



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2016 – 06:25 PM EDT

PDB ID : 4UMB  
Title : Structural analysis of substrate-mimicking inhibitors in complex with *Neisseria meningitidis* 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase - the importance of accommodating the active site water  
Authors : Heyes, L.C.; Reichau, S.; Cross, P.J.; Parker, E.J.  
Deposited on : 2014-05-16  
Resolution : 2.17 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) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

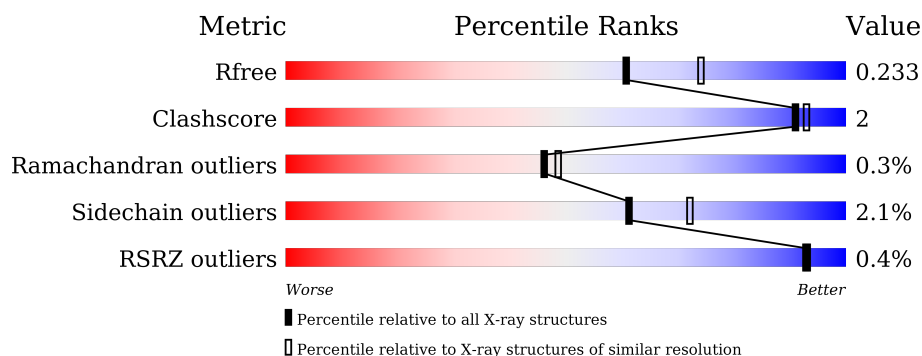
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.17 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))
$R_{free}$	91344	5130 (2.20-2.16)
Clashscore	102246	5965 (2.20-2.16)
Ramachandran outliers	100387	5863 (2.20-2.16)
Sidechain outliers	100360	5864 (2.20-2.16)
RSRZ outliers	91569	5142 (2.20-2.16)

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.

Mol	Chain	Length	Quality of chain
1	A	351	<div> <div>91%</div> <div> <div></div> <div>5%</div> </div> </div>
1	B	351	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>5%</div> </div> </div>
1	C	351	<div> <div>91%</div> <div> <div></div> <div>5%</div> </div> </div>
1	D	351	<div> <div>91%</div> <div> <div></div> <div>5%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	1352	-	-	-	X
3	PO4	C	1352	-	-	-	X
3	PO4	D	1352	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10942 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 PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	3	0
			2584	1615	468	486	15			
1	B	333	Total	C	N	O	S	0	1	0
			2558	1597	460	487	14			
1	C	333	Total	C	N	O	S	0	2	0
			2554	1596	460	483	15			
1	D	333	Total	C	N	O	S	0	2	0
			2548	1593	456	484	15			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

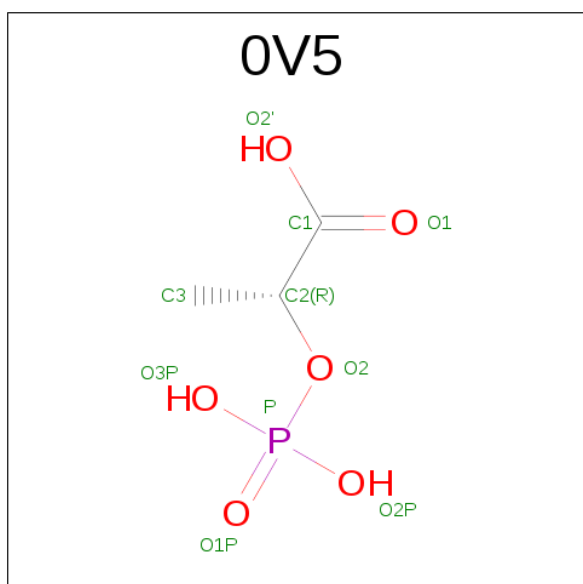
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 4 is (2R)-2-(PHOSPHONOOXY)PROPANOIC ACID (three-letter code: 0V5) (formula: C<sub>3</sub>H<sub>7</sub>O<sub>6</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			10	3	6	1		
4	B	1	Total	C	O	P	0	0
			10	3	6	1		
4	C	1	Total	C	O	P	0	0
			10	3	6	1		
4	D	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	197	Total	O	0	1
			198	198		
5	B	139	Total	O	0	0
			139	139		
5	C	164	Total	O	0	0
			164	164		
5	D	133	Total	O	0	0
			133	133		



● Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

MT	THR	HIS	HIS	THR	THR	PRO	ASP	ASP	ILE	LVS	LVS	GLU	VAL	K16	R40	R52	R77	K93	D148	N189	R219	R236	D267	C268	V283	D294	V301	N302	H306	K329	A350	ASP
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Chain B:  91% 5%

MET	THR	HIS	HIS	TYR	PRO	THR	ASP	ASP	LEU	LYS	ILE	LYS	GLU	VAL	LYS	E17	R52	R77	R94	D148	N189	H219	R236	E250	E292	Q293	D294	R306	L307	V308	R329	A348	R349	ALA	ASP
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Chain C:  91% • 5%

MET	THR	HIS	HIS	TVR	PRO	THR	ASP	ASP	IIE	LYS	LYS	GLU	VAL	LYS	E17	I30	D148	N189	H219	R236	E250	D267	R274	D294	V301	R302	H306	R349	ALA	SFR
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Chain D:  91% • 5%

MET	THR	HIS	HIS	TYR	PRO	THR	ASP	ASP	ILE	LVS	ILE	LVS	GLU	VAL	LVS	E17	R40	D148	T151	P152	N189	E219	R236	E246	M265	D266	D267	E292	Q293	D294	M302	H306	R311	R349	ALA	ASP
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.44Å 133.73Å 147.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.99 – 2.17 48.32 – 2.17	Depositor EDS
% Data completeness (in resolution range)	99.9 (98.99-2.17) 99.9 (48.32-2.17)	Depositor EDS
$R_{merge}$	0.30	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.201 , 0.227 0.208 , 0.233	Depositor DCC
$R_{free}$ test set	4166 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.9	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 34.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 83527 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10942	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: PO4, MN, OV5

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	0.58	0/2632	0.71	3/3561 (0.1%)
1	B	0.54	0/2606	0.70	2/3529 (0.1%)
1	C	0.54	0/2602	0.69	1/3524 (0.0%)
1	D	0.55	0/2596	0.69	2/3517 (0.1%)
All	All	0.55	0/10436	0.70	8/14131 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	D	311	ARG	NE-CZ-NH2	6.02	123.31	120.30
1	C	274	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	94	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	294	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	40[A]	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	40[B]	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	D	40	ARG	NE-CZ-NH1	5.29	122.94	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2584	0	2555	18	0
1	B	2558	0	2518	15	0
1	C	2554	0	2512	16	0
1	D	2548	0	2499	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	10	0	6	0	0
4	B	10	0	6	0	0
4	C	10	0	6	0	0
4	D	10	0	6	0	0
5	A	198	0	0	6	0
5	B	139	0	0	4	0
5	C	164	0	0	5	0
5	D	133	0	0	1	0
All	All	10942	0	10108	44	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 2.

All (44) 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:B:148[A]:ASP:OD1	5:B:2070:HOH:O	1.79	1.00
1:A:219:HIS:CD2	1:B:219:HIS:NE2	2.33	0.97
1:C:219:HIS:NE2	1:D:219:HIS:CD2	2.46	0.83
1:A:219:HIS:NE2	1:B:219:HIS:CD2	2.46	0.83
1:C:302[A]:MET:HG2	5:C:2050:HOH:O	1.77	0.83
1:C:148[A]:ASP:OD2	5:C:2082:HOH:O	1.98	0.81
1:A:219:HIS:HE2	1:C:219:HIS:HE2	0.83	0.80
5:C:2124:HOH:O	1:D:148[A]:ASP:OD2	1.99	0.80
5:A:2146:HOH:O	1:B:148[A]:ASP:OD2	1.98	0.80
1:C:219:HIS:CD2	1:D:219:HIS:CD2	2.71	0.78
1:A:219:HIS:CD2	1:B:219:HIS:CD2	2.72	0.78
1:C:219:HIS:NE2	1:D:219:HIS:HD2	1.84	0.73
1:C:148[A]:ASP:OD1	5:C:2080:HOH:O	2.10	0.69
1:B:148[B]:ASP:OD1	5:B:2071:HOH:O	0.68	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:HIS:NE2	1:D:219:HIS:NE2	2.43	0.65
1:C:219:HIS:HE2	1:D:219:HIS:HD2	1.45	0.65
1:A:219:HIS:HD2	1:B:219:HIS:NE2	1.90	0.64
1:A:148[A]:ASP:OD1	5:A:2096:HOH:O	2.14	0.64
1:A:52:ARG:HD3	5:A:2024:HOH:O	1.99	0.63
1:C:267:ASP:HA	1:C:302[B]:MET:HB2	1.80	0.62
1:C:219:HIS:CD2	1:D:219:HIS:NE2	2.68	0.61
1:A:219:HIS:NE2	1:C:219:HIS:NE2	2.17	0.59
1:B:219:HIS:CD2	1:C:219:HIS:CD2	2.92	0.58
1:A:267:ASP:HA	1:A:302[B]:MET:HB2	1.87	0.56
1:A:219:HIS:CD2	1:C:219:HIS:HE2	2.20	0.54
1:B:308:VAL:HG22	5:B:2119:HOH:O	2.09	0.53
1:A:219:HIS:HE2	1:B:219:HIS:CD2	2.25	0.51
1:C:219:HIS:HE2	1:D:219:HIS:CD2	2.22	0.49
1:D:267:ASP:HA	1:D:302[B]:MET:HB2	1.96	0.48
1:B:148[A]:ASP:CG	5:B:2070:HOH:O	2.44	0.46
1:A:148[A]:ASP:OD2	5:A:2097:HOH:O	2.20	0.46
1:A:83:LYS:HD3	5:A:2046:HOH:O	2.15	0.46
1:A:219:HIS:NE2	1:B:219:HIS:HD2	2.07	0.46
1:A:148[A]:ASP:OD2	5:A:2095:HOH:O	2.20	0.46
1:A:219:HIS:CD2	1:D:219:HIS:CD2	3.04	0.45
1:B:219:HIS:CE1	1:D:219:HIS:HE2	2.36	0.42
1:C:30:ILE:HD13	5:C:2005:HOH:O	2.21	0.41
1:B:77:ARG:HB3	1:B:329:TRP:CZ2	2.55	0.41
1:D:151:THR:N	1:D:152:PRO:CD	2.84	0.41
1:D:246:GLU:HB2	5:D:2110:HOH:O	2.20	0.41
1:D:265:MET:SD	1:D:302[B]:MET:HG3	2.61	0.41
1:C:302[A]:MET:HB2	1:C:302[A]:MET:HE2	1.93	0.41
1:A:268:CYS:HA	1:A:283:VAL:HG11	2.03	0.40
1:A:77:ARG:HB3	1:A:329:TRP:CZ2	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	336/351 (96%)	330 (98%)	5 (2%)	1 (0%)	46	48
1	B	332/351 (95%)	326 (98%)	5 (2%)	1 (0%)	46	48
1	C	333/351 (95%)	328 (98%)	4 (1%)	1 (0%)	46	48
1	D	333/351 (95%)	327 (98%)	5 (2%)	1 (0%)	46	48
All	All	1334/1404 (95%)	1311 (98%)	19 (1%)	4 (0%)	46	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	ASP
1	B	294	ASP
1	C	294	ASP
1	D	294	ASP

### 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	270/289 (93%)	265 (98%)	5 (2%)	65	75
1	B	269/289 (93%)	263 (98%)	6 (2%)	60	70
1	C	267/289 (92%)	260 (97%)	7 (3%)	54	63
1	D	266/289 (92%)	262 (98%)	4 (2%)	72	82
All	All	1072/1156 (93%)	1050 (98%)	22 (2%)	61	72

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	ASN
1	A	219	HIS
1	A	236	ARG
1	A	301	VAL

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Mol	Chain	Res	Type
1	A	306	HIS
1	B	52	ARG
1	B	189	ASN
1	B	219	HIS
1	B	236	ARG
1	B	250	GLU
1	B	306	HIS
1	C	189	ASN
1	C	219	HIS
1	C	236	ARG
1	C	250	GLU
1	C	301	VAL
1	C	306	HIS
1	C	349	ARG
1	D	189	ASN
1	D	219	HIS
1	D	236	ARG
1	D	306	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PO4	A	1352	-	4,4,4	0.51	0	6,6,6	0.28	0
4	0V5	A	1353	2	4,9,9	1.81	1 (25%)	7,13,13	3.01	4 (57%)
4	0V5	B	1351	2	4,9,9	1.63	1 (25%)	7,13,13	1.98	3 (42%)
3	PO4	B	1352	-	4,4,4	0.39	0	6,6,6	0.27	0
4	0V5	C	1351	2	4,9,9	2.20	1 (25%)	7,13,13	1.55	2 (28%)
3	PO4	C	1352	-	4,4,4	0.62	0	6,6,6	0.28	0
4	0V5	D	1351	2	4,9,9	1.71	1 (25%)	7,13,13	1.88	3 (42%)
3	PO4	D	1352	-	4,4,4	0.65	0	6,6,6	0.35	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	PO4	A	1352	-	-	0/0/0/0	0/0/0/0
4	0V5	A	1353	2	-	0/5/9/9	0/0/0/0
4	0V5	B	1351	2	-	0/5/9/9	0/0/0/0
3	PO4	B	1352	-	-	0/0/0/0	0/0/0/0
4	0V5	C	1351	2	-	0/5/9/9	0/0/0/0
3	PO4	C	1352	-	-	0/0/0/0	0/0/0/0
4	0V5	D	1351	2	-	0/5/9/9	0/0/0/0
3	PO4	D	1352	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1353	0V5	P-O1P	2.81	1.59	1.50
4	D	1351	0V5	P-O1P	2.87	1.59	1.50
4	B	1351	0V5	P-O1P	3.09	1.60	1.50
4	C	1351	0V5	P-O1P	3.78	1.62	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	A	1353	0V5	C3-C2-C1	-6.41	105.28	113.19
4	D	1351	0V5	C3-C2-C1	-2.81	109.72	113.19
4	D	1351	0V5	O2P-P-O1P	-2.80	101.47	110.63
4	B	1351	0V5	O2-P-O1P	-2.71	101.02	107.48
4	C	1351	0V5	O2P-P-O1P	-2.32	103.07	110.63
4	B	1351	0V5	C3-C2-C1	-2.09	110.61	113.19
4	A	1353	0V5	O2-P-O1P	-2.08	102.51	107.48
4	D	1351	0V5	O3P-P-O2P	2.13	115.25	107.44
4	A	1353	0V5	O3P-P-O2	2.21	113.22	106.62
4	C	1351	0V5	O3P-P-O2P	2.31	115.92	107.44
4	B	1351	0V5	O2P-P-O2	3.11	115.91	106.62
4	A	1353	0V5	O3P-P-O2P	3.11	118.86	107.44

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	335/351 (95%)	-0.33	0 100 100	15, 22, 30, 47	0
1	B	333/351 (94%)	-0.19	4 (1%) 81 81	17, 24, 37, 50	0
1	C	333/351 (94%)	-0.22	0 100 100	17, 24, 34, 49	0
1	D	333/351 (94%)	-0.16	1 (0%) 94 94	18, 24, 37, 48	0
All	All	1334/1404 (95%)	-0.23	5 (0%) 93 93	15, 24, 36, 50	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	292	GLU	2.9
1	B	348	ALA	2.2
1	B	293	GLN	2.1
1	D	292	GLU	2.1
1	B	349	ARG	2.0

### 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.



The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	PO4	C	1352	5/5	0.94	0.16	6.13	51,52,55,57	0
3	PO4	A	1352	5/5	0.93	0.19	6.13	41,45,50,50	0
3	PO4	D	1352	5/5	0.94	0.18	2.63	43,45,48,48	0
3	PO4	B	1352	5/5	0.93	0.17	1.92	35,36,40,40	0
4	0V5	C	1351	10/10	0.97	0.09	-0.89	20,25,26,27	0
4	0V5	B	1351	10/10	0.98	0.09	-0.91	18,20,21,21	0
2	MN	B	1350	1/1	0.99	0.08	-0.92	20,20,20,20	0
4	0V5	A	1353	10/10	0.98	0.08	-1.06	18,20,21,22	0
4	0V5	D	1351	10/10	0.98	0.11	-1.08	22,24,25,26	0
2	MN	A	1351	1/1	0.99	0.06	-1.61	18,18,18,18	0
2	MN	D	1350	1/1	0.99	0.07	-2.10	20,20,20,20	0
2	MN	C	1350	1/1	0.99	0.05	-2.65	21,21,21,21	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.