



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:43 PM GMT

PDB ID : 3UPI  
Title : Synthesis of novel 4,5-dihydrofurano indoles and their evaluation as HCV NS5B polymerase inhibitors  
Authors : Velazquez, F.; Venkataraman, S.; Lesburg, C.A.; Duca, J.S.; Rosenblum, S.B.; Kozlowski, J.A.; Njoroge, F.G.  
Deposited on : 2011-11-18  
Resolution : 2.00 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

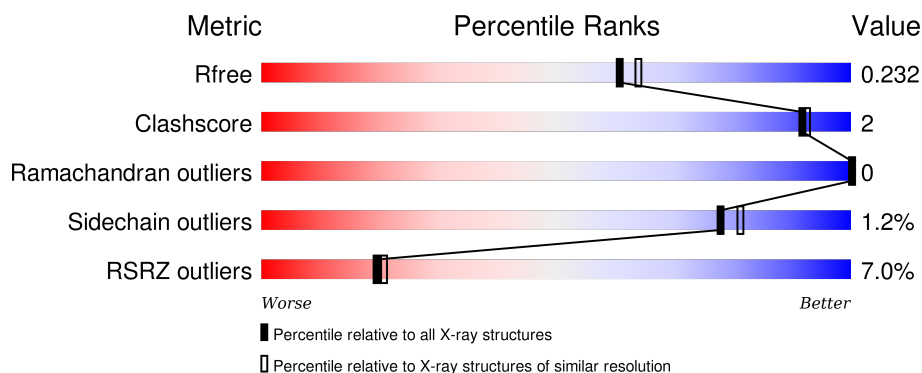
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

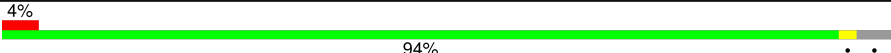

The reported resolution of this entry is 2.00 Å.

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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	585	 4% 94% . .
1	B	585	 9% 90% 5% 5%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9854 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 RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	563	Total	C	N	O	S	0	2	0
			4406	2772	783	816	35			
1	B	558	Total	C	N	O	S	0	2	0
			4365	2748	772	810	35			

There are 34 discrepancies between the modelled and reference sequences:

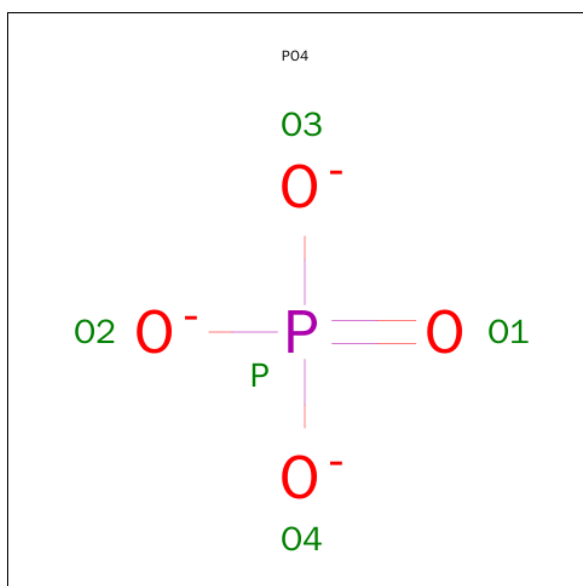
Chain	Residue	Modelled	Actual	Comment	Reference
A	440	GLY	GLU	CONFLICT	UNP O92972
A	520	ILE	THR	CONFLICT	UNP O92972
A	571	GLU	-	EXPRESSION TAG	UNP O92972
A	572	ASN	-	EXPRESSION TAG	UNP O92972
A	573	LEU	-	EXPRESSION TAG	UNP O92972
A	574	TYR	-	EXPRESSION TAG	UNP O92972
A	575	PHE	-	EXPRESSION TAG	UNP O92972
A	576	GLN	-	EXPRESSION TAG	UNP O92972
A	577	GLY	-	EXPRESSION TAG	UNP O92972
A	578	LEU	-	EXPRESSION TAG	UNP O92972
A	579	GLU	-	EXPRESSION TAG	UNP O92972
A	580	HIS	-	EXPRESSION TAG	UNP O92972
A	581	HIS	-	EXPRESSION TAG	UNP O92972
A	582	HIS	-	EXPRESSION TAG	UNP O92972
A	583	HIS	-	EXPRESSION TAG	UNP O92972
A	584	HIS	-	EXPRESSION TAG	UNP O92972
A	585	HIS	-	EXPRESSION TAG	UNP O92972
B	440	GLY	GLU	CONFLICT	UNP O92972
B	520	ILE	THR	CONFLICT	UNP O92972
B	571	GLU	-	EXPRESSION TAG	UNP O92972
B	572	ASN	-	EXPRESSION TAG	UNP O92972
B	573	LEU	-	EXPRESSION TAG	UNP O92972
B	574	TYR	-	EXPRESSION TAG	UNP O92972
B	575	PHE	-	EXPRESSION TAG	UNP O92972
B	576	GLN	-	EXPRESSION TAG	UNP O92972

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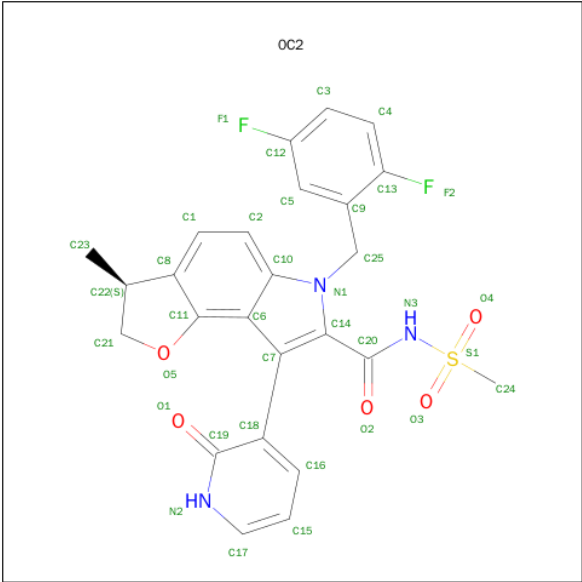
Chain	Residue	Modelled	Actual	Comment	Reference
B	577	GLY	-	EXPRESSION TAG	UNP O92972
B	578	LEU	-	EXPRESSION TAG	UNP O92972
B	579	GLU	-	EXPRESSION TAG	UNP O92972
B	580	HIS	-	EXPRESSION TAG	UNP O92972
B	581	HIS	-	EXPRESSION TAG	UNP O92972
B	582	HIS	-	EXPRESSION TAG	UNP O92972
B	583	HIS	-	EXPRESSION TAG	UNP O92972
B	584	HIS	-	EXPRESSION TAG	UNP O92972
B	585	HIS	-	EXPRESSION TAG	UNP O92972

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



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

- Molecule 3 is (3S)-6-(2,5-DIFLUOROBENZYL)-3-METHYL-N-(METHYLSULFONYL)-8-(2-OXO-1,2-DIHYDROPYRIDIN-3-YL)-3,6-DIHYDRO-2H-FURO[2,3-E]INDOLE-7-CARBOXAMIDE (three-letter code: 0C2) (formula: C<sub>25</sub>H<sub>21</sub>F<sub>2</sub>N<sub>3</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	1
			72	50	4	6	10	2		
3	B	1	Total	C	F	N	O	S	0	1
			72	50	4	6	10	2		

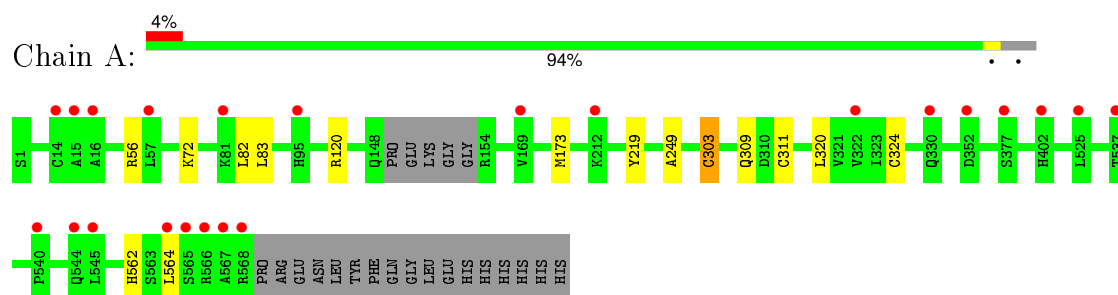
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	520	Total	O	0	0
			520	520		
4	B	414	Total	O	0	0
			414	414		

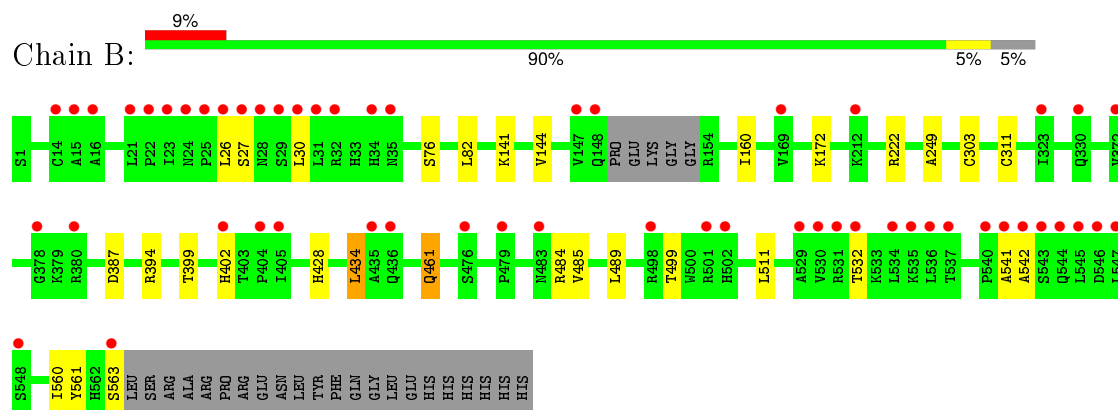
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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: RNA-directed RNA polymerase



#### • Molecule 1: RNA-directed RNA polymerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.82Å 106.54Å 134.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.00) 99.8 (19.99-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.01Å)	Xtriage
Refinement program	BUSTER 2.9.4	Depositor
R, $R_{free}$	0.189 , 0.235 0.186 , 0.232	Depositor DCC
$R_{free}$ test set	4345 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.4	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 87262 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9854	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: 0C2, 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	0.50	0/4500	0.61	0/6104
1	B	0.50	0/4459	0.64	0/6050
All	All	0.50	0/8959	0.63	0/12154

There are no bond length outliers.

There are no bond angle outliers.

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	4406	0	4425	9	0
1	B	4365	0	4378	20	0
2	A	5	0	0	0	0
3	A	72	0	42	4	0
3	B	72	0	42	4	0
4	A	520	0	0	0	0
4	B	414	0	0	1	0
All	All	9854	0	8887	36	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 (36) 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)
3:A:587[A]:OC2:H20	3:A:587[A]:OC2:H21	1.14	1.12
3:B:586[A]:OC2:H20	3:B:586[A]:OC2:H21	1.10	1.07
3:B:586[A]:OC2:C25	3:B:586[A]:OC2:H21	1.88	0.87
1:B:303[A]:CYS:HG	1:B:311:CYS:CB	1.87	0.86
1:A:303[A]:CYS:HG	1:A:311:CYS:HG	1.22	0.85
3:B:586[A]:OC2:N3	3:B:586[A]:OC2:H20	1.93	0.83
3:A:587[A]:OC2:H21	3:A:587[A]:OC2:C25	1.90	0.83
3:A:587[A]:OC2:H20	3:A:587[A]:OC2:N3	1.97	0.77
1:B:141:LYS:HD2	1:B:160:ILE:HD11	1.72	0.72
1:A:303[A]:CYS:HG	1:A:311:CYS:CB	2.19	0.56
3:B:586[A]:OC2:N3	3:B:586[A]:OC2:C25	2.58	0.55
1:A:219:TYR:HB3	1:A:320:LEU:HD23	1.93	0.51
3:A:587[A]:OC2:C25	3:A:587[A]:OC2:N3	2.60	0.50
1:B:303[B]:CYS:SG	1:B:311:CYS:SG	3.08	0.49
1:A:303[B]:CYS:SG	1:A:311:CYS:SG	3.02	0.49
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.95	0.49
1:B:303[C]:CYS:SG	1:B:311:CYS:SG	3.09	0.48
1:A:303[C]:CYS:SG	1:A:311:CYS:SG	3.03	0.48
1:B:144:VAL:HB	1:B:394:ARG:HG2	1.95	0.47
1:B:82:LEU:HD13	1:B:249:ALA:HB2	1.96	0.47
1:B:461:GLN:HG2	1:B:541:ALA:HB3	1.97	0.47
1:B:27:SER:HB2	1:B:399:THR:HB	1.98	0.46
1:A:83:LEU:HB2	1:A:173:MET:HA	1.98	0.45
1:A:309:GLN:O	1:A:324:CYS:HB2	2.17	0.45
1:A:72:LYS:HB3	1:B:76:SER:HB2	1.98	0.45
1:B:303[A]:CYS:SG	1:B:311:CYS:CB	2.96	0.45
1:B:561:TYR:CZ	1:B:563:SER:HB2	2.52	0.45
1:B:434:LEU:HD11	1:B:511:LEU:HG	2.00	0.43
1:B:30:LEU:HB2	1:B:428:HIS:CE1	2.54	0.43
1:B:26:LEU:O	1:B:27:SER:HB3	2.19	0.43
1:B:160:ILE:HD12	4:B:965:HOH:O	2.18	0.43
1:B:461:GLN:HB3	1:B:542:ALA:HA	2.01	0.42
1:B:303[A]:CYS:SG	1:B:311:CYS:HB2	2.60	0.42
1:B:387:ASP:HA	1:B:484:ARG:HD3	2.01	0.41
1:B:172:LYS:HE3	1:B:560:ILE:HD13	2.03	0.41
1:B:485:VAL:O	1:B:489:LEU:HG	2.20	0.41

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	562/585 (96%)	554 (99%)	8 (1%)	0	100	100
1	B	557/585 (95%)	543 (98%)	14 (2%)	0	100	100
All	All	1119/1170 (96%)	1097 (98%)	22 (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	482/498 (97%)	475 (98%)	7 (2%)	72	75
1	B	478/498 (96%)	472 (99%)	6 (1%)	76	79
All	All	960/996 (96%)	947 (99%)	13 (1%)	78	77

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ARG
1	A	120	ARG
1	A	303[A]	CYS
1	A	303[B]	CYS
1	A	303[C]	CYS
1	A	562	HIS
1	A	564	LEU
1	B	222	ARG

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Mol	Chain	Res	Type
1	B	402	HIS
1	B	434	LEU
1	B	461	GLN
1	B	499	THR
1	B	532	THR

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](#)

5 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	586	-	4,4,4	2.20	1 (25%)	6,6,6	0.27	0
3	0C2	A	587[A]	-	36,40,40	1.63	7 (19%)	40,61,61	1.92	7 (17%)
3	0C2	A	587[B]	-	36,40,40	1.87	8 (22%)	40,61,61	1.56	8 (20%)
3	0C2	B	586[A]	-	36,40,40	1.75	8 (22%)	40,61,61	1.82	8 (20%)
3	0C2	B	586[B]	-	36,40,40	1.87	8 (22%)	40,61,61	1.53	7 (17%)

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	586	-	-	0/0/0/0	0/0/0/0
3	0C2	A	587[A]	-	-	0/13/26/26	0/5/5/5
3	0C2	A	587[B]	-	-	0/13/26/26	0/5/5/5
3	0C2	B	586[A]	-	-	0/13/26/26	0/5/5/5
3	0C2	B	586[B]	-	-	0/13/26/26	0/5/5/5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	586[B]	0C2	C18-C7	-3.06	1.44	1.49
3	A	587[B]	0C2	C18-C7	-2.99	1.44	1.49
3	B	586[A]	0C2	C18-C7	-2.77	1.44	1.49
3	A	587[A]	0C2	C18-C7	-2.63	1.45	1.49
3	B	586[A]	0C2	C8-C22	-2.61	1.48	1.52
3	A	587[A]	0C2	C16-C18	-2.54	1.35	1.39
3	A	587[A]	0C2	C8-C22	-2.50	1.48	1.52
3	A	587[B]	0C2	C16-C18	-2.47	1.35	1.39
3	B	586[B]	0C2	C8-C22	-2.44	1.48	1.52
3	A	587[B]	0C2	C8-C22	-2.30	1.48	1.52
3	B	586[B]	0C2	C16-C18	-2.21	1.36	1.39
3	B	586[A]	0C2	C16-C18	-2.15	1.36	1.39
3	A	587[B]	0C2	C20-N3	2.44	1.41	1.39
3	B	586[B]	0C2	C20-N3	2.58	1.42	1.39
3	A	587[B]	0C2	C15-C16	2.86	1.44	1.38
3	A	587[A]	0C2	C15-C16	3.00	1.45	1.38
3	B	586[A]	0C2	C20-N3	3.06	1.42	1.39
3	B	586[B]	0C2	C15-C16	3.12	1.45	1.38
3	B	586[A]	0C2	C15-C16	3.17	1.45	1.38
3	A	587[A]	0C2	S1-N3	3.17	1.68	1.63
3	A	587[B]	0C2	C19-N2	3.38	1.39	1.33
3	A	587[A]	0C2	C19-N2	3.44	1.39	1.33
3	B	586[B]	0C2	C19-N2	3.45	1.39	1.33
2	A	586	PO4	P-O4	3.52	1.66	1.53
3	B	586[A]	0C2	C19-N2	3.54	1.39	1.33
3	B	586[B]	0C2	C19-C18	3.61	1.52	1.44
3	A	587[B]	0C2	C19-C18	3.68	1.52	1.44
3	B	586[A]	0C2	C19-C18	3.87	1.52	1.44
3	B	586[A]	0C2	S1-N3	4.09	1.69	1.63
3	A	587[A]	0C2	C19-C18	4.10	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	586[B]	0C2	S1-N3	6.06	1.72	1.63
3	A	587[B]	0C2	S1-N3	6.23	1.72	1.63

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	587[A]	0C2	C24-S1-N3	-7.50	97.04	106.72
3	B	586[A]	0C2	C24-S1-N3	-6.39	98.47	106.72
3	B	586[B]	0C2	C24-S1-N3	-4.23	101.26	106.72
3	A	587[B]	0C2	C24-S1-N3	-4.05	101.50	106.72
3	B	586[A]	0C2	C9-C25-N1	-2.92	108.47	113.31
3	A	587[B]	0C2	C18-C19-N2	-2.63	116.04	123.89
3	B	586[B]	0C2	C18-C19-N2	-2.57	116.21	123.89
3	A	587[A]	0C2	C18-C19-N2	-2.56	116.25	123.89
3	B	586[A]	0C2	C18-C19-N2	-2.54	116.30	123.89
3	B	586[B]	0C2	C9-C25-N1	-2.28	109.53	113.31
3	A	587[B]	0C2	C9-C25-N1	-2.26	109.56	113.31
3	A	587[B]	0C2	O2-C20-N3	-2.18	118.78	120.80
3	A	587[A]	0C2	C16-C18-C7	2.16	123.91	119.16
3	B	586[A]	0C2	C16-C18-C7	2.17	123.92	119.16
3	A	587[A]	0C2	C25-C9-C5	2.24	123.21	119.51
3	B	586[B]	0C2	C25-C9-C5	2.24	123.22	119.51
3	A	587[B]	0C2	C25-C9-C5	2.35	123.39	119.51
3	B	586[B]	0C2	O4-S1-N3	2.41	112.22	107.14
3	A	587[B]	0C2	O4-S1-N3	2.43	112.26	107.14
3	B	586[A]	0C2	O2-C20-N3	2.48	123.09	120.80
3	B	586[A]	0C2	O4-S1-O3	2.65	122.62	118.77
3	A	587[A]	0C2	C17-N2-C19	2.83	123.78	116.57
3	A	587[B]	0C2	C17-N2-C19	2.87	123.89	116.57
3	B	586[A]	0C2	C17-N2-C19	2.93	124.03	116.57
3	B	586[B]	0C2	C17-N2-C19	2.97	124.14	116.57
3	A	587[B]	0C2	C1-C8-C11	3.27	121.67	119.47
3	B	586[B]	0C2	C1-C8-C11	3.41	121.76	119.47
3	B	586[A]	0C2	C1-C8-C11	3.41	121.76	119.47
3	A	587[A]	0C2	C1-C8-C11	3.46	121.80	119.47
3	A	587[A]	0C2	O4-S1-O3	3.50	123.86	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	587[A]	0C2	4	0
3	B	586[A]	0C2	4	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

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	563/585 (96%)	0.09	23 (4%) 41 42	25, 34, 56, 132	0
1	B	558/585 (95%)	0.47	55 (9%) 9 10	26, 40, 70, 112	0
All	All	1121/1170 (95%)	0.28	78 (6%) 19 21	25, 37, 66, 132	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	532	THR	9.7
1	B	26	LEU	8.3
1	B	24	ASN	7.8
1	B	23	ILE	7.8
1	B	544	GLN	7.6
1	B	545	LEU	7.4
1	B	25	PRO	7.3
1	A	568	ARG	6.7
1	B	14	CYS	6.4
1	B	542	ALA	6.3
1	B	548	SER	6.1
1	A	567	ALA	6.0
1	B	502	HIS	5.6
1	B	404	PRO	5.6
1	B	531	ARG	5.4
1	B	22	PRO	5.1
1	B	535	LYS	5.0
1	B	543	SER	4.8
1	B	16	ALA	4.5
1	B	541	ALA	4.5
1	B	15	ALA	4.3
1	B	29	SER	4.2
1	B	402	HIS	4.1
1	A	169	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	27	SER	3.9
1	B	35	ASN	3.8
1	A	16	ALA	3.8
1	B	540	PRO	3.8
1	A	402	HIS	3.8
1	B	32	ARG	3.6
1	B	30	LEU	3.6
1	B	34	HIS	3.6
1	B	537	THR	3.6
1	B	147	VAL	3.5
1	A	564	LEU	3.4
1	B	536	LEU	3.4
1	A	15	ALA	3.3
1	A	352	ASP	3.2
1	A	525	LEU	3.1
1	A	14	CYS	2.9
1	B	534	LEU	2.9
1	A	95	HIS	2.7
1	B	380	ARG	2.7
1	B	405	ILE	2.7
1	B	435	ALA	2.6
1	A	566	ARG	2.6
1	B	169	VAL	2.6
1	B	547	LEU	2.6
1	B	483	ASN	2.6
1	B	563	SER	2.5
1	B	28	ASN	2.5
1	A	540	PRO	2.4
1	B	330	GLN	2.4
1	B	372	VAL	2.4
1	A	545	LEU	2.4
1	B	476	SER	2.4
1	B	546	ASP	2.3
1	B	436	GLN	2.3
1	B	498	ARG	2.3
1	B	21	LEU	2.3
1	A	565	SER	2.3
1	B	323	ILE	2.3
1	A	212	LYS	2.2
1	A	322	VAL	2.2
1	A	57	LEU	2.2
1	B	501	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	529	ALA	2.2
1	B	148	GLN	2.1
1	A	544	GLN	2.1
1	B	378	GLY	2.1
1	B	31	LEU	2.1
1	A	330	GLN	2.1
1	A	377	SER	2.1
1	B	479	PRO	2.1
1	A	81	LYS	2.1
1	A	537	THR	2.0
1	B	212	LYS	2.0
1	B	530	VAL	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( $\text{\AA}^2$ )	Q<0.9
3	0C2	B	586[A]	36/36	0.91	0.15	0.86	33,36,38,39	36
3	0C2	B	586[B]	36/36	0.91	0.15	0.80	29,39,44,45	36
3	0C2	A	587[B]	36/36	0.92	0.14	0.71	27,35,43,44	36
3	0C2	A	587[A]	36/36	0.92	0.14	0.71	23,31,41,44	36
2	PO4	A	586	5/5	0.96	0.13	0.39	40,41,42,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.