



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:43 AM UTC

PDB ID : 4EEC / pdb_00004eec
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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

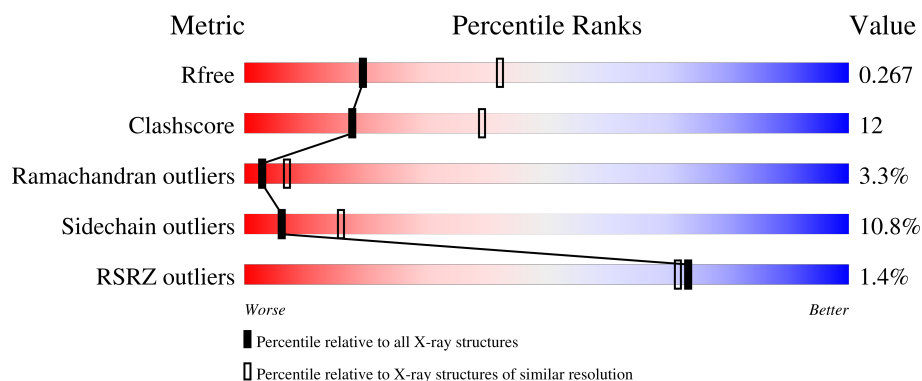
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	286	<div> <div></div> <div>62% 21% 6% 12%</div> </div>
1	B	286	<div> <div></div> <div>63% 18% . . 15%</div> </div>
2	C	7	<div> <div></div> <div>14% 57% 29%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3899 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 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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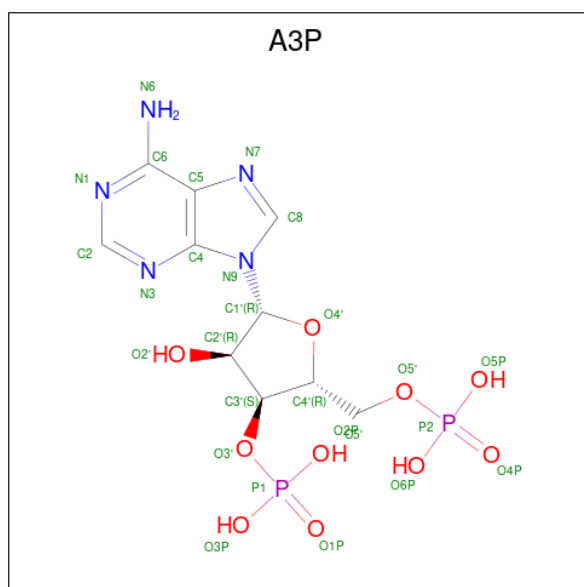
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	HIS	-	expression tag	UNP Q8KLM3
B	-8	HIS	-	expression tag	UNP Q8KLM3
B	-7	HIS	-	expression tag	UNP Q8KLM3
B	-6	HIS	-	expression tag	UNP Q8KLM3
B	-5	SER	-	expression tag	UNP Q8KLM3
B	-4	SER	-	expression 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 (CCD ID: A3P) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

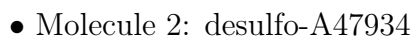


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- 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

- Molecule 1: StaL



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.44Å 82.58Å 123.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.70) 99.3 (50.00-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.10 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.223 , 0.272 0.215 , 0.267	Depositor DCC
R_{free} test set	778 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.978	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3899	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GHP, 0UZ, A3P, 3MY, 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	0.97	2/1985 (0.1%)	1.16	9/2701 (0.3%)
1	B	0.89	0/1885	1.04	2/2566 (0.1%)
All	All	0.93	2/3870 (0.1%)	1.10	11/5267 (0.2%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	LYS	CE-NZ	5.97	1.67	1.49
1	A	57	ASP	CA-C	5.15	1.59	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	PHE	N-CA-C	7.53	120.44	111.33
1	B	158	VAL	N-CA-C	6.90	117.77	108.11
1	A	34	TRP	CA-C-N	-6.78	112.92	120.45
1	A	34	TRP	C-N-CA	-6.78	112.92	120.45
1	A	208	SER	N-CA-C	-5.47	105.00	110.97
1	A	7	ILE	CB-CA-C	-5.37	106.56	112.68
1	A	18	LEU	N-CA-C	-5.24	105.57	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	LEU	N-CA-C	5.24	119.77	112.90
1	A	93	ARG	N-CA-C	-5.16	105.84	111.82
1	B	257	THR	N-CA-C	5.10	118.27	110.36
1	A	63	LEU	N-CA-C	5.03	116.60	108.41

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
2	C	406	OMY	Mainchain,Peptide

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	1937	0	1823	50	0
1	B	1839	0	1713	40	0
2	C	86	0	37	5	0
3	A	27	0	11	1	0
4	A	3	0	0	0	0
4	B	7	0	0	1	0
All	All	3899	0	3584	92	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 12.

All (92) 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:21:MET:HE2	1:B:174:LEU:HD22	1.41	0.99
1:A:242:GLY:HA2	1:A:245:ILE:HG13	1.53	0.90
1:B:33:THR:HG23	1:B:34:TRP:H	1.35	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:PRO:HA	1:A:76:ARG:HD3	1.60	0.83
1:B:73:PRO:O	1:B:76:ARG:HB2	1.79	0.83
1:B:33:THR:CG2	1:B:34:TRP:H	1.92	0.83
1:A:205:GLU:OE1	1:A:229:VAL:HG22	1.82	0.80
1:B:185:GLY:O	1:B:186:ARG:HB2	1.85	0.77
1:B:21:MET:CE	1:B:174:LEU:HD22	2.14	0.77
1:B:114:ARG:HD3	1:B:245:ILE:HD11	1.67	0.74
1:B:186:ARG:HH11	1:B:186:ARG:HG3	1.53	0.72
1:A:49:ARG:HG3	2:C:402:3MY:CD2	2.21	0.71
1:B:33:THR:CG2	1:B:34:TRP:N	2.52	0.70
1:A:197:THR:HG23	1:A:198:LEU:HG	1.74	0.69
1:A:4:MET:SD	1:A:64:LEU:HD11	2.32	0.69
1:B:32:GLU:O	1:B:33:THR:HB	1.94	0.67
1:A:73:PRO:HA	1:A:76:ARG:CD	2.25	0.65
1:A:197:THR:CG2	1:A:198:LEU:HG	2.26	0.65
1:B:242:GLY:O	1:B:244:ASP:N	2.30	0.65
1:B:34:TRP:HB3	1:B:35:PRO:CD	2.30	0.62
1:A:242:GLY:CA	1:A:245:ILE:HG13	2.28	0.62
1:A:228:PHE:CD2	1:A:228:PHE:C	2.78	0.61
1:B:170:PRO:HB2	1:B:193:VAL:HG11	1.81	0.61
1:A:21:MET:CE	1:A:193:VAL:HG22	2.32	0.59
1:A:5:CYS:HB2	1:A:63:LEU:HD23	1.83	0.58
2:C:407:3FG:OXT	2:C:407:3FG:HG2	2.02	0.58
1:A:72:ARG:NH1	1:B:50:ASP:O	2.35	0.58
1:A:171:GLU:OE2	1:A:186:ARG:NH2	2.36	0.57
1:A:69:THR:OG1	1:A:72:ARG:HG2	2.05	0.57
1:B:90:ARG:HB2	1:B:163:TYR:HB3	1.87	0.57
1:A:197:THR:HG22	1:A:199:GLU:H	1.70	0.56
1:B:21:MET:HE3	1:B:193:VAL:HG22	1.86	0.56
1:B:175:TRP:CD2	1:B:186:ARG:HG2	2.40	0.56
1:A:4:MET:SD	1:A:64:LEU:CD1	2.94	0.56
1:B:60:GLU:O	1:B:62:VAL:HG23	2.07	0.55
1:B:189:VAL:O	1:B:193:VAL:HG23	2.06	0.55
1:A:98:SER:HA	1:A:101:ARG:NH1	2.22	0.55
1:A:49:ARG:HG3	2:C:402:3MY:CE2	2.38	0.54
1:A:187:ASP:OD1	1:A:187:ASP:N	2.35	0.53
1:A:175:TRP:CE3	1:A:186:ARG:HG3	2.43	0.53
1:B:79:ARG:HD2	4:B:301:HOH:O	2.09	0.52
1:B:98:SER:HA	1:B:101:ARG:NH1	2.25	0.52
1:A:211:LEU:O	1:A:212:GLY:C	2.53	0.52
1:A:228:PHE:CD2	1:A:228:PHE:O	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:GLU:O	1:A:137:SER:HB2	2.10	0.51
1:A:25:TYR:OH	1:A:185:GLY:N	2.44	0.50
1:A:73:PRO:O	1:A:76:ARG:HB2	2.11	0.50
1:B:83:ALA:O	1:B:156:ALA:HA	2.10	0.50
1:A:148:SER:O	1:A:149:VAL:C	2.55	0.49
1:A:117:ALA:O	1:A:121:ILE:HG13	2.12	0.49
1:B:32:GLU:O	1:B:33:THR:CB	2.60	0.49
1:A:22:LEU:O	1:A:26:VAL:HG23	2.13	0.49
1:B:186:ARG:HH11	1:B:186:ARG:CG	2.24	0.48
1:A:31:VAL:O	1:A:204:MET:HE2	2.15	0.47
1:B:187:ASP:OD1	1:B:187:ASP:N	2.45	0.47
1:B:33:THR:HA	1:B:204:MET:HG2	1.96	0.46
1:A:106:PRO:HB2	1:A:108:GLU:OE2	2.15	0.46
1:A:175:TRP:CD2	1:A:186:ARG:HG3	2.49	0.46
2:C:402:3MY:CE1	2:C:404:GHP:C2	2.83	0.46
1:B:10:TYR:CG	1:B:11:PRO:HD2	2.50	0.46
1:A:148:SER:O	1:A:150:HIS:N	2.48	0.46
1:B:4:MET:HB3	1:B:82:THR:HA	1.98	0.45
1:A:197:THR:HG22	1:A:199:GLU:N	2.31	0.45
1:B:25:TYR:OH	1:B:185:GLY:N	2.49	0.45
1:A:241:MET:HG3	1:A:245:ILE:HD12	1.99	0.45
1:B:33:THR:HG22	1:B:34:TRP:N	2.30	0.45
1:B:34:TRP:HB3	1:B:35:PRO:HD3	1.99	0.45
1:A:249:TYR:HE2	1:A:253:LEU:HD22	1.82	0.44
1:B:20:CYS:SG	1:B:204:MET:HE1	2.57	0.44
1:A:93:ARG:O	1:A:97:LEU:HD22	2.17	0.44
2:C:401:GHP:C2	2:C:403:3FG:CG1	2.91	0.44
1:B:4:MET:HE2	1:B:4:MET:HB2	1.49	0.44
1:B:33:THR:HG23	1:B:204:MET:O	2.18	0.44
1:B:106:PRO:O	1:B:108:GLU:N	2.51	0.43
1:B:21:MET:HE2	1:B:174:LEU:CD2	2.29	0.43
1:A:17:TRP:HA	1:A:201:MET:HE1	2.01	0.43
1:A:202:ARG:HA	1:A:229:VAL:HG21	2.00	0.43
1:B:137:SER:OG	1:B:140:GLU:HB2	2.18	0.43
1:B:105:ILE:H	1:B:105:ILE:HG13	1.59	0.42
1:A:21:MET:HE3	1:A:193:VAL:HG22	1.99	0.42
1:A:15:GLY:O	1:A:19:ARG:HG3	2.19	0.42
1:A:72:ARG:HA	1:A:72:ARG:HE	1.83	0.42
1:B:238:LEU:HD23	1:B:238:LEU:HA	1.75	0.42
1:A:186:ARG:HA	1:A:189:VAL:HG23	2.02	0.42
1:A:92:PRO:HG3	1:A:138:TRP:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:HG3	1:A:229:VAL:CG2	2.50	0.41
1:B:20:CYS:C	1:B:196:CYS:SG	3.04	0.41
1:A:137:SER:O	1:A:138:TRP:C	2.64	0.41
1:A:4:MET:HB3	1:A:82:THR:HA	2.01	0.41
1:A:73:PRO:HA	1:A:76:ARG:NE	2.36	0.41
1:A:12:LYS:HD2	3:A:301:A3P:O6P	2.21	0.40
1:A:38:GLN:HA	1:A:38:GLN:OE1	2.21	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	247/286 (86%)	226 (92%)	15 (6%)	6 (2%)	4	12
1	B	238/286 (83%)	203 (85%)	25 (10%)	10 (4%)	2	4
All	All	485/572 (85%)	429 (88%)	40 (8%)	16 (3%)	3	7

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
1	B	185	GLY

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Mol	Chain	Res	Type
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%)	176 (90%)	19 (10%)	8	20
1	B	183/234 (78%)	161 (88%)	22 (12%)	5	12
All	All	378/468 (81%)	337 (89%)	41 (11%)	6	16

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	SER
1	A	49	ARG
1	A	76	ARG
1	A	97	LEU
1	A	98	SER
1	A	135	GLU
1	A	161	VAL
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

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Mol	Chain	Res	Type
1	A	265	LEU
1	B	3	SER
1	B	32	GLU
1	B	33	THR
1	B	64	LEU
1	B	76	ARG
1	B	80	GLU
1	B	90	ARG
1	B	97	LEU
1	B	98	SER
1	B	108	GLU
1	B	143	ARG
1	B	151	GLU
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	209	LYS
1	B	237	SER
1	B	244	ASP

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

Mol	Chain	Res	Type
1	A	261	HIS
1	B	43	HIS
1	B	61	GLN
1	B	141	ASN
1	B	261	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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	10,11,12	1.08	1 (10%)	11,14,16	1.45	2 (18%)
2	0UZ	C	405	2	11,12,13	1.78	3 (27%)	12,16,18	1.25	1 (8%)
2	OMY	C	406	2	12,14,15	3.45	2 (16%)	17,19,21	1.91	4 (23%)
2	3FG	C	403	2	11,12,13	1.40	1 (9%)	11,16,18	0.43	0
2	3MY	C	402	2	12,13,14	1.39	1 (8%)	12,17,19	0.91	0
2	GHP	C	404	2	10,11,12	1.44	1 (10%)	11,14,16	0.66	0
2	3FG	C	407	2	12,13,13	1.64	4 (33%)	14,18,18	1.16	2 (14%)

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	-	2/4/6/8	0/1/1/1
2	0UZ	C	405	2	-	0/4/6/8	0/1/1/1
2	OMY	C	406	2	-	1/9/10/12	0/1/1/1
2	3FG	C	403	2	-	0/4/6/8	0/1/1/1
2	3MY	C	402	2	-	2/5/6/8	0/1/1/1
2	GHP	C	404	2	-	0/4/6/8	0/1/1/1
2	3FG	C	407	2	-	6/8/8/8	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	406	OMY	CZ-CE1	10.91	1.50	1.39
2	C	403	3FG	CB-CA	-3.73	1.48	1.52
2	C	406	OMY	CE1-CL	3.30	1.81	1.73
2	C	402	3MY	CE2-CL	3.24	1.81	1.73
2	C	404	GHP	C1-CA	-3.20	1.49	1.52
2	C	405	0UZ	C1-CA	-3.16	1.49	1.52
2	C	405	0UZ	C3-CL3	2.76	1.80	1.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	407	3FG	CG1-CB	2.72	1.43	1.39
2	C	407	3FG	CG2-CB	2.56	1.42	1.39
2	C	405	0UZ	CA-C	2.49	1.55	1.51
2	C	401	GHP	C1-CA	-2.34	1.50	1.52
2	C	407	3FG	CG1-CD1	2.20	1.42	1.39
2	C	407	3FG	CG2-CD2	2.02	1.42	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	406	OMY	CG-CB-CA	-5.45	104.42	111.58
2	C	406	OMY	CD1-CE1-CZ	-3.31	119.00	120.92
2	C	401	GHP	C2-C1-CA	-3.08	115.84	120.64
2	C	407	3FG	CB-CA-C	2.93	116.42	110.10
2	C	406	OMY	CD1-CE1-CL	2.59	122.69	118.45
2	C	401	GHP	C6-C1-CA	2.52	124.55	120.64
2	C	407	3FG	CG2-CB-CA	2.32	123.35	119.79
2	C	406	OMY	O-C-CA	-2.23	119.03	124.77
2	C	405	0UZ	C4-C3-CL3	2.16	123.28	119.43

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	402	3MY	C-CA-CB-CG
2	C	407	3FG	C-CA-CB-CG2
2	C	401	GHP	C6-C1-CA-C
2	C	407	3FG	O-C-CA-N
2	C	407	3FG	C-CA-CB-CG1
2	C	407	3FG	OXT-C-CA-N
2	C	407	3FG	O-C-CA-CB
2	C	407	3FG	OXT-C-CA-CB
2	C	401	GHP	C2-C1-CA-C
2	C	402	3MY	CA-CB-CG-CD2
2	C	406	OMY	O-C-CA-CB

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	GHP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	403	3FG	1	0
2	C	402	3MY	3	0
2	C	404	GHP	1	0
2	C	407	3FG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	1.48	3 (10%)	44,45,45	2.13	14 (31%)

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	-	-	1/15/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	A3P	C5-C4	5.41	1.48	1.39
3	A	301	A3P	C5-C6	2.78	1.48	1.41
3	A	301	A3P	C8-N7	2.53	1.36	1.31

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	A3P	C5-C4-N3	-6.07	118.36	126.72
3	A	301	A3P	N3-C4-N9	5.37	136.30	127.17
3	A	301	A3P	O4'-C1'-N9	4.19	116.14	108.09
3	A	301	A3P	C2-N3-C4	3.65	120.73	111.83
3	A	301	A3P	C4-C5-N7	-3.43	106.66	110.58
3	A	301	A3P	C5-N7-C8	3.36	108.73	103.45
3	A	301	A3P	N3-C2-N1	-3.35	123.51	128.58
3	A	301	A3P	C4-N9-C8	3.09	108.98	105.74
3	A	301	A3P	O4'-C1'-C2'	-2.65	100.94	106.62
3	A	301	A3P	N9-C8-N7	-2.57	110.29	113.94
3	A	301	A3P	O6P-P2-O5P	2.27	116.31	107.80
3	A	301	A3P	C2-N1-C6	2.11	122.19	118.73
3	A	301	A3P	O6P-P2-O5'	-2.08	101.24	106.67
3	A	301	A3P	O3P-P1-O2P	2.00	115.31	107.80

There are no chirality outliers.

All (1) torsion outliers are listed below:

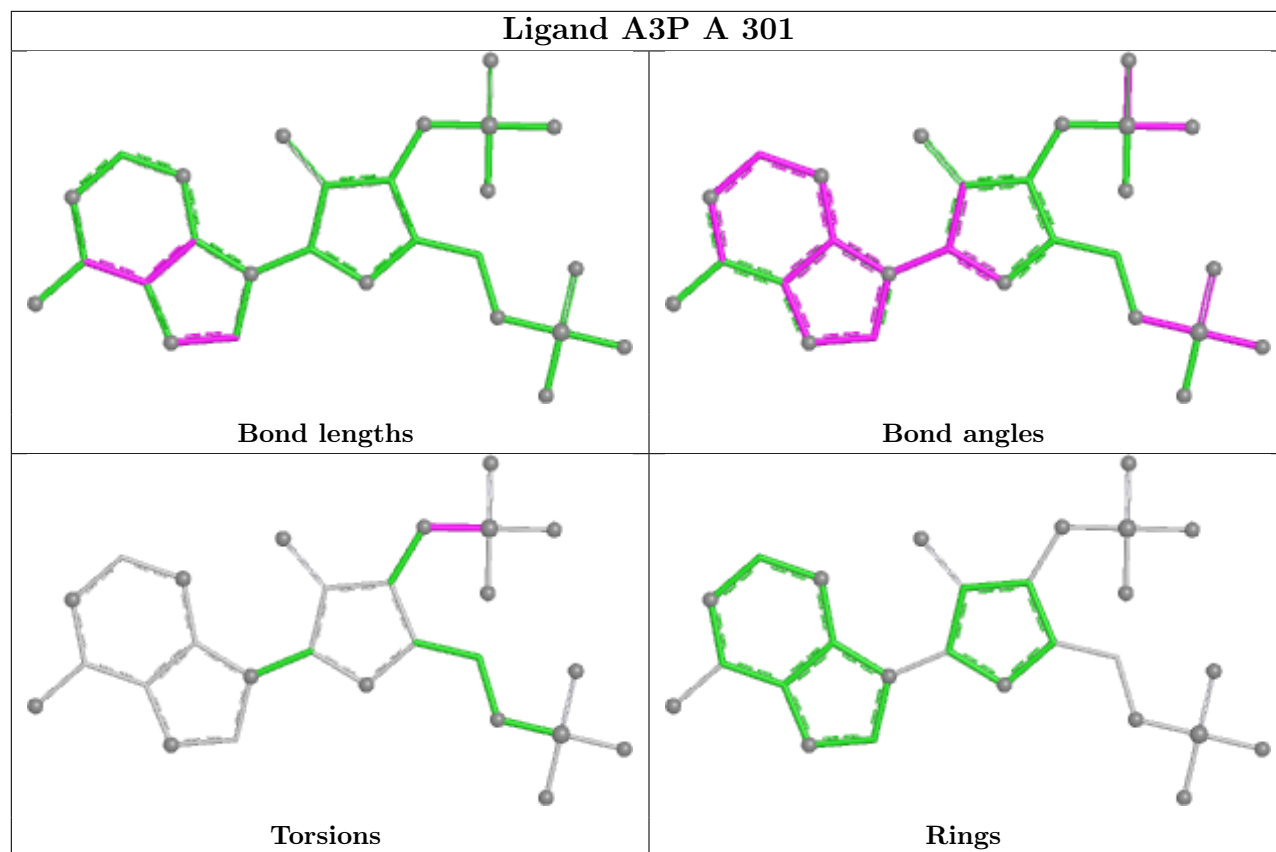
Mol	Chain	Res	Type	Atoms
3	A	301	A3P	C3'-O3'-P1-O1P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	A3P	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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, 95th 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 ²)	Q<0.9
1	A	253/286 (88%)	-0.04	3 (1%) 76 75	38, 59, 94, 105	0
1	B	242/286 (84%)	0.03	4 (1%) 69 67	39, 66, 114, 127	0
2	C	0/7	-	-	-	-
All	All	495/579 (85%)	-0.01	7 (1%) 73 72	38, 61, 103, 127	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	243	ASP	3.4
1	A	238	LEU	3.1
1	A	236	LYS	2.5
1	B	2	GLY	2.5
1	B	200	ARG	2.4
1	B	110	VAL	2.3
1	A	216	THR	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
2	3FG	C	407	13/13	0.15	0.15	104,105,107,108	0
2	OMY	C	406	14/15	0.71	0.11	93,97,101,101	0
2	OUZ	C	405	12/13	0.71	0.12	93,97,100,103	0
2	3MY	C	402	13/14	0.80	0.12	66,68,72,72	0
2	GHP	C	404	11/12	0.84	0.09	80,82,85,86	0
2	3FG	C	403	12/13	0.86	0.10	70,74,76,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GHP	C	401	11/12	0.94	0.07	62,64,65,65	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

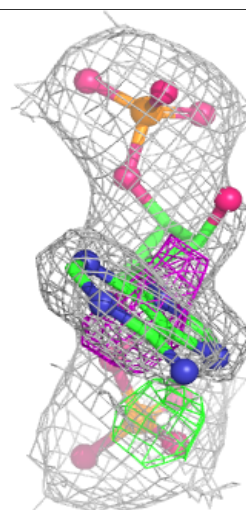
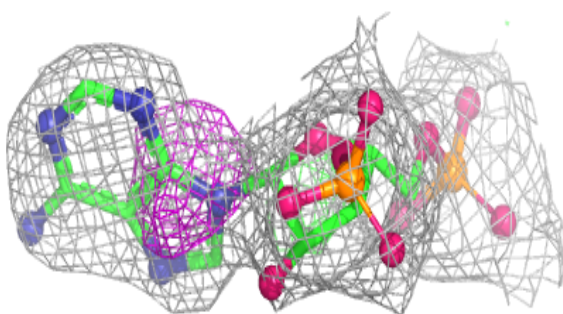
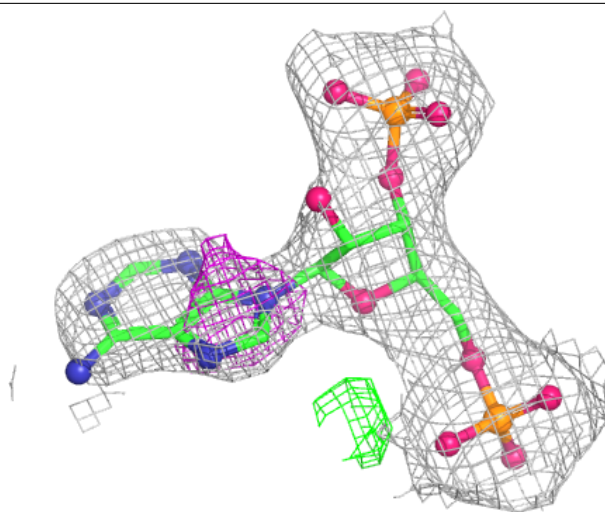
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	A3P	A	301	27/27	0.89	0.09	52,58,61,62	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A3P A 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.