



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:47 am GMT

PDB ID : 3MKW  
Title : Structure of sopB(155-272)-18mer complex, I23 form  
Authors : Schumacher, M.A.; Piro, K.; Xu, W.  
Deposited on : 2010-04-15  
Resolution : 2.99 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

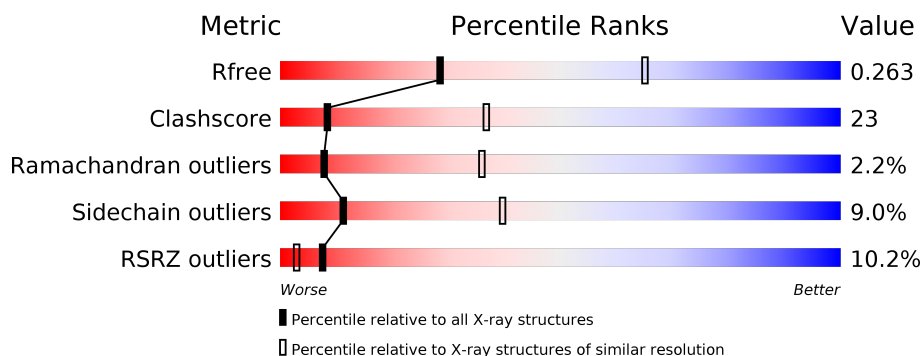
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.99 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))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	T	18	<div> <div>6%</div> <div>28%</div> <div>61%</div> <div>11%</div> </div>
1	U	18	<div> <div>39%</div> <div>56%</div> <div>6%</div> </div>
2	B	138	<div> <div>9%</div> <div>51%</div> <div>28%</div> <div>5%</div> <div>17%</div> </div>
2	P	138	<div> <div>10%</div> <div>49%</div> <div>31%</div> <div>•</div> <div>17%</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	SO4	B	835	-	-	-	X
3	SO4	P	335	-	-	-	X
3	SO4	P	865	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2530 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 DNA chain called DNA (5'-D(\*CP\*TP\*GP\*GP\*GP\*AP\*CP\*CP\*AP\*TP\*GP\*GP\*TP\*CP\*CP\*CP\*AP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	U	18	Total	C	N	O	P	0	0	0
			365	174	69	105	17			
1	T	18	Total	C	N	O	P	0	0	0
			366	174	69	106	17			

- Molecule 2 is a protein called Protein sopB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	115	Total	C	N	O	S	0	0	0
			877	546	157	173	1			
2	P	115	Total	C	N	O	S	0	0	0
			877	546	157	173	1			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	135	MET	-	EXPRESSION TAG	UNP P62558
B	136	GLY	-	EXPRESSION TAG	UNP P62558
B	137	SER	-	EXPRESSION TAG	UNP P62558
B	138	SER	-	EXPRESSION TAG	UNP P62558
B	139	HIS	-	EXPRESSION TAG	UNP P62558
B	140	HIS	-	EXPRESSION TAG	UNP P62558
B	141	HIS	-	EXPRESSION TAG	UNP P62558
B	142	HIS	-	EXPRESSION TAG	UNP P62558
B	143	HIS	-	EXPRESSION TAG	UNP P62558
B	144	HIS	-	EXPRESSION TAG	UNP P62558
B	145	SER	-	EXPRESSION TAG	UNP P62558
B	146	SER	-	EXPRESSION TAG	UNP P62558
B	147	GLY	-	EXPRESSION TAG	UNP P62558
B	148	LEU	-	EXPRESSION TAG	UNP P62558
B	149	VAL	-	EXPRESSION TAG	UNP P62558

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Chain	Residue	Modelled	Actual	Comment	Reference
B	150	PRO	-	EXPRESSION TAG	UNP P62558
B	151	ARG	-	EXPRESSION TAG	UNP P62558
B	152	GLY	-	EXPRESSION TAG	UNP P62558
B	153	SER	-	EXPRESSION TAG	UNP P62558
B	154	HIS	-	EXPRESSION TAG	UNP P62558
B	255	ASP	GLU	CONFLICT	UNP P62558
P	135	MET	-	EXPRESSION TAG	UNP P62558
P	136	GLY	-	EXPRESSION TAG	UNP P62558
P	137	SER	-	EXPRESSION TAG	UNP P62558
P	138	SER	-	EXPRESSION TAG	UNP P62558
P	139	HIS	-	EXPRESSION TAG	UNP P62558
P	140	HIS	-	EXPRESSION TAG	UNP P62558
P	141	HIS	-	EXPRESSION TAG	UNP P62558
P	142	HIS	-	EXPRESSION TAG	UNP P62558
P	143	HIS	-	EXPRESSION TAG	UNP P62558
P	144	HIS	-	EXPRESSION TAG	UNP P62558
P	145	SER	-	EXPRESSION TAG	UNP P62558
P	146	SER	-	EXPRESSION TAG	UNP P62558
P	147	GLY	-	EXPRESSION TAG	UNP P62558
P	148	LEU	-	EXPRESSION TAG	UNP P62558
P	149	VAL	-	EXPRESSION TAG	UNP P62558
P	150	PRO	-	EXPRESSION TAG	UNP P62558
P	151	ARG	-	EXPRESSION TAG	UNP P62558
P	152	GLY	-	EXPRESSION TAG	UNP P62558
P	153	SER	-	EXPRESSION TAG	UNP P62558
P	154	HIS	-	EXPRESSION TAG	UNP P62558
P	255	ASP	GLU	CONFLICT	UNP P62558

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



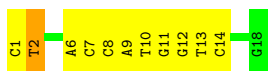
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	P	1	Total	O	S	0	0
			5	4	1		
3	P	1	Total	O	S	0	0
			5	4	1		
3	P	1	Total	O	S	0	0
			5	4	1		
3	P	1	Total	O	S	0	0
			5	4	1		
3	P	1	Total	O	S	0	0
			5	4	1		

### 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 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.

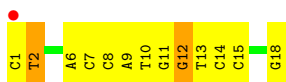
- Molecule 1: DNA (5'-D(\*CP\*TP\*GP\*GP\*GP\*AP\*CP\*CP\*AP\*TP\*GP\*GP\*TP\*CP\*CP\*CP\*AP\*G)-3')

Chain U: 



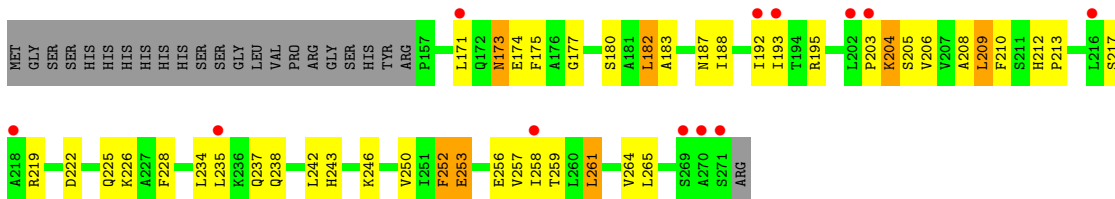
- Molecule 1: DNA (5'-D(\*CP\*TP\*GP\*GP\*GP\*AP\*CP\*CP\*AP\*TP\*GP\*GP\*TP\*CP\*CP\*CP\*AP\*G)-3')

Chain T: 



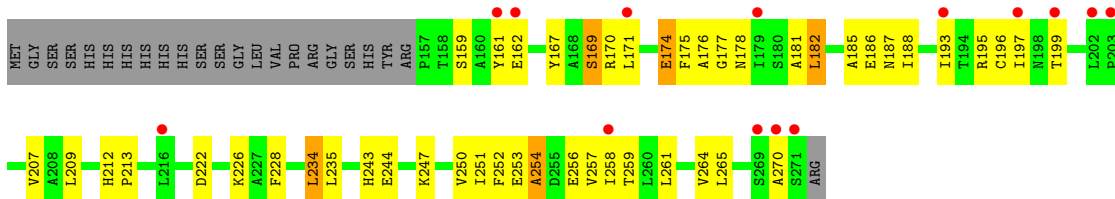
- Molecule 2: Protein sopB

Chain B: 



- Molecule 2: Protein sopB

Chain P: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	200.46Å 200.46Å 200.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.23 – 2.99 100.23 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.5 (100.23-2.99) 98.6 (100.23-2.99)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.233 , 0.268 0.233 , 0.263	Depositor DCC
$R_{free}$ test set	2666 reflections (11.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 73.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.031 for -l,-k,-h	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	2530	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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, 0.333 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: SO4

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	T	0.54	0/410	0.80	0/631
1	U	0.51	0/409	0.79	0/630
2	B	0.33	0/887	0.55	0/1194
2	P	0.34	0/887	0.60	0/1194
All	All	0.40	0/2593	0.66	0/3649

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	T	0	3
1	U	0	2
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	T	12	DG	Sidechain
1	T	18	DG	Sidechain
1	T	2	DT	Sidechain
1	U	12	DG	Sidechain
1	U	2	DT	Sidechain

## 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	T	366	0	203	22	0
1	U	365	0	200	14	0
2	B	877	0	892	41	0
2	P	877	0	892	37	0
3	B	15	0	0	1	0
3	P	30	0	0	0	0
All	All	2530	0	2187	107	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 23.

All (107) 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:T:6:DA:H2''	1:T:7:DC:H5''	1.37	1.03
1:T:11:DG:H2''	1:T:12:DG:C5'	1.92	0.97
1:T:11:DG:H2''	1:T:12:DG:H5''	1.52	0.89
1:T:6:DA:C2'	1:T:7:DC:H5''	2.02	0.88
2:B:204:LYS:H	2:B:204:LYS:HD3	1.40	0.87
1:T:11:DG:C2'	1:T:12:DG:H5''	2.07	0.83
1:T:11:DG:H2''	1:T:12:DG:H5'	1.61	0.82
1:U:6:DA:H2''	1:U:7:DC:C5'	2.14	0.78
1:U:10:DT:H2''	1:U:11:DG:C8	2.18	0.77
2:B:238:GLN:HE22	2:P:270:ALA:HB1	1.49	0.77
1:T:6:DA:H2''	1:T:7:DC:C5'	2.12	0.76
1:T:10:DT:H2''	1:T:11:DG:C8	2.22	0.74
2:B:238:GLN:NE2	2:P:270:ALA:HB1	2.03	0.74
2:P:228:PHE:CZ	2:P:265:LEU:HD21	2.23	0.72
1:U:6:DA:H2''	1:U:7:DC:H5'	1.74	0.69
2:B:264:VAL:HG13	2:B:265:LEU:HD22	1.74	0.69
2:B:258:ILE:HG13	2:B:259:THR:N	2.09	0.68
2:P:188:ILE:HD12	2:P:188:ILE:O	1.94	0.67
2:P:212:HIS:ND1	2:P:213:PRO:HD2	2.10	0.67
1:U:6:DA:C2'	1:U:7:DC:H5''	2.25	0.67
1:T:11:DG:N7	2:B:219:ARG:NH1	2.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:258:ILE:HD12	2:P:259:THR:N	2.11	0.65
2:B:237:GLN:HG3	2:P:234:LEU:HD11	1.79	0.64
2:P:193:ILE:O	2:P:197:ILE:HG12	1.97	0.63
1:U:6:DA:H1'	1:U:7:DC:H5''	1.80	0.63
1:U:6:DA:H2''	1:U:7:DC:H5''	1.81	0.62
2:P:222:ASP:OD1	2:P:226:LYS:HE3	1.99	0.62
2:P:167:TYR:HB3	2:P:197:ILE:HD11	1.83	0.60
2:P:171:LEU:CD1	2:P:177:GLY:HA2	2.32	0.59
1:U:13:DT:H2''	1:U:14:DC:H5'	1.85	0.59
2:B:212:HIS:ND1	2:B:213:PRO:HD2	2.18	0.59
2:P:209:LEU:HD12	2:P:243:HIS:NE2	2.17	0.59
2:P:161:TYR:CE1	2:P:207:VAL:HG21	2.38	0.59
2:B:171:LEU:HG	2:B:182:LEU:HD12	1.84	0.58
2:B:222:ASP:OD1	2:B:226:LYS:HE3	2.04	0.58
2:B:252:PHE:N	2:B:252:PHE:CD2	2.70	0.57
2:P:188:ILE:HD11	2:P:193:ILE:HD11	1.86	0.57
2:B:195:ARG:HA	2:B:222:ASP:OD2	2.04	0.57
1:T:1:DC:C6	1:T:2:DT:H72	2.40	0.56
1:T:13:DT:H2''	1:T:14:DC:H5'	1.88	0.56
2:B:209:LEU:HD12	2:B:243:HIS:CE1	2.41	0.55
2:P:171:LEU:HD11	2:P:177:GLY:HA2	1.88	0.55
1:T:1:DC:H2'	1:T:2:DT:C7	2.37	0.55
2:P:195:ARG:HA	2:P:222:ASP:OD2	2.06	0.55
2:B:188:ILE:CD1	2:B:192:ILE:HG21	2.37	0.55
2:P:265:LEU:HD22	2:P:265:LEU:H	1.72	0.54
1:T:8:DC:H2''	1:T:9:DA:C8	2.44	0.53
1:U:1:DC:H2''	1:U:2:DT:O5'	2.09	0.53
2:B:242:LEU:HD12	2:B:261:LEU:HD13	1.89	0.53
2:P:228:PHE:HE2	2:P:234:LEU:HD13	1.74	0.53
1:T:14:DC:H5'	1:T:14:DC:H6	1.72	0.53
2:P:209:LEU:HD12	2:P:243:HIS:CE1	2.43	0.53
2:P:244:GLU:O	2:P:247:LYS:HB3	2.09	0.52
1:U:6:DA:C1'	1:U:7:DC:H5''	2.40	0.52
2:P:234:LEU:HD21	2:P:264:VAL:HG11	1.91	0.52
1:T:1:DC:H2'	1:T:2:DT:H72	1.91	0.52
2:B:253:GLU:N	2:B:253:GLU:OE1	2.42	0.51
2:B:204:LYS:H	2:B:204:LYS:CD	2.10	0.51
1:U:1:DC:C6	1:U:2:DT:H72	2.45	0.51
2:B:219:ARG:NH2	3:B:836:SO4:S	2.83	0.51
2:B:238:GLN:NE2	2:B:264:VAL:HB	2.25	0.51
2:P:186:GLU:HB2	2:P:188:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:253:GLU:OE1	2:P:253:GLU:N	2.45	0.50
1:U:8:DC:H2''	1:U:9:DA:C8	2.48	0.48
1:T:10:DT:OP1	2:B:217:SER:OG	2.29	0.48
2:P:252:PHE:HA	2:P:256:GLU:OE1	2.14	0.47
1:T:10:DT:H2''	1:T:11:DG:H8	1.73	0.47
2:B:171:LEU:HD22	2:B:177:GLY:HA2	1.96	0.47
2:P:159:SER:OG	2:P:162:GLU:HG3	2.15	0.46
2:B:257:VAL:O	2:B:261:LEU:HB2	2.15	0.46
2:B:246:LYS:HA	2:B:250:VAL:O	2.16	0.46
2:B:188:ILE:HD13	2:B:192:ILE:HG21	1.97	0.46
2:B:209:LEU:HD12	2:B:243:HIS:NE2	2.31	0.46
2:P:209:LEU:HD23	2:P:257:VAL:HG13	1.99	0.45
1:T:14:DC:C6	1:T:14:DC:H5'	2.52	0.45
2:B:188:ILE:HD11	2:B:192:ILE:HG21	1.99	0.45
2:B:228:PHE:CE2	2:B:265:LEU:HD21	2.52	0.45
2:P:171:LEU:HD13	2:P:177:GLY:HA2	1.98	0.45
2:P:178:ASN:OD1	2:P:181:ALA:N	2.46	0.44
2:P:167:TYR:CE1	2:P:193:ILE:HD13	2.52	0.44
2:P:196:CYS:O	2:P:199:THR:HB	2.18	0.44
2:P:174:GLU:HB3	2:P:175:PHE:CE1	2.53	0.43
2:B:238:GLN:HB3	2:B:261:LEU:HD12	2.00	0.43
2:B:183:ALA:HA	2:B:193:ILE:HD11	2.00	0.43
1:T:11:DG:C1'	1:T:12:DG:H5''	2.48	0.43
2:B:171:LEU:HA	2:B:171:LEU:HD23	1.82	0.43
1:U:1:DC:H2'	1:U:2:DT:H72	1.99	0.43
2:B:228:PHE:CZ	2:B:265:LEU:CD2	3.01	0.42
2:B:252:PHE:HB3	2:B:256:GLU:OE1	2.20	0.42
2:B:209:LEU:HD23	2:B:257:VAL:HG13	2.02	0.42
1:T:11:DG:OP2	2:B:219:ARG:HB2	2.20	0.42
1:U:1:DC:H2'	1:U:2:DT:C7	2.50	0.42
2:B:203:PRO:HB2	2:B:206:VAL:HG23	2.02	0.42
2:B:237:GLN:O	2:B:238:GLN:C	2.57	0.42
2:B:238:GLN:HG3	2:B:264:VAL:HG11	2.02	0.42
2:P:169:SER:OG	2:P:170:ARG:N	2.53	0.41
2:P:182:LEU:O	2:P:185:ALA:HB3	2.20	0.41
2:P:171:LEU:HB2	2:P:182:LEU:HD12	2.02	0.41
1:T:14:DC:H2''	1:T:15:DC:O5'	2.21	0.41
1:U:1:DC:H3'	2:B:180:SER:OG	2.20	0.41
1:T:7:DC:H2''	1:T:8:DC:O5'	2.21	0.41
2:B:208:ALA:O	2:B:210:PHE:N	2.54	0.41
2:P:250:VAL:HG12	2:P:251:ILE:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:ASN:O	2:B:175:PHE:N	2.54	0.40
2:P:253:GLU:O	2:P:254:ALA:C	2.59	0.40
2:B:261:LEU:HA	2:B:261:LEU:HD12	1.90	0.40
2:P:182:LEU:CD2	2:P:186:GLU:HG2	2.51	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	
2	B	113/138 (82%)	98 (87%)	13 (12%)	2 (2%)	10	43
2	P	113/138 (82%)	98 (87%)	12 (11%)	3 (3%)	6	30
All	All	226/276 (82%)	196 (87%)	25 (11%)	5 (2%)	8	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	174	GLU
2	P	174	GLU
2	P	176	ALA
2	P	254	ALA
2	B	209	LEU

### 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	
2	B	94/115 (82%)	83 (88%)	11 (12%)	6	25
2	P	94/115 (82%)	88 (94%)	6 (6%)	20	57
All	All	188/230 (82%)	171 (91%)	17 (9%)	11	40

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	173	ASN
2	B	182	LEU
2	B	187	ASN
2	B	204	LYS
2	B	205	SER
2	B	225	GLN
2	B	234	LEU
2	B	235	LEU
2	B	252	PHE
2	B	253	GLU
2	B	261	LEU
2	P	169	SER
2	P	182	LEU
2	P	187	ASN
2	P	234	LEU
2	P	235	LEU
2	P	261	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	172	GLN
2	B	187	ASN
2	B	238	GLN
2	P	165	GLN
2	P	187	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 ⓘ

9 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	$\# Z  > 2$
3	SO4	B	835	-	4,4,4	0.37	0	6,6,6	0.09	0
3	SO4	B	836	-	4,4,4	0.29	0	6,6,6	0.16	0
3	SO4	B	936	-	4,4,4	0.32	0	6,6,6	0.07	0
3	SO4	P	273	-	4,4,4	0.29	0	6,6,6	0.20	0
3	SO4	P	274	-	4,4,4	0.35	0	6,6,6	0.06	0
3	SO4	P	335	-	4,4,4	0.36	0	6,6,6	0.09	0
3	SO4	P	435	-	4,4,4	0.37	0	6,6,6	0.09	0
3	SO4	P	865	-	4,4,4	0.39	0	6,6,6	0.09	0
3	SO4	P	965	-	4,4,4	0.40	0	6,6,6	0.08	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	SO4	B	835	-	-	0/0/0/0	0/0/0/0
3	SO4	B	836	-	-	0/0/0/0	0/0/0/0
3	SO4	B	936	-	-	0/0/0/0	0/0/0/0
3	SO4	P	273	-	-	0/0/0/0	0/0/0/0
3	SO4	P	274	-	-	0/0/0/0	0/0/0/0
3	SO4	P	335	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	P	435	-	-	0/0/0/0	0/0/0/0
3	SO4	P	865	-	-	0/0/0/0	0/0/0/0
3	SO4	P	965	-	-	0/0/0/0	0/0/0/0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	836	SO4	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

### 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	T	18/18 (100%)	1.12	1 (5%) 25 10	41, 51, 58, 61	0
1	U	18/18 (100%)	1.11	0 100 100	42, 50, 60, 60	0
2	B	115/138 (83%)	0.93	12 (10%) 7 3	47, 71, 102, 140	0
2	P	115/138 (83%)	0.97	14 (12%) 5 2	45, 69, 95, 129	0
All	All	266/312 (85%)	0.97	27 (10%) 7 3	41, 67, 100, 140	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	270	ALA	5.1
2	B	269	SER	3.5
2	P	271	SER	3.0
2	P	269	SER	3.0
2	P	270	ALA	3.0
2	P	258	ILE	2.7
2	B	258	ILE	2.6
2	P	161	TYR	2.5
2	B	216	LEU	2.5
2	B	202	LEU	2.4
2	B	203	PRO	2.4
2	P	197	ILE	2.3
2	B	218	ALA	2.3
2	B	171	LEU	2.3
2	B	192	ILE	2.3
1	T	1	DC	2.2
2	B	271	SER	2.2
2	P	162	GLU	2.2
2	P	216	LEU	2.2
2	B	193	ILE	2.2
2	P	203	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	235	LEU	2.1
2	P	179	ILE	2.1
2	P	171	LEU	2.1
2	P	199	THR	2.1
2	P	193	ILE	2.1
2	P	202	LEU	2.1

## 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	SO4	B	835	5/5	0.80	0.99	8.23	150,150,151,151	0
3	SO4	P	865	5/5	0.86	0.64	5.25	144,145,146,146	0
3	SO4	P	335	5/5	0.81	0.42	3.07	154,154,155,155	0
3	SO4	P	274	5/5	0.95	0.30	0.62	84,86,87,88	0
3	SO4	B	936	5/5	0.96	0.28	0.22	80,81,83,84	0
3	SO4	P	273	5/5	0.96	0.28	-0.09	81,81,84,85	0
3	SO4	B	836	5/5	0.97	0.26	-0.65	78,79,81,82	0
3	SO4	P	435	5/5	0.88	0.23	-2.32	138,138,138,139	0
3	SO4	P	965	5/5	0.78	0.13	-	160,161,162,162	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.