



# Full wwPDB X-ray Structure Validation Report

Mar 5, 2026 – 05:58 PM UTC

PDB ID : 2BFD / pdb\_00002bfd  
Title : Reactivity modulation of human branched-chain alpha-ketoacid dehydrogenase by an internal molecular switch  
Authors : Machius, M.; Wynn, R.M.; Chuang, J.L.; Tomchick, D.R.; Brautigam, C.A.; Chuang, D.T.  
Deposited on : 2004-12-06  
Resolution : 1.39 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.

The types of validation reports are described at

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

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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)  
Xtrriage (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

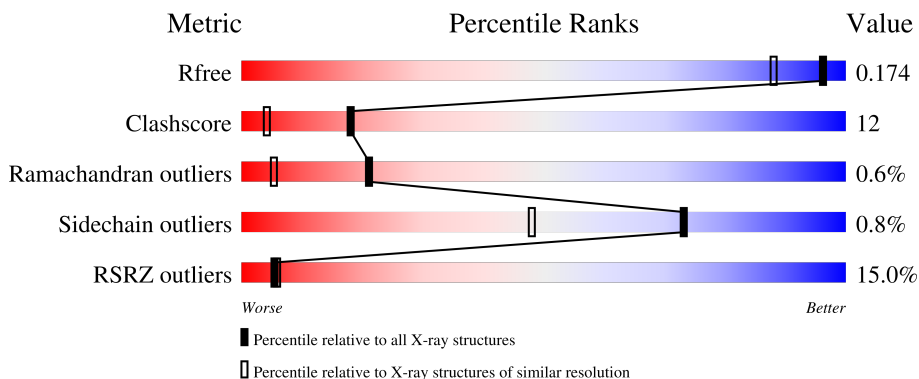
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.39 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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  $\geq 3$ , 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	400	 12% (red), 75% (green), 16% (yellow), 6% (grey)
2	B	342	 17% (red), 88% (green), 8% (yellow), 6% (grey)

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6678 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 2-OXOISOVALERATE DEHYDROGENASE ALPHA SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	374	3312	2085	596	609	22	0	32	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	ALA	TYR	engineered mutation	UNP P12694
A	292	SER	HIS	conflict	UNP P12694
A	300	PHE	TYR	conflict	UNP P12694

- Molecule 2 is a protein called 2-OXOISOVALERATE DEHYDROGENASE BETA SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	332	2721	1746	458	501	16	0	14	0

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total K 1 1	0	0
3	B	1	Total K 1 1	0	0

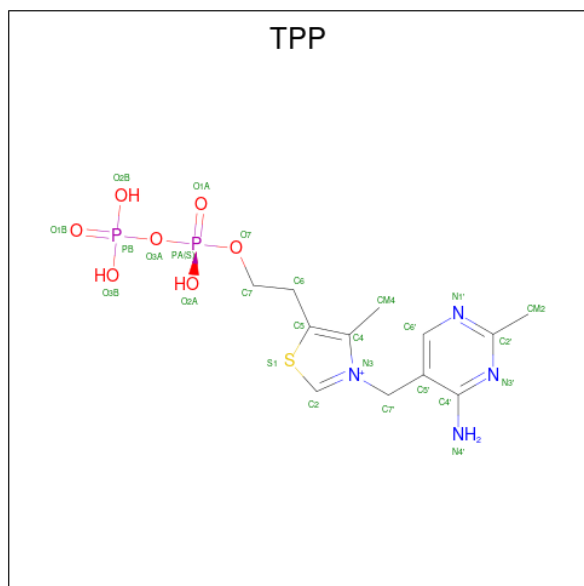
- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mn 1 1	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

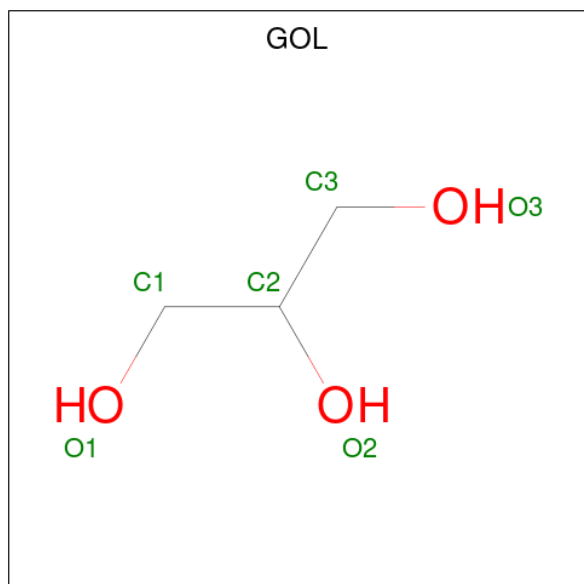
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



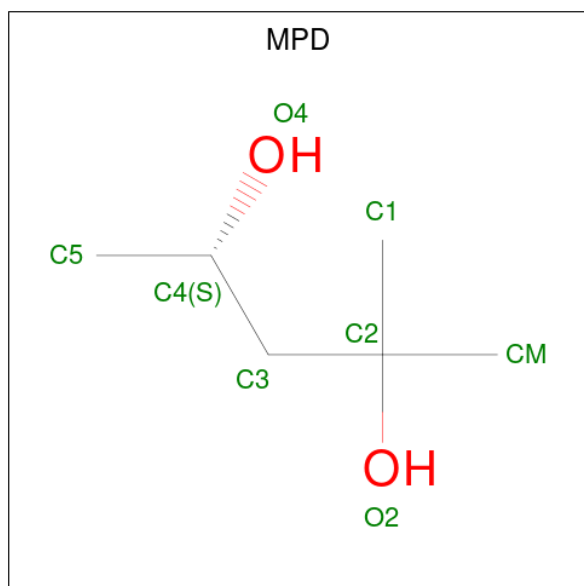
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O P S 26 12 4 7 2 1	0	0

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			8	6	2		

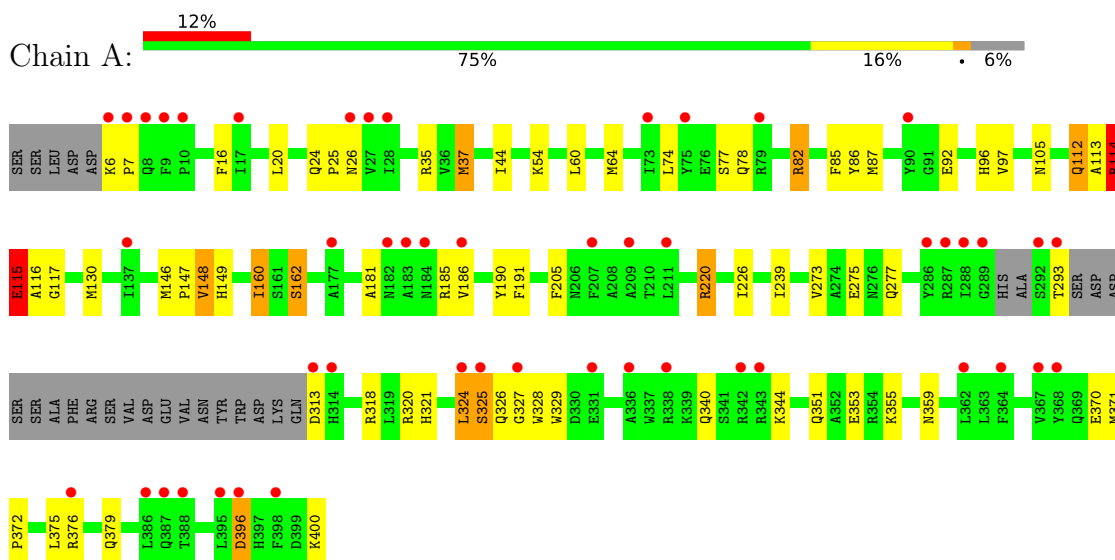
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	340	Total	O	0	0
			340	340		
9	B	261	Total	O	0	0
			261	261		

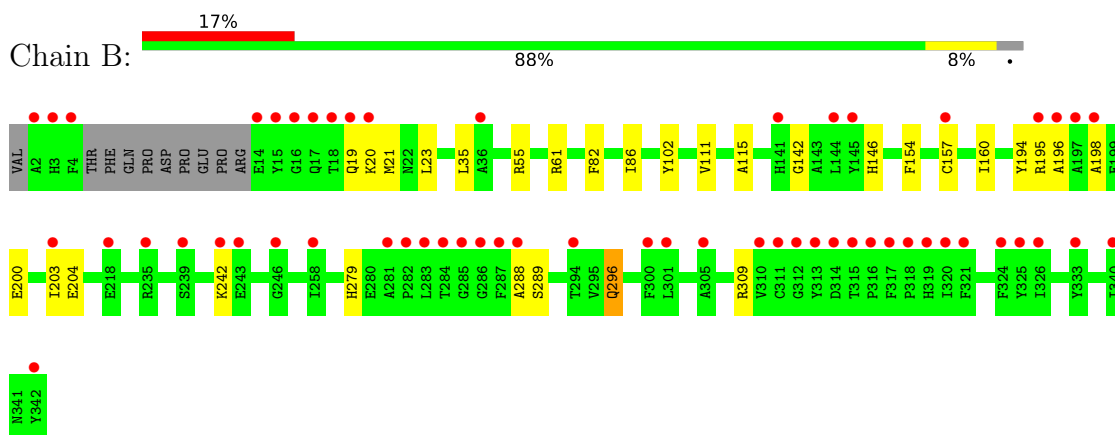
### 3 Residue-property plots

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: 2-OXOISOVALERATE DEHYDROGENASE ALPHA SUBUNIT



- Molecule 2: 2-OXOISOVALERATE DEHYDROGENASE BETA SUBUNIT



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.84Å 144.84Å 69.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.39 30.00 – 1.39	Depositor EDS
% Data completeness (in resolution range)	97.8 (30.00-1.39) 97.7 (30.00-1.39)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 1.39Å)	Xtrriage
Refinement program	REFMAC 5.2.0003	Depositor
R, $R_{free}$	0.149 , 0.170 0.151 , 0.174	Depositor DCC
$R_{free}$ test set	1633 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.8	Xtrriage
Anisotropy	0.320	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 48.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6678	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, GOL, CL, MPD, TPP, MN

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	1.12	6/3390 (0.2%)	1.13	5/4576 (0.1%)
2	B	1.05	1/2790 (0.0%)	1.06	2/3788 (0.1%)
All	All	1.09	7/6180 (0.1%)	1.10	7/8364 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	220	ARG	NE-CZ	9.66	1.43	1.33
1	A	162	SER	CA-CB	7.98	1.64	1.53
1	A	82	ARG	CD-NE	-5.71	1.38	1.46
2	B	61	ARG	CZ-NH1	5.49	1.40	1.32
1	A	114[A]	ARG	N-CA	-5.24	1.40	1.46
1	A	114[B]	ARG	N-CA	-5.24	1.40	1.46
1	A	160	ILE	CG1-CD1	-5.19	1.31	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115[A]	GLU	N-CA-C	-8.30	102.73	112.86
1	A	115[B]	GLU	N-CA-C	-8.30	102.73	112.86
1	A	396	ASP	N-CA-C	5.59	118.14	111.71
1	A	37	MET	CG-SD-CE	-5.50	88.80	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	ALA	N-CA-C	-5.49	106.54	113.18
2	B	61	ARG	NE-CZ-NH1	5.31	126.81	121.50
2	B	242	LYS	N-CA-C	-5.19	105.54	111.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112[B]	GLN	Peptide

## 5.2 Too-close contacts [i](#)

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	3312	0	3187	118	1
2	B	2721	0	2667	29	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	26	0	16	0	0
7	B	6	0	8	0	0
8	B	8	0	14	0	0
9	A	340	0	0	16	0
9	B	261	0	0	2	0
All	All	6678	0	5892	147	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (147) 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:92[A]:GLU:OE2	1:A:114[A]:ARG:HD2	1.28	1.32
1:A:186[B]:VAL:CG2	1:A:273[B]:VAL:CG2	2.08	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92[A]:GLU:OE2	1:A:114[A]:ARG:CD	1.85	1.21
1:A:92[A]:GLU:OE1	1:A:220:ARG:HD2	1.34	1.20
1:A:186[B]:VAL:CG2	1:A:273[B]:VAL:HG23	1.67	1.20
1:A:186[B]:VAL:HG23	1:A:273[B]:VAL:CG2	1.75	1.12
1:A:92[A]:GLU:OE1	1:A:220:ARG:CD	2.07	1.02
1:A:26:ASN:HB3	9:A:2035:HOH:O	1.62	1.00
1:A:149[A]:HIS:CE1	9:A:2162:HOH:O	2.16	0.97
1:A:112[A]:GLN:HE21	1:A:220:ARG:NH2	1.62	0.96
1:A:186[B]:VAL:HG22	1:A:273[B]:VAL:CG2	1.93	0.96
1:A:186[B]:VAL:HG23	1:A:273[B]:VAL:HG21	1.51	0.90
1:A:74:LEU:HD21	1:A:130[A]:MET:SD	2.12	0.88
1:A:112[A]:GLN:NE2	1:A:220:ARG:NH2	2.22	0.87
1:A:92[A]:GLU:OE2	1:A:114[A]:ARG:HD3	1.72	0.86
2:B:111:VAL:HG22	2:B:157[B]:CYS:SG	2.14	0.86
1:A:205[A]:PHE:CD2	9:A:2232:HOH:O	2.28	0.85
1:A:186[B]:VAL:HG21	1:A:273[B]:VAL:HG23	1.55	0.85
1:A:185:ARG:HG2	9:A:2194:HOH:O	1.75	0.84
1:A:149[A]:HIS:ND1	9:A:2162:HOH:O	2.08	0.83
1:A:186[B]:VAL:CG2	1:A:273[B]:VAL:HG22	2.08	0.83
1:A:186[B]:VAL:HG22	1:A:273[B]:VAL:HG23	1.57	0.82
1:A:326:GLN:HB3	1:A:328[A]:TRP:CE2	2.17	0.80
1:A:96[C]:HIS:CE1	1:A:220:ARG:HD3	2.19	0.78
1:A:324[C]:LEU:CD1	1:A:329:TRP:HB3	2.15	0.76
1:A:112[A]:GLN:HB3	1:A:190:TYR:O	1.86	0.76
1:A:112[B]:GLN:HG3	1:A:113[B]:ALA:N	2.01	0.76
1:A:325[A]:SER:C	1:A:327[A]:GLY:H	1.93	0.76
1:A:351:GLN:HG2	1:A:355:LYS:HE3	1.67	0.75
1:A:186[B]:VAL:HG22	1:A:273[B]:VAL:HG22	1.65	0.74
1:A:105:ASN:ND2	9:A:2114:HOH:O	2.21	0.74
1:A:64[B]:MET:SD	1:A:97[B]:VAL:HG21	2.29	0.72
2:B:19:GLN:HE21	2:B:203:ILE:CD1	2.02	0.72
2:B:289[B]:SER:OG	2:B:309:ARG:NH1	2.22	0.72
1:A:112[A]:GLN:HE21	1:A:220:ARG:HH21	1.37	0.72
1:A:82:ARG:NH2	9:A:2090:HOH:O	2.25	0.69
1:A:396:ASP:HB2	9:A:2331:HOH:O	1.94	0.68
1:A:6:LYS:HB3	1:A:7:PRO:HD3	1.75	0.68
1:A:324[C]:LEU:HD11	1:A:329:TRP:HB3	1.75	0.68
1:A:96[A]:HIS:HD1	1:A:117:GLY:H	1.41	0.68
2:B:55[A]:ARG:HD2	2:B:195:ARG:HH22	1.58	0.68
1:A:112[A]:GLN:NE2	1:A:220:ARG:HH22	1.90	0.67
1:A:92[C]:GLU:OE2	1:A:220:ARG:HD2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96[C]:HIS:HE1	1:A:220:ARG:HD3	1.60	0.66
2:B:20:LYS:HE2	2:B:198:ALA:HB3	1.76	0.66
1:A:92[C]:GLU:OE1	9:A:2105:HOH:O	2.15	0.65
1:A:205[A]:PHE:HD2	9:A:2232:HOH:O	1.74	0.65
1:A:112[A]:GLN:HG3	1:A:115[A]:GLU:OE1	1.96	0.65
2:B:55[A]:ARG:HD2	2:B:195:ARG:NH2	2.12	0.64
1:A:371[A]:MET:HE1	1:A:379[A]:GLN:HE21	1.63	0.64
1:A:112[C]:GLN:HB2	1:A:191:PHE:HA	1.78	0.64
1:A:149[A]:HIS:HE1	1:A:162:SER:OG	1.82	0.62
1:A:92[B]:GLU:OE2	1:A:220:ARG:NH1	2.32	0.62
1:A:92[B]:GLU:HB3	1:A:96[B]:HIS:CE1	2.35	0.62
1:A:112[B]:GLN:HA	1:A:160:ILE:HG23	1.81	0.62
2:B:23[B]:LEU:HB3	2:B:194:TYR:HA	1.80	0.62
1:A:112[A]:GLN:HB2	1:A:191:PHE:HA	1.82	0.61
1:A:359:ASN:ND2	1:A:400:LYS:HB3	2.15	0.61
2:B:279:HIS:CE1	2:B:288:ALA:H	2.19	0.60
1:A:112[B]:GLN:CG	1:A:113[B]:ALA:N	2.64	0.60
1:A:324[C]:LEU:HD12	1:A:329:TRP:HB3	1.81	0.60
1:A:87[B]:MET:CE	1:A:148[B]:VAL:HG21	2.32	0.60
1:A:351:GLN:CG	1:A:355:LYS:HE3	2.32	0.59
1:A:92[C]:GLU:CD	9:A:2105:HOH:O	2.45	0.59
1:A:85:PHE:CZ	1:A:87[B]:MET:HG3	2.38	0.59
2:B:19:GLN:HE21	2:B:203:ILE:HD11	1.68	0.58
2:B:19:GLN:NE2	2:B:203:ILE:CD1	2.66	0.58
1:A:376:ARG:NH1	9:A:2315:HOH:O	2.37	0.57
1:A:321:HIS:HA	1:A:324[B]:LEU:HD12	1.86	0.57
2:B:19:GLN:NE2	2:B:203:ILE:HD11	2.20	0.57
2:B:20:LYS:HG3	2:B:200:GLU:OE2	2.03	0.57
1:A:37:MET:O	1:A:318[A]:ARG:NH2	2.35	0.56
1:A:112[B]:GLN:HG3	9:A:2120:HOH:O	2.06	0.56
1:A:87[B]:MET:HE2	1:A:148[B]:VAL:CG2	2.36	0.56
1:A:85:PHE:CE2	1:A:87[B]:MET:HG3	2.41	0.55
1:A:112[A]:GLN:NE2	1:A:220:ARG:HH21	1.97	0.55
1:A:205[A]:PHE:CE2	9:A:2232:HOH:O	2.55	0.55
1:A:35[A]:ARG:HG2	1:A:44:ILE:HD12	1.88	0.54
1:A:325[A]:SER:C	1:A:327[A]:GLY:N	2.65	0.54
2:B:279:HIS:HE1	2:B:288:ALA:H	1.53	0.54
1:A:64[B]:MET:CG	1:A:97[B]:VAL:HG21	2.38	0.54
1:A:87[B]:MET:HE3	1:A:148[B]:VAL:HG21	1.90	0.54
1:A:326:GLN:CB	1:A:328[A]:TRP:CE2	2.90	0.53
2:B:19:GLN:HE21	2:B:203:ILE:HD12	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLN:NE2	9:A:2084:HOH:O	2.42	0.53
2:B:55[A]:ARG:HH11	2:B:195:ARG:HH22	1.57	0.53
1:A:112[A]:GLN:CB	1:A:190:TYR:O	2.56	0.53
1:A:92[C]:GLU:CD	1:A:220:ARG:HD2	2.34	0.53
1:A:324[C]:LEU:HD12	1:A:324[C]:LEU:N	2.24	0.52
1:A:340:GLN:HE21	1:A:344:LYS:HE3	1.76	0.51
1:A:324[A]:LEU:HD12	1:A:329:TRP:HB3	1.93	0.51
1:A:275:GLU:OE1	1:A:277:GLN:NE2	2.43	0.51
1:A:326:GLN:HB2	1:A:328[A]:TRP:CD2	2.46	0.51
1:A:326:GLN:HB3	1:A:328[A]:TRP:NE1	2.26	0.51
2:B:204:GLU:OE1	9:B:2169:HOH:O	2.20	0.50
2:B:146[C]:HIS:CE1	9:B:2127:HOH:O	2.64	0.50
1:A:326:GLN:HB2	1:A:328[A]:TRP:CG	2.46	0.50
1:A:186[B]:VAL:HG23	1:A:273[B]:VAL:HG22	1.80	0.50
1:A:326:GLN:CB	1:A:328[A]:TRP:CD2	2.96	0.49
1:A:113[B]:ALA:O	1:A:114[B]:ARG:HB2	2.13	0.49
2:B:35[B]:LEU:CD2	2:B:35[B]:LEU:N	2.76	0.49
1:A:87[B]:MET:CE	1:A:148[B]:VAL:CG2	2.91	0.48
1:A:370[A]:GLU:O	1:A:372:PRO:HD3	2.12	0.48
2:B:35[B]:LEU:N	2:B:35[B]:LEU:HD23	2.29	0.48
1:A:87[B]:MET:HE2	1:A:148[B]:VAL:HG21	1.96	0.47
1:A:396:ASP:CB	9:A:2331:HOH:O	2.55	0.47
1:A:86:TYR:O	1:A:293:THR:HG23	2.14	0.47
1:A:92[A]:GLU:OE1	1:A:220:ARG:NE	2.47	0.47
1:A:146[B]:MET:O	1:A:149[B]:HIS:HD2	1.98	0.47
1:A:147:PRO:O	1:A:149[C]:HIS:HD2	1.97	0.47
2:B:21:MET:CE	2:B:203:ILE:HD13	2.45	0.47
1:A:114[B]:ARG:C	1:A:116:ALA:N	2.72	0.46
1:A:149[A]:HIS:CE1	1:A:162:SER:OG	2.66	0.46
1:A:146[B]:MET:HG3	1:A:149[B]:HIS:CD2	2.50	0.46
1:A:359:ASN:HD21	1:A:400:LYS:HD2	1.79	0.46
1:A:359:ASN:ND2	1:A:400:LYS:HD2	2.30	0.46
1:A:371[A]:MET:HE3	1:A:375:LEU:HG	1.96	0.46
1:A:115[A]:GLU:N	1:A:115[A]:GLU:CD	2.72	0.45
2:B:19:GLN:NE2	2:B:203:ILE:HD12	2.30	0.45
1:A:92[B]:GLU:OE1	1:A:96[B]:HIS:HE1	2.00	0.45
1:A:113[B]:ALA:HB1	1:A:114[B]:ARG:CZ	2.47	0.45
1:A:82:ARG:HD3	1:A:353:GLU:OE2	2.17	0.44
1:A:96[B]:HIS:CD2	1:A:115[B]:GLU:HA	2.52	0.44
1:A:371[A]:MET:SD	1:A:379[A]:GLN:NE2	2.90	0.44
1:A:77:SER:OG	1:A:82:ARG:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92[B]:GLU:HB3	1:A:96[B]:HIS:ND1	2.32	0.44
1:A:147:PRO:O	1:A:148[B]:VAL:HG22	2.19	0.43
1:A:20:LEU:C	1:A:20:LEU:HD23	2.43	0.43
1:A:313:ASP:OD1	1:A:318[B]:ARG:NH2	2.50	0.43
1:A:113[B]:ALA:C	1:A:114[B]:ARG:HG3	2.43	0.43
1:A:54:LYS:HA	1:A:328[B]:TRP:CZ3	2.55	0.42
1:A:78:GLN:OE1	1:A:293:THR:HB	2.18	0.42
2:B:55[B]:ARG:HG3	2:B:195:ARG:NH2	2.35	0.42
2:B:142:GLY:O	2:B:146[B]:HIS:HB2	2.19	0.42
2:B:102:TYR:OH	2:B:146[C]:HIS:HE1	2.03	0.42
1:A:82:ARG:HD3	1:A:82:ARG:HH11	1.73	0.41
2:B:296[A]:GLN:HE21	2:B:296[A]:GLN:HB3	1.60	0.41
2:B:82:PHE:CE2	2:B:86:ILE:HD11	2.55	0.41
1:A:6:LYS:HD3	1:A:16:PHE:HD2	1.85	0.41
1:A:60:LEU:O	1:A:64[B]:MET:HG3	2.21	0.41
1:A:112[A]:GLN:HB3	1:A:190:TYR:C	2.44	0.41
2:B:115:ALA:HB2	2:B:160:ILE:HG23	2.03	0.41
1:A:320:ARG:O	1:A:324[C]:LEU:HD13	2.21	0.41
1:A:24:GLN:HA	1:A:25:PRO:HD3	1.78	0.40
1:A:115[A]:GLU:OE2	1:A:115[A]:GLU:CA	2.66	0.40
2:B:55[A]:ARG:HH11	2:B:195:ARG:NH2	2.20	0.40
2:B:154:PHE:O	2:B:157[B]:CYS:HB2	2.21	0.40

All (1) 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:326:GLN:OE1	1:A:370[A]:GLU:CG[3_664]	1.88	0.32

## 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	407/400 (102%)	387 (95%)	14 (3%)	6 (2%)	8 1
2	B	344/342 (101%)	333 (97%)	10 (3%)	1 (0%)	36 16
All	All	751/742 (101%)	720 (96%)	24 (3%)	7 (1%)	21 2

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	325[A]	SER
1	A	325[B]	SER
1	A	325[C]	SER
1	A	226	ILE
2	B	196	ALA
1	A	114[A]	ARG
1	A	114[B]	ARG

### 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	346/334 (104%)	338 (98%)	8 (2%)	44 13
2	B	295/289 (102%)	293 (99%)	2 (1%)	76 52
All	All	641/623 (103%)	631 (98%)	10 (2%)	73 23

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115[A]	GLU
1	A	115[B]	GLU
1	A	148[A]	VAL
1	A	148[B]	VAL
1	A	239	ILE
1	A	324[A]	LEU
1	A	324[B]	LEU
1	A	324[C]	LEU
2	B	296[A]	GLN

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Mol	Chain	Res	Type
2	B	296[B]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	HIS
1	A	182	ASN
1	A	321	HIS
1	A	351	GLN
1	A	387	GLN
2	B	19	GLN
2	B	77	GLN
2	B	279	HIS
2	B	302	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](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

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
8	MPD	B	901	-	7,7,7	0.37	0	9,10,10	1.20	1 (11%)
6	TPP	A	601	4	26,27,27	1.78	6 (23%)	38,40,40	2.01	9 (23%)
7	GOL	B	701	-	5,5,5	0.45	0	5,5,5	0.36	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
8	MPD	B	901	-	-	0/5/5/5	-
6	TPP	A	601	4	-	1/17/17/17	0/2/2/2
7	GOL	B	701	-	-	0/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	601	TPP	C2-S1	4.66	1.83	1.69
6	A	601	TPP	C2-N3	4.08	1.42	1.32
6	A	601	TPP	C7'-C5'	2.88	1.56	1.51
6	A	601	TPP	PA-O2A	-2.34	1.44	1.55
6	A	601	TPP	C4'-N3'	2.06	1.37	1.35
6	A	601	TPP	C6-C5	-2.06	1.46	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	601	TPP	S1-C2-N3	-6.78	103.71	112.30
6	A	601	TPP	C2-S1-C5	5.03	94.54	91.22
6	A	601	TPP	C7'-N3-C2	-3.89	115.37	123.48
6	A	601	TPP	CM2-C2'-N1'	3.83	121.28	117.20
6	A	601	TPP	C6'-N1'-C2'	3.05	121.08	116.07
8	B	901	MPD	CM-C2-C1	-2.81	104.32	110.63
6	A	601	TPP	N1'-C2'-N3'	-2.44	121.48	125.53
6	A	601	TPP	C5-C4-N3	2.39	116.02	111.67
6	A	601	TPP	C2-N3-C4	2.12	116.93	114.06
6	A	601	TPP	C7'-N3-C4	2.00	127.67	122.36

There are no chirality outliers.

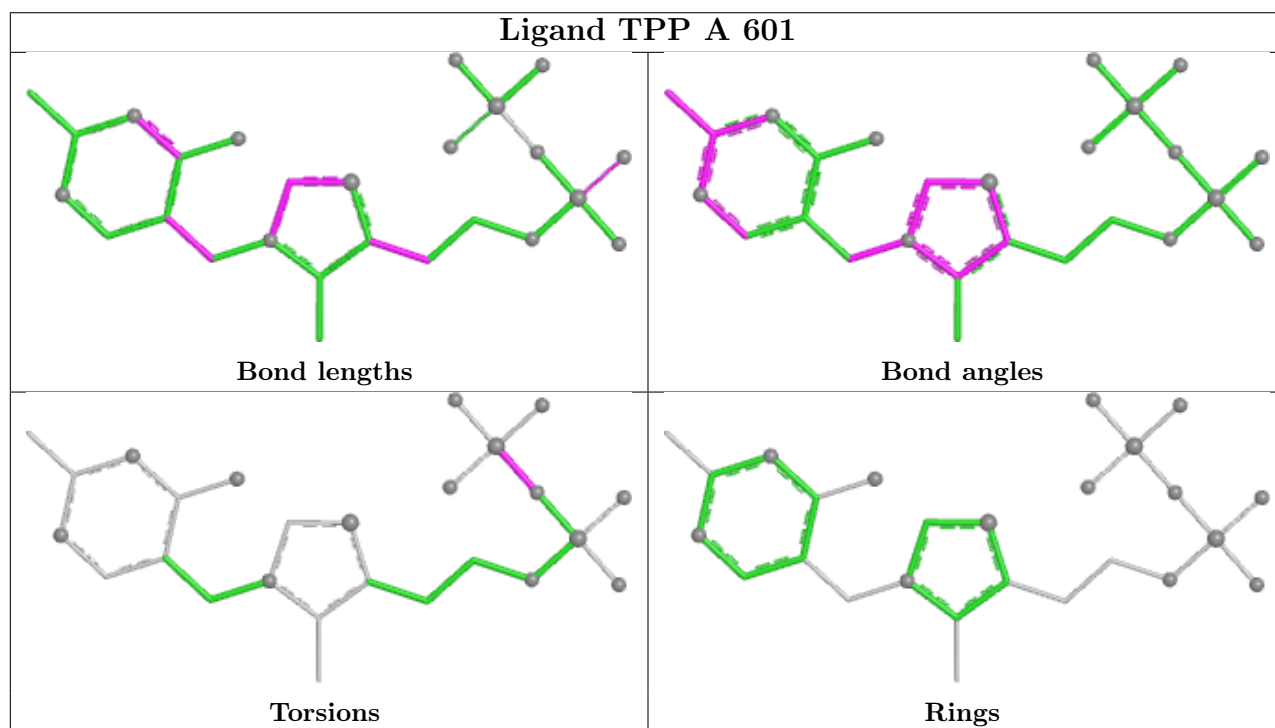
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	601	TPP	PA-O3A-PB-O2B

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.



## 5.7 Other polymers [\(i\)](#)

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, 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	374/400 (93%)	0.90	49 (13%) <b>7</b> <b>8</b>	4, 14, 31, 51	32 (8%)
2	B	332/342 (97%)	0.96	57 (17%) <b>4</b> <b>4</b>	3, 13, 24, 37	14 (4%)
All	All	706/742 (95%)	0.93	106 (15%) <b>5</b> <b>6</b>	3, 13, 28, 51	46 (6%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	288	ILE	7.9
1	A	28	ILE	6.4
1	A	292	SER	5.7
1	A	286	TYR	5.7
2	B	4	PHE	5.6
1	A	293	THR	5.3
2	B	321	PHE	5.0
2	B	315	THR	4.9
2	B	3	HIS	4.5
2	B	2	ALA	4.4
2	B	284	THR	4.4
2	B	317	PHE	4.3
2	B	18	THR	4.2
2	B	316	PRO	4.2
2	B	15	TYR	4.1
2	B	14	GLU	4.1
2	B	286	GLY	4.0
1	A	90	TYR	3.9
2	B	325	TYR	3.8
1	A	26	ASN	3.8
2	B	320	ILE	3.7
1	A	324[A]	LEU	3.7
2	B	281	ALA	3.7
2	B	283	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	312	GLY	3.7
2	B	318	PRO	3.6
1	A	331	GLU	3.5
1	A	287	ARG	3.5
1	A	289	GLY	3.5
2	B	196	ALA	3.5
1	A	183	ALA	3.4
2	B	305	ALA	3.4
2	B	285	GLY	3.3
2	B	197	ALA	3.3
2	B	198	ALA	3.3
2	B	246	GLY	3.2
2	B	287	PHE	3.1
2	B	340	ILE	3.1
1	A	325[A]	SER	3.1
1	A	396	ASP	3.1
1	A	395	LEU	3.0
2	B	319	HIS	3.0
1	A	9	PHE	3.0
2	B	243	GLU	2.9
1	A	79	ARG	2.9
1	A	368	TYR	2.9
2	B	20	LYS	2.9
2	B	17	GLN	2.8
1	A	314	HIS	2.8
2	B	16	GLY	2.8
2	B	300	PHE	2.8
2	B	235	ARG	2.7
2	B	313	TYR	2.7
2	B	144	LEU	2.7
1	A	6	LYS	2.7
2	B	314	ASP	2.6
2	B	19	GLN	2.6
2	B	310	VAL	2.6
1	A	367	VAL	2.6
1	A	342	ARG	2.6
2	B	294	THR	2.6
1	A	10	PRO	2.6
1	A	327[A]	GLY	2.5
1	A	211	LEU	2.5
1	A	184	ASN	2.5
2	B	311	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	282	PRO	2.4
2	B	326	ILE	2.4
1	A	75	TYR	2.4
2	B	324	PHE	2.4
2	B	145	TYR	2.3
2	B	342	TYR	2.3
1	A	7	PRO	2.3
1	A	17	ILE	2.3
1	A	73	ILE	2.3
2	B	203	ILE	2.3
1	A	362	LEU	2.3
1	A	338	ARG	2.3
1	A	177	ALA	2.3
1	A	336	ALA	2.3
1	A	8	GLN	2.3
1	A	387	GLN	2.3
1	A	343	ARG	2.2
1	A	182	ASN	2.2
1	A	388	THR	2.2
2	B	218	GLU	2.2
1	A	207	PHE	2.2
2	B	195	ARG	2.2
2	B	141[A]	HIS	2.1
2	B	301	LEU	2.1
1	A	313	ASP	2.1
1	A	364	PHE	2.1
1	A	137	ILE	2.1
2	B	258	ILE	2.1
1	A	209	ALA	2.1
1	A	186[A]	VAL	2.1
2	B	36	ALA	2.1
2	B	288	ALA	2.1
1	A	376	ARG	2.1
1	A	398	PHE	2.1
2	B	242	LYS	2.1
1	A	386	LEU	2.0
2	B	157[A]	CYS	2.0
2	B	239	SER	2.0
2	B	333	TYR	2.0
1	A	27	VAL	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](#)

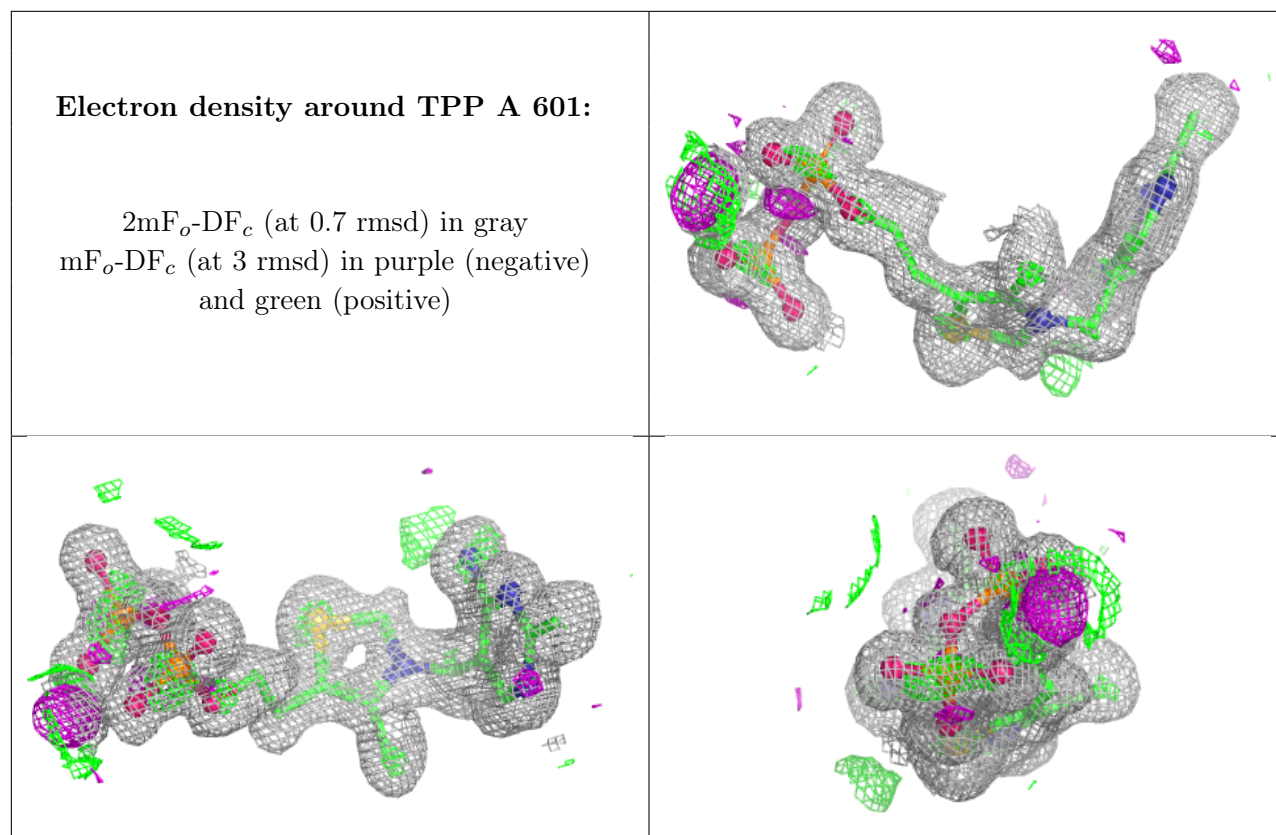
There are no oligosaccharides in this entry.

## 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, 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(Å <sup>2</sup> )	Q<0.9
8	MPD	B	901	8/8	0.83	0.15	28,35,37,38	0
7	GOL	B	701	6/6	0.95	0.06	14,16,16,16	0
5	CL	A	504	1/1	0.97	0.16	24,24,24,24	0
3	K	B	502	1/1	0.98	0.11	11,11,11,11	0
6	TPP	A	601	26/26	0.98	0.07	8,10,13,16	0
3	K	A	501	1/1	0.99	0.10	10,10,10,10	0
4	MN	A	503	1/1	1.00	0.09	9,9,9,9	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.