



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:26 PM GMT

PDB ID : 1AQY
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

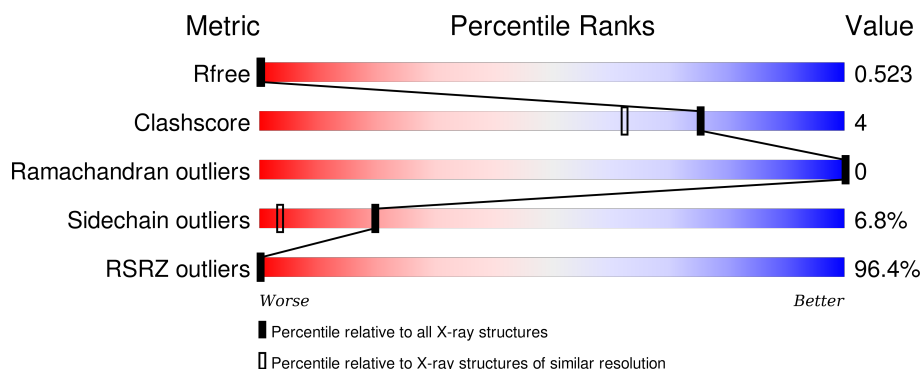
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	297	<div> <div>91%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>• 5%</div> </div> </div>
1	B	297	<div> <div>92%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>• 6%</div> </div> </div>

2 Entry composition [i](#)

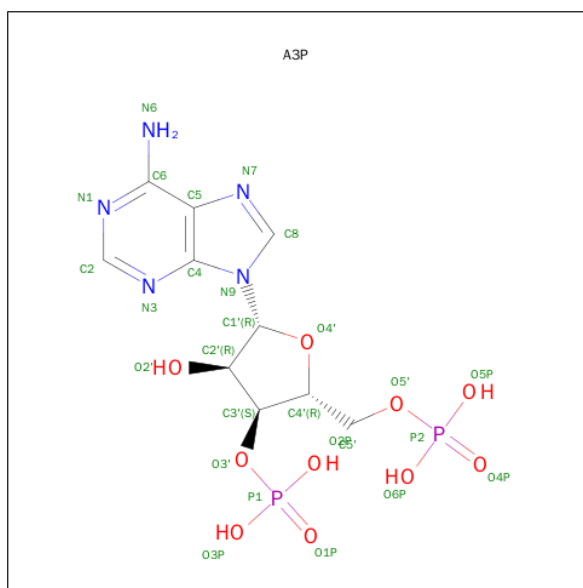
There are 3 unique types of molecules in this entry. The entry contains 5108 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: 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		

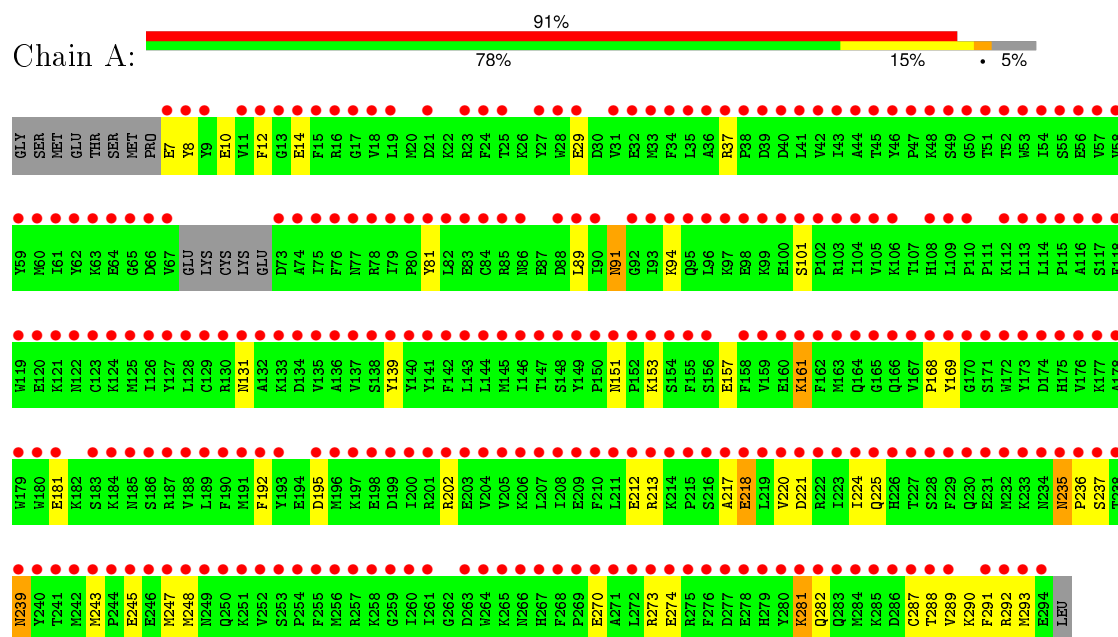
- Molecule 3 is water.

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

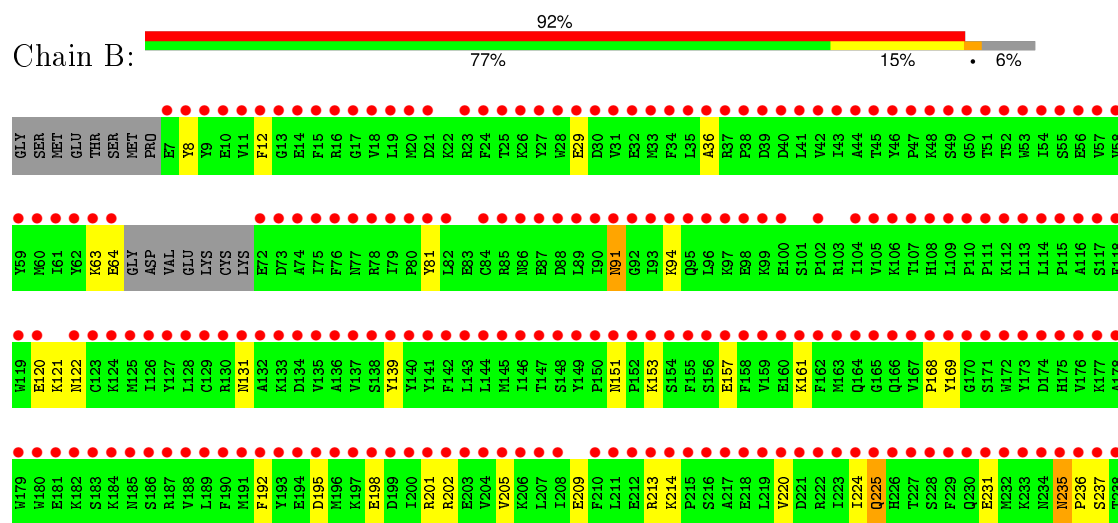
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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



N239	Y240	T241	M242	M243	P244	E245	E246	M247	M248	N249	Q250	K251	V252	S253	P254	F255	N256	R257	K258	G259	I260	I261	G262	D263	N264	K265	N266	H267	F268	P269	E270	A271	L272	R273	E274	R275	F276	D277	E278	H279	Y280	K281	Q282	Q283	M284	K285	D286	C287	T288	V289	K290	F291	R292	M293	GIU	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 18.47 – 1.70	Depositor EDS
% Data completeness (in resolution range)	91.1 (50.00-1.75) 90.3 (18.47-1.70)	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 0.505 , 0.523	Depositor DCC
R_{free} test set	2948 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	15.7	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.8	EDS
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 62618 reflections	Xtriage
F_o, F_c correlation	0.58	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.54	0/2468	0.61	0/3323
1	B	0.54	0/2448	0.59	0/3296
All	All	0.54	0/4916	0.60	0/6619

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2401	0	2359	17	36
1	B	2381	0	2341	22	33
2	A	27	0	11	0	0
2	B	27	0	11	0	0
3	A	136	0	0	1	6
3	B	136	0	0	1	4
All	All	5108	0	4722	37	43

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 (37) 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:A:243:MET:HG2	1:A:248:MET:HE3	1.72	0.71
1:B:243:MET:HG2	1:B:248:MET:HE3	1.75	0.68
1:A:89:LEU:HD23	1:B:244:PRO:HG2	1.83	0.60
1:A:235:ASN:ND2	1:A:237:SER:H	2.01	0.58
1:B:235:ASN:ND2	1:B:237:SER:H	2.01	0.57
1:B:151:ASN:ND2	3:B:399:HOH:O	2.38	0.56
1:A:235:ASN:HD22	1:A:235:ASN:C	2.09	0.55
1:B:235:ASN:HD22	1:B:235:ASN:C	2.10	0.55
1:A:91:ASN:HD22	1:A:91:ASN:C	2.11	0.54
1:B:225:GLN:O	1:B:231:GLU:HG3	2.08	0.54
1:A:151:ASN:ND2	3:A:324:HOH:O	2.40	0.53
1:B:91:ASN:C	1:B:91:ASN:HD22	2.13	0.53
1:B:168:PRO:O	1:B:169:TYR:HB2	2.09	0.51
1:A:168:PRO:O	1:A:169:TYR:HB2	2.12	0.50
1:B:12:PHE:CE1	1:B:168:PRO:HG3	2.47	0.50
1:B:29:GLU:CD	1:B:29:GLU:H	2.15	0.50
1:B:202:ARG:HH11	1:B:202:ARG:HG3	1.78	0.48
1:A:29:GLU:H	1:A:29:GLU:CD	2.17	0.48
1:A:239:ASN:C	1:A:239:ASN:HD22	2.17	0.47
1:B:239:ASN:HD22	1:B:239:ASN:C	2.18	0.47
1:A:8:TYR:CZ	1:A:161:LYS:HE3	2.50	0.46
1:A:202:ARG:HH11	1:A:202:ARG:HG3	1.80	0.46
1:B:36:ALA:O	1:B:121:LYS:HE3	2.16	0.46
1:B:281:LYS:NZ	1:B:285:LYS:HG2	2.31	0.45
1:B:63:LYS:O	1:B:64:GLU:HB2	2.16	0.45
1:B:8:TYR:CZ	1:B:161:LYS:HE3	2.51	0.44
1:A:235:ASN:HD22	1:A:237:SER:H	1.66	0.44
1:B:220:VAL:O	1:B:224:ILE:HG13	2.17	0.44
1:B:235:ASN:HD22	1:B:237:SER:H	1.66	0.43
1:B:235:ASN:HD22	1:B:236:PRO:N	2.17	0.42
1:A:89:LEU:CD2	1:B:244:PRO:HG2	2.47	0.42
1:B:281:LYS:HZ3	1:B:285:LYS:HG2	1.84	0.42
1:A:220:VAL:O	1:A:224:ILE:HG13	2.19	0.41
1:A:12:PHE:CE1	1:A:168:PRO:HG3	2.55	0.41
1:A:235:ASN:HD22	1:A:236:PRO:N	2.18	0.40
1:B:205:VAL:O	1:B:209:GLU:HG3	2.22	0.40

All (43) 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:212:GLU:OE1	1:B:282:GLN:CB[3_546]	1.27	0.93
1:A:274:GLU:OE2	1:B:274:GLU:OE2[2_566]	1.30	0.90
3:A:401:HOH:O	3:A:401:HOH:O[2_565]	1.35	0.85
1:A:289:VAL:O	1:B:292:ARG:NH1[1_556]	1.40	0.80
1:A:217:ALA:CB	1:A:282:GLN:CG[4_557]	1.48	0.72
1:A:218:GLU:OE2	1:A:281:LYS:NZ[4_557]	1.48	0.72
1:A:292:ARG:NH1	1:B:289:VAL:O[1_556]	1.51	0.69
1:A:37:ARG:CD	3:B:305:HOH:O[3_546]	1.57	0.63
1:B:120:GLU:CB	3:A:322:HOH:O[4_556]	1.63	0.57
1:A:274:GLU:CD	1:B:274:GLU:OE2[2_566]	1.70	0.50
1:A:274:GLU:OE1	1:B:274:GLU:OE1[2_566]	1.75	0.45
1:A:212:GLU:CD	1:B:282:GLN:CB[3_546]	1.79	0.41
1:A:291:PHE:O	1:B:292:ARG:CA[1_556]	1.81	0.39
1:A:101:SER:CB	3:B:313:HOH:O[3_546]	1.83	0.37
1:A:292:ARG:CA	1:B:291:PHE:O[1_556]	1.87	0.33
1:A:270:GLU:OE2	1:A:273:ARG:NH1[2_565]	1.88	0.32
1:A:10:GLU:CG	3:B:320:HOH:O[4_456]	1.90	0.30
1:A:274:GLU:OE1	1:B:274:GLU:CD[2_566]	1.90	0.30
1:B:120:GLU:OE1	3:A:321:HOH:O[4_556]	1.91	0.29
1:A:290:LYS:CD	1:B:195:ASP:OD1[1_556]	1.92	0.28
1:A:212:GLU:OE1	1:B:282:GLN:CG[3_546]	1.93	0.27
1:A:7:GLU:OE2	1:B:121:LYS:NZ[4_456]	1.95	0.25
1:A:293:MET:N	1:B:291:PHE:O[1_556]	1.98	0.22
1:A:293:MET:CE	3:B:353:HOH:O[1_556]	1.99	0.21
1:A:7:GLU:OE1	1:B:121:LYS:NZ[4_456]	2.00	0.20
1:A:192:PHE:CD1	1:B:290:LYS:NZ[1_556]	2.00	0.20
1:A:218:GLU:CD	1:A:281:LYS:NZ[4_557]	2.03	0.17
1:A:290:LYS:NZ	1:B:192:PHE:CD1[1_556]	2.03	0.17
1:B:225:GLN:OE1	1:B:225:GLN:OE1[2_555]	2.05	0.15
1:A:8:TYR:CB	1:B:120:GLU:CG[4_456]	2.06	0.14
1:A:290:LYS:NZ	1:B:195:ASP:OD2[1_556]	2.06	0.14
1:A:195:ASP:OD1	1:B:290:LYS:CD[1_556]	2.06	0.14
1:A:289:VAL:C	1:B:292:ARG:NH1[1_556]	2.07	0.13
1:A:274:GLU:OE1	1:B:274:GLU:OE2[2_566]	2.09	0.11
1:B:120:GLU:OE2	3:A:321:HOH:O[4_556]	2.09	0.11
1:A:212:GLU:CG	1:B:282:GLN:CD[3_546]	2.10	0.10
3:A:431:HOH:O	3:A:431:HOH:O[2_565]	2.11	0.09
1:A:212:GLU:CB	1:B:282:GLN:NE2[3_546]	2.12	0.08
1:A:291:PHE:O	1:B:293:MET:N[1_556]	2.13	0.07
1:A:288:THR:CG2	1:B:198:GLU:O[1_556]	2.13	0.07
1:B:120:GLU:CD	3:A:321:HOH:O[4_556]	2.14	0.06
1:A:7:GLU:CD	1:B:121:LYS:NZ[4_456]	2.18	0.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ASP:OD2	1:B:290:LYS:NZ[1_556]	2.19	0.01

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%)	245 (93%)	19 (7%)	18	3
1	B	262/278 (94%)	245 (94%)	17 (6%)	21	4
All	All	526/556 (95%)	490 (93%)	36 (7%)	20	3

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	81	TYR

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Mol	Chain	Res	Type
1	A	91	ASN
1	A	94	LYS
1	A	131	ASN
1	A	139	TYR
1	A	153	LYS
1	A	157	GLU
1	A	161	LYS
1	A	181	GLU
1	A	213	ARG
1	A	218	GLU
1	A	221	ASP
1	A	225	GLN
1	A	235	ASN
1	A	239	ASN
1	A	245	GLU
1	A	247	MET
1	A	281	LYS
1	B	81	TYR
1	B	91	ASN
1	B	94	LYS
1	B	122	ASN
1	B	131	ASN
1	B	139	TYR
1	B	153	LYS
1	B	157	GLU
1	B	201	ARG
1	B	213	ARG
1	B	214	LYS
1	B	225	GLN
1	B	235	ASN
1	B	239	ASN
1	B	245	GLU
1	B	247	MET
1	B	281	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	95	GLN
1	A	131	ASN
1	A	151	ASN

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Mol	Chain	Res	Type
1	A	166	GLN
1	A	234	ASN
1	A	235	ASN
1	A	239	ASN
1	B	91	ASN
1	B	95	GLN
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 carbohydrates 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	A	301	-	24,29,29	1.20	2 (8%)	28,45,45	0.91	0
2	A3P	B	302	-	24,29,29	1.12	1 (4%)	28,45,45	0.93	1 (3%)

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	A	301	-	-	0/11/31/31	0/3/3/3
2	A3P	B	302	-	-	0/11/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	A3P	P2-O5P	-2.12	1.47	1.54
2	B	302	A3P	C2-N3	2.29	1.36	1.32
2	A	301	A3P	C2-N3	2.42	1.36	1.32

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	A3P	P1-O3'-C3'	2.30	127.08	121.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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%)	5.02	269 (95%) 0 0	9, 18, 37, 57	0
1	B	280/297 (94%)	4.89	274 (97%) 0 0	9, 20, 39, 49	0
All	All	563/594 (94%)	4.95	543 (96%) 0 0	9, 19, 38, 57	0

All (543) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	VAL	16.3
1	A	217	ALA	15.0
1	B	35	LEU	14.7
1	B	93	ILE	12.6
1	A	61	ILE	12.4
1	A	287	CYS	12.3
1	A	233	LYS	11.6
1	B	142	PHE	11.1
1	B	271	ALA	10.9
1	A	50	GLY	10.9
1	A	190	PHE	10.7
1	A	264	TRP	10.4
1	B	244	PRO	10.3
1	A	200	ILE	10.3
1	A	65	GLY	10.0
1	A	224	ILE	9.7
1	B	240	TYR	9.5
1	A	54	ILE	9.5
1	B	119	TRP	9.5
1	A	248	MET	9.4
1	A	291	PHE	9.3
1	A	137	VAL	9.2
1	A	223	ILE	9.2
1	A	132	ALA	9.1

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Mol	Chain	Res	Type	RSRZ
1	B	219	LEU	9.0
1	B	207	LEU	9.0
1	A	162	PHE	8.9
1	A	144	LEU	8.9
1	A	240	TYR	8.9
1	A	255	PHE	8.9
1	B	59	TYR	8.8
1	A	104	ILE	8.7
1	B	255	PHE	8.6
1	A	227	THR	8.5
1	B	118	PHE	8.5
1	B	169	TYR	8.5
1	A	261	ILE	8.4
1	B	275	ARG	8.4
1	A	35	LEU	8.3
1	A	149	TYR	8.3
1	A	205	VAL	8.3
1	A	214	LYS	8.3
1	A	118	PHE	8.2
1	A	204	VAL	8.2
1	A	66	ASP	8.2
1	B	161	LYS	8.2
1	B	215	PRO	8.1
1	B	237	SER	8.0
1	A	53	TRP	7.9
1	B	167	VAL	7.9
1	A	220	VAL	7.9
1	A	219	LEU	7.8
1	A	293	MET	7.8
1	B	291	PHE	7.8
1	A	192	PHE	7.7
1	B	38	PRO	7.7
1	B	28	TRP	7.7
1	A	76	PHE	7.7
1	A	155	PHE	7.7
1	A	129	CYS	7.7
1	B	179	TRP	7.6
1	A	79	ILE	7.6
1	A	176	VAL	7.6
1	A	152	PRO	7.6
1	A	93	ILE	7.6
1	A	140	TYR	7.6

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Mol	Chain	Res	Type	RSRZ
1	B	41	LEU	7.6
1	B	113	LEU	7.5
1	B	186	SER	7.5
1	B	268	PHE	7.4
1	B	261	ILE	7.4
1	A	193	TYR	7.4
1	B	173	TYR	7.3
1	B	223	ILE	7.3
1	B	76	PHE	7.3
1	B	148	SER	7.3
1	B	208	ILE	7.3
1	B	13	GLY	7.3
1	B	241	THR	7.2
1	A	24	PHE	7.2
1	B	9	TYR	7.2
1	B	146	ILE	7.2
1	B	159	VAL	7.1
1	B	16	ARG	7.0
1	B	172	TRP	7.0
1	A	102	PRO	7.0
1	A	136	ALA	7.0
1	B	162	PHE	7.0
1	B	156	SER	6.9
1	B	15	PHE	6.9
1	A	116	ALA	6.9
1	B	217	ALA	6.9
1	A	243	MET	6.9
1	B	105	VAL	6.9
1	A	126	ILE	6.9
1	A	234	ASN	6.9
1	B	114	LEU	6.8
1	B	276	PHE	6.8
1	A	280	TYR	6.8
1	A	271	ALA	6.8
1	B	64	GLU	6.8
1	A	156	SER	6.8
1	B	141	TYR	6.8
1	B	90	ILE	6.7
1	A	60	MET	6.7
1	B	279	HIS	6.7
1	B	33	MET	6.7
1	A	95	GLN	6.6

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Mol	Chain	Res	Type	RSRZ
1	A	260	ILE	6.6
1	B	79	ILE	6.6
1	A	254	PRO	6.6
1	A	135	VAL	6.6
1	A	173	TYR	6.6
1	B	272	LEU	6.6
1	B	46	TYR	6.5
1	B	132	ALA	6.5
1	A	59	TYR	6.5
1	B	260	ILE	6.5
1	B	29	GLU	6.5
1	A	41	LEU	6.5
1	A	189	LEU	6.4
1	A	42	VAL	6.4
1	A	146	ILE	6.4
1	B	24	PHE	6.4
1	A	272	LEU	6.3
1	A	208	ILE	6.3
1	B	54	ILE	6.3
1	B	123	CYS	6.3
1	B	127	TYR	6.3
1	B	289	VAL	6.3
1	A	229	PHE	6.2
1	B	188	VAL	6.2
1	B	224	ILE	6.2
1	A	15	PHE	6.2
1	B	189	LEU	6.2
1	A	57	VAL	6.2
1	B	228	SER	6.2
1	B	128	LEU	6.2
1	B	43	ILE	6.2
1	B	176	VAL	6.1
1	A	242	MET	6.1
1	B	18	VAL	6.1
1	A	46	TYR	6.1
1	A	288	THR	6.1
1	B	75	ILE	6.0
1	A	210	PHE	6.0
1	B	139	TYR	6.0
1	A	90	ILE	6.0
1	B	274	GLU	6.0
1	A	289	VAL	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	269	PRO	6.0
1	B	262	GLY	6.0
1	B	140	TYR	5.9
1	B	264	TRP	5.9
1	B	158	PHE	5.9
1	A	92	GLY	5.9
1	B	8	TYR	5.9
1	A	58	VAL	5.9
1	A	211	LEU	5.9
1	A	235	ASN	5.9
1	B	126	ILE	5.9
1	B	34	PHE	5.8
1	B	116	ALA	5.8
1	B	171	SER	5.8
1	B	84	CYS	5.8
1	A	34	PHE	5.8
1	A	212	GLU	5.8
1	B	229	PHE	5.8
1	A	199	ASP	5.8
1	B	27	TYR	5.7
1	A	241	THR	5.7
1	B	220	VAL	5.7
1	B	192	PHE	5.7
1	A	25	THR	5.7
1	A	8	TYR	5.7
1	B	222	ARG	5.7
1	B	155	PHE	5.7
1	A	27	TYR	5.6
1	B	104	ILE	5.6
1	B	180	TRP	5.6
1	B	17	GLY	5.6
1	B	252	VAL	5.6
1	A	143	LEU	5.6
1	B	144	LEU	5.6
1	A	122	ASN	5.6
1	A	188	VAL	5.6
1	B	31	VAL	5.6
1	B	80	PRO	5.6
1	B	99	LYS	5.6
1	B	284	MET	5.6
1	B	204	VAL	5.5
1	A	141	TYR	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	268	PHE	5.5
1	B	199	ASP	5.4
1	A	159	VAL	5.4
1	A	249	ASN	5.4
1	A	270	GLU	5.3
1	A	36	ALA	5.3
1	A	148	SER	5.3
1	A	89	LEU	5.3
1	A	256	MET	5.3
1	A	109	LEU	5.3
1	B	100	GLU	5.3
1	A	228	SER	5.3
1	B	60	MET	5.3
1	A	75	ILE	5.2
1	B	249	ASN	5.2
1	A	180	TRP	5.2
1	A	105	VAL	5.2
1	B	170	GLY	5.2
1	B	210	PHE	5.2
1	A	172	TRP	5.1
1	B	57	VAL	5.1
1	B	193	TYR	5.1
1	A	213	ARG	5.1
1	A	232	MET	5.1
1	A	28	TRP	5.1
1	B	187	ARG	5.1
1	A	236	PRO	5.1
1	B	53	TRP	5.1
1	A	62	TYR	5.1
1	B	288	THR	5.1
1	B	122	ASN	5.1
1	A	218	GLU	5.1
1	B	61	ILE	5.1
1	B	257	ARG	5.0
1	B	137	VAL	5.0
1	B	256	MET	5.0
1	A	267	HIS	5.0
1	A	179	TRP	5.0
1	A	158	PHE	5.0
1	B	243	MET	5.0
1	B	273	ARG	5.0
1	B	214	LYS	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	96	LEU	5.0
1	B	62	TYR	5.0
1	B	149	TYR	4.9
1	A	84	CYS	4.9
1	B	20	MET	4.9
1	B	12	PHE	4.9
1	A	278	GLU	4.9
1	A	39	ASP	4.9
1	A	81	TYR	4.9
1	B	135	VAL	4.9
1	A	281	LYS	4.9
1	B	280	TYR	4.9
1	B	286	ASP	4.9
1	A	142	PHE	4.8
1	B	82	LEU	4.8
1	A	222	ARG	4.8
1	B	7	GLU	4.8
1	B	250	GLN	4.8
1	A	244	PRO	4.8
1	B	185	ASN	4.8
1	B	236	PRO	4.8
1	A	170	GLY	4.8
1	B	259	GLY	4.8
1	A	139	TYR	4.8
1	B	72	GLU	4.7
1	B	97	LYS	4.7
1	A	231	GLU	4.7
1	A	207	LEU	4.7
1	B	39	ASP	4.7
1	A	31	VAL	4.7
1	A	165	GLY	4.7
1	B	233	LYS	4.7
1	A	239	ASN	4.7
1	B	213	ARG	4.7
1	B	52	THR	4.7
1	B	92	GLY	4.7
1	B	147	THR	4.7
1	A	196	MET	4.7
1	B	178	ALA	4.7
1	A	225	GLN	4.7
1	A	127	TYR	4.6
1	B	111	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	251	LYS	4.6
1	B	73	ASP	4.6
1	B	10	GLU	4.6
1	B	81	TYR	4.6
1	A	164	GLN	4.6
1	A	215	PRO	4.6
1	A	9	TYR	4.6
1	A	169	TYR	4.5
1	A	128	LEU	4.5
1	A	273	ARG	4.5
1	A	49	SER	4.5
1	A	18	VAL	4.5
1	A	185	ASN	4.5
1	A	119	TRP	4.5
1	B	153	LYS	4.4
1	A	121	LYS	4.4
1	A	19	LEU	4.4
1	B	285	LYS	4.4
1	A	202	ARG	4.4
1	B	129	CYS	4.4
1	B	165	GLY	4.4
1	B	230	GLN	4.4
1	B	234	ASN	4.3
1	B	58	VAL	4.3
1	B	205	VAL	4.3
1	B	36	ALA	4.3
1	B	25	THR	4.3
1	A	237	SER	4.3
1	B	287	CYS	4.3
1	A	52	THR	4.3
1	A	38	PRO	4.3
1	A	257	ARG	4.3
1	B	248	MET	4.3
1	A	150	PRO	4.3
1	B	225	GLN	4.3
1	A	51	THR	4.3
1	B	78	ARG	4.3
1	A	123	CYS	4.3
1	B	206	LYS	4.2
1	A	186	SER	4.2
1	A	195	ASP	4.2
1	B	23	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	294	GLU	4.2
1	B	143	LEU	4.2
1	B	190	PHE	4.2
1	A	183	SER	4.2
1	A	216	SER	4.2
1	A	134	ASP	4.2
1	A	201	ARG	4.2
1	A	154	SER	4.2
1	B	182	LYS	4.1
1	A	11	VAL	4.1
1	B	200	ILE	4.1
1	A	101	SER	4.1
1	A	77	ASN	4.1
1	A	47	PRO	4.1
1	B	110	PRO	4.1
1	A	258	LYS	4.1
1	B	212	GLU	4.1
1	A	131	ASN	4.1
1	A	238	THR	4.1
1	B	131	ASN	4.1
1	A	245	GLU	4.1
1	B	120	GLU	4.1
1	A	145	MET	4.0
1	A	113	LEU	4.0
1	B	202	ARG	4.0
1	B	211	LEU	4.0
1	B	77	ASN	4.0
1	A	153	LYS	4.0
1	A	177	LYS	4.0
1	B	96	LEU	4.0
1	B	246	GLU	4.0
1	B	227	THR	4.0
1	B	44	ALA	4.0
1	A	191	MET	4.0
1	B	98	GLU	4.0
1	A	230	GLN	4.0
1	B	221	ASP	4.0
1	A	226	HIS	4.0
1	A	63	LYS	4.0
1	A	13	GLY	3.9
1	A	99	LYS	3.9
1	B	164	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	285	LYS	3.9
1	A	266	ASN	3.9
1	A	44	ALA	3.9
1	B	163	MET	3.9
1	B	11	VAL	3.9
1	B	254	PRO	3.9
1	B	19	LEU	3.9
1	B	239	ASN	3.9
1	A	277	ASP	3.9
1	B	14	GLU	3.9
1	B	216	SER	3.9
1	A	94	LYS	3.9
1	B	37	ARG	3.8
1	A	115	PRO	3.8
1	A	97	LYS	3.8
1	B	151	ASN	3.8
1	B	30	ASP	3.8
1	A	184	LYS	3.8
1	A	167	VAL	3.8
1	B	45	THR	3.8
1	B	138	SER	3.8
1	B	191	MET	3.8
1	B	293	MET	3.8
1	A	74	ALA	3.8
1	B	247	MET	3.8
1	B	166	GLN	3.8
1	B	89	LEU	3.7
1	B	112	LYS	3.7
1	B	117	SER	3.7
1	A	16	ARG	3.7
1	B	251	LYS	3.7
1	B	115	PRO	3.7
1	B	152	PRO	3.7
1	B	168	PRO	3.7
1	A	138	SER	3.7
1	A	187	ARG	3.7
1	A	174	ASP	3.7
1	A	151	ASN	3.7
1	A	246	GLU	3.7
1	B	283	GLN	3.7
1	A	114	LEU	3.7
1	B	157	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	178	ALA	3.7
1	B	136	ALA	3.7
1	A	284	MET	3.6
1	B	232	MET	3.6
1	A	166	GLN	3.6
1	A	125	MET	3.6
1	B	245	GLU	3.6
1	A	259	GLY	3.6
1	B	269	PRO	3.6
1	B	196	MET	3.6
1	A	147	THR	3.6
1	A	86	ASN	3.6
1	A	197	LYS	3.6
1	B	51	THR	3.5
1	A	250	GLN	3.5
1	B	85	ARG	3.5
1	A	33	MET	3.5
1	B	145	MET	3.5
1	B	174	ASP	3.5
1	A	82	LEU	3.5
1	B	32	GLU	3.5
1	B	242	MET	3.5
1	A	276	PHE	3.5
1	A	221	ASP	3.4
1	A	64	GLU	3.4
1	B	86	ASN	3.4
1	B	292	ARG	3.4
1	A	274	GLU	3.4
1	A	279	HIS	3.4
1	B	154	SER	3.4
1	B	270	GLU	3.4
1	B	201	ARG	3.4
1	B	197	LYS	3.4
1	A	163	MET	3.4
1	A	206	LYS	3.3
1	A	14	GLU	3.3
1	A	98	GLU	3.3
1	A	106	LYS	3.3
1	B	26	LYS	3.3
1	A	12	PHE	3.3
1	A	286	ASP	3.3
1	B	124	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	258	LYS	3.3
1	A	209	GLU	3.2
1	A	292	ARG	3.2
1	B	183	SER	3.2
1	B	109	LEU	3.2
1	A	73	ASP	3.2
1	B	42	VAL	3.2
1	A	171	SER	3.2
1	B	253	SER	3.2
1	A	32	GLU	3.2
1	B	50	GLY	3.2
1	A	124	LYS	3.2
1	A	263	ASP	3.1
1	B	175	HIS	3.1
1	B	130	ARG	3.1
1	B	195	ASP	3.1
1	A	29	GLU	3.1
1	A	282	GLN	3.1
1	B	281	LYS	3.1
1	B	125	MET	3.1
1	A	55	SER	3.1
1	B	49	SER	3.1
1	B	238	THR	3.1
1	B	91	ASN	3.1
1	B	266	ASN	3.1
1	B	231	GLU	3.0
1	A	45	THR	3.0
1	A	198	GLU	3.0
1	B	277	ASP	3.0
1	B	74	ALA	3.0
1	A	265	LYS	3.0
1	B	160	GLU	2.9
1	B	94	LYS	2.9
1	A	78	ARG	2.9
1	A	283	GLN	2.9
1	A	181	GLU	2.9
1	A	43	ILE	2.9
1	B	102	PRO	2.9
1	A	21	ASP	2.9
1	A	161	LYS	2.9
1	B	226	HIS	2.8
1	A	80	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	181	GLU	2.8
1	B	198	GLU	2.8
1	A	168	PRO	2.8
1	A	247	MET	2.8
1	A	133	LYS	2.8
1	A	7	GLU	2.8
1	A	37	ARG	2.8
1	A	110	PRO	2.8
1	A	103	ARG	2.8
1	A	252	VAL	2.7
1	A	253	SER	2.7
1	A	83	GLU	2.7
1	B	267	HIS	2.7
1	B	177	LYS	2.6
1	A	175	HIS	2.6
1	B	133	LYS	2.6
1	A	85	ARG	2.6
1	B	282	GLN	2.6
1	A	108	HIS	2.5
1	B	56	GLU	2.5
1	A	130	ARG	2.5
1	A	275	ARG	2.5
1	A	117	SER	2.5
1	B	278	GLU	2.5
1	A	40	ASP	2.5
1	B	134	ASP	2.5
1	A	56	GLU	2.5
1	A	100	GLU	2.5
1	B	48	LYS	2.5
1	A	120	GLU	2.4
1	A	112	LYS	2.4
1	B	88	ASP	2.4
1	B	263	ASP	2.4
1	B	21	ASP	2.4
1	B	107	THR	2.4
1	B	87	GLU	2.3
1	B	235	ASN	2.3
1	B	194	GLU	2.3
1	A	203	GLU	2.3
1	B	218	GLU	2.3
1	A	17	GLY	2.3
1	B	95	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	23	ARG	2.3
1	B	106	LYS	2.2
1	B	63	LYS	2.2
1	B	55	SER	2.2
1	B	203	GLU	2.2
1	B	265	LYS	2.2
1	B	40	ASP	2.2
1	B	184	LYS	2.1
1	B	290	LYS	2.1
1	B	150	PRO	2.1
1	B	47	PRO	2.1
1	B	108	HIS	2.1
1	A	88	ASP	2.1
1	A	160	GLU	2.0
1	A	48	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
2	A3P	A	301	27/27	0.71	0.31	-0.37	9,12,16,17	0
2	A3P	B	302	27/27	0.70	0.23	-1.34	10,16,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.