



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:25 PM GMT

PDB ID : 1AQU  
Title : ESTROGEN SULFOTRANSFERASE WITH BOUND INACTIVE COFAC-  
TOR PAP AND 17-BETA ESTRADIOL  
Authors : Kakuta, Y.; Negishi, M.; Pedersen, L.C.  
Deposited on : 1997-08-01  
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

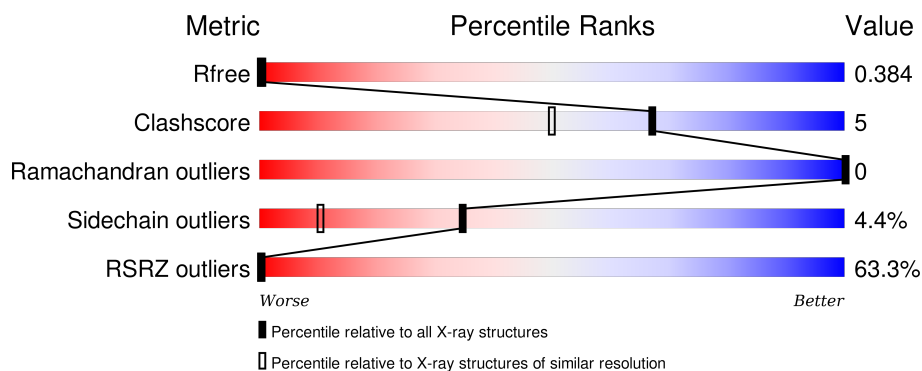
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	297	<div> <div>69%</div> <div>83% 10% • 5%</div> </div>
1	B	297	<div> <div>51%</div> <div>81% 11% • 6%</div> </div>

## 2 Entry composition [i](#)

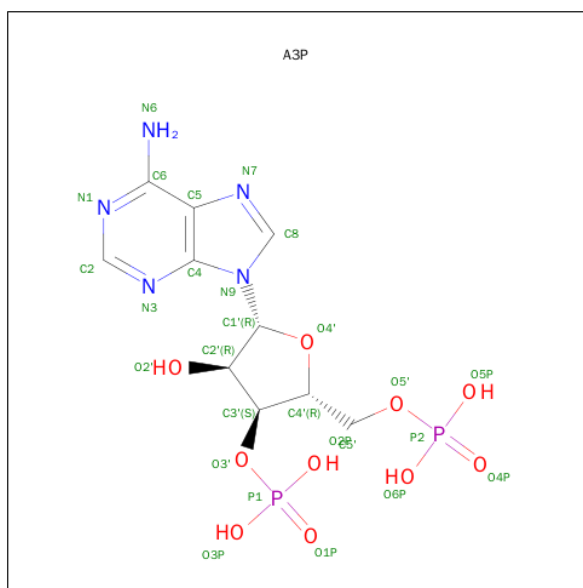
There are 4 unique types of molecules in this entry. The entry contains 5143 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

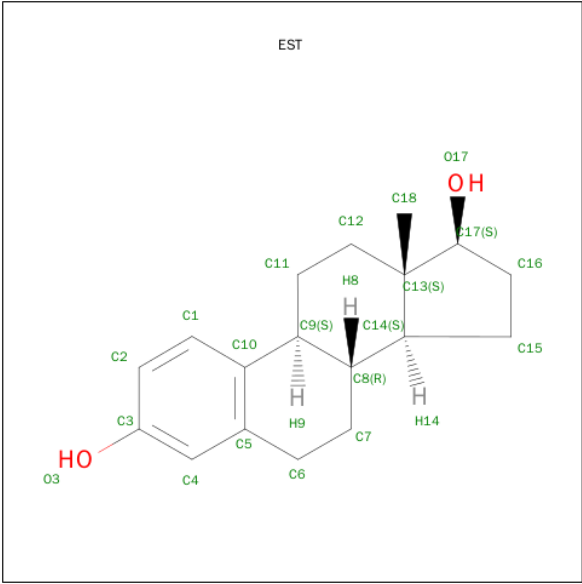
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2389	1549	393	427	20			
1	B	280	Total	C	N	O	S	0	0	0
			2381	1545	392	424	20			

- 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 ESTRADIOL (three-letter code: EST) (formula:  $C_{18}H_{24}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			20	18	2		
3	A	1	Total	C	O	0	0
			20	18	2		

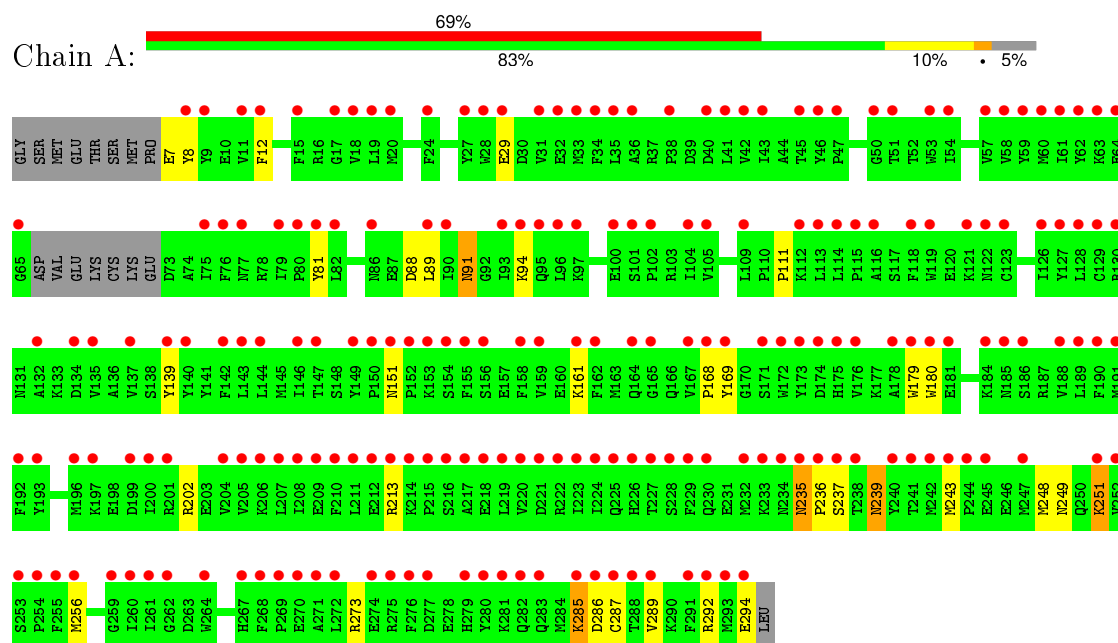
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	154	Total	O	0	0
			154	154		
4	B	125	Total	O	0	0
			125	125		

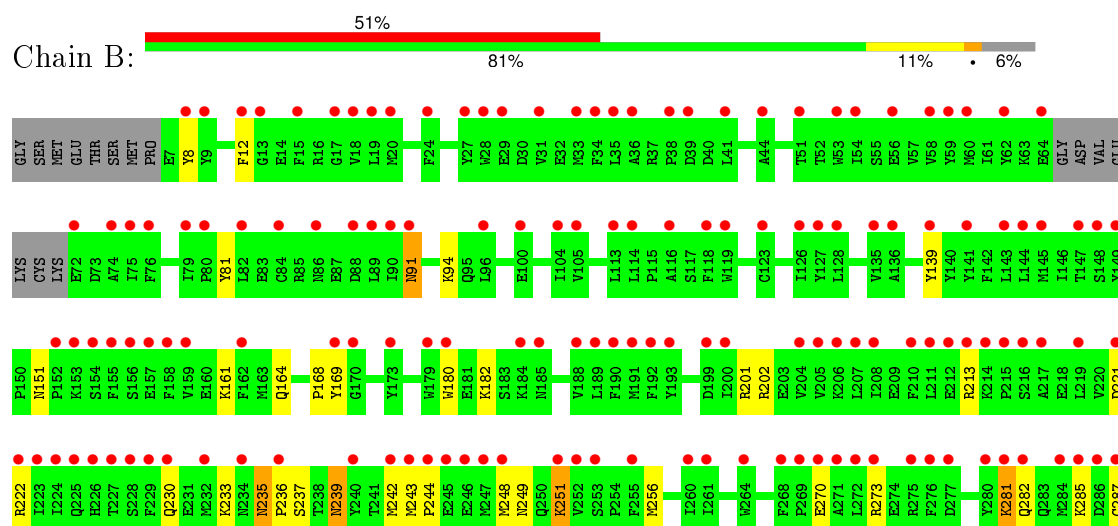
### 3 Residue-property plots

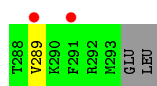
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). 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





A residue validation plot for the protein structure 1AQU. The plot shows a vertical bar chart of residues from T288 to L290. The residues are color-coded: T288 (yellow), V289 (green), K290 (green), F291 (green), R292 (green), N293 (green), Q294 (grey), and L290 (grey). Two red dots are positioned above the bars for residues T288 and V289, indicating specific validation points or outliers.

Residue	Color
T288	Yellow
V289	Green
K290	Green
F291	Green
R292	Green
N293	Green
Q294	Grey
L290	Grey

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.38Å 80.39Å 80.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.60 19.13 – 1.58	Depositor EDS
% Data completeness (in resolution range)	81.7 (50.00-1.60) 78.6 (19.13-1.58)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.17 (at 1.58Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.218 , 0.251 0.383 , 0.384	Depositor DCC
$R_{free}$ test set	7000 reflections (11.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	14.6	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 38.0	EDS
Estimated twinning fraction	0.024 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 71412 reflections	Xtriage
$F_o, F_c$ correlation	0.79	EDS
Total number of atoms	5143	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 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, EST

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	0.51	0/2456	0.60	0/3306
1	B	0.49	0/2448	0.59	0/3296
All	All	0.50	0/4904	0.60	0/6602

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	2389	0	2348	22	1
1	B	2381	0	2341	26	2
2	A	27	0	11	1	0
2	B	27	0	11	0	0
3	A	20	0	24	0	0
3	B	20	0	24	0	0
4	A	154	0	0	1	1
4	B	125	0	0	2	1
All	All	5143	0	4759	46	3

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 5.

All (46) 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:287:CYS:SG	1:B:289:VAL:HG23	2.19	0.82
1:B:202:ARG:HH11	1:B:202:ARG:HG3	1.47	0.80
1:A:202:ARG:HH11	1:A:202:ARG:HG3	1.47	0.79
1:A:287:CYS:SG	1:A:289:VAL:HG23	2.22	0.79
1:B:233:LYS:HA	1:B:256:MET:HG3	1.76	0.67
1:B:151:ASN:ND2	4:B:371:HOH:O	2.30	0.65
1:A:151:ASN:ND2	4:A:328:HOH:O	2.32	0.62
1:B:202:ARG:NH1	1:B:202:ARG:HG3	2.14	0.59
1:A:202:ARG:NH1	1:A:202:ARG:HG3	2.14	0.57
1:A:235:ASN:ND2	1:A:237:SER:H	2.05	0.55
1:A:29:GLU:H	1:A:29:GLU:CD	2.11	0.54
1:B:239:ASN:C	1:B:239:ASN:HD22	2.11	0.53
1:A:89:LEU:HD23	1:B:244:PRO:HG2	1.89	0.53
1:A:243:MET:HG2	1:A:248:MET:SD	2.49	0.53
1:A:235:ASN:HD22	1:A:235:ASN:C	2.12	0.53
1:A:91:ASN:C	1:A:91:ASN:HD22	2.12	0.53
1:B:235:ASN:ND2	1:B:237:SER:H	2.06	0.53
1:A:239:ASN:C	1:A:239:ASN:HD22	2.13	0.52
1:B:235:ASN:HD22	1:B:235:ASN:C	2.13	0.51
1:B:282:GLN:HE22	1:B:285:LYS:NZ	2.09	0.51
1:B:180:TRP:CG	1:B:289:VAL:HG22	2.46	0.50
1:B:91:ASN:HD22	1:B:91:ASN:C	2.14	0.50
1:B:243:MET:HG2	1:B:248:MET:SD	2.51	0.50
1:A:256:MET:CE	2:A:301:A3P:H8	2.42	0.50
1:A:12:PHE:CE1	1:A:168:PRO:HG3	2.46	0.50
1:B:12:PHE:CE1	1:B:168:PRO:HG3	2.47	0.50
1:B:180:TRP:CD2	1:B:289:VAL:HG22	2.46	0.49
1:B:249:ASN:OD1	1:B:251:LYS:HB2	2.13	0.48
1:A:249:ASN:OD1	1:A:251:LYS:HB2	2.13	0.48
1:B:282:GLN:OE1	1:B:285:LYS:HE3	2.14	0.48
1:B:281:LYS:O	1:B:285:LYS:HG3	2.14	0.47
1:A:180:TRP:CD2	1:A:289:VAL:HG22	2.50	0.47
1:B:201:ARG:NH2	1:B:221:ASP:OD1	2.45	0.46
1:A:168:PRO:O	1:A:169:TYR:HB2	2.17	0.45
1:A:111:PRO:HD3	1:A:179:TRP:CD1	2.52	0.45
1:A:8:TYR:CZ	1:A:161:LYS:HE2	2.51	0.45
1:B:235:ASN:HD22	1:B:236:PRO:N	2.16	0.44
1:A:88:ASP:HB2	1:B:242:MET:HB3	1.99	0.44
1:B:287:CYS:SG	1:B:289:VAL:CG2	3.01	0.44
1:B:281:LYS:HE3	1:B:285:LYS:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ASN:HD22	1:A:236:PRO:N	2.16	0.43
1:B:168:PRO:O	1:B:169:TYR:HB2	2.18	0.42
1:A:292:ARG:O	1:A:294:GLU:HG2	2.19	0.42
1:B:8:TYR:CZ	1:B:161:LYS:HE2	2.55	0.41
1:B:182:LYS:HE2	4:B:407:HOH:O	2.21	0.41
1:A:285:LYS:H	1:A:285:LYS:HG3	1.50	0.41

All (3) 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:7:GLU:OE1	4:B:367:HOH:O[4_456]	1.51	0.69
1:B:270:GLU:CG	1:B:270:GLU:CG[2_565]	1.86	0.34
1:B:164:GLN:O	4:A:308:HOH:O[3_556]	1.90	0.30

## 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	277/297 (93%)	267 (96%)	10 (4%)	0	100	100
1	B	276/297 (93%)	262 (95%)	14 (5%)	0	100	100
All	All	553/594 (93%)	529 (96%)	24 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	263/278 (95%)	252 (96%)	11 (4%)	36	11
1	B	262/278 (94%)	250 (95%)	12 (5%)	33	9
All	All	525/556 (94%)	502 (96%)	23 (4%)	35	10

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	TYR
1	A	91	ASN
1	A	94	LYS
1	A	139	TYR
1	A	213	ARG
1	A	235	ASN
1	A	239	ASN
1	A	251	LYS
1	A	273	ARG
1	A	285	LYS
1	A	286	ASP
1	B	81	TYR
1	B	91	ASN
1	B	94	LYS
1	B	139	TYR
1	B	213	ARG
1	B	222	ARG
1	B	230	GLN
1	B	235	ASN
1	B	239	ASN
1	B	251	LYS
1	B	273	ARG
1	B	281	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	122	ASN
1	A	151	ASN
1	A	166	GLN

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Mol	Chain	Res	Type
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	151	ASN
1	B	166	GLN
1	B	226	HIS
1	B	235	ASN
1	B	239	ASN
1	B	282	GLN

### 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](#)

4 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	1.18	3 (12%)	28,45,45	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EST	A	304	-	23,23,23	1.91	7 (30%)	36,36,36	1.07	2 (5%)
2	A3P	B	302	-	24,29,29	1.14	1 (4%)	28,45,45	0.91	2 (7%)
3	EST	B	303	-	23,23,23	2.03	9 (39%)	36,36,36	1.05	2 (5%)

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
3	EST	A	304	-	-	0/0/40/40	0/4/4/4
2	A3P	B	302	-	-	0/11/31/31	0/3/3/3
3	EST	B	303	-	-	0/0/40/40	0/4/4/4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	A3P	P1-O2P	-2.17	1.46	1.54
2	A	301	A3P	P2-O5P	-2.15	1.47	1.54
3	B	303	EST	C18-C13	2.00	1.58	1.54
3	B	303	EST	C16-C17	2.07	1.57	1.53
3	B	303	EST	C4-C3	2.14	1.42	1.39
3	A	304	EST	C18-C13	2.20	1.58	1.54
3	B	303	EST	C13-C14	2.22	1.59	1.55
2	A	301	A3P	C2-N3	2.26	1.36	1.32
3	A	304	EST	C4-C5	2.35	1.43	1.39
2	B	302	A3P	C2-N3	2.53	1.36	1.32
3	B	303	EST	C4-C5	2.54	1.44	1.39
3	A	304	EST	C4-C3	2.56	1.43	1.39
3	A	304	EST	C8-C14	2.72	1.59	1.53
3	B	303	EST	C8-C14	2.89	1.59	1.53
3	A	304	EST	C9-C8	3.08	1.57	1.54
3	A	304	EST	C1-C10	3.10	1.44	1.39
3	B	303	EST	C1-C10	3.23	1.44	1.39
3	B	303	EST	C9-C8	3.47	1.58	1.54
3	A	304	EST	C5-C10	3.53	1.45	1.39
3	B	303	EST	C5-C10	3.81	1.46	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	302	A3P	O2'-C2'-C3'	2.09	117.19	111.16
2	B	302	A3P	P1-O3'-C3'	2.13	126.66	121.56
3	B	303	EST	C16-C17-C13	2.21	106.29	104.58
3	A	304	EST	C16-C17-C13	2.39	106.44	104.58
3	B	303	EST	C15-C14-C8	2.51	122.99	119.03
3	A	304	EST	C15-C14-C8	2.68	123.26	119.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	281/297 (94%)	3.00	204 (72%) <b>0</b> <b>0</b>	9, 17, 35, 53	0
1	B	280/297 (94%)	2.26	151 (53%) <b>0</b> <b>0</b>	11, 19, 37, 52	0
All	All	561/594 (94%)	2.63	355 (63%) <b>0</b> <b>0</b>	9, 18, 36, 53	0

All (355) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	271	ALA	10.4
1	B	64	GLU	8.2
1	A	287	CYS	7.9
1	A	220	VAL	7.8
1	A	65	GLY	7.5
1	A	208	ILE	7.0
1	A	252	VAL	6.8
1	B	228	SER	6.7
1	A	139	TYR	6.6
1	A	219	LEU	6.6
1	A	214	LYS	6.5
1	A	53	TRP	6.3
1	A	204	VAL	6.0
1	A	229	PHE	5.9
1	A	276	PHE	5.8
1	A	146	ILE	5.7
1	B	252	VAL	5.6
1	A	256	MET	5.6
1	A	135	VAL	5.6
1	B	13	GLY	5.5
1	A	264	TRP	5.5
1	A	57	VAL	5.4
1	A	9	TYR	5.4
1	A	260	ILE	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	230	GLN	5.2
1	A	212	GLU	5.1
1	A	282	GLN	5.1
1	A	180	TRP	5.0
1	A	104	ILE	5.0
1	A	240	TYR	5.0
1	B	59	TYR	5.0
1	B	217	ALA	5.0
1	A	223	ILE	4.8
1	A	59	TYR	4.8
1	B	236	PRO	4.7
1	A	210	PHE	4.7
1	A	62	TYR	4.7
1	A	164	GLN	4.7
1	A	215	PRO	4.7
1	B	208	ILE	4.6
1	A	285	LYS	4.6
1	A	255	PHE	4.6
1	A	81	TYR	4.5
1	A	41	LEU	4.5
1	B	189	LEU	4.5
1	A	245	GLU	4.4
1	A	200	ILE	4.4
1	A	153	LYS	4.4
1	A	186	SER	4.4
1	A	152	PRO	4.4
1	A	270	GLU	4.4
1	B	105	VAL	4.4
1	B	216	SER	4.4
1	A	222	ARG	4.4
1	A	102	PRO	4.3
1	A	289	VAL	4.3
1	B	260	ILE	4.3
1	A	279	HIS	4.3
1	A	224	ILE	4.3
1	A	61	ILE	4.2
1	A	105	VAL	4.2
1	B	119	TRP	4.2
1	A	192	PHE	4.2
1	B	243	MET	4.2
1	A	137	VAL	4.2
1	A	143	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	268	PHE	4.2
1	A	235	ASN	4.1
1	A	43	ILE	4.1
1	A	144	LEU	4.1
1	B	128	LEU	4.1
1	A	42	VAL	4.1
1	A	63	LYS	4.0
1	A	167	VAL	4.0
1	A	196	MET	4.0
1	A	291	PHE	4.0
1	B	229	PHE	4.0
1	A	234	ASN	4.0
1	B	205	VAL	4.0
1	A	243	MET	4.0
1	A	162	PHE	4.0
1	A	64	GLU	4.0
1	A	216	SER	3.9
1	A	176	VAL	3.9
1	B	31	VAL	3.9
1	B	270	GLU	3.9
1	A	173	TYR	3.9
1	A	217	ALA	3.9
1	A	24	PHE	3.9
1	A	184	LYS	3.9
1	B	141	TYR	3.8
1	A	54	ILE	3.8
1	A	76	PHE	3.8
1	A	142	PHE	3.8
1	B	155	PHE	3.8
1	A	140	TYR	3.8
1	B	18	VAL	3.7
1	A	158	PHE	3.7
1	A	277	ASP	3.7
1	A	193	TYR	3.7
1	B	190	PHE	3.7
1	A	115	PRO	3.7
1	A	254	PRO	3.7
1	A	280	TYR	3.7
1	B	272	LEU	3.7
1	A	28	TRP	3.6
1	B	248	MET	3.6
1	A	189	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	286	ASP	3.6
1	A	190	PHE	3.6
1	B	147	THR	3.6
1	A	89	LEU	3.6
1	B	211	LEU	3.6
1	B	224	ILE	3.6
1	B	179	TRP	3.6
1	A	60	MET	3.6
1	B	79	ILE	3.6
1	B	90	ILE	3.6
1	A	213	ARG	3.6
1	B	153	LYS	3.5
1	B	247	MET	3.5
1	A	225	GLN	3.5
1	A	113	LEU	3.5
1	B	275	ARG	3.5
1	B	28	TRP	3.5
1	A	199	ASP	3.4
1	B	185	ASN	3.4
1	A	179	TRP	3.4
1	A	233	LYS	3.4
1	A	292	ARG	3.4
1	A	293	MET	3.4
1	A	269	PRO	3.4
1	A	132	ALA	3.4
1	A	31	VAL	3.4
1	A	205	VAL	3.4
1	A	155	PHE	3.4
1	B	158	PHE	3.3
1	A	218	GLU	3.3
1	B	180	TRP	3.3
1	A	126	ILE	3.3
1	A	127	TYR	3.3
1	A	244	PRO	3.3
1	A	51	THR	3.3
1	A	18	VAL	3.3
1	A	114	LEU	3.3
1	A	90	ILE	3.3
1	A	36	ALA	3.2
1	A	109	LEU	3.2
1	B	8	TYR	3.2
1	B	51	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	262	GLY	3.2
1	A	149	TYR	3.2
1	B	244	PRO	3.2
1	B	280	TYR	3.2
1	B	223	ILE	3.2
1	B	245	GLU	3.2
1	A	19	LEU	3.2
1	B	154	SER	3.2
1	A	169	TYR	3.2
1	A	226	HIS	3.2
1	B	213	ARG	3.2
1	A	100	GLU	3.1
1	B	123	CYS	3.1
1	B	114	LEU	3.1
1	B	156	SER	3.1
1	B	188	VAL	3.1
1	A	238	THR	3.1
1	A	96	LEU	3.1
1	A	129	CYS	3.1
1	A	185	ASN	3.1
1	A	259	GLY	3.1
1	A	29	GLU	3.1
1	A	45	THR	3.1
1	B	144	LEU	3.1
1	B	287	CYS	3.1
1	A	242	MET	3.1
1	B	169	TYR	3.1
1	A	236	PRO	3.0
1	A	17	GLY	3.0
1	B	234	ASN	3.0
1	B	148	SER	3.0
1	A	50	GLY	3.0
1	B	126	ILE	3.0
1	A	251	LYS	3.0
1	A	294	GLU	3.0
1	B	289	VAL	3.0
1	A	207	LEU	3.0
1	B	273	ARG	3.0
1	B	225	GLN	3.0
1	A	8	TYR	3.0
1	B	34	PHE	3.0
1	A	211	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	219	LEU	3.0
1	B	29	GLU	3.0
1	A	191	MET	3.0
1	A	288	THR	3.0
1	A	121	LYS	3.0
1	A	247	MET	2.9
1	B	139	TYR	2.9
1	A	119	TRP	2.9
1	B	41	LEU	2.9
1	A	275	ARG	2.9
1	A	253	SER	2.9
1	A	27	TYR	2.9
1	B	27	TYR	2.9
1	A	261	ILE	2.9
1	A	172	TRP	2.9
1	B	38	PRO	2.9
1	B	242	MET	2.9
1	A	118	PHE	2.9
1	A	168	PRO	2.9
1	B	104	ILE	2.9
1	B	226	HIS	2.9
1	A	123	CYS	2.9
1	B	255	PHE	2.9
1	A	134	ASP	2.9
1	B	39	ASP	2.9
1	B	136	ALA	2.9
1	B	232	MET	2.9
1	A	75	ILE	2.9
1	B	204	VAL	2.9
1	A	128	LEU	2.8
1	A	188	VAL	2.8
1	A	230	GLN	2.8
1	B	118	PHE	2.8
1	B	291	PHE	2.8
1	A	58	VAL	2.8
1	B	113	LEU	2.8
1	A	201	ARG	2.8
1	A	12	PHE	2.8
1	A	94	LYS	2.8
1	B	285	LYS	2.8
1	B	74	ALA	2.8
1	B	214	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	145	MET	2.8
1	A	82	LEU	2.7
1	A	112	LYS	2.7
1	A	272	LEU	2.7
1	B	17	GLY	2.7
1	A	181	GLU	2.7
1	A	227	THR	2.7
1	B	36	ALA	2.7
1	A	150	PRO	2.7
1	A	32	GLU	2.7
1	B	222	ARG	2.7
1	A	15	PHE	2.7
1	B	15	PHE	2.7
1	B	276	PHE	2.7
1	B	135	VAL	2.7
1	A	281	LYS	2.7
1	B	284	MET	2.7
1	A	35	LEU	2.7
1	B	35	LEU	2.7
1	A	178	ALA	2.7
1	B	53	TRP	2.6
1	A	11	VAL	2.6
1	B	269	PRO	2.6
1	B	200	ILE	2.6
1	B	116	ALA	2.6
1	A	154	SER	2.6
1	B	12	PHE	2.6
1	A	79	ILE	2.6
1	B	271	ALA	2.6
1	A	122	ASN	2.6
1	A	130	ARG	2.6
1	A	147	THR	2.6
1	A	237	SER	2.5
1	B	191	MET	2.5
1	B	76	PHE	2.5
1	B	152	PRO	2.5
1	A	101	SER	2.5
1	B	227	THR	2.5
1	A	159	VAL	2.5
1	B	143	LEU	2.5
1	B	210	PHE	2.5
1	A	38	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	44	ALA	2.5
1	B	159	VAL	2.5
1	B	19	LEU	2.5
1	B	170	GLY	2.5
1	B	162	PHE	2.5
1	A	46	TYR	2.4
1	B	221	ASP	2.4
1	B	212	GLU	2.4
1	A	97	LYS	2.4
1	B	96	LEU	2.4
1	B	24	PHE	2.4
1	A	80	PRO	2.4
1	B	58	VAL	2.4
1	B	33	MET	2.4
1	A	95	GLN	2.4
1	A	232	MET	2.4
1	A	171	SER	2.4
1	B	215	PRO	2.4
1	B	268	PHE	2.4
1	A	274	GLU	2.3
1	B	72	GLU	2.3
1	B	246	GLU	2.3
1	B	60	MET	2.3
1	A	283	GLN	2.3
1	B	91	ASN	2.3
1	B	149	TYR	2.3
1	A	174	ASP	2.3
1	A	175	HIS	2.3
1	B	54	ILE	2.3
1	B	253	SER	2.3
1	A	165	GLY	2.3
1	B	88	ASP	2.3
1	B	207	LEU	2.3
1	B	206	LYS	2.3
1	B	199	ASP	2.3
1	B	84	CYS	2.3
1	B	82	LEU	2.2
1	A	93	ILE	2.2
1	B	173	TYR	2.2
1	A	34	PHE	2.2
1	B	192	PHE	2.2
1	A	116	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	89	LEU	2.2
1	B	261	ILE	2.2
1	B	264	TRP	2.2
1	A	77	ASN	2.2
1	A	86	ASN	2.2
1	B	56	GLU	2.2
1	B	184	LYS	2.2
1	A	20	MET	2.2
1	A	206	LYS	2.2
1	B	127	TYR	2.2
1	B	193	TYR	2.2
1	A	47	PRO	2.1
1	B	80	PRO	2.1
1	B	282	GLN	2.1
1	A	228	SER	2.1
1	B	277	ASP	2.1
1	B	86	ASN	2.1
1	B	157	GLU	2.1
1	B	100	GLU	2.1
1	B	62	TYR	2.1
1	B	240	TYR	2.1
1	A	267	HIS	2.1
1	B	20	MET	2.1
1	A	151	ASN	2.1
1	B	75	ILE	2.1
1	B	9	TYR	2.1
1	A	209	GLU	2.0
1	B	286	ASP	2.0
1	A	161	LYS	2.0
1	A	33	MET	2.0
1	A	156	SER	2.0
1	A	40	ASP	2.0
1	A	221	ASP	2.0
1	A	241	THR	2.0
1	A	197	LYS	2.0
1	B	251	LYS	2.0
1	B	281	LYS	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EST	B	303	20/20	0.55	0.28	1.76	23,26,31,31	0
3	EST	A	304	20/20	0.61	0.20	-0.33	17,20,25,29	0
2	A3P	A	301	27/27	0.77	0.20	-0.70	9,12,16,17	0
2	A3P	B	302	27/27	0.85	0.14	-1.02	12,17,20,23	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.