



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:22 AM UTC

PDB ID : 1AQY / pdb_00001aqy
Title : ESTROGEN SULFOTRANSFERASE WITH PAP
Authors : Kakuta, Y.; Pedersen, L.G.; Carter, C.W.; Negishi, M.; Pedersen, L.C.
Deposited on : 1997-08-04
Resolution : 1.75 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

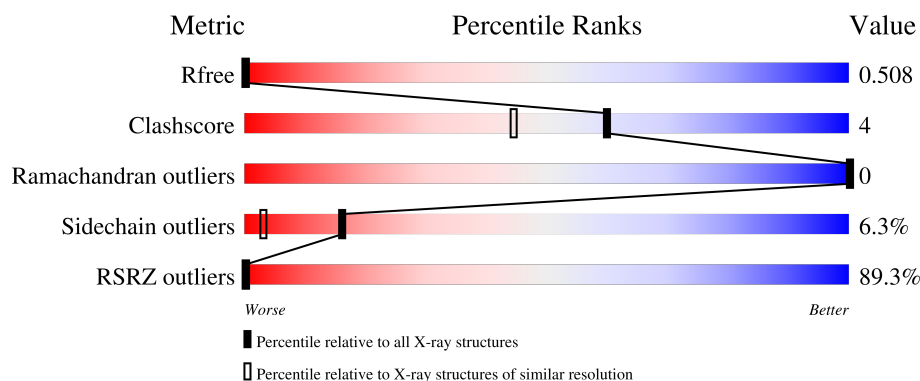
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	297	82% 75%20%• 5%
1	B	297	88% 74%18%• 6%

2 Entry composition [i](#)

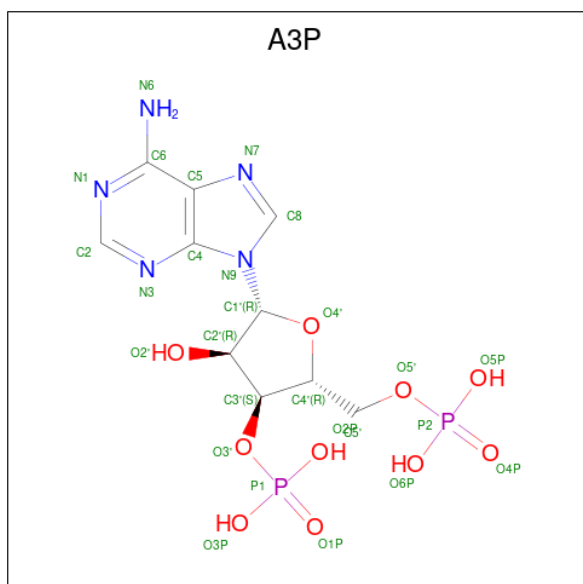
There are 3 unique types of molecules in this entry. The entry contains 5108 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ESTROGEN SULFOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2401	1557	395	429	20			
1	B	280	Total	C	N	O	S	0	0	0
			2381	1545	392	424	20			

- Molecule 2 is ADENOSINE-3'-5'-DIPHOSPHATE (CCD ID: A3P) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

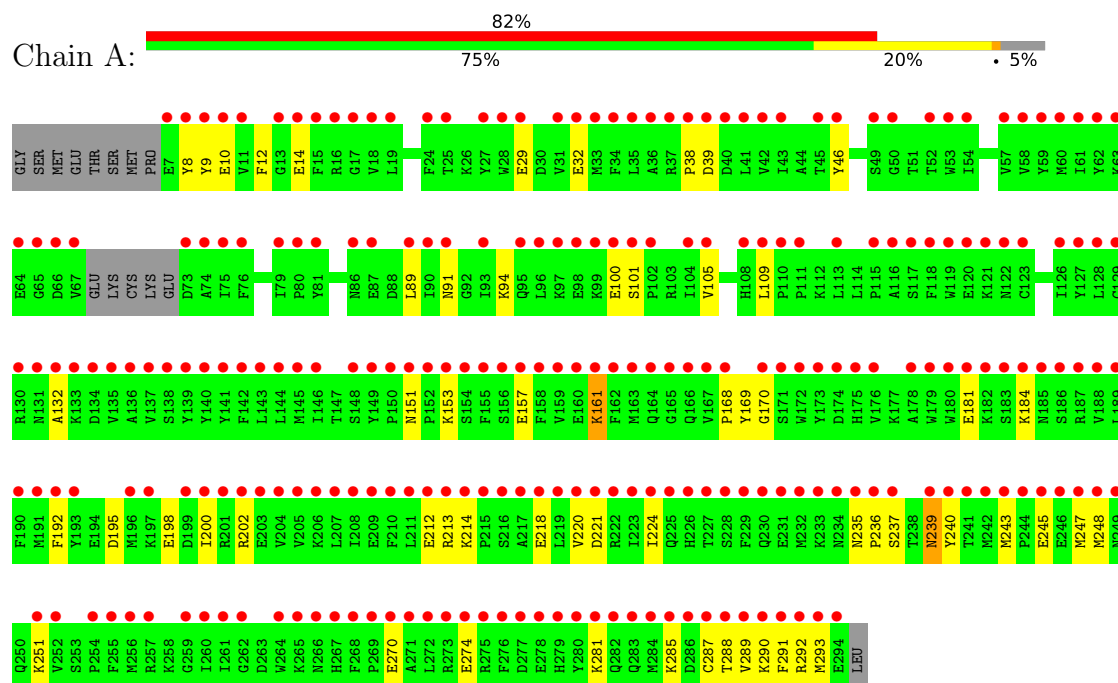
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	136	Total 136	O 136	0	0
3	B	136	Total 136	O 136	0	0

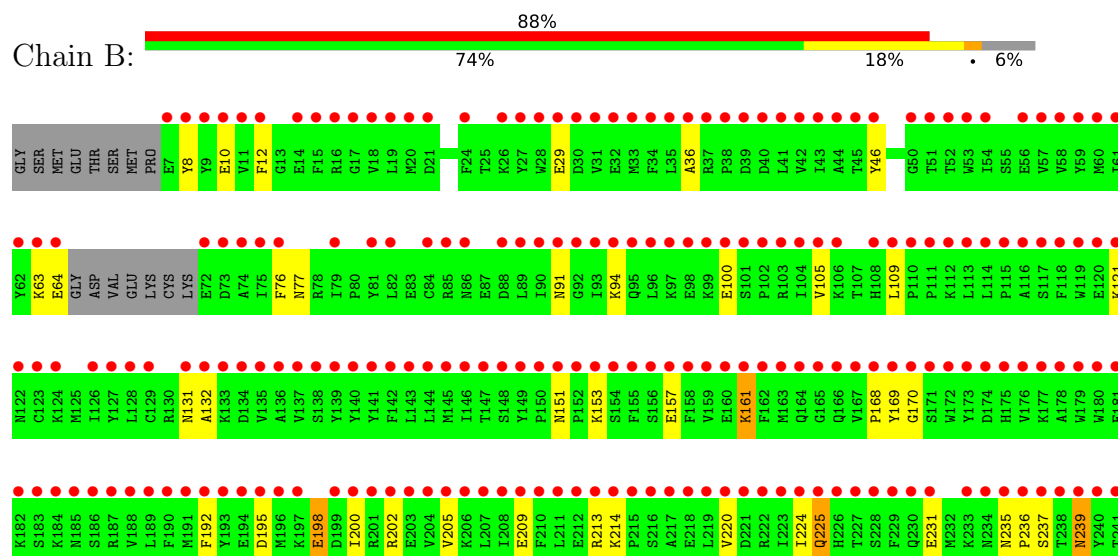
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: ESTROGEN SULFOTRANSFERASE



• Molecule 1: ESTROGEN SULFOTRANSFERASE



M242	M243	P244	E245	E246	M247	M248	R249	Q250	K251	V252	S253	P254	F255	M256	G259	I260	I261	G262	D263	W264	K265	N266	H267	F268	F269	E270	A271	L272	R273	E274	R275	F276	D277	E278	H279	Y280	K281	Q282	Q283	M284	K285	D286	C287	T288	V289	K290	F291	R292	K293	GLU	LEU
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	96.44Å 79.18Å 80.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.75 50.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	91.1 (50.00-1.75) 91.6 (50.00-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.58 (at 1.70Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.218 , 0.248 0.507 , 0.508	Depositor DCC
R_{free} test set	3165 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	15.7	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 19.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	5108	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: A3P

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	0.66	0/2468	0.95	10/3323 (0.3%)
1	B	0.65	0/2448	0.94	11/3296 (0.3%)
All	All	0.65	0/4916	0.94	21/6619 (0.3%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	TYR	N-CA-C	-8.60	99.23	110.07
1	A	46	TYR	N-CA-C	-8.42	99.46	110.07
1	A	132	ALA	N-CA-C	7.28	120.14	111.33
1	B	132	ALA	N-CA-C	7.13	119.95	111.33
1	A	10	GLU	N-CA-C	-6.95	102.79	112.45
1	A	200	ILE	N-CA-C	6.71	117.46	110.62
1	B	200	ILE	N-CA-C	6.66	117.41	110.62
1	B	10	GLU	N-CA-C	-6.55	103.34	112.45
1	A	109	LEU	N-CA-C	6.03	117.41	109.93
1	B	251	LYS	N-CA-C	-5.82	104.90	112.23
1	B	109	LEU	N-CA-C	5.67	116.96	109.93
1	A	105	VAL	N-CA-C	5.58	115.99	108.17
1	A	170	GLY	N-CA-C	5.53	122.31	112.02
1	B	170	GLY	N-CA-C	5.46	122.17	112.02
1	A	251	LYS	N-CA-C	-5.35	105.49	112.23
1	B	290	LYS	N-CA-C	5.15	117.76	107.62
1	B	286	ASP	N-CA-C	5.08	118.62	112.93
1	B	105	VAL	N-CA-C	5.06	115.26	108.17
1	A	240	TYR	N-CA-C	5.06	119.03	112.86
1	A	184	LYS	N-CA-C	-5.06	105.95	111.82
1	B	77	ASN	N-CA-C	-5.01	107.23	113.55

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	2401	0	2359	19	23
1	B	2381	0	2341	24	19
2	A	27	0	11	0	0
2	B	27	0	11	0	0
3	A	136	0	0	1	1
3	B	136	0	0	1	5
All	All	5108	0	4722	41	26

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 4.

All (41) 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:A:287:CYS:SG	1:A:289:VAL:HG23	2.18	0.83
1:B:243:MET:HG2	1:B:248:MET:HE3	1.73	0.69
1:A:243:MET:HG2	1:A:248:MET:HE3	1.74	0.69
1:B:281:LYS:HZ3	1:B:285:LYS:HG2	1.65	0.61
1:A:89:LEU:HD23	1:B:244:PRO:HG2	1.83	0.60
1:A:235:ASN:C	1:A:235:ASN:HD22	2.09	0.60
1:B:235:ASN:HD22	1:B:235:ASN:C	2.10	0.59
1:B:235:ASN:ND2	1:B:237:SER:H	2.01	0.59
1:A:91:ASN:HD22	1:A:91:ASN:C	2.11	0.58
1:A:235:ASN:ND2	1:A:237:SER:H	2.01	0.58
1:B:91:ASN:HD22	1:B:91:ASN:C	2.13	0.57
1:B:151:ASN:ND2	3:B:399:HOH:O	2.38	0.56
1:A:151:ASN:ND2	3:A:324:HOH:O	2.40	0.54
1:B:29:GLU:H	1:B:29:GLU:CD	2.15	0.54
1:B:225:GLN:O	1:B:231:GLU:HG3	2.08	0.54
1:B:168:PRO:O	1:B:169:TYR:HB2	2.09	0.53
1:A:29:GLU:H	1:A:29:GLU:CD	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ASN:C	1:A:239:ASN:HD22	2.17	0.52
1:B:239:ASN:C	1:B:239:ASN:HD22	2.18	0.50
1:B:12:PHE:CE1	1:B:168:PRO:HG3	2.47	0.49
1:A:168:PRO:O	1:A:169:TYR:HB2	2.12	0.48
1:B:202:ARG:HH11	1:B:202:ARG:HG3	1.78	0.47
1:A:202:ARG:HG3	1:A:202:ARG:HH11	1.80	0.47
1:A:8:TYR:CZ	1:A:161:LYS:HE3	2.50	0.46
1:B:8:TYR:CZ	1:B:161:LYS:HE3	2.51	0.46
1:B:36:ALA:O	1:B:121:LYS:HE3	2.16	0.45
1:B:63:LYS:O	1:B:64:GLU:HB2	2.16	0.44
1:B:220:VAL:O	1:B:224:ILE:HG13	2.17	0.44
1:B:281:LYS:NZ	1:B:285:LYS:HG2	2.31	0.43
1:A:235:ASN:C	1:A:235:ASN:ND2	2.76	0.43
1:B:76:PHE:CE2	1:B:243:MET:HE2	2.54	0.42
1:A:220:VAL:O	1:A:224:ILE:HG13	2.19	0.42
1:A:89:LEU:CD2	1:B:244:PRO:HG2	2.47	0.42
1:B:235:ASN:HD22	1:B:237:SER:H	1.66	0.42
1:A:235:ASN:HD22	1:A:236:PRO:N	2.18	0.42
1:B:235:ASN:C	1:B:235:ASN:ND2	2.77	0.41
1:B:235:ASN:HD22	1:B:236:PRO:N	2.17	0.41
1:A:12:PHE:CE1	1:A:168:PRO:HG3	2.55	0.41
1:A:243:MET:HE2	1:A:243:MET:HB2	1.97	0.41
1:A:235:ASN:HD22	1:A:237:SER:H	1.66	0.40
1:B:205:VAL:O	1:B:209:GLU:HG3	2.21	0.40

All (26) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:GLU:OE2	1:B:274:GLU:OE2[2_564]	1.25	0.95
1:A:289:VAL:O	1:B:292:ARG:NH1[1_554]	1.38	0.82
1:A:292:ARG:NH1	1:B:289:VAL:O[1_554]	1.50	0.70
1:A:274:GLU:OE1	1:B:274:GLU:OE1[2_564]	1.67	0.53
1:A:291:PHE:O	1:B:292:ARG:CA[1_554]	1.82	0.38
1:A:274:GLU:OE2	1:B:274:GLU:CD[2_564]	1.87	0.33
1:A:292:ARG:CA	1:B:291:PHE:O[1_554]	1.87	0.33
1:A:290:LYS:NZ	1:B:192:PHE:CD1[1_554]	1.92	0.28
1:A:192:PHE:CD1	1:B:290:LYS:NZ[1_554]	1.93	0.27
1:A:212:GLU:OE1	1:B:283:GLN:NE2[3_445]	1.96	0.24
1:A:293:MET:N	1:B:291:PHE:O[1_554]	1.98	0.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:MET:CE	3:B:353:HOH:O[1_554]	1.99	0.21
1:A:39:ASP:OD2	3:B:313:HOH:O[3_445]	2.00	0.20
1:A:9:TYR:O	3:B:321:HOH:O[4_555]	2.02	0.18
1:A:274:GLU:CD	1:B:274:GLU:OE1[2_564]	2.03	0.17
1:A:290:LYS:CD	1:B:195:ASP:OD1[1_554]	2.03	0.17
3:A:401:HOH:O	3:A:401:HOH:O[2_565]	2.05	0.15
1:A:289:VAL:C	1:B:292:ARG:NH1[1_554]	2.10	0.10
1:A:288:THR:CG2	1:B:198:GLU:O[1_554]	2.11	0.09
1:A:101:SER:N	3:B:304:HOH:O[3_445]	2.12	0.08
1:B:270:GLU:OE2	1:B:273:ARG:NH1[2_565]	2.12	0.08
1:A:32:GLU:CG	1:A:32:GLU:CD[2_555]	2.13	0.07
1:A:195:ASP:OD1	1:B:290:LYS:CD[1_554]	2.15	0.05
1:A:38:PRO:CG	3:B:415:HOH:O[3_445]	2.17	0.03
1:A:290:LYS:NZ	1:B:195:ASP:OD2[1_554]	2.17	0.03
1:B:225:GLN:OE1	1:B:225:GLN:OE1[2_555]	2.18	0.02

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	279/297 (94%)	270 (97%)	9 (3%)	0	100	100
1	B	276/297 (93%)	266 (96%)	10 (4%)	0	100	100
All	All	555/594 (93%)	536 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	A	264/278 (95%)	246 (93%)	18 (7%)	14	3
1	B	262/278 (94%)	247 (94%)	15 (6%)	18	4
All	All	526/556 (95%)	493 (94%)	33 (6%)	16	3

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	94	LYS
1	A	100	GLU
1	A	153	LYS
1	A	157	GLU
1	A	161	LYS
1	A	181	GLU
1	A	198	GLU
1	A	213	ARG
1	A	214	LYS
1	A	218	GLU
1	A	221	ASP
1	A	239	ASN
1	A	245	GLU
1	A	247	MET
1	A	270	GLU
1	A	281	LYS
1	A	285	LYS
1	B	94	LYS
1	B	100	GLU
1	B	131	ASN
1	B	153	LYS
1	B	157	GLU
1	B	161	LYS
1	B	198	GLU
1	B	213	ARG
1	B	214	LYS
1	B	225	GLN
1	B	239	ASN
1	B	245	GLU
1	B	247	MET
1	B	270	GLU
1	B	281	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	131	ASN
1	A	151	ASN
1	A	234	ASN
1	A	235	ASN
1	A	239	ASN
1	B	91	ASN
1	B	122	ASN
1	B	131	ASN
1	B	151	ASN
1	B	235	ASN
1	B	239	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	A3P	B	302	-	29,29,29	1.07	0	44,45,45	0.72	1 (2%)
2	A3P	A	301	-	29,29,29	1.12	1 (3%)	44,45,45	0.70	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
2	A3P	B	302	-	-	0/15/31/31	0/3/3/3
2	A3P	A	301	-	-	0/15/31/31	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	A3P	P2-O5P	-2.09	1.47	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	A3P	O2'-C2'-C3'	2.01	116.81	111.19

There are no chirality outliers.

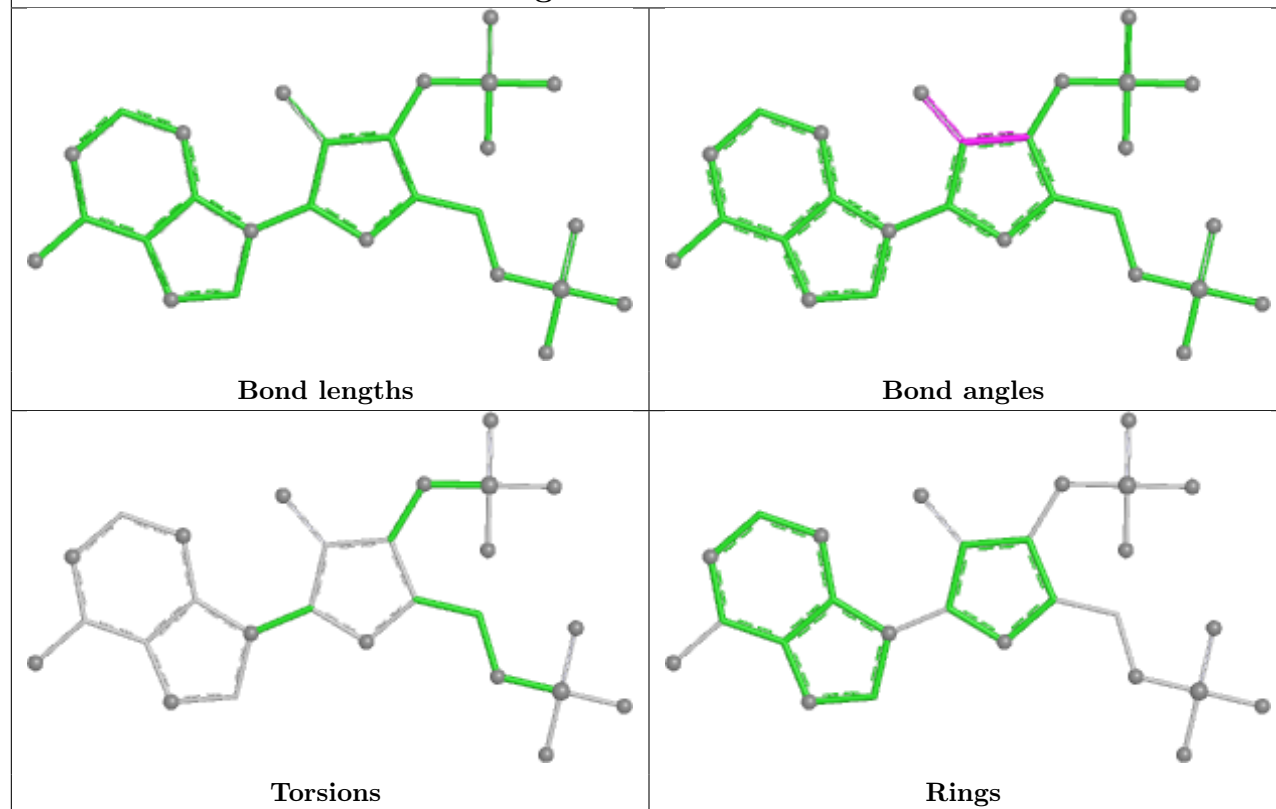
There are no torsion outliers.

There are no ring outliers.

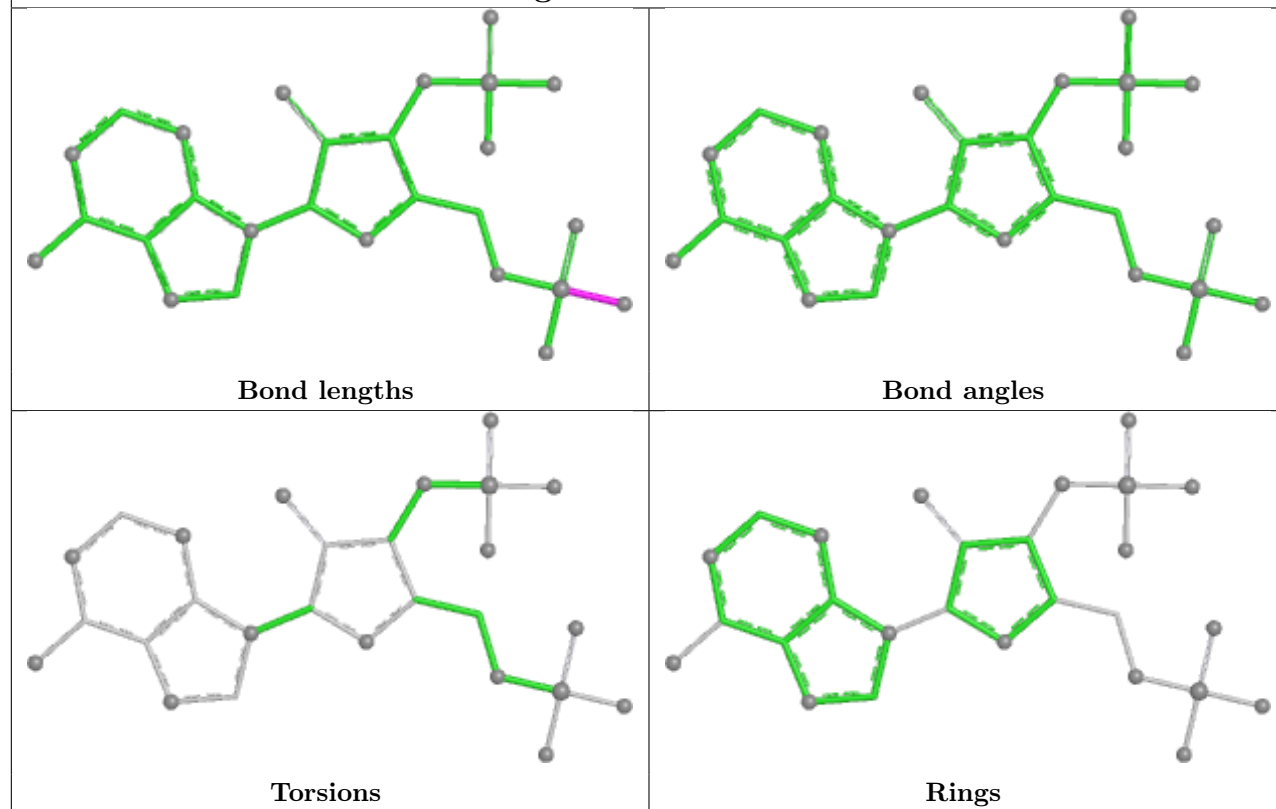
No monomer is involved in short contacts.

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.

Ligand A3P B 302



Ligand A3P A 301



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, 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	283/297 (95%)	3.32	243 (85%) 0 0	9, 18, 37, 57	0
1	B	280/297 (94%)	3.68	260 (92%) 0 0	9, 20, 39, 49	0
All	All	563/594 (94%)	3.50	503 (89%) 0 0	9, 19, 38, 57	0

All (503) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	VAL	11.1
1	A	217	ALA	9.0
1	B	220	VAL	8.0
1	A	220	VAL	7.9
1	B	58	VAL	7.5
1	A	271	ALA	7.4
1	B	208	ILE	7.2
1	B	268	PHE	7.1
1	A	219	LEU	7.0
1	B	214	LYS	7.0
1	B	287	CYS	6.9
1	B	212	GLU	6.9
1	B	188	VAL	6.5
1	B	183	SER	6.4
1	B	217	ALA	6.3
1	B	224	ILE	6.3
1	B	269	PRO	6.3
1	B	216	SER	6.2
1	B	173	TYR	6.2
1	B	282	GLN	6.2
1	B	199	ASP	6.2
1	B	123	CYS	6.2
1	B	229	PHE	6.1
1	B	213	ARG	6.1

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Mol	Chain	Res	Type	RSRZ
1	B	288	THR	6.0
1	A	223	ILE	6.0
1	B	207	LEU	6.0
1	A	216	SER	5.8
1	B	254	PRO	5.7
1	B	105	VAL	5.7
1	A	270	GLU	5.7
1	B	275	ARG	5.7
1	A	102	PRO	5.7
1	A	192	PHE	5.7
1	B	61	ILE	5.7
1	B	200	ILE	5.6
1	B	215	PRO	5.6
1	B	185	ASN	5.6
1	B	271	ALA	5.6
1	B	225	GLN	5.6
1	A	229	PHE	5.5
1	A	282	GLN	5.5
1	A	212	GLU	5.5
1	B	211	LEU	5.5
1	B	15	PHE	5.5
1	B	270	GLU	5.5
1	A	199	ASP	5.4
1	B	180	TRP	5.4
1	A	188	VAL	5.3
1	A	224	ILE	5.3
1	B	189	LEU	5.3
1	A	132	ALA	5.3
1	B	272	LEU	5.3
1	A	244	PRO	5.2
1	A	208	ILE	5.2
1	B	219	LEU	5.2
1	A	62	TYR	5.2
1	A	200	ILE	5.2
1	B	122	ASN	5.2
1	B	64	GLU	5.2
1	A	9	TYR	5.2
1	B	285	LYS	5.1
1	B	178	ALA	5.1
1	B	227	THR	5.1
1	A	214	LYS	5.1
1	A	15	PHE	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	137	VAL	5.1
1	B	119	TRP	5.1
1	B	90	ILE	5.1
1	A	286	ASP	5.1
1	A	210	PHE	5.1
1	B	17	GLY	5.1
1	A	38	PRO	5.0
1	B	289	VAL	5.0
1	B	59	TYR	5.0
1	A	268	PHE	5.0
1	B	159	VAL	5.0
1	A	269	PRO	5.0
1	B	184	LYS	4.9
1	B	228	SER	4.9
1	A	205	VAL	4.9
1	B	276	PHE	4.9
1	B	286	ASP	4.8
1	B	264	TRP	4.8
1	B	252	VAL	4.8
1	A	8	TYR	4.8
1	B	8	TYR	4.8
1	A	90	ILE	4.8
1	B	190	PHE	4.8
1	A	101	SER	4.7
1	B	293	MET	4.7
1	B	244	PRO	4.7
1	B	192	PHE	4.7
1	B	193	TYR	4.7
1	A	241	THR	4.7
1	B	238	THR	4.7
1	A	218	GLU	4.7
1	A	285	LYS	4.7
1	A	190	PHE	4.7
1	B	113	LEU	4.7
1	B	274	GLU	4.7
1	A	119	TRP	4.7
1	A	287	CYS	4.6
1	A	289	VAL	4.6
1	B	62	TYR	4.6
1	B	149	TYR	4.6
1	A	274	GLU	4.6
1	B	261	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	281	LYS	4.6
1	B	280	TYR	4.6
1	A	36	ALA	4.6
1	B	135	VAL	4.6
1	A	245	GLU	4.6
1	A	243	MET	4.6
1	A	186	SER	4.5
1	B	201	ARG	4.5
1	A	234	ASN	4.5
1	A	215	PRO	4.5
1	A	225	GLN	4.5
1	A	66	ASP	4.5
1	B	24	PHE	4.4
1	A	61	ILE	4.4
1	B	139	TYR	4.4
1	A	204	VAL	4.4
1	B	222	ARG	4.4
1	B	35	LEU	4.4
1	B	210	PHE	4.4
1	B	143	LEU	4.4
1	A	65	GLY	4.4
1	A	127	TYR	4.3
1	B	127	TYR	4.3
1	A	18	VAL	4.3
1	A	272	LEU	4.3
1	A	16	ARG	4.3
1	B	205	VAL	4.3
1	B	242	MET	4.3
1	B	223	ILE	4.3
1	A	179	TRP	4.3
1	A	276	PHE	4.3
1	B	115	PRO	4.3
1	B	236	PRO	4.3
1	A	275	ARG	4.3
1	A	32	GLU	4.3
1	B	267	HIS	4.3
1	A	17	GLY	4.2
1	B	141	TYR	4.2
1	A	142	PHE	4.2
1	A	294	GLU	4.2
1	A	31	VAL	4.2
1	A	277	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	228	SER	4.2
1	B	28	TRP	4.2
1	A	207	LEU	4.2
1	B	187	ARG	4.2
1	A	53	TRP	4.2
1	A	183	SER	4.1
1	B	255	PHE	4.1
1	B	54	ILE	4.1
1	A	64	GLU	4.1
1	A	158	PHE	4.1
1	B	160	GLU	4.1
1	A	221	ASP	4.1
1	B	16	ARG	4.1
1	B	260	ILE	4.1
1	B	132	ALA	4.1
1	A	293	MET	4.1
1	A	59	TYR	4.1
1	A	278	GLU	4.1
1	B	253	SER	4.1
1	B	278	GLU	4.1
1	A	202	ARG	4.1
1	A	236	PRO	4.0
1	B	89	LEU	4.0
1	B	281	LYS	4.0
1	B	155	PHE	4.0
1	A	28	TRP	4.0
1	A	180	TRP	4.0
1	B	53	TRP	4.0
1	B	153	LYS	4.0
1	B	9	TYR	4.0
1	A	60	MET	4.0
1	A	159	VAL	4.0
1	A	201	ARG	4.0
1	B	169	TYR	4.0
1	B	291	PHE	4.0
1	B	129	CYS	4.0
1	A	252	VAL	4.0
1	B	221	ASP	4.0
1	A	27	TYR	3.9
1	A	267	HIS	3.9
1	A	140	TYR	3.9
1	A	172	TRP	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	76	PHE	3.9
1	A	288	THR	3.9
1	A	153	LYS	3.9
1	B	100	GLU	3.9
1	A	35	LEU	3.9
1	A	266	ASN	3.9
1	B	102	PRO	3.9
1	A	126	ILE	3.8
1	A	261	ILE	3.8
1	B	279	HIS	3.8
1	B	92	GLY	3.8
1	A	254	PRO	3.8
1	B	150	PRO	3.8
1	A	230	GLN	3.8
1	B	234	ASN	3.8
1	A	291	PHE	3.8
1	B	126	ILE	3.8
1	B	31	VAL	3.8
1	B	121	LYS	3.8
1	B	38	PRO	3.8
1	A	232	MET	3.8
1	A	123	CYS	3.8
1	B	182	LYS	3.7
1	B	259	GLY	3.7
1	B	41	LEU	3.7
1	A	100	GLU	3.7
1	A	185	ASN	3.7
1	A	7	GLU	3.7
1	A	89	LEU	3.7
1	A	143	LEU	3.7
1	B	251	LYS	3.7
1	B	283	GLN	3.7
1	B	39	ASP	3.7
1	B	131	ASN	3.7
1	B	152	PRO	3.7
1	B	82	LEU	3.7
1	A	203	GLU	3.7
1	B	7	GLU	3.7
1	A	226	HIS	3.6
1	B	277	ASP	3.6
1	A	247	MET	3.6
1	A	14	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	46	TYR	3.6
1	A	280	TYR	3.6
1	A	54	ILE	3.6
1	B	51	THR	3.6
1	B	60	MET	3.6
1	B	11	VAL	3.6
1	B	230	GLN	3.6
1	A	279	HIS	3.6
1	A	242	MET	3.6
1	B	284	MET	3.6
1	B	273	ARG	3.6
1	A	19	LEU	3.6
1	A	29	GLU	3.6
1	A	171	SER	3.5
1	B	156	SER	3.5
1	A	176	VAL	3.5
1	B	231	GLU	3.5
1	A	211	LEU	3.5
1	B	226	HIS	3.5
1	B	63	LYS	3.5
1	A	139	TYR	3.5
1	B	186	SER	3.5
1	A	79	ILE	3.5
1	A	255	PHE	3.5
1	B	202	ARG	3.5
1	B	18	VAL	3.5
1	B	168	PRO	3.5
1	B	104	ILE	3.5
1	A	118	PHE	3.5
1	A	290	LYS	3.5
1	B	57	VAL	3.5
1	B	161	LYS	3.4
1	B	151	ASN	3.4
1	A	33	MET	3.4
1	B	33	MET	3.4
1	B	247	MET	3.4
1	B	101	SER	3.4
1	B	248	MET	3.4
1	B	114	LEU	3.4
1	A	137	VAL	3.4
1	A	283	GLN	3.4
1	A	222	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	290	LYS	3.4
1	B	142	PHE	3.4
1	A	167	VAL	3.4
1	B	176	VAL	3.4
1	A	240	TYR	3.3
1	B	140	TYR	3.3
1	B	237	SER	3.3
1	B	206	LYS	3.3
1	B	88	ASP	3.3
1	B	266	ASN	3.3
1	A	227	THR	3.3
1	A	113	LEU	3.3
1	A	111	PRO	3.3
1	A	231	GLU	3.3
1	B	265	LYS	3.3
1	B	250	GLN	3.3
1	A	173	TYR	3.3
1	A	259	GLY	3.3
1	A	264	TRP	3.3
1	B	172	TRP	3.3
1	B	179	TRP	3.3
1	B	191	MET	3.3
1	A	154	SER	3.3
1	A	121	LYS	3.3
1	B	147	THR	3.2
1	B	162	PHE	3.2
1	A	116	ALA	3.2
1	A	248	MET	3.2
1	A	39	ASP	3.2
1	A	144	LEU	3.2
1	A	181	GLU	3.2
1	B	32	GLU	3.2
1	B	112	LYS	3.2
1	A	156	SER	3.2
1	B	195	ASP	3.2
1	B	27	TYR	3.1
1	A	161	LYS	3.1
1	A	146	ILE	3.1
1	B	43	ILE	3.1
1	B	233	LYS	3.1
1	B	262	GLY	3.1
1	A	256	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	158	PHE	3.1
1	A	105	VAL	3.1
1	A	174	ASP	3.1
1	B	50	GLY	3.1
1	A	233	LYS	3.1
1	A	265	LYS	3.1
1	B	12	PHE	3.1
1	B	157	GLU	3.1
1	B	110	PRO	3.0
1	A	164	GLN	3.0
1	B	94	LYS	3.0
1	B	124	LYS	3.0
1	A	213	ARG	3.0
1	B	246	GLU	3.0
1	B	118	PHE	3.0
1	A	184	LYS	3.0
1	B	97	LYS	3.0
1	B	197	LYS	3.0
1	A	209	GLU	3.0
1	A	74	ALA	3.0
1	A	178	ALA	3.0
1	B	10	GLU	3.0
1	A	149	TYR	3.0
1	A	193	TYR	3.0
1	A	138	SER	3.0
1	B	128	LEU	3.0
1	A	237	SER	2.9
1	B	95	GLN	2.9
1	B	164	GLN	2.9
1	A	292	ARG	2.9
1	B	256	MET	2.9
1	A	63	LYS	2.9
1	A	97	LYS	2.9
1	B	116	ALA	2.9
1	B	218	GLU	2.9
1	B	40	ASP	2.9
1	B	196	MET	2.9
1	B	243	MET	2.9
1	B	98	GLU	2.9
1	B	36	ALA	2.9
1	A	239	ASN	2.9
1	A	99	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	251	LYS	2.9
1	B	245	GLU	2.9
1	B	249	ASN	2.9
1	A	50	GLY	2.9
1	B	21	ASP	2.8
1	A	117	SER	2.8
1	A	152	PRO	2.8
1	B	79	ILE	2.8
1	A	122	ASN	2.8
1	B	52	THR	2.8
1	B	241	THR	2.8
1	A	157	GLU	2.8
1	A	24	PHE	2.8
1	B	163	MET	2.8
1	B	263	ASP	2.8
1	B	75	ILE	2.8
1	B	181	GLU	2.8
1	A	34	PHE	2.8
1	A	155	PHE	2.8
1	B	34	PHE	2.8
1	B	76	PHE	2.8
1	A	115	PRO	2.8
1	A	41	LEU	2.8
1	B	14	GLU	2.8
1	B	19	LEU	2.8
1	B	209	GLU	2.8
1	B	30	ASP	2.8
1	A	175	HIS	2.8
1	A	170	GLY	2.8
1	A	87	GLU	2.7
1	A	110	PRO	2.7
1	A	168	PRO	2.7
1	A	284	MET	2.7
1	B	204	VAL	2.7
1	A	75	ILE	2.7
1	B	146	ILE	2.7
1	A	45	THR	2.7
1	A	37	ARG	2.7
1	A	187	ARG	2.7
1	B	203	GLU	2.7
1	A	197	LYS	2.7
1	B	26	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	73	ASP	2.7
1	A	57	VAL	2.7
1	B	166	GLN	2.7
1	A	150	PRO	2.7
1	B	111	PRO	2.7
1	B	29	GLU	2.7
1	B	240	TYR	2.7
1	A	235	ASN	2.7
1	A	131	ASN	2.6
1	A	129	CYS	2.6
1	A	42	VAL	2.6
1	B	42	VAL	2.6
1	B	46	TYR	2.6
1	B	56	GLU	2.6
1	A	136	ALA	2.6
1	B	117	SER	2.6
1	A	273	ARG	2.6
1	A	98	GLU	2.6
1	A	25	THR	2.6
1	B	170	GLY	2.6
1	A	96	LEU	2.6
1	A	135	VAL	2.6
1	A	43	ILE	2.6
1	A	260	ILE	2.6
1	A	151	ASN	2.6
1	B	91	ASN	2.6
1	B	120	GLU	2.6
1	B	154	SER	2.5
1	A	40	ASP	2.5
1	B	175	HIS	2.5
1	A	249	ASN	2.5
1	B	292	ARG	2.5
1	B	235	ASN	2.5
1	A	109	LEU	2.5
1	B	134	ASP	2.5
1	B	136	ALA	2.5
1	A	165	GLY	2.5
1	A	93	ILE	2.5
1	B	93	ILE	2.5
1	A	133	LYS	2.4
1	A	108	HIS	2.4
1	B	108	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	13	GLY	2.4
1	A	128	LEU	2.4
1	A	262	GLY	2.4
1	A	148	SER	2.4
1	A	81	TYR	2.4
1	A	11	VAL	2.4
1	B	194	GLU	2.4
1	A	206	LYS	2.4
1	B	144	LEU	2.4
1	A	120	GLU	2.4
1	A	182	LYS	2.4
1	B	37	ARG	2.3
1	B	174	ASP	2.3
1	B	133	LYS	2.3
1	B	167	VAL	2.3
1	B	72	GLU	2.3
1	B	85	ARG	2.3
1	A	191	MET	2.3
1	B	138	SER	2.3
1	A	73	ASP	2.3
1	A	134	ASP	2.3
1	A	196	MET	2.3
1	B	109	LEU	2.3
1	A	257	ARG	2.3
1	B	148	SER	2.3
1	B	171	SER	2.3
1	A	58	VAL	2.3
1	B	145	MET	2.3
1	B	103	ARG	2.2
1	A	189	LEU	2.2
1	B	177	LYS	2.2
1	A	145	MET	2.2
1	B	239	ASN	2.2
1	B	44	ALA	2.2
1	A	49	SER	2.2
1	A	10	GLU	2.2
1	B	45	THR	2.2
1	B	86	ASN	2.2
1	A	163	MET	2.2
1	B	84	CYS	2.2
1	B	96	LEU	2.2
1	B	106	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	81	TYR	2.1
1	A	86	ASN	2.1
1	A	91	ASN	2.1
1	A	52	THR	2.1
1	A	130	ARG	2.1
1	B	74	ALA	2.1
1	B	99	LYS	2.1
1	A	160	GLU	2.1
1	A	246	GLU	2.1
1	B	20	MET	2.1
1	A	166	GLN	2.1
1	A	80	PRO	2.1
1	A	162	PHE	2.1
1	B	165	GLY	2.0
1	A	95	GLN	2.0
1	A	104	ILE	2.0
1	A	141	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

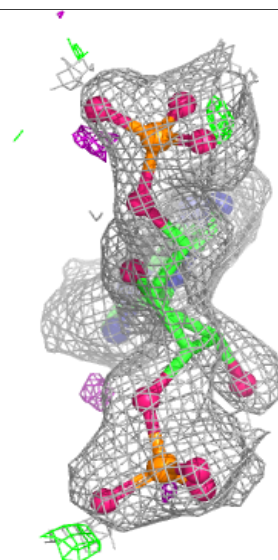
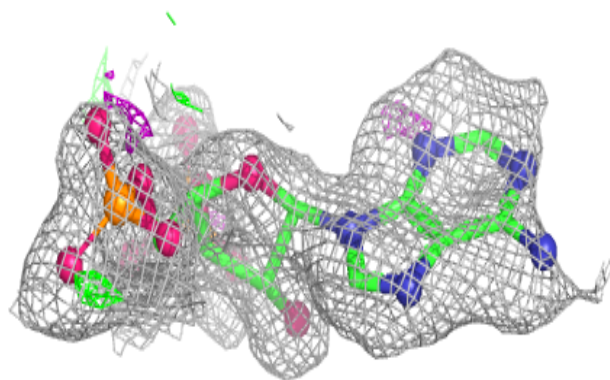
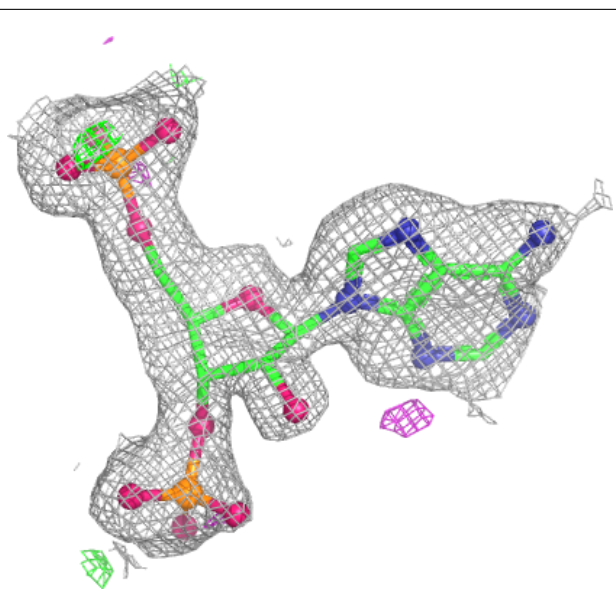
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	A3P	B	302	27/27	0.79	0.16	10,16,20,20	0
2	A3P	A	301	27/27	0.85	0.13	9,12,16,17	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.

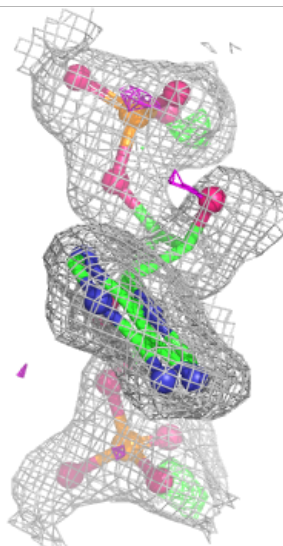
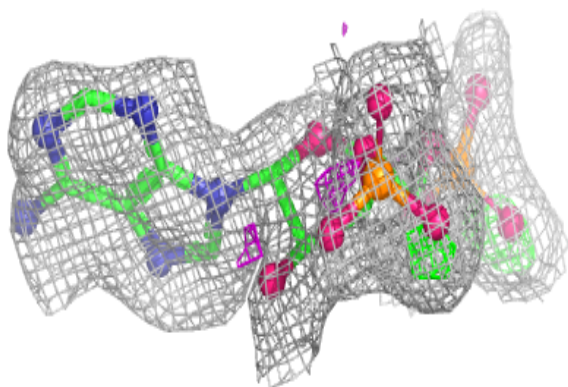
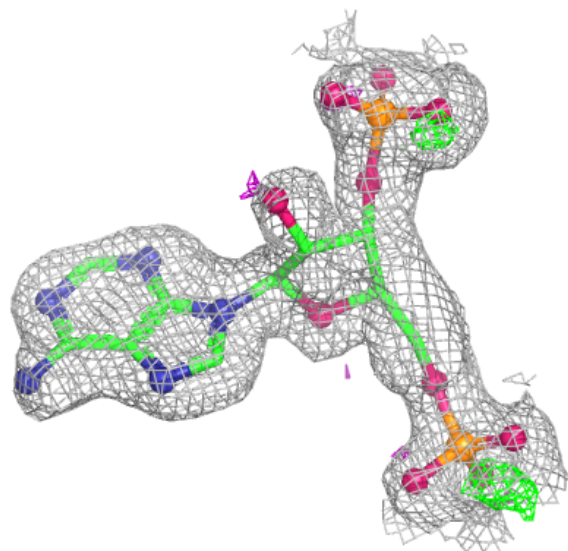
Electron density around A3P B 302:

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



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.