



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 03:30 AM GMT

PDB ID : 4EEC  
Title : Crystal Structure of the glycopeptide antibiotic sulfotransferase StaL complexed with A3P and desulfo-A47934.  
Authors : Shi, R.; Cygler, M.  
Deposited on : 2012-03-28  
Resolution : 2.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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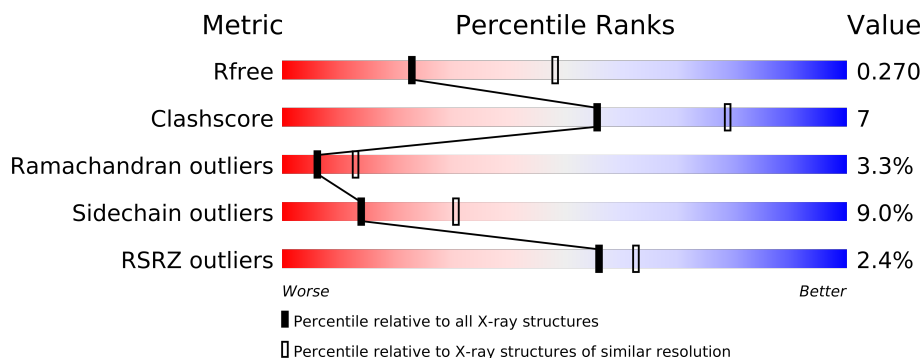
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.70 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))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	286	
1	B	286	
2	C	7	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3899 atoms, of which 0 are hydrogen and 0 are deuterium.

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 StaL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1937	1228	333	363	13			
1	B	242	Total	C	N	O	S	0	0	0
			1839	1162	315	350	12			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	INITIATING METHIONINE	UNP Q8KLM3
A	-14	GLY	-	EXPRESSION TAG	UNP Q8KLM3
A	-13	SER	-	EXPRESSION TAG	UNP Q8KLM3
A	-12	SER	-	EXPRESSION TAG	UNP Q8KLM3
A	-11	HIS	-	EXPRESSION TAG	UNP Q8KLM3
A	-10	HIS	-	EXPRESSION TAG	UNP Q8KLM3
A	-9	HIS	-	EXPRESSION TAG	UNP Q8KLM3
A	-8	HIS	-	EXPRESSION TAG	UNP Q8KLM3
A	-7	HIS	-	EXPRESSION TAG	UNP Q8KLM3
A	-6	HIS	-	EXPRESSION TAG	UNP Q8KLM3
A	-5	SER	-	EXPRESSION TAG	UNP Q8KLM3
A	-4	SER	-	EXPRESSION TAG	UNP Q8KLM3
A	-3	GLY	-	EXPRESSION TAG	UNP Q8KLM3
A	-2	LEU	-	EXPRESSION TAG	UNP Q8KLM3
A	-1	VAL	-	EXPRESSION TAG	UNP Q8KLM3
A	0	PRO	-	EXPRESSION TAG	UNP Q8KLM3
A	1	ARG	-	EXPRESSION TAG	UNP Q8KLM3
A	2	GLY	-	EXPRESSION TAG	UNP Q8KLM3
A	3	SER	-	EXPRESSION TAG	UNP Q8KLM3
B	-15	MET	-	INITIATING METHIONINE	UNP Q8KLM3
B	-14	GLY	-	EXPRESSION TAG	UNP Q8KLM3
B	-13	SER	-	EXPRESSION TAG	UNP Q8KLM3
B	-12	SER	-	EXPRESSION TAG	UNP Q8KLM3
B	-11	HIS	-	EXPRESSION TAG	UNP Q8KLM3
B	-10	HIS	-	EXPRESSION TAG	UNP Q8KLM3

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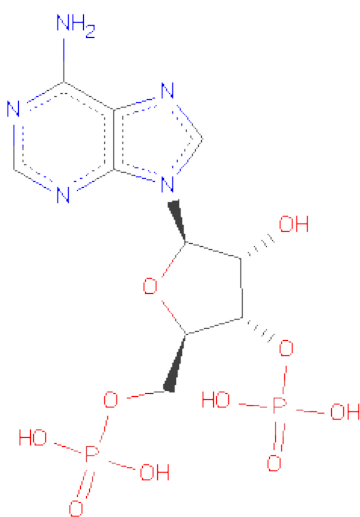
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	HIS	-	EXPRESSION TAG	UNP Q8KLM3
B	-8	HIS	-	EXPRESSION TAG	UNP Q8KLM3
B	-7	HIS	-	EXPRESSION TAG	UNP Q8KLM3
B	-6	HIS	-	EXPRESSION TAG	UNP Q8KLM3
B	-5	SER	-	EXPRESSION TAG	UNP Q8KLM3
B	-4	SER	-	EXPRESSION TAG	UNP Q8KLM3
B	-3	GLY	-	EXPRESSION TAG	UNP Q8KLM3
B	-2	LEU	-	EXPRESSION TAG	UNP Q8KLM3
B	-1	VAL	-	EXPRESSION TAG	UNP Q8KLM3
B	0	PRO	-	EXPRESSION TAG	UNP Q8KLM3
B	1	ARG	-	EXPRESSION TAG	UNP Q8KLM3
B	2	GLY	-	EXPRESSION TAG	UNP Q8KLM3
B	3	SER	-	EXPRESSION TAG	UNP Q8KLM3

- Molecule 2 is a protein called desulfo-A47934.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	7	Total	C	Cl	N	O	0	0	0
			86	58	3	7	18			

- Molecule 3 is ADENOSINE-3'-5'-DIPHOSPHATE (three-letter code: A3P) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total 3	O 3	0	0
4	B	7	Total 7	O 7	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.44Å 82.58Å 123.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 44.87 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.70) 99.4 (44.87-2.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.10 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.223 , 0.272 0.216 , 0.270	Depositor DCC
$R_{free}$ test set	773 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.5	Xtriage
Anisotropy	0.978	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 29.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 15490 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3899	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.24% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A3P, GHP, 3MY, 0UZ, 3FG, OMY

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	0.80	3/1985 (0.2%)	0.82	0/2701
1	B	0.71	0/1885	0.77	0/2566
All	All	0.76	3/3870 (0.1%)	0.80	0/5267

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	A	0	1
2	C	0	4
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	LYS	CE-NZ	7.28	1.67	1.49
1	A	256	GLU	CG-CD	5.63	1.60	1.51
1	A	256	GLU	CB-CG	5.30	1.62	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	MET	Peptide
2	C	401	GHP	Mainchain
2	C	404	GHP	Peptide

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Mol	Chain	Res	Type	Group
2	C	406	OMY	Mainchain,Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1937	0	0	13	0
1	B	1839	0	0	11	0
2	C	86	0	37	3	0
3	A	27	0	11	0	0
4	A	3	0	0	0	0
4	B	7	0	0	0	0
All	All	3899	0	48	26	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (26) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:33:THR:CG2	1:B:34:TRP:N	2.52	0.72
1:B:242:GLY:O	1:B:244:ASP:N	2.30	0.65
1:A:187:ASP:N	1:A:187:ASP:OD1	2.35	0.59
1:A:72:ARG:NH1	1:B:50:ASP:O	2.35	0.58
2:C:407:3FG:HG2	2:C:407:3FG:OXT	2.02	0.58
1:A:171:GLU:OE2	1:A:186:ARG:NH2	2.36	0.57
1:A:228:PHE:CD2	1:A:228:PHE:C	2.78	0.56
1:A:4:MET:SD	1:A:64:LEU:CD1	2.94	0.56
1:A:228:PHE:CD2	1:A:228:PHE:O	2.63	0.51
1:A:25:TYR:OH	1:A:185:GLY:N	2.44	0.50
1:B:187:ASP:OD1	1:B:187:ASP:N	2.45	0.49
1:B:114:ARG:O	1:B:118:GLU:N	2.45	0.49
1:B:32:GLU:O	1:B:33:THR:CB	2.60	0.49
1:A:110:VAL:O	1:A:114:ARG:N	2.46	0.48
1:A:211:LEU:O	1:A:212:GLY:C	2.53	0.47
2:C:402:3MY:CE1	2:C:404:GHP:C2	2.83	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:89:ILE:O	1:B:163:TYR:N	2.48	0.46
1:A:148:SER:O	1:A:150:HIS:N	2.48	0.46
1:B:25:TYR:OH	1:B:185:GLY:N	2.49	0.45
1:A:148:SER:O	1:A:149:VAL:C	2.55	0.45
1:B:185:GLY:O	1:B:186:ARG:CB	2.65	0.44
2:C:401:GHP:C2	2:C:403:3FG:CG1	2.91	0.44
1:B:106:PRO:O	1:B:108:GLU:N	2.51	0.43
1:A:16:HIS:O	1:A:20:CYS:N	2.52	0.42
1:A:205:GLU:OE1	1:A:229:VAL:CG2	2.69	0.41
1:B:191:ASP:O	1:B:195:ASN:N	2.55	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	247/286 (86%)	226 (92%)	15 (6%)	6 (2%)	9	22
1	B	238/286 (83%)	203 (85%)	25 (10%)	10 (4%)	4	8
All	All	485/572 (85%)	429 (88%)	40 (8%)	16 (3%)	6	13

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	ARG
1	B	33	THR
1	B	110	VAL
1	B	243	ASP
1	A	105	ILE
1	A	149	VAL
1	A	185	GLY
1	A	212	GLY
1	B	186	ARG
1	A	243	ASP

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Mol	Chain	Res	Type
1	B	185	GLY
1	B	207	ARG
1	B	103	LYS
1	B	107	PRO
1	B	105	ILE
1	B	242	GLY

### 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	195/234 (83%)	178 (91%)	17 (9%)	15	33
1	B	183/234 (78%)	166 (91%)	17 (9%)	13	29
All	All	378/468 (81%)	344 (91%)	34 (9%)	14	31

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	SER
1	A	49	ARG
1	A	72	ARG
1	A	97	LEU
1	A	98	SER
1	A	135	GLU
1	A	162	ARG
1	A	171	GLU
1	A	186	ARG
1	A	187	ASP
1	A	198	LEU
1	A	199	GLU
1	A	201	MET
1	A	207	ARG
1	A	226	LEU
1	A	244	ASP
1	A	245	ILE
1	B	3	SER
1	B	32	GLU

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Mol	Chain	Res	Type
1	B	76	ARG
1	B	80	GLU
1	B	90	ARG
1	B	98	SER
1	B	108	GLU
1	B	143	ARG
1	B	167	ARG
1	B	171	GLU
1	B	186	ARG
1	B	187	ASP
1	B	205	GLU
1	B	206	GLU
1	B	208	SER
1	B	237	SER
1	B	244	ASP

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

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

7 non-standard protein/DNA/RNA residues 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	GHP	C	401	2	11,11,12	5.72	2 (18%)	12,14,16	3.64	3 (25%)
2	3MY	C	402	2	13,13,14	5.17	3 (23%)	15,17,19	2.09	2 (13%)
2	3FG	C	403	2	12,12,13	4.89	3 (25%)	14,16,18	4.84	1 (7%)
2	GHP	C	404	2	11,11,12	6.45	3 (27%)	12,14,16	7.84	1 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	0UZ	C	405	2	12,12,13	5.92	4 (33%)	14,16,18	7.85	1 (7%)
2	OMY	C	406	2	14,14,15	6.07	4 (28%)	17,19,21	1.91	4 (23%)
2	3FG	C	407	2	13,13,13	1.40	3 (23%)	18,18,18	1.33	3 (16%)

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	GHP	C	401	2	-	0/4/6/8	0/1/1/1
2	3MY	C	402	2	-	0/4/6/8	0/1/1/1
2	3FG	C	403	2	-	0/4/6/8	0/1/1/1
2	GHP	C	404	2	-	0/4/6/8	0/1/1/1
2	0UZ	C	405	2	-	0/4/6/8	0/1/1/1
2	OMY	C	406	2	-	0/8/10/12	0/1/1/1
2	3FG	C	407	2	-	0/8/8/8	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	404	GHP	O-C	20.85	1.25	1.11
2	C	406	OMY	O-C	19.30	1.24	1.11
2	C	405	0UZ	O-C	19.00	1.24	1.11
2	C	401	GHP	O-C	18.58	1.24	1.11
2	C	402	3MY	O-C	17.95	1.23	1.11
2	C	403	3FG	O-C	16.19	1.22	1.11
2	C	406	OMY	CZ-CE1	10.76	1.50	1.39
2	C	405	0UZ	CA-C	6.26	1.55	1.48
2	C	403	3FG	CA-C	3.48	1.52	1.48
2	C	404	GHP	CA-C	3.37	1.52	1.48
2	C	406	OMY	CE1-CL	3.06	1.81	1.73
2	C	402	3MY	CE2-CL	3.00	1.81	1.73
2	C	406	OMY	CA-C	2.92	1.53	1.48
2	C	403	3FG	CB-CA	-2.75	1.48	1.52
2	C	402	3MY	CA-C	2.65	1.53	1.48
2	C	401	GHP	CA-C	2.65	1.51	1.48
2	C	405	0UZ	C3-CL3	2.55	1.80	1.73
2	C	404	GHP	C1-CA	-2.36	1.49	1.52
2	C	407	3FG	CG1-CB	2.35	1.43	1.38
2	C	405	0UZ	C1-CA	-2.33	1.49	1.52
2	C	407	3FG	CG2-CB	2.22	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	407	3FG	CG1-CD1	2.04	1.42	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	405	0UZ	C-CA-N	29.17	116.57	113.27
2	C	404	GHP	C-CA-N	-27.05	110.20	113.27
2	C	403	3FG	C-CA-N	-17.98	111.23	113.27
2	C	401	GHP	C-CA-N	-11.63	111.95	113.27
2	C	402	3MY	C-CA-N	-7.05	106.78	113.83
2	C	406	OMY	CG-CB-CA	-4.95	104.42	111.75
2	C	406	OMY	CD1-CE1-CZ	-4.10	119.00	121.13
2	C	401	GHP	C2-C1-CA	-3.44	115.84	120.60
2	C	407	3FG	CG2-CB-CA	2.97	123.35	119.22
2	C	407	3FG	OXT-C-CA	2.90	121.09	113.75
2	C	401	GHP	C6-C1-CA	2.86	124.55	120.60
2	C	407	3FG	CB-CA-C	2.72	116.42	110.14
2	C	406	OMY	CD1-CE1-CL	2.63	122.69	118.55
2	C	402	3MY	CG-CB-CA	-2.28	109.03	114.42
2	C	406	OMY	CB-CA-N	2.04	112.28	109.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	A3P	A	301	-	29,29,29	1.09	2 (6%)	45,45,45	2.32	9 (20%)

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	A3P	A	301	-	-	0/15/31/31	0/1/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	A3P	C5-C4	3.65	1.48	1.40
3	A	301	A3P	O4'-C1'	2.32	1.44	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	A3P	O4'-C1'-N9	8.28	116.14	108.44
3	A	301	A3P	N3-C2-N1	-6.22	123.51	128.71
3	A	301	A3P	N3-C4-N9	6.02	136.30	125.43
3	A	301	A3P	O4'-C1'-C2'	-3.80	100.94	106.77
3	A	301	A3P	C5-C4-N3	-3.37	118.36	125.70
3	A	301	A3P	C4-C5-N7	-3.34	106.66	109.52
3	A	301	A3P	C8-N9-C4	2.73	108.98	106.90
3	A	301	A3P	C2-N3-C4	2.36	120.73	114.01
3	A	301	A3P	O6P-P2-O5P	2.23	116.31	107.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	253/286 (88%)	-0.03	2 (0%) 83 87	38, 59, 94, 105	0
1	B	242/286 (84%)	0.04	10 (4%) 35 40	39, 66, 114, 127	0
2	C	6/7 (85%)	0.22	0 100 100	65, 75, 98, 106	0
All	All	501/579 (86%)	0.00	12 (2%) 56 62	38, 61, 103, 127	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	215	THR	4.9
1	B	110	VAL	3.5
1	B	201	MET	3.4
1	B	2	GLY	3.3
1	A	214	GLU	3.1
1	B	102	MET	2.5
1	B	22	LEU	2.5
1	B	120	PHE	2.4
1	B	103	LYS	2.3
1	B	96	MET	2.1
1	B	99	LEU	2.1
1	B	34	TRP	2.0

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

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	3MY	C	402	13/14	0.23	2.92	66,68,72,72	0
2	GHP	C	401	11/12	0.18	1.14	62,64,65,65	0
2	3FG	C	403	12/13	0.16	-0.16	70,74,76,80	0
2	0UZ	C	405	12/13	0.16	-0.51	93,97,100,103	0
2	GHP	C	404	11/12	0.11	-1.76	80,82,85,86	0
2	3FG	C	407	13/13	0.24	-	104,105,107,108	0
2	OMY	C	406	14/15	0.27	-	93,97,101,101	0

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	A3P	A	301	27/27	0.14	-0.27	52,58,61,62	0

### 6.5 Other polymers

There are no such residues in this entry.