. The entry contains 5949 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 6,7-Dimethyl-8-ribityllumazine Synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	11	1	0
			1129	718	199	208	4			
1	B	147	Total	C	N	O	S	20	1	0
			1129	718	199	208	4			
1	C	149	Total	C	N	O	S	10	1	0
			1147	730	201	212	4			
1	D	147	Total	C	N	O	S	11	1	0
			1129	718	199	208	4			
1	E	152	Total	C	N	O	S	16	1	0
			1161	737	205	215	4			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



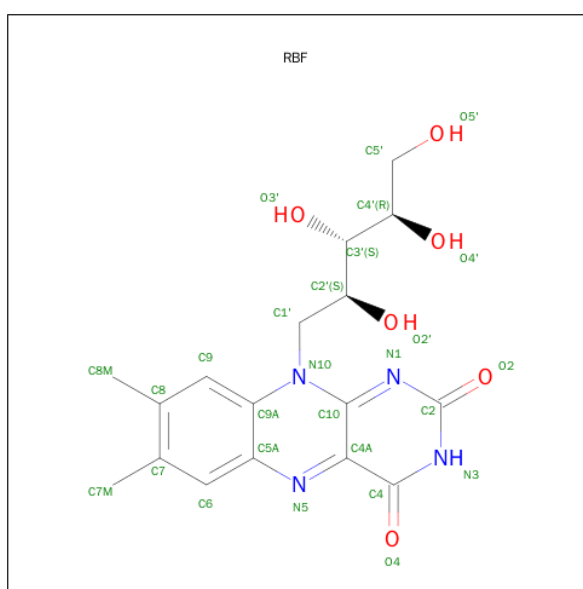
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		

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

- Molecule 3 is RIBOFLAVIN (three-letter code: RBF) (formula:  $C_{17}H_{20}N_4O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			27	17	4	6		
3	B	1	Total	C	N	O	0	0
			27	17	4	6		
3	C	1	Total	C	N	O	0	0
			27	17	4	6		
3	D	1	Total	C	N	O	0	0
			27	17	4	6		
3	E	1	Total	C	N	O	0	0
			27	17	4	6		

- Molecule 4 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total 23	O 23	0	0
4	B	16	Total 16	O 16	0	0
4	C	21	Total 21	O 21	0	0
4	D	16	Total 16	O 16	0	0
4	E	18	Total 18	O 18	0	0

### 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.

Note EDS was not executed.

- Molecule 1: 6,7-Dimethyl-8-ribityllumazine Synthase

Chain A: 




- Molecule 1: 6,7-Dimethyl-8-ribityllumazine Synthase

Chain B: 




TYR

- Molecule 1: 6,7-Dimethyl-8-ribityllumazine Synthase

Chain C: 




- Molecule 1: 6,7-Dimethyl-8-ribityllumazine Synthase

Chain D: 



- Molecule 1: 6,7-Dimethyl-8-ribityllumazine Synthase

Chain E: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.50Å 145.52Å 128.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.03 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (16.03-2.40)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.180 , 0.213	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5949	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

## 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: RBF, 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	0.51	0/1150	0.70	0/1560
1	B	0.52	0/1150	0.75	2/1560 (0.1%)
1	C	0.53	0/1169	0.76	2/1586 (0.1%)
1	D	0.49	0/1150	0.66	0/1560
1	E	0.50	0/1184	0.68	0/1608
All	All	0.51	0/5803	0.71	4/7874 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	26	ARG	NE-CZ-NH2	-7.71	116.45	120.30
1	B	26	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	C	158	LEU	CA-CB-CG	-6.12	101.22	115.30
1	C	158	LEU	CA-C-N	-5.65	104.76	117.20

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	A	1129	0	1143	15	0
1	B	1129	0	1143	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1147	0	1157	18	0
1	D	1129	0	1143	8	0
1	E	1161	0	1171	11	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
3	A	27	0	20	2	0
3	B	27	0	19	5	0
3	C	27	0	19	5	0
3	D	27	0	19	2	0
3	E	27	0	19	1	0
4	A	23	0	0	0	0
4	B	16	0	0	1	0
4	C	21	0	0	1	0
4	D	16	0	0	0	0
4	E	18	0	0	0	0
All	All	5949	0	5853	75	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 6.

All (75) 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:158:LEU:HD22	1:C:159:TYR:H	1.05	1.10
1:C:158:LEU:HD22	1:C:159:TYR:N	1.72	1.01
1:B:67:GLN:HG3	4:B:1015:HOH:O	1.65	0.95
1:C:158:LEU:HD13	1:C:158:LEU:C	1.91	0.91
1:D:157:ALA:O	1:D:158:LEU:HB2	1.74	0.87
1:B:15:GLY:HA3	1:B:18:LEU:HD12	1.61	0.81
1:B:157:ALA:O	1:B:158:LEU:HB2	1.80	0.80
1:E:157:ALA:O	1:E:158:LEU:HB2	1.80	0.79
1:A:152:GLU:OE2	1:B:26:ARG:NH2	2.16	0.77
1:A:157:ALA:O	1:A:158:LEU:HB2	1.84	0.76
1:C:158:LEU:HD13	1:C:159:TYR:N	2.09	0.68
1:C:158:LEU:CD2	1:C:159:TYR:N	2.53	0.68
1:A:142:HIS:HD2	3:B:502:RBF:HC82	1.59	0.68
1:B:15:GLY:CA	1:B:18:LEU:HD12	2.24	0.68
1:C:158:LEU:CD1	1:C:158:LEU:C	2.62	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:GLY:HA3	1:B:18:LEU:CD1	2.25	0.66
1:A:142:HIS:CD2	3:B:502:RBF:HC82	2.32	0.65
1:B:63:TRP:HB3	3:B:502:RBF:HC3'	1.80	0.62
1:D:12:ASP:N	1:D:12:ASP:OD2	2.34	0.61
1:A:152:GLU:CD	1:B:26:ARG:HH22	2.04	0.58
1:C:157:ALA:O	1:C:158:LEU:HB2	2.05	0.57
1:A:157:ALA:O	1:A:158:LEU:CB	2.52	0.57
1:B:142:HIS:CD2	3:C:503:RBF:HC82	2.39	0.56
1:B:142:HIS:HD2	3:C:503:RBF:HC82	1.71	0.55
1:E:33:GLU:HB2	1:E:34:PRO:HD3	1.88	0.55
1:C:87:LEU:HD21	1:C:98:ILE:HD11	1.89	0.55
1:D:51:LEU:HD23	1:D:51:LEU:O	2.07	0.55
1:D:89:LYS:HE3	1:D:90:GLY:O	2.07	0.54
1:B:157:ALA:O	1:B:158:LEU:CB	2.53	0.54
1:D:157:ALA:O	1:D:158:LEU:CB	2.51	0.53
1:B:31:ALA:O	1:B:34:PRO:HD2	2.08	0.53
1:C:31:ALA:O	1:C:34:PRO:HD2	2.09	0.53
1:E:11:SER:OG	1:E:13:LEU:HD12	2.09	0.53
1:C:33:GLU:HB2	1:C:34:PRO:HD3	1.91	0.52
1:C:142:HIS:HD2	3:D:504:RBF:HC82	1.75	0.52
1:E:157:ALA:O	1:E:158:LEU:CB	2.53	0.52
1:A:31:ALA:O	1:A:34:PRO:HD2	2.09	0.52
1:A:63:TRP:HB3	3:A:501:RBF:HC3'	1.92	0.52
1:B:18:LEU:HD11	1:B:155:LEU:CD2	2.41	0.51
1:B:119:LEU:O	3:C:503:RBF:HC51	2.11	0.51
1:B:12:ASP:OD2	1:B:12:ASP:N	2.43	0.51
1:D:33:GLU:HB2	1:D:34:PRO:HD3	1.92	0.50
1:C:89:LYS:HE3	1:C:90:GLY:O	2.12	0.50
1:B:33:GLU:HB2	1:B:34:PRO:HD3	1.92	0.50
1:C:158:LEU:HD13	1:C:158:LEU:O	2.11	0.49
1:E:89:LYS:HE3	1:E:90:GLY:O	2.12	0.48
1:E:51:LEU:O	1:E:51:LEU:HD23	2.13	0.48
3:C:503:RBF:HC72	4:C:1024:HOH:O	2.13	0.47
1:E:87:LEU:HD21	1:E:98:ILE:HD11	1.95	0.47
1:C:24:HIS:O	1:C:58:SER:HA	2.14	0.47
1:C:158:LEU:CD1	1:C:159:TYR:N	2.78	0.46
1:A:84:ILE:HA	1:A:120:GLY:O	2.15	0.46
1:B:119:LEU:HB3	3:C:503:RBF:HC52	1.98	0.46
1:C:158:LEU:O	1:C:159:TYR:CD2	2.70	0.45
1:D:103:VAL:HG12	1:E:101:ALA:HB2	1.98	0.45
1:D:87:LEU:HD21	1:D:98:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ASP:OD2	1:A:12:ASP:N	2.51	0.44
1:A:33:GLU:HB2	1:A:34:PRO:HD3	1.99	0.44
1:B:66:PRO:HG3	1:B:106:LEU:HD13	1.99	0.44
1:A:89:LYS:HE3	1:A:90:GLY:O	2.18	0.44
1:C:142:HIS:CD2	3:D:504:RBF:HC82	2.52	0.43
1:B:24:HIS:HA	1:B:84:ILE:O	2.17	0.43
1:A:119:LEU:O	3:B:502:RBF:HC52	2.19	0.42
2:A:1004:PO4:O1	3:A:501:RBF:HC6	2.19	0.42
1:B:18:LEU:HD23	1:B:79:ASP:CB	2.50	0.42
1:C:158:LEU:O	1:C:159:TYR:CG	2.73	0.41
1:B:37:LYS:HG2	1:B:41:GLU:OE2	2.19	0.41
1:B:87:LEU:HD23	3:B:502:RBF:N3	2.36	0.41
1:E:31:ALA:O	1:E:34:PRO:HD2	2.20	0.41
1:A:103:VAL:HG12	1:B:101:ALA:HB2	2.03	0.41
1:B:18:LEU:HD11	1:B:155:LEU:HD21	2.03	0.41
1:B:24:HIS:O	1:B:58:SER:HA	2.21	0.41
1:E:87:LEU:HD23	3:E:505:RBF:C4	2.51	0.40
1:E:37:LYS:HG2	1:E:41:GLU:OE2	2.21	0.40
1:A:87:LEU:HD21	1:A:98:ILE:HD11	2.02	0.40

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	146/159 (92%)	143 (98%)	3 (2%)	0	100	100
1	B	146/159 (92%)	143 (98%)	3 (2%)	0	100	100
1	C	148/159 (93%)	144 (97%)	4 (3%)	0	100	100
1	D	146/159 (92%)	143 (98%)	3 (2%)	0	100	100
1	E	151/159 (95%)	148 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	737/795 (93%)	721 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	119/128 (93%)	114 (96%)	5 (4%)	36	56
1	B	119/128 (93%)	112 (94%)	7 (6%)	24	38
1	C	121/128 (94%)	118 (98%)	3 (2%)	55	76
1	D	119/128 (93%)	114 (96%)	5 (4%)	36	56
1	E	123/128 (96%)	120 (98%)	3 (2%)	57	76
All	All	601/640 (94%)	578 (96%)	23 (4%)	39	60

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	70	ARG
1	A	98	ILE
1	A	136	LEU
1	A	158	LEU
1	B	12	ASP
1	B	18	LEU
1	B	51	LEU
1	B	65	LEU
1	B	106	LEU
1	B	136	LEU
1	B	158	LEU
1	C	65	LEU
1	C	70	ARG
1	C	127	GLU
1	D	12	ASP

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Mol	Chain	Res	Type
1	D	65	LEU
1	D	70	ARG
1	D	136	LEU
1	D	158	LEU
1	E	70	ARG
1	E	136	LEU
1	E	158	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	142	HIS
1	A	144	ASN
1	B	53	ASN
1	B	142	HIS
1	C	47	HIS
1	C	142	HIS
1	C	144	ASN
1	D	28	ASN
1	D	47	HIS
1	D	53	ASN
1	D	144	ASN
1	E	144	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

10 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	A	1004	-	4,4,4	1.46	0	6,6,6	0.23	0
3	RBF	A	501	-	28,29,29	2.62	12 (42%)	30,43,43	4.16	13 (43%)
2	PO4	B	1001	-	4,4,4	1.58	0	6,6,6	0.23	0
3	RBF	B	502	-	28,29,29	2.69	11 (39%)	30,43,43	4.33	14 (46%)
2	PO4	C	1003	-	4,4,4	1.52	0	6,6,6	0.23	0
3	RBF	C	503	-	28,29,29	2.81	11 (39%)	30,43,43	4.65	15 (50%)
2	PO4	D	1005	-	4,4,4	1.50	0	6,6,6	0.23	0
3	RBF	D	504	-	28,29,29	2.70	11 (39%)	30,43,43	4.23	13 (43%)
2	PO4	E	1002	-	4,4,4	1.53	0	6,6,6	0.23	0
3	RBF	E	505	-	28,29,29	2.86	12 (42%)	30,43,43	4.31	14 (46%)

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
2	PO4	A	1004	-	-	0/0/0/0	0/0/0/0
3	RBF	A	501	-	-	0/14/14/14	0/3/3/3
2	PO4	B	1001	-	-	0/0/0/0	0/0/0/0
3	RBF	B	502	-	-	0/14/14/14	0/3/3/3
2	PO4	C	1003	-	-	0/0/0/0	0/0/0/0
3	RBF	C	503	-	-	0/14/14/14	0/3/3/3
2	PO4	D	1005	-	-	0/0/0/0	0/0/0/0
3	RBF	D	504	-	-	0/14/14/14	0/3/3/3
2	PO4	E	1002	-	-	0/0/0/0	0/0/0/0
3	RBF	E	505	-	-	0/14/14/14	0/3/3/3

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	504	RBF	C10-N10	-2.74	1.36	1.39
3	A	501	RBF	C4'-C3'	-2.25	1.49	1.53
3	A	501	RBF	C9-C9A	2.00	1.45	1.40
3	B	502	RBF	C5'-C4'	2.01	1.58	1.52
3	E	505	RBF	C4A-C10	2.15	1.44	1.40
3	B	502	RBF	C9-C9A	2.20	1.45	1.40
3	B	502	RBF	C7M-C7	2.20	1.55	1.51
3	D	504	RBF	C9-C9A	2.29	1.45	1.40
3	E	505	RBF	C9-C9A	2.31	1.45	1.40
3	A	501	RBF	C5'-C4'	2.34	1.58	1.52
3	E	505	RBF	C5'-C4'	2.34	1.58	1.52
3	C	503	RBF	C5'-C4'	2.37	1.59	1.52
3	A	501	RBF	C7M-C7	2.39	1.55	1.51
3	C	503	RBF	C7M-C7	2.39	1.55	1.51
3	C	503	RBF	C9-C9A	2.45	1.46	1.40
3	D	504	RBF	C5'-C4'	2.48	1.59	1.52
3	E	505	RBF	C7M-C7	2.52	1.56	1.51
3	B	502	RBF	C10-N1	2.60	1.40	1.35
3	C	503	RBF	C8-C7	2.70	1.48	1.41
3	C	503	RBF	C10-N1	2.78	1.40	1.35
3	E	505	RBF	C10-N1	2.84	1.40	1.35
3	D	504	RBF	C8-C7	2.85	1.48	1.41
3	A	501	RBF	C10-N1	2.91	1.40	1.35
3	D	504	RBF	C10-N1	2.91	1.40	1.35
3	A	501	RBF	C8M-C8	3.07	1.57	1.51
3	A	501	RBF	C8-C7	3.12	1.49	1.41
3	B	502	RBF	C8M-C8	3.13	1.57	1.51
3	B	502	RBF	C8-C7	3.16	1.49	1.41
3	E	505	RBF	C8-C7	3.32	1.49	1.41
3	D	504	RBF	C8M-C8	3.34	1.57	1.51
3	C	503	RBF	C8M-C8	3.40	1.57	1.51
3	B	502	RBF	C6-C5A	3.46	1.47	1.41
3	D	504	RBF	C6-C5A	3.46	1.47	1.41
3	C	503	RBF	C6-C5A	3.56	1.47	1.41
3	A	501	RBF	C6-C5A	3.56	1.47	1.41
3	E	505	RBF	C6-C5A	3.58	1.47	1.41
3	E	505	RBF	C8M-C8	3.70	1.58	1.51
3	A	501	RBF	C5A-N5	4.27	1.42	1.35
3	D	504	RBF	C5A-N5	4.43	1.42	1.35
3	A	501	RBF	C4-N3	4.54	1.41	1.33
3	C	503	RBF	C4-N3	4.73	1.41	1.33
3	D	504	RBF	C4-N3	4.99	1.42	1.33
3	B	502	RBF	C5A-N5	5.00	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	RBF	C4-N3	5.14	1.42	1.33
3	E	505	RBF	C5A-N5	5.22	1.43	1.35
3	E	505	RBF	C4-N3	5.37	1.42	1.33
3	C	503	RBF	C5A-N5	5.66	1.44	1.35
3	D	504	RBF	C4-C4A	5.94	1.53	1.41
3	B	502	RBF	C4-C4A	5.94	1.53	1.41
3	A	501	RBF	C4-C4A	5.96	1.53	1.41
3	E	505	RBF	C4-C4A	6.15	1.53	1.41
3	A	501	RBF	C9A-N10	6.50	1.48	1.38
3	C	503	RBF	C9A-N10	6.64	1.48	1.38
3	B	502	RBF	C9A-N10	6.72	1.48	1.38
3	D	504	RBF	C9A-N10	6.88	1.48	1.38
3	C	503	RBF	C4-C4A	6.89	1.55	1.41
3	E	505	RBF	C9A-N10	7.09	1.48	1.38

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	503	RBF	C4A-C4-N3	-8.33	112.64	123.52
3	A	501	RBF	C4A-C4-N3	-8.28	112.70	123.52
3	E	505	RBF	C4A-C4-N3	-8.00	113.06	123.52
3	B	502	RBF	C4A-C4-N3	-7.92	113.16	123.52
3	D	504	RBF	C4A-C4-N3	-7.82	113.30	123.52
3	B	502	RBF	N3-C2-N1	-7.36	115.29	127.69
3	D	504	RBF	N3-C2-N1	-7.35	115.31	127.69
3	C	503	RBF	N3-C2-N1	-7.26	115.47	127.69
3	C	503	RBF	O5'-C5'-C4'	-7.24	95.02	111.07
3	E	505	RBF	N3-C2-N1	-7.23	115.51	127.69
3	A	501	RBF	N3-C2-N1	-7.16	115.63	127.69
3	B	502	RBF	O4'-C4'-C5'	-5.78	95.48	109.23
3	C	503	RBF	O4'-C4'-C5'	-5.46	96.24	109.23
3	C	503	RBF	C4-C4A-C10	-4.21	117.25	119.94
3	D	504	RBF	O3'-C3'-C4'	-4.15	97.97	108.73
3	E	505	RBF	O4'-C4'-C5'	-4.12	99.44	109.23
3	E	505	RBF	O3'-C3'-C4'	-3.95	98.48	108.73
3	C	503	RBF	O3'-C3'-C4'	-3.82	98.82	108.73
3	D	504	RBF	C4-C4A-C10	-3.62	117.62	119.94
3	E	505	RBF	C4-C4A-C10	-3.56	117.66	119.94
3	B	502	RBF	C4-C4A-C10	-3.54	117.67	119.94
3	A	501	RBF	C7-C6-C5A	-3.43	115.30	120.90
3	D	504	RBF	C7-C6-C5A	-3.40	115.34	120.90
3	B	502	RBF	O3'-C3'-C4'	-3.31	100.15	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	RBF	C7-C6-C5A	-3.27	115.57	120.90
3	E	505	RBF	C7-C6-C5A	-3.26	115.58	120.90
3	C	503	RBF	C7-C6-C5A	-2.88	116.20	120.90
3	A	501	RBF	C6-C5A-N5	-2.80	115.43	118.92
3	A	501	RBF	C4-C4A-C10	-2.63	118.26	119.94
3	E	505	RBF	O2'-C2'-C1'	-2.62	103.45	109.93
3	B	502	RBF	O5'-C5'-C4'	-2.59	105.31	111.07
3	B	502	RBF	C6-C5A-N5	-2.50	115.80	118.92
3	D	504	RBF	C6-C5A-N5	-2.47	115.84	118.92
3	A	501	RBF	O3'-C3'-C4'	-2.39	102.53	108.73
3	D	504	RBF	O4'-C4'-C5'	-2.38	103.58	109.23
3	E	505	RBF	C6-C5A-N5	-2.32	116.02	118.92
3	A	501	RBF	O4'-C4'-C5'	-2.30	103.76	109.23
3	C	503	RBF	C6-C5A-N5	-2.16	116.22	118.92
3	B	502	RBF	O2'-C2'-C1'	-2.13	104.68	109.93
3	C	503	RBF	C4A-N5-C5A	2.02	119.10	116.72
3	A	501	RBF	C5'-C4'-C3'	2.13	117.69	112.43
3	C	503	RBF	O2'-C2'-C3'	2.26	114.76	108.96
3	A	501	RBF	O3'-C3'-C2'	2.45	115.08	108.73
3	A	501	RBF	C4A-N5-C5A	2.56	119.74	116.72
3	E	505	RBF	O2'-C2'-C3'	2.72	115.96	108.96
3	D	504	RBF	O2'-C2'-C3'	2.77	116.08	108.96
3	C	503	RBF	C9-C8-C7	2.78	125.41	119.97
3	C	503	RBF	C6-C5A-C9A	2.78	122.17	119.11
3	E	505	RBF	C9-C8-C7	2.80	125.45	119.97
3	D	504	RBF	C5'-C4'-C3'	2.84	119.45	112.43
3	D	504	RBF	C9-C8-C7	2.95	125.74	119.97
3	B	502	RBF	C9-C8-C7	3.01	125.86	119.97
3	A	501	RBF	C9-C8-C7	3.10	126.04	119.97
3	E	505	RBF	C6-C5A-C9A	3.19	122.63	119.11
3	D	504	RBF	C6-C5A-C9A	3.28	122.72	119.11
3	B	502	RBF	C6-C5A-C9A	3.28	122.72	119.11
3	B	502	RBF	O3'-C3'-C2'	3.45	117.67	108.73
3	E	505	RBF	C5'-C4'-C3'	3.46	120.97	112.43
3	A	501	RBF	C6-C5A-C9A	3.52	122.99	119.11
3	C	503	RBF	C5'-C4'-C3'	4.38	123.24	112.43
3	C	503	RBF	O3'-C3'-C2'	4.69	120.88	108.73
3	D	504	RBF	O3'-C3'-C2'	4.73	121.00	108.73
3	B	502	RBF	C5'-C4'-C3'	4.80	124.29	112.43
3	E	505	RBF	O3'-C3'-C2'	4.97	121.61	108.73
3	B	502	RBF	C4-N3-C2	16.76	129.14	115.16
3	D	504	RBF	C4-N3-C2	16.95	129.30	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	505	RBF	C4-N3-C2	16.97	129.32	115.16
3	A	501	RBF	C4-N3-C2	17.24	129.54	115.16
3	C	503	RBF	C4-N3-C2	17.68	129.91	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1004	PO4	1	0
3	A	501	RBF	2	0
3	B	502	RBF	5	0
3	C	503	RBF	5	0
3	D	504	RBF	2	0
3	E	505	RBF	1	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.