



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 09:01 pm BST

PDB ID : 4L9Q  
Title : X-ray study of human serum albumin complexed with teniposide  
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Deposited on : 2013-06-18  
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](mailto: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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

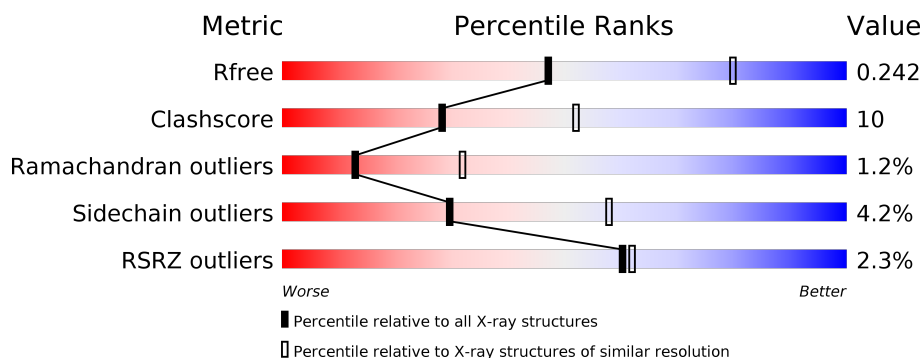
# 1 Overall quality at a glance

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))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	585	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 20%, green 77%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>77%</span> <span>20%</span> <span>..</span> </div> </div>
1	B	585	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 1%, yellow 18%, green 78%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>78%</span> <span>18%</span> <span>..</span> </div> </div>

## 2 Entry composition [i](#)

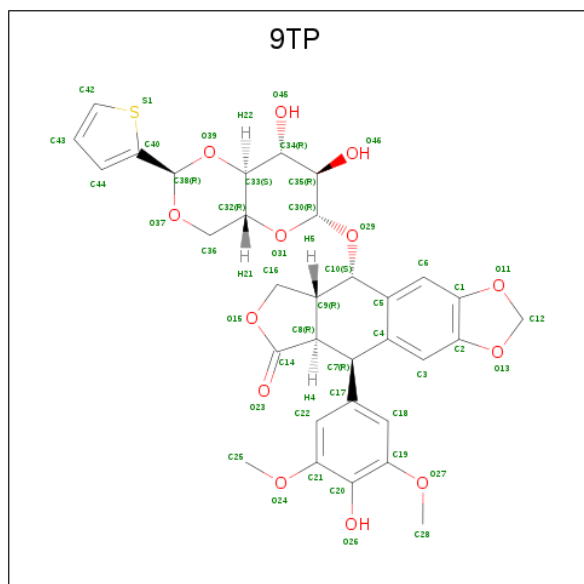
There are 3 unique types of molecules in this entry. The entry contains 9423 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SERUM ALBUMIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4623	2918	782	882	41			
1	B	578	Total	C	N	O	S	0	0	0
			4599	2903	776	879	41			

- Molecule 2 is (5S,5aR,8aR,9R)-9-(4-hydroxy-3,5-dimethoxyphenyl)-8-oxo-5,5a,6,8,8a,9-hexahydrofuro[3',4':6,7]naphtho[2,3-d][1,3]dioxol-5-yl 4,6-O-(thiophen-2-ylmethylidene)-beta-D-glucopyranoside (three-letter code: 9TP) (formula: C<sub>32</sub>H<sub>32</sub>O<sub>13</sub>S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			46	32	13	1		
2	B	1	Total	C	O	S	0	0
			46	32	13	1		

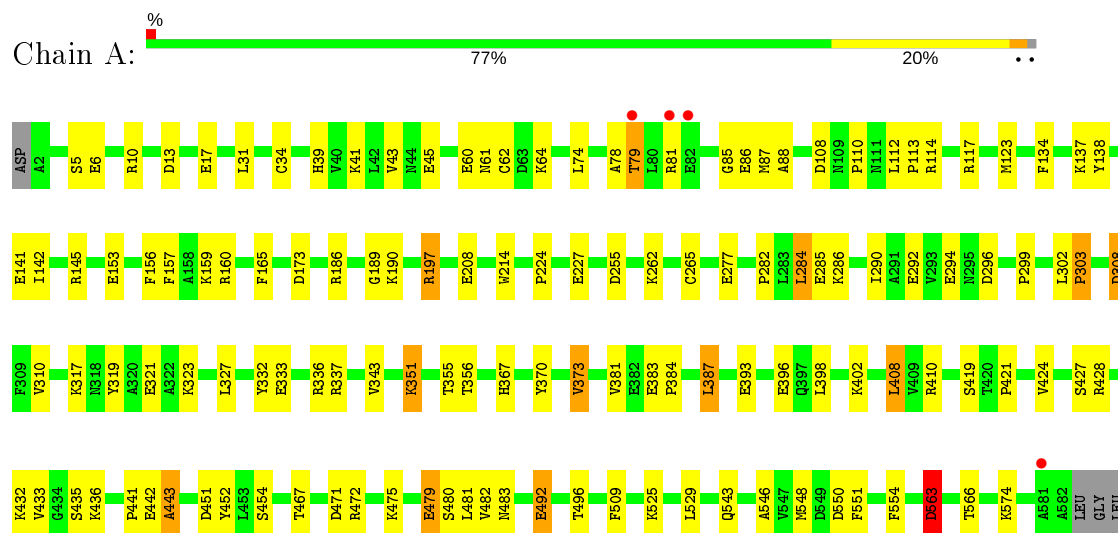
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	69	Total 69	O 69	0	0
3	B	40	Total 40	O 40	0	0

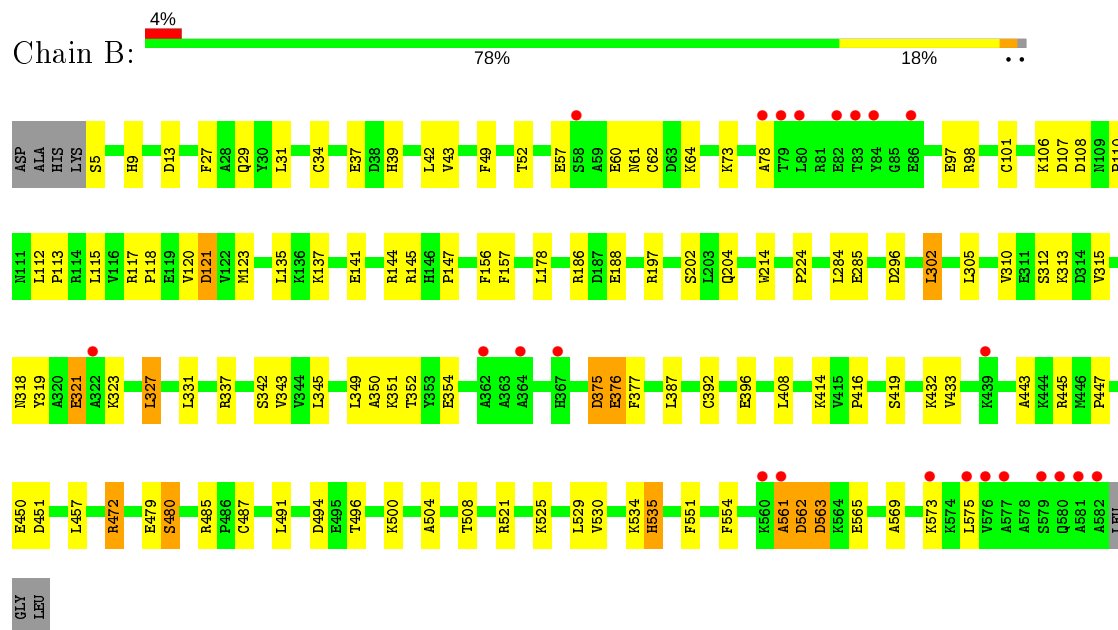
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: SERUM ALBUMIN



#### • Molecule 1: SERUM ALBUMIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.35Å 59.59Å 95.54Å 73.17° 83.45° 73.93°	Depositor
Resolution (Å)	29.66 – 2.70 29.66 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.7 (29.66-2.70) 90.8 (29.66-2.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.10 (at 2.68Å)	Xtriage
Refinement program	PHENIX 1.8.2 _1309	Depositor
R, $R_{free}$	0.187 , 0.243 0.187 , 0.242	Depositor DCC
$R_{free}$ test set	1530 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.011 for -h,-k,-k+l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9423	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% 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, 0.333 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: 9TP

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	0/4713	0.68	0/6357
1	B	0.46	0/4688	0.64	0/6324
All	All	0.49	0/9401	0.66	0/12681

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	4623	0	4543	95	0
1	B	4599	0	4518	85	0
2	A	46	0	29	10	0
2	B	46	0	30	7	0
3	A	69	0	0	13	0
3	B	40	0	0	10	0
All	All	9423	0	9120	180	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 10.

All (180) 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:525:LYS:NZ	1:A:548:MET:SD	2.35	0.97
1:B:186:ARG:HD2	2:B:601:9TP:H1	1.47	0.94
1:A:31:LEU:HD11	1:A:78:ALA:HB2	1.56	0.86
1:A:142:ILE:HD13	2:A:601:9TP:H15	1.60	0.81
1:A:173:ASP:OD1	1:B:117:ARG:NH1	2.11	0.81
1:B:408:LEU:HD23	1:B:529:LEU:HD23	1.64	0.78
1:B:375:ASP:O	3:B:724:HOH:O	2.04	0.75
1:A:299:PRO:HB2	1:A:302:LEU:HD11	1.66	0.75
1:B:327:LEU:HD21	1:B:354:GLU:HB2	1.68	0.74
1:A:110:PRO:HB2	1:A:112:LEU:HG	1.68	0.73
1:A:138:TYR:CD1	2:A:601:9TP:H10	2.24	0.73
1:A:356:THR:HG21	1:A:373:VAL:HG12	1.72	0.71
1:A:113:PRO:O	1:A:145:ARG:NH2	2.24	0.70
1:B:416:PRO:O	3:B:710:HOH:O	2.10	0.70
1:B:61:ASN:HB3	1:B:64:LYS:HD2	1.72	0.69
1:A:308:ASP:OD1	1:A:308:ASP:N	2.25	0.69
1:A:208:GLU:OE1	3:A:738:HOH:O	2.11	0.69
1:A:333:GLU:OE1	1:A:337:ARG:NH2	2.26	0.68
1:B:57:GLU:OE2	3:B:714:HOH:O	2.11	0.68
1:A:79:THR:HA	1:A:88:ALA:HB2	1.77	0.67
1:A:393:GLU:OE1	3:A:747:HOH:O	2.13	0.65
1:A:81:ARG:NH2	1:A:88:ALA:HB3	2.13	0.64
1:B:569:ALA:O	1:B:573:LYS:HG3	1.98	0.64
1:B:186:ARG:HH11	2:B:601:9TP:H1	1.63	0.64
1:B:392:CYS:O	1:B:396:GLU:HG2	1.98	0.64
1:A:525:LYS:HE2	1:A:551:PHE:HD1	1.63	0.63
1:A:529:LEU:HD13	1:A:548:MET:HE1	1.79	0.63
2:A:601:9TP:H9	2:A:601:9TP:O31	1.99	0.62
1:A:332:TYR:O	1:A:336:ARG:HG3	1.99	0.62
1:A:480:SER:OG	1:A:481:LEU:N	2.28	0.61
1:B:375:ASP:O	1:B:377:PHE:N	2.32	0.60
1:A:433:VAL:HG22	1:A:452:TYR:HD2	1.66	0.60
1:B:141:GLU:OE1	1:B:145:ARG:NH1	2.34	0.60
1:B:137:LYS:HB3	2:B:601:9TP:H27	1.82	0.60
1:A:563:ASP:OD1	1:A:566:THR:OG1	2.12	0.60
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.84	0.59
1:A:292:GLU:O	3:A:737:HOH:O	2.17	0.58
1:A:134:PHE:CD1	2:A:601:9TP:H30	2.37	0.58
1:A:299:PRO:HB2	1:A:302:LEU:CD1	2.33	0.57
1:B:42:LEU:HD22	1:B:73:LYS:HG3	1.85	0.57
1:A:156:PHE:HE1	1:A:285:GLU:HG3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:GLN:NE2	3:B:730:HOH:O	2.29	0.56
1:B:97:GLU:OE2	3:B:705:HOH:O	2.18	0.56
1:A:419:SER:OG	1:A:421:PRO:HD2	2.04	0.56
1:A:141:GLU:OE1	1:A:145:ARG:NH1	2.32	0.56
1:A:408:LEU:HD13	1:A:427:SER:HB2	1.87	0.56
1:A:381:VAL:O	1:A:384:PRO:HD2	2.05	0.56
1:B:525:LYS:HG2	1:B:551:PHE:HE2	1.71	0.56
1:A:551:PHE:HA	1:A:554:PHE:CE2	2.39	0.56
1:A:81:ARG:HH21	1:A:88:ALA:HB3	1.71	0.55
1:A:302:LEU:HB3	1:A:337:ARG:NH1	2.21	0.55
1:A:433:VAL:HG22	1:A:452:TYR:CD2	2.40	0.55
1:B:110:PRO:HB2	1:B:112:LEU:HG	1.88	0.55
1:B:342:SER:HA	1:B:447:PRO:HA	1.89	0.54
1:B:186:ARG:NH1	2:B:601:9TP:H3	2.23	0.54
1:A:509:PHE:CD2	1:A:554:PHE:HZ	2.26	0.54
1:A:156:PHE:HD1	1:A:284:LEU:HB3	1.74	0.53
1:A:441:PRO:O	1:A:443:ALA:N	2.41	0.53
1:B:120:VAL:HG13	1:B:178:LEU:HD23	1.90	0.53
1:B:504:ALA:O	1:B:508:THR:HG23	2.07	0.53
1:A:551:PHE:HD2	1:A:554:PHE:HE2	1.56	0.53
1:B:5:SER:HA	1:B:62:CYS:O	2.08	0.53
1:B:521:ARG:O	1:B:525:LYS:HG3	2.10	0.52
1:B:186:ARG:HD2	2:B:601:9TP:C3	2.32	0.52
1:A:432:LYS:HE3	3:A:763:HOH:O	2.10	0.51
1:A:351:LYS:HE2	1:A:355:THR:HG23	1.93	0.51
1:A:186:ARG:HD2	2:A:601:9TP:H1	1.92	0.51
1:B:351:LYS:NZ	1:B:354:GLU:OE1	2.27	0.50
1:A:17:GLU:O	3:A:720:HOH:O	2.19	0.50
1:A:61:ASN:HB3	1:A:64:LYS:HD2	1.93	0.50
1:B:352:THR:HG23	1:B:377:PHE:HE1	1.76	0.50
1:A:31:LEU:HD13	1:A:34:CYS:SG	2.51	0.50
1:A:398:LEU:O	1:A:402:LYS:HB2	2.12	0.50
1:A:134:PHE:HD1	2:A:601:9TP:H30	1.76	0.49
1:A:302:LEU:HD23	1:A:337:ARG:CZ	2.42	0.49
1:B:331:LEU:HD13	1:B:350:ALA:HB2	1.94	0.49
1:B:319:TYR:CZ	1:B:323:LYS:HD3	2.47	0.49
1:B:563:ASP:OD1	1:B:563:ASP:N	2.45	0.49
1:A:286:LYS:O	1:A:290:ILE:HG13	2.12	0.49
1:B:312:SER:HB3	1:B:315:VAL:HG23	1.94	0.49
1:B:39:HIS:O	1:B:43:VAL:HG23	2.13	0.49
1:A:472:ARG:NH2	1:A:492:GLU:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:PHE:HD2	1:A:554:PHE:HZ	1.59	0.48
1:B:551:PHE:HA	1:B:575:LEU:HD21	1.95	0.48
1:A:383:GLU:OE1	1:A:387:LEU:HD11	2.13	0.48
1:A:475:LYS:O	1:A:479:GLU:HB2	2.14	0.48
1:B:107:ASP:O	1:B:110:PRO:HD3	2.13	0.48
1:B:49:PHE:O	1:B:52:THR:HB	2.13	0.48
1:B:157:PHE:CZ	1:B:188:GLU:HG2	2.49	0.48
1:B:432:LYS:NZ	3:B:701:HOH:O	2.43	0.48
1:B:313:LYS:HB2	3:B:719:HOH:O	2.13	0.47
1:B:224:PRO:HD2	1:B:296:ASP:HB3	1.95	0.47
1:A:408:LEU:HD13	1:A:427:SER:CB	2.44	0.47
1:A:108:ASP:OD1	1:A:197:ARG:HD2	2.14	0.47
1:A:39:HIS:O	1:A:43:VAL:HG23	2.15	0.47
1:B:214:TRP:CD1	1:B:343:VAL:HG11	2.49	0.47
1:A:332:TYR:CE2	1:A:336:ARG:HD2	2.50	0.47
1:B:487:CYS:O	1:B:491:LEU:HD13	2.15	0.46
1:B:525:LYS:HG2	1:B:551:PHE:CE2	2.50	0.46
1:A:428:ARG:NH2	3:A:732:HOH:O	2.43	0.46
1:B:9:HIS:NE2	1:B:13:ASP:OD2	2.49	0.46
1:B:318:ASN:HA	1:B:321:GLU:OE1	2.16	0.45
1:A:137:LYS:HG2	2:A:601:9TP:C38	2.47	0.45
1:A:319:TYR:O	1:A:323:LYS:HG2	2.17	0.45
1:A:138:TYR:HD1	2:A:601:9TP:H10	1.75	0.45
1:B:457:LEU:HA	1:B:457:LEU:HD23	1.71	0.45
1:A:160:ARG:NH1	3:A:750:HOH:O	2.31	0.45
1:A:262:LYS:NZ	3:A:740:HOH:O	2.38	0.45
1:B:186:ARG:HH11	2:B:601:9TP:C3	2.29	0.44
1:B:349:LEU:HA	1:B:352:THR:HG22	1.98	0.44
1:B:375:ASP:C	1:B:377:PHE:H	2.20	0.44
1:A:5:SER:HA	1:A:62:CYS:O	2.17	0.44
1:B:106:LYS:HD3	1:B:147:PRO:HB2	1.99	0.44
1:A:428:ARG:NE	3:A:732:HOH:O	2.47	0.44
1:B:117:ARG:HA	1:B:118:PRO:HD3	1.88	0.44
1:B:115:LEU:HD22	2:B:601:9TP:H24	2.00	0.44
1:A:189:GLY:HA3	2:A:601:9TP:C25	2.48	0.44
1:A:159:LYS:NZ	1:A:285:GLU:OE1	2.49	0.44
1:A:31:LEU:HD12	1:A:74:LEU:HD22	2.00	0.44
1:A:303:PRO:O	1:A:337:ARG:NH1	2.51	0.44
1:A:410:ARG:NH1	3:A:746:HOH:O	2.50	0.44
1:B:345:LEU:O	1:B:349:LEU:HG	2.18	0.44
1:A:543:GLN:O	1:A:546:ALA:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:VAL:HG12	1:B:534:LYS:HE3	1.99	0.44
1:A:451:ASP:O	1:A:454:SER:HB2	2.18	0.43
1:B:108:ASP:OD2	1:B:197:ARG:NH1	2.51	0.43
1:A:574:LYS:NZ	3:A:736:HOH:O	2.51	0.43
1:B:31:LEU:HD11	1:B:78:ALA:HB2	1.99	0.43
1:A:410:ARG:NH2	3:A:746:HOH:O	2.52	0.43
1:A:6:GLU:O	1:A:10:ARG:HG2	2.18	0.43
1:A:31:LEU:HD23	1:A:31:LEU:HA	1.82	0.43
1:B:60:GLU:HG3	1:B:61:ASN:H	1.84	0.43
1:B:29:GLN:HG2	1:B:147:PRO:HA	2.01	0.43
1:B:534:LYS:HD3	3:B:710:HOH:O	2.17	0.43
1:A:367:HIS:HA	1:A:370:TYR:CE1	2.53	0.43
1:A:81:ARG:NE	1:A:85:GLY:O	2.52	0.43
1:A:197:ARG:NH2	3:A:709:HOH:O	2.52	0.42
1:B:494:ASP:OD2	1:B:496:THR:OG1	2.22	0.42
1:A:265:CYS:SG	1:A:286:LYS:HD2	2.59	0.42
1:A:529:LEU:HD22	1:A:548:MET:HE1	2.00	0.42
1:A:525:LYS:CE	1:A:548:MET:SD	3.07	0.42
1:B:414:LYS:O	1:B:472:ARG:NH1	2.53	0.42
1:B:500:LYS:O	1:B:535:HIS:HB2	2.19	0.42
1:B:5:SER:N	3:B:706:HOH:O	2.53	0.42
1:B:121:ASP:OD1	1:B:121:ASP:N	2.41	0.42
1:B:144:ARG:NH1	1:B:145:ARG:HH12	2.18	0.42
1:B:31:LEU:HB2	1:B:39:HIS:CE1	2.54	0.42
1:A:13:ASP:HB3	1:A:255:ASP:OD1	2.18	0.42
1:B:98:ARG:O	1:B:101:CYS:HB3	2.20	0.42
1:B:113:PRO:O	1:B:145:ARG:NH2	2.52	0.42
1:B:305:LEU:HD21	1:B:337:ARG:CZ	2.50	0.42
1:A:317:LYS:O	1:A:321:GLU:HB2	2.20	0.42
1:A:41:LYS:O	1:A:45:GLU:HG3	2.20	0.42
1:A:480:SER:HG	1:A:483:ASN:H	1.65	0.41
1:B:352:THR:CG2	1:B:377:PHE:HE1	2.33	0.41
1:B:302:LEU:HD13	1:B:337:ARG:HD3	2.02	0.41
1:A:153:GLU:O	1:A:157:PHE:HD1	2.03	0.41
1:A:383:GLU:O	1:A:387:LEU:HG	2.21	0.41
1:B:156:PHE:HA	1:B:284:LEU:HD23	2.02	0.41
1:B:156:PHE:HD1	1:B:284:LEU:HB3	1.85	0.41
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.56	0.41
1:B:156:PHE:CE1	1:B:285:GLU:HG3	2.55	0.41
1:B:27:PHE:HE2	1:B:42:LEU:HB3	1.86	0.41
1:B:141:GLU:OE1	1:B:144:ARG:NH1	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:MET:HB3	1:A:165:PHE:HE1	1.85	0.41
1:B:31:LEU:HD23	1:B:31:LEU:HA	1.73	0.41
1:B:479:GLU:O	1:B:480:SER:HB3	2.20	0.41
1:B:561:ALA:O	1:B:562:ASP:HB2	2.21	0.41
1:A:190:LYS:HE2	1:A:190:LYS:HB3	1.76	0.41
1:A:142:ILE:CD1	2:A:601:9TP:H15	2.41	0.41
1:B:31:LEU:HB2	1:B:39:HIS:HE1	1.86	0.41
1:A:408:LEU:HD11	1:A:424:VAL:HA	2.03	0.41
1:A:156:PHE:CD1	1:A:284:LEU:HB3	2.56	0.40
1:A:435:SER:HB2	1:A:436:LYS:HZ2	1.86	0.40
1:B:447:PRO:O	1:B:451:ASP:HB2	2.21	0.40
1:B:313:LYS:N	3:B:719:HOH:O	2.52	0.40
1:B:450:GLU:OE2	1:B:485:ARG:NH2	2.52	0.40
1:B:561:ALA:HB1	1:B:563:ASP:OD1	2.21	0.40
1:B:60:GLU:CG	1:B:61:ASN:H	2.33	0.40
1:A:282:PRO:HB2	1:A:285:GLU:OE1	2.22	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	579/585 (99%)	554 (96%)	17 (3%)	8 (1%)	11	28
1	B	576/585 (98%)	554 (96%)	16 (3%)	6 (1%)	15	37
All	All	1155/1170 (99%)	1108 (96%)	33 (3%)	14 (1%)	13	32

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	373	VAL
1	A	443	ALA

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Mol	Chain	Res	Type
1	B	376	GLU
1	B	561	ALA
1	B	562	ASP
1	A	563	ASP
1	B	443	ALA
1	B	563	ASP
1	A	60	GLU
1	A	117	ARG
1	A	479	GLU
1	B	480	SER
1	A	442	GLU
1	A	303	PRO

### 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	508/511 (99%)	485 (96%)	23 (4%)	27	55
1	B	506/511 (99%)	486 (96%)	20 (4%)	31	60
All	All	1014/1022 (99%)	971 (96%)	43 (4%)	30	58

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	THR
1	A	86	GLU
1	A	87	MET
1	A	114	ARG
1	A	197	ARG
1	A	227	GLU
1	A	277	GLU
1	A	284	LEU
1	A	294	GLU
1	A	308	ASP
1	A	310	VAL

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Mol	Chain	Res	Type
1	A	327	LEU
1	A	351	LYS
1	A	387	LEU
1	A	396	GLU
1	A	408	LEU
1	A	467	THR
1	A	471	ASP
1	A	482	VAL
1	A	492	GLU
1	A	496	THR
1	A	550	ASP
1	A	563	ASP
1	B	34	CYS
1	B	37	GLU
1	B	121	ASP
1	B	123	MET
1	B	135	LEU
1	B	202	SER
1	B	302	LEU
1	B	310	VAL
1	B	321	GLU
1	B	327	LEU
1	B	375	ASP
1	B	376	GLU
1	B	387	LEU
1	B	419	SER
1	B	433	VAL
1	B	445	ARG
1	B	472	ARG
1	B	535	HIS
1	B	554	PHE
1	B	565	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	429	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	9TP	A	601	-	52,53,53	4.81	31 (59%)	74,80,80	5.11	32 (43%)
2	9TP	B	601	-	52,53,53	4.78	32 (61%)	74,80,80	3.98	22 (29%)

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	9TP	A	601	-	-	2/12/80/80	0/8/8/8
2	9TP	B	601	-	-	0/12/80/80	0/8/8/8

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	9TP	C8-C14	-19.07	1.26	1.51
2	A	601	9TP	C8-C14	-18.60	1.27	1.51
2	A	601	9TP	C16-C9	-13.38	1.29	1.53
2	B	601	9TP	C16-C9	-12.76	1.30	1.53
2	B	601	9TP	O15-C14	11.90	1.61	1.35
2	A	601	9TP	O15-C14	11.61	1.60	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	9TP	C4-C7	8.41	1.63	1.51
2	B	601	9TP	O24-C21	7.25	1.48	1.37
2	A	601	9TP	O24-C21	7.22	1.48	1.37
2	B	601	9TP	C4-C7	7.14	1.61	1.51
2	A	601	9TP	C3-C2	6.33	1.50	1.38
2	B	601	9TP	C3-C2	6.02	1.49	1.38
2	B	601	9TP	C8-C7	-5.96	1.45	1.56
2	A	601	9TP	C8-C7	-5.46	1.45	1.56
2	A	601	9TP	O27-C19	5.44	1.45	1.37
2	B	601	9TP	O39-C38	5.39	1.50	1.42
2	A	601	9TP	O39-C38	5.34	1.50	1.42
2	A	601	9TP	C43-C44	4.98	1.55	1.39
2	B	601	9TP	C43-C44	4.94	1.55	1.39
2	B	601	9TP	O27-C19	4.88	1.44	1.37
2	B	601	9TP	C6-C1	4.76	1.47	1.38
2	A	601	9TP	C6-C1	4.50	1.47	1.38
2	A	601	9TP	O13-C2	4.34	1.44	1.38
2	B	601	9TP	O13-C2	4.27	1.44	1.38
2	B	601	9TP	C9-C10	4.17	1.59	1.53
2	A	601	9TP	O31-C30	4.07	1.52	1.41
2	A	601	9TP	O37-C38	4.03	1.48	1.41
2	B	601	9TP	C43-C42	4.02	1.46	1.34
2	A	601	9TP	C43-C42	3.94	1.46	1.34
2	B	601	9TP	O39-C33	3.90	1.50	1.44
2	A	601	9TP	C5-C4	3.85	1.47	1.40
2	B	601	9TP	C40-S1	-3.84	1.65	1.73
2	B	601	9TP	O31-C30	3.70	1.51	1.41
2	B	601	9TP	C5-C4	3.61	1.46	1.40
2	A	601	9TP	O39-C33	3.59	1.49	1.44
2	B	601	9TP	C6-C5	3.54	1.45	1.39
2	A	601	9TP	C40-S1	-3.50	1.66	1.73
2	A	601	9TP	O11-C1	3.30	1.43	1.38
2	A	601	9TP	O26-C20	3.26	1.44	1.37
2	A	601	9TP	C19-C20	3.23	1.44	1.40
2	A	601	9TP	C3-C4	3.13	1.44	1.39
2	B	601	9TP	O29-C30	-3.11	1.33	1.41
2	B	601	9TP	O37-C38	3.11	1.46	1.41
2	A	601	9TP	C9-C10	3.10	1.57	1.53
2	B	601	9TP	C21-C20	-3.07	1.36	1.40
2	A	601	9TP	C6-C5	3.06	1.44	1.39
2	B	601	9TP	O11-C1	2.99	1.42	1.38
2	B	601	9TP	O26-C20	2.99	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	9TP	C36-C32	-2.92	1.46	1.51
2	A	601	9TP	C22-C21	2.87	1.44	1.38
2	A	601	9TP	C36-C32	-2.87	1.46	1.51
2	A	601	9TP	O29-C30	-2.85	1.33	1.41
2	B	601	9TP	C8-C9	2.79	1.60	1.54
2	B	601	9TP	C3-C4	2.56	1.43	1.39
2	A	601	9TP	C22-C17	2.49	1.43	1.39
2	B	601	9TP	O29-C10	-2.48	1.39	1.44
2	A	601	9TP	C21-C20	-2.48	1.37	1.40
2	B	601	9TP	C5-C10	2.46	1.55	1.50
2	B	601	9TP	C22-C17	2.45	1.42	1.39
2	A	601	9TP	C8-C9	2.38	1.59	1.54
2	A	601	9TP	C5-C10	2.24	1.54	1.50
2	B	601	9TP	C17-C7	2.22	1.55	1.52
2	B	601	9TP	C44-C40	2.06	1.47	1.38

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	9TP	O37-C38-C40	37.91	153.41	108.57
2	B	601	9TP	O37-C38-C40	28.88	142.73	108.57
2	A	601	9TP	O27-C19-C20	9.51	124.13	114.54
2	B	601	9TP	O39-C38-O37	6.36	117.88	110.85
2	B	601	9TP	O24-C21-C20	6.28	120.87	114.54
2	A	601	9TP	O39-C38-O37	5.65	117.09	110.85
2	B	601	9TP	O15-C14-O23	4.93	126.53	121.42
2	B	601	9TP	C16-C9-C8	4.74	108.64	101.79
2	A	601	9TP	C36-O37-C38	-4.58	106.02	111.22
2	A	601	9TP	O15-C14-C8	-4.57	102.97	109.52
2	A	601	9TP	C16-C9-C8	4.33	108.05	101.79
2	A	601	9TP	C4-C7-C8	4.23	113.69	106.58
2	A	601	9TP	C43-C42-S1	-4.17	109.60	112.98
2	A	601	9TP	O27-C19-C18	-4.13	117.01	124.12
2	B	601	9TP	C9-C8-C14	4.13	108.59	103.07
2	A	601	9TP	C9-C8-C14	4.05	108.50	103.07
2	B	601	9TP	O15-C14-C8	-3.93	103.89	109.52
2	A	601	9TP	C17-C7-C4	3.92	118.78	112.86
2	B	601	9TP	O39-C33-C34	3.91	116.77	109.75
2	A	601	9TP	C5-C10-C9	-3.89	106.77	111.51
2	A	601	9TP	O15-C14-O23	3.70	125.25	121.42
2	B	601	9TP	C5-C4-C7	3.64	124.01	114.40
2	A	601	9TP	C36-C32-C33	3.63	114.82	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	9TP	C17-C7-C8	-3.50	107.74	113.31
2	A	601	9TP	O24-C21-C20	3.37	117.94	114.54
2	B	601	9TP	C17-C7-C4	-3.37	107.78	112.86
2	B	601	9TP	O27-C19-C20	3.28	117.85	114.54
2	B	601	9TP	C43-C42-S1	-3.23	110.36	112.98
2	A	601	9TP	C18-C17-C7	-3.21	114.12	120.39
2	A	601	9TP	C30-O31-C32	-3.14	107.53	113.69
2	A	601	9TP	C22-C17-C7	3.06	126.37	120.39
2	A	601	9TP	O37-C36-C32	-3.02	103.28	109.41
2	A	601	9TP	O13-C2-C3	3.01	131.88	127.85
2	A	601	9TP	C5-C4-C7	2.98	122.28	114.40
2	A	601	9TP	C16-O15-C14	-2.85	107.68	110.28
2	B	601	9TP	C4-C7-C8	2.79	111.27	106.58
2	B	601	9TP	C25-O24-C21	-2.78	113.33	117.53
2	B	601	9TP	C30-O29-C10	-2.67	110.65	114.99
2	B	601	9TP	O24-C21-C22	-2.64	119.58	124.12
2	A	601	9TP	O31-C30-C35	-2.55	104.96	110.35
2	B	601	9TP	C16-O15-C14	-2.49	108.01	110.28
2	A	601	9TP	O29-C30-C35	2.43	114.38	108.10
2	B	601	9TP	O31-C32-C33	2.34	114.69	109.75
2	B	601	9TP	O11-C1-C6	2.33	130.97	127.85
2	A	601	9TP	O11-C1-C6	2.29	130.92	127.85
2	B	601	9TP	O13-C2-C3	2.25	130.87	127.85
2	A	601	9TP	O15-C16-C9	2.22	107.94	104.71
2	A	601	9TP	C28-O27-C19	-2.17	114.25	117.53
2	A	601	9TP	O31-C32-C33	2.17	114.32	109.75
2	A	601	9TP	O13-C2-C1	-2.16	107.32	109.78
2	A	601	9TP	O31-C32-C36	2.13	112.07	108.78
2	A	601	9TP	O39-C33-C32	2.13	112.11	108.88
2	B	601	9TP	C36-C32-C33	2.09	112.53	109.40
2	B	601	9TP	O31-C32-C36	-2.09	105.54	108.78

There are no chirality outliers.

All (2) torsion outliers are listed below:

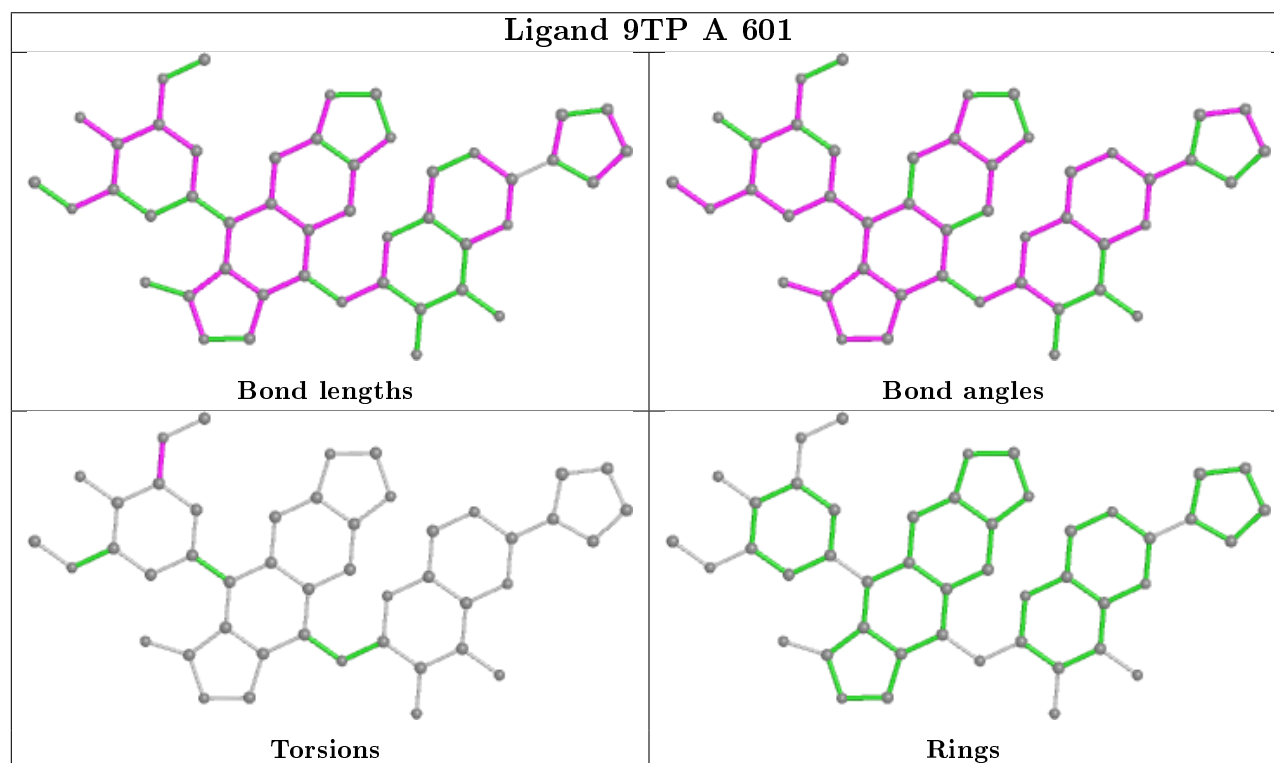
Mol	Chain	Res	Type	Atoms
2	A	601	9TP	C22-C21-O24-C25
2	A	601	9TP	C20-C21-O24-C25

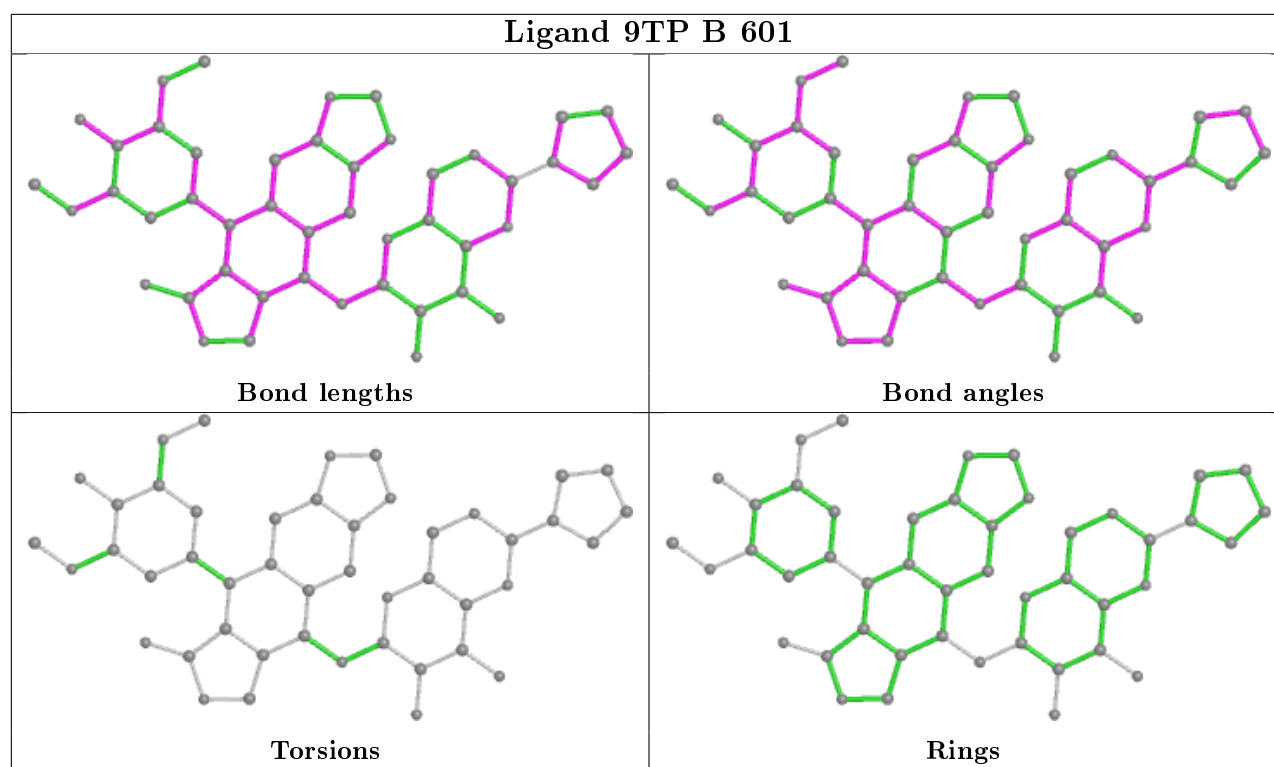
There are no ring outliers.

2 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	9TP	10	0
2	B	601	9TP	7	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 ⓘ

### 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	581/585 (99%)	-0.37	4 (0%) 87 89	12, 29, 60, 84	0
1	B	578/585 (98%)	-0.13	23 (3%) 38 37	21, 40, 69, 90	0
All	All	1159/1170 (99%)	-0.25	27 (2%) 60 62	12, 34, 65, 90	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	582	ALA	5.7
1	B	84	TYR	5.7
1	B	86	GLU	5.5
1	B	581	ALA	5.1
1	B	83	THR	4.8
1	B	580	GLN	4.8
1	B	79	THR	4.2
1	A	82	GLU	4.1
1	B	579	SER	4.1
1	B	575	LEU	4.0
1	B	82	GLU	3.8
1	B	364	ALA	3.3
1	B	80	LEU	3.1
1	B	577	ALA	3.1
1	B	78	ALA	2.8
1	A	79	THR	2.8
1	B	561	ALA	2.7
1	B	362	ALA	2.4
1	A	581	ALA	2.4
1	B	573	LYS	2.4
1	B	322	ALA	2.3
1	A	81	ARG	2.2
1	B	576	VAL	2.2
1	B	439	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	58	SER	2.1
1	B	560	LYS	2.1
1	B	367	HIS	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](#)

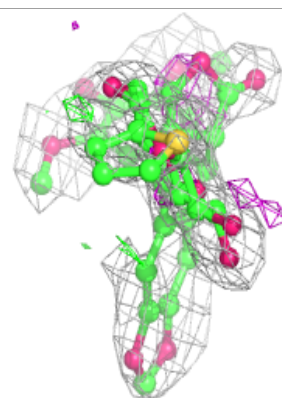
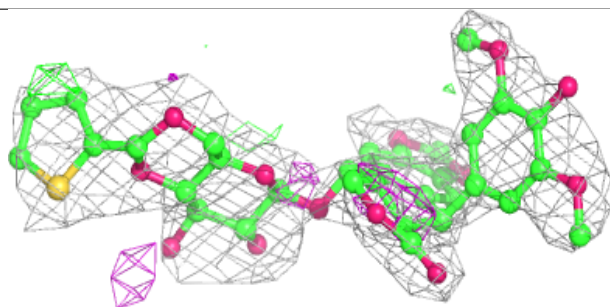
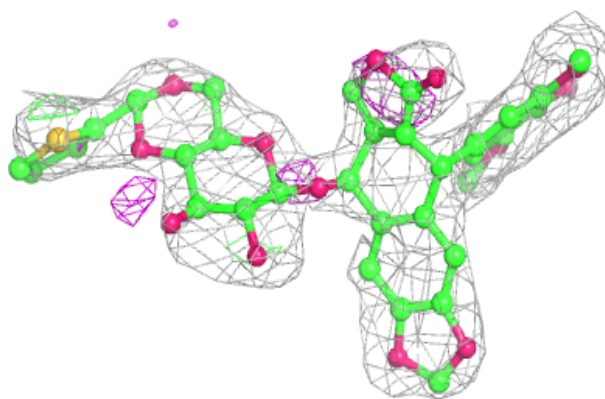
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	9TP	B	601	46/46	0.85	0.26	36,56,69,86	0
2	9TP	A	601	46/46	0.87	0.26	29,53,66,85	0

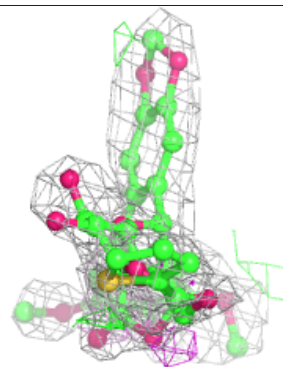
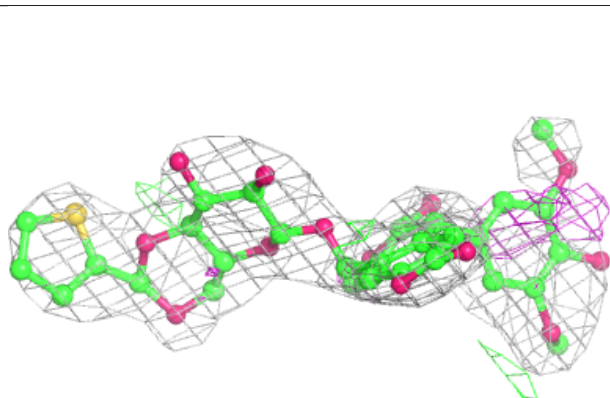
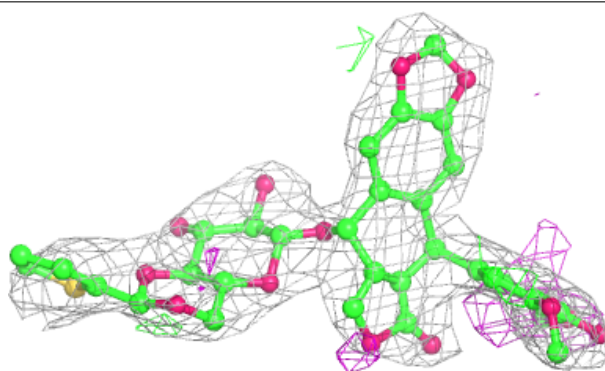
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 9TP B 601:**

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

**Electron density around 9TP A 601:**

$2mF_o-DF_c$  (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.