Full wwPDB X-ray Structure Validation Report (i)

May 25, 2020 – 05:48 am BST

PDB ID	:	5TUS
Title	:	Potent competitive inhibition of human ribonucleotide reductase by a novel non-nucleoside small molecule
Authors	:	Mohammed, F.A.; Alam, I.; Dealwis, C.G.
Deposited on	:	2016-11-07
Resolution	:	2.66 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

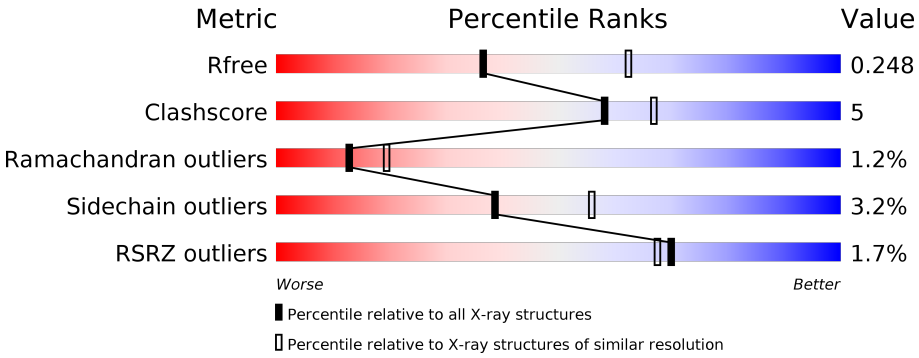
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 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 <=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	792	2% 79% 10% • 9%
1	B	792	2% 80% 10% • 8%

2 Entry composition

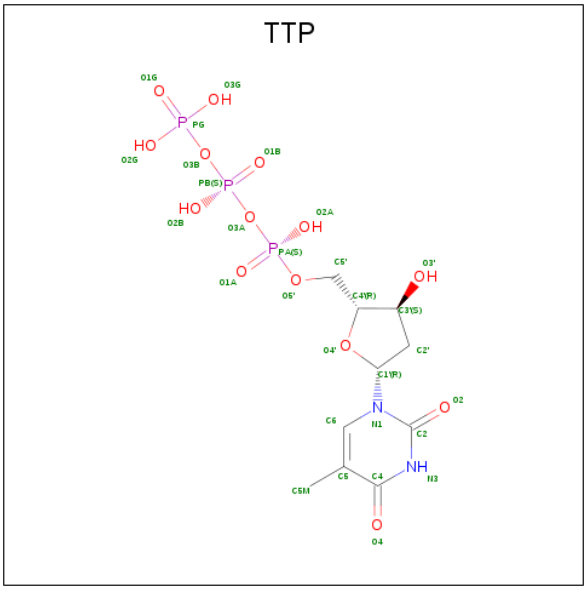
There are 5 unique types of molecules in this entry. The entry contains 11713 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ribonucleoside-diphosphate reductase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	720	Total	C	N	O	S	0	0	0
			5752	3674	964	1081	33			
1	B	731	Total	C	N	O	S	0	0	0
			5845	3729	986	1096	34			

- Molecule 2 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).

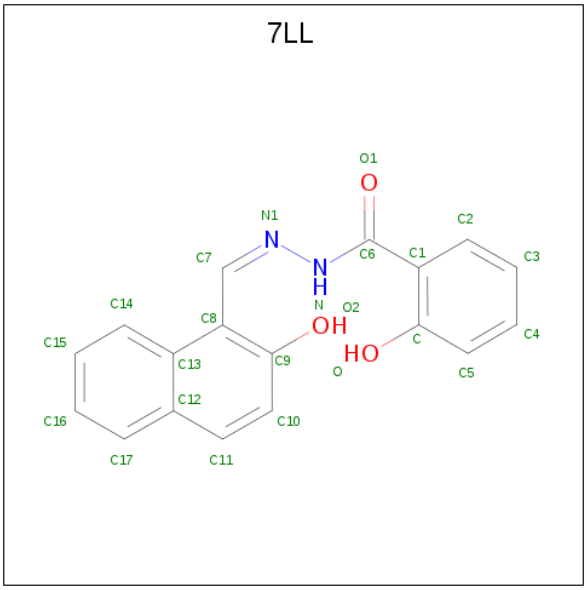


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is 2-hydroxy-N'-[(Z)-(2-hydroxynaphthalen-1-yl)methylidene]benzohydrazide (three-letter code: 7LL) (formula: $C_{18}H_{14}N_2O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 23 18 2 3	0	0

- Molecule 5 is water.

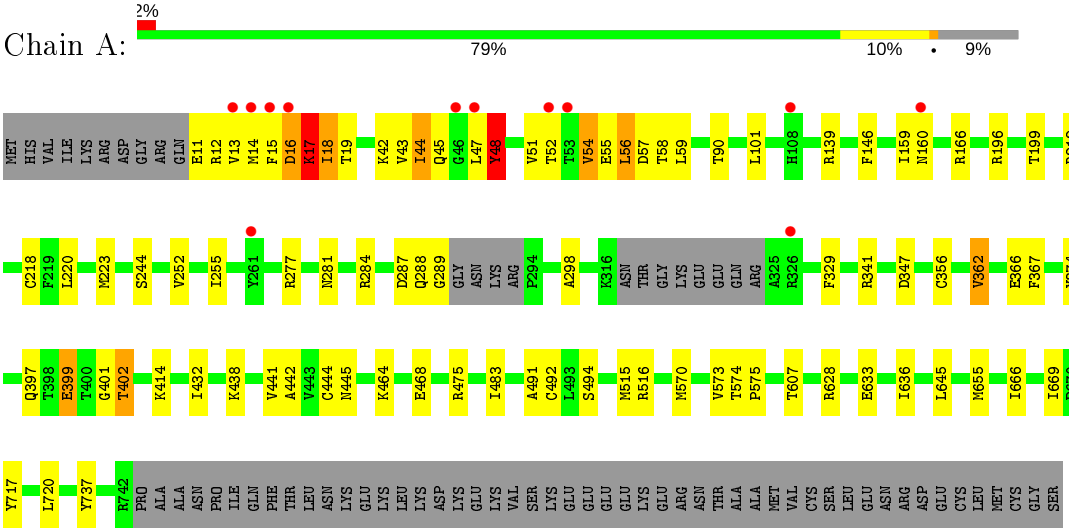
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	28	Total O 28 28	0	0
5	B	5	Total O 5 5	0	0

3 Residue-property plots (i)

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.

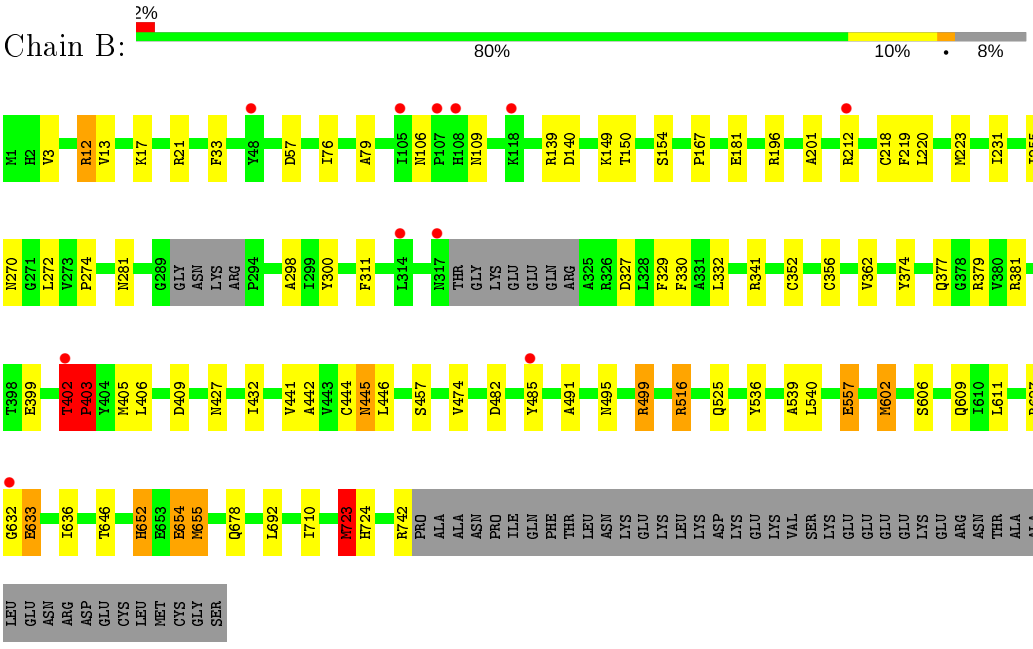
- Molecule 1: Ribonucleoside-diphosphate reductase large subunit

Chain A:



- Molecule 1: Ribonucleoside-diphosphate reductase large subunit

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.52Å 114.28Å 220.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	110.18 – 2.66 101.45 – 2.66	Depositor EDS
% Data completeness (in resolution range)	98.7 (110.18-2.66) 98.7 (101.45-2.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.199 , 0.250 0.205 , 0.248	Depositor DCC
R_{free} test set	1998 reflections (3.94%)	wwPDB-VP
Wilson B-factor (Å^2)	58.0	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 32.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11713	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, TTP, 7LL

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	0.73	0/5877	0.85	9/7962 (0.1%)
1	B	0.70	0/5971	0.85	9/8086 (0.1%)
All	All	0.71	0/11848	0.85	18/16048 (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
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	402	THR	C-N-CD	-14.54	88.61	120.60
1	B	629	VAL	CB-CA-C	-8.52	95.22	111.40
1	B	341	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	A	139	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	629	VAL	N-CA-C	6.10	127.46	111.00
1	A	402	THR	C-N-CD	-6.07	107.24	120.60
1	A	139	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	A	475	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	284	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	B	742	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	403	PRO	CA-N-CD	-5.33	104.04	111.50
1	A	16	ASP	CB-CG-OD2	5.23	123.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	341	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	B	409	ASP	CB-CG-OD1	5.17	122.96	118.30
1	A	48	TYR	N-CA-C	5.13	124.84	111.00
1	B	723	MET	CG-SD-CE	5.05	108.28	100.20
1	B	139	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	277	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	402	THR	Peptide
1	B	402	THR	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	5752	0	5728	51	1
1	B	5845	0	5827	61	1
2	A	29	0	13	0	0
2	B	29	0	13	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	23	0	0	2	0
5	A	28	0	0	4	0
5	B	5	0	0	0	0
All	All	11713	0	11581	112	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 5.

All (112) 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:654:GLU:HG3	1:B:655:MET:H	1.06	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LYS:HD3	1:A:18:ILE:N	1.71	1.04
1:B:446:LEU:HB3	1:B:602:MET:HE1	1.45	0.98
1:A:575:PRO:HD3	5:A:1701:HOH:O	1.64	0.94
1:A:17:LYS:HD3	1:A:18:ILE:H	1.33	0.92
1:A:16:ASP:O	1:A:19:THR:N	2.02	0.92
1:B:654:GLU:HG3	1:B:655:MET:N	1.90	0.86
1:B:652:HIS:HB2	1:B:654:GLU:HG2	1.58	0.84
1:B:654:GLU:CG	1:B:655:MET:H	1.89	0.82
1:B:218:CYS:HB2	1:B:444:CYS:SG	2.20	0.81
1:A:17:LYS:CD	1:A:18:ILE:H	1.92	0.81
1:A:492:CYS:SG	5:A:1727:HOH:O	2.39	0.80
1:A:56:LEU:O	1:A:59:LEU:N	2.15	0.79
1:B:652:HIS:CB	1:B:654:GLU:HG2	2.14	0.77
1:B:629:VAL:HG11	1:B:633:GLU:N	2.01	0.76
1:A:90:THR:HG21	1:A:166:ARG:HG3	1.72	0.72
1:A:218:CYS:HB3	1:A:444:CYS:SG	2.34	0.67
1:A:16:ASP:O	1:A:18:ILE:N	2.28	0.67
1:A:56:LEU:O	1:A:57:ASP:C	2.33	0.67
1:A:574:THR:HA	5:A:1701:HOH:O	1.96	0.66
1:A:573:VAL:O	5:A:1701:HOH:O	2.13	0.65
1:B:446:LEU:HB3	1:B:602:MET:CE	2.25	0.64
1:A:281:ASN:OD1	1:B:281:ASN:ND2	2.30	0.64
1:B:630:LEU:C	1:B:630:LEU:HD12	2.19	0.63
1:B:630:LEU:HD12	1:B:630:LEU:O	1.99	0.63
1:B:201:ALA:HA	4:B:1603:7LL:C16	2.31	0.61
1:B:150:THR:OG1	1:B:609:GLN:OE1	2.14	0.60
1:A:223:MET:HG2	1:A:255:ILE:HD11	1.83	0.60
1:B:627:ARG:HG3	1:B:636:ILE:HD12	1.83	0.59
1:B:260:SER:OG	1:B:381:ARG:NH1	2.36	0.59
1:A:17:LYS:HD3	1:A:18:ILE:HB	1.84	0.58
1:B:330:PHE:O	1:B:403:PRO:HA	2.04	0.58
1:A:52:THR:HG23	1:A:54:VAL:HG12	1.85	0.57
1:B:629:VAL:CG1	1:B:633:GLU:N	2.66	0.57
1:A:17:LYS:HE2	1:A:18:ILE:HD12	1.87	0.56
1:B:557:GLU:CD	1:B:557:GLU:H	2.09	0.56
1:B:405:MET:HG3	1:B:724:HIS:CE1	2.42	0.55
1:B:220:LEU:HD11	1:B:427:ASN:HB3	1.90	0.54
1:A:17:LYS:CD	1:A:18:ILE:HB	2.37	0.54
1:B:270:ASN:HB3	1:B:274:PRO:HG2	1.90	0.54
1:A:220:LEU:HB2	1:A:442:ALA:HB3	1.90	0.53
1:B:106:ASN:HD21	1:B:109:ASN:HB3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LYS:CD	1:A:18:ILE:N	2.53	0.53
1:A:362:VAL:HG22	1:A:366:GLU:HB3	1.91	0.53
1:A:199:THR:HG21	1:A:607:THR:HB	1.91	0.53
1:B:311:PHE:CZ	1:B:330:PHE:HD1	2.27	0.52
1:A:48:TYR:CD1	1:A:51:VAL:HB	2.46	0.51
1:A:101:LEU:HD23	1:A:159:ILE:HD11	1.92	0.51
1:A:287:ASP:C	1:A:289:GLY:H	2.15	0.51
1:B:652:HIS:HB3	1:B:654:GLU:HG2	1.93	0.50
1:A:56:LEU:O	1:A:58:THR:N	2.45	0.50
1:A:666:ILE:HA	1:A:669:ILE:HD12	1.94	0.50
1:B:654:GLU:CG	1:B:655:MET:N	2.63	0.49
1:A:146:PHE:CE2	1:A:636:ILE:HD11	2.49	0.48
1:B:710:ILE:HG21	1:B:723:MET:SD	2.53	0.48
1:B:220:LEU:HB2	1:B:442:ALA:HB3	1.94	0.48
1:A:214:GLN:HG2	1:A:244:SER:HB3	1.95	0.48
1:A:432:ILE:HG13	1:A:444:CYS:SG	2.54	0.48
1:A:394:ILE:HD11	1:A:717:TYR:HB3	1.96	0.48
1:B:482:ASP:OD2	1:B:499:ARG:NH2	2.47	0.48
1:B:394:ILE:HA	1:B:397:GLN:HG3	1.96	0.47
1:B:393:ILE:O	1:B:397:GLN:HG3	2.14	0.47
1:B:223:MET:HE3	1:B:223:MET:HB3	1.57	0.47
1:A:43:VAL:C	1:A:44:ILE:O	2.53	0.47
1:A:159:ILE:O	1:A:160:ASN:CB	2.62	0.47
1:B:223:MET:HE1	1:B:231:ILE:HA	1.97	0.46
1:B:17:LYS:O	1:B:21:ARG:HG3	2.16	0.46
1:B:377:GLN:OE1	1:B:379:ARG:NH1	2.49	0.45
1:B:432:ILE:HG13	1:B:444:CYS:SG	2.57	0.45
1:B:402:THR:C	1:B:403:PRO:O	2.54	0.45
1:B:140:ASP:OD2	1:B:167:PRO:HB2	2.17	0.45
1:A:56:LEU:N	1:A:56:LEU:CD1	2.79	0.45
1:B:21:ARG:NH2	1:B:57:ASP:OD1	2.50	0.45
1:A:47:LEU:HB3	1:A:48:TYR:H	1.54	0.44
1:B:76:ILE:O	1:B:79:ALA:HB3	2.18	0.44
1:A:362:VAL:HG13	1:A:367:PHE:HA	2.00	0.44
1:B:196:ARG:HG2	1:B:611:LEU:HD22	2.00	0.44
1:A:44:ILE:O	1:A:45:GLN:CB	2.66	0.44
1:A:414:LYS:HG2	1:A:570:MET:HB3	1.99	0.43
1:B:219:PHE:C	1:B:220:LEU:HD12	2.38	0.43
1:A:397:GLN:O	1:A:401:GLY:HA2	2.18	0.43
1:B:474:VAL:HG21	1:B:539:ALA:HA	2.01	0.43
1:B:300:TYR:HE2	1:B:406:LEU:HD13	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:629:VAL:HG13	1:B:633:GLU:HA	2.00	0.43
1:A:464:LYS:HE3	1:A:468:GLU:OE1	2.18	0.43
1:A:441:VAL:O	1:A:491:ALA:HA	2.19	0.43
1:A:15:PHE:O	1:A:15:PHE:CG	2.70	0.43
1:B:3:VAL:HG22	1:B:13:VAL:HG22	2.01	0.43
4:B:1603:7LL:O2	4:B:1603:7LL:N	2.53	0.42
1:B:627:ARG:HG3	1:B:636:ILE:CD1	2.48	0.42
1:B:256:ARG:HH22	2:B:1601:TTP:PG	2.42	0.42
1:A:159:ILE:O	1:A:160:ASN:HB3	2.20	0.42
1:A:515:MET:O	1:A:516:ARG:HB2	2.18	0.42
1:B:298:ALA:HA	1:B:329:PHE:O	2.19	0.42
1:A:356:CYS:HB3	1:A:374:TYR:CD1	2.54	0.42
1:A:483:ILE:O	1:A:483:ILE:HG22	2.20	0.42
1:B:33:PHE:CE2	1:B:646:THR:HB	2.54	0.41
1:A:42:LYS:O	1:A:44:ILE:O	2.37	0.41
1:A:146:PHE:CD2	1:A:636:ILE:HD11	2.56	0.41
1:A:298:ALA:HA	1:A:329:PHE:O	2.20	0.41
1:B:482:ASP:CG	1:B:499:ARG:HH22	2.24	0.41
1:B:692:LEU:HD11	1:B:723:MET:HG2	2.02	0.41
1:B:445:ASN:HD21	1:B:495:ASN:HD21	1.68	0.41
1:B:255:ILE:HB	1:B:272:LEU:HD21	2.03	0.41
1:B:629:VAL:CG1	1:B:633:GLU:H	2.34	0.41
1:A:645:LEU:HD13	1:A:655:MET:CE	2.51	0.40
1:B:516:ARG:HD2	1:B:516:ARG:HA	1.84	0.40
1:B:536:TYR:CZ	1:B:540:LEU:HD11	2.56	0.40
1:B:356:CYS:HB3	1:B:374:TYR:CD1	2.56	0.40
1:B:441:VAL:O	1:B:491:ALA:HA	2.21	0.40
1:B:332:LEU:HG	1:B:403:PRO:HB2	2.03	0.40
1:B:106:ASN:ND2	1:B:109:ASN:HB3	2.36	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:399:GLU:OE1	1:B:12:ARG:NH2[3_554]	2.12	0.08

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	714/792 (90%)	671 (94%)	34 (5%)	9 (1%)	12	18
1	B	725/792 (92%)	693 (96%)	24 (3%)	8 (1%)	14	21
All	All	1439/1584 (91%)	1364 (95%)	58 (4%)	17 (1%)	13	19

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	288	GLN
1	B	403	PRO
1	B	633	GLU
1	B	654	GLU
1	B	655	MET
1	A	48	TYR
1	A	54	VAL
1	B	402	THR
1	A	12	ARG
1	A	737	TYR
1	B	631	SER
1	A	13	VAL
1	B	632	GLY
1	A	196	ARG
1	A	44	ILE
1	B	212	ARG

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	629/693 (91%)	611 (97%)	18 (3%)	42 60
1	B	639/693 (92%)	616 (96%)	23 (4%)	35 51
All	All	1268/1386 (92%)	1227 (97%)	41 (3%)	39 56

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	14	MET
1	A	17	LYS
1	A	18	ILE
1	A	55	GLU
1	A	56	LEU
1	A	212	ARG
1	A	252	VAL
1	A	347	ASP
1	A	362	VAL
1	A	399	GLU
1	A	438	LYS
1	A	445	ASN
1	A	494	SER
1	A	628	ARG
1	A	633	GLU
1	A	671	GLU
1	A	720	LEU
1	B	12	ARG
1	B	149	LYS
1	B	154	SER
1	B	181	GLU
1	B	327	ASP
1	B	352	CYS
1	B	362	VAL
1	B	397	GLN
1	B	399	GLU
1	B	445	ASN
1	B	457	SER
1	B	485	TYR
1	B	499	ARG
1	B	516	ARG
1	B	525	GLN
1	B	557	GLU

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Mol	Chain	Res	Type
1	B	602	MET
1	B	606	SER
1	B	628	ARG
1	B	630	LEU
1	B	652	HIS
1	B	678	GLN
1	B	723	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	445	ASN
1	B	495	ASN
1	B	663	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)

Of 5 ligands modelled in this entry, 2 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	$\#\|Z\|>2$
4	7LL	B	1603	-	25,25,25	1.45	4 (16%)	34,34,34	2.20	10 (29%)
2	TTP	B	1601	3	23,30,30	0.94	1 (4%)	29,47,47	1.89	3 (10%)
2	TTP	A	1601	3	23,30,30	0.90	1 (4%)	29,47,47	2.28	5 (17%)

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
4	7LL	B	1603	-	-	4/10/10/10	0/3/3/3
2	TTP	B	1601	3	-	4/19/34/34	0/2/2/2
2	TTP	A	1601	3	-	1/19/34/34	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1603	7LL	N-N1	3.99	1.43	1.38
2	B	1601	TTP	C4-C5	2.55	1.46	1.41
4	B	1603	7LL	C8-C7	2.53	1.50	1.44
2	A	1601	TTP	C4-C5	2.44	1.46	1.41
4	B	1603	7LL	C13-C12	-2.20	1.39	1.43
4	B	1603	7LL	C16-C17	2.06	1.41	1.36

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1601	TTP	C4-N3-C2	9.41	123.09	115.14
2	B	1601	TTP	C4-N3-C2	7.91	121.82	115.14
4	B	1603	7LL	C7-N1-N	6.91	128.14	115.96
4	B	1603	7LL	C8-C7-N1	4.39	130.06	121.54
2	A	1601	TTP	PB-O3A-PA	-4.37	117.85	132.83
4	B	1603	7LL	C9-C8-C7	4.13	124.03	120.02
2	A	1601	TTP	O3G-PG-O3B	-3.63	92.45	104.64
4	B	1603	7LL	C16-C17-C12	3.21	125.45	120.44
2	A	1601	TTP	O3G-PG-O2G	3.16	119.71	107.64
4	B	1603	7LL	C11-C12-C13	3.08	123.17	119.12
4	B	1603	7LL	O2-C9-C8	-3.07	118.64	122.40
4	B	1603	7LL	C15-C14-C13	2.76	124.72	120.89
4	B	1603	7LL	C16-C15-C14	-2.72	116.62	120.44
2	B	1601	TTP	PB-O3A-PA	-2.66	123.69	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1603	7LL	O1-C6-N	-2.63	118.82	122.64
4	B	1603	7LL	C10-C11-C12	-2.36	117.16	120.82
2	B	1601	TTP	O3B-PG-O1G	-2.12	99.43	111.19
2	A	1601	TTP	O2B-PB-O1B	2.07	122.50	112.24

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1603	7LL	C6-N-N1-C7
4	B	1603	7LL	N1-C7-C8-C9
4	B	1603	7LL	N1-C7-C8-C13
4	B	1603	7LL	C8-C7-N1-N
2	B	1601	TTP	PG-O3B-PB-O1B
2	B	1601	TTP	PA-O3A-PB-O1B
2	B	1601	TTP	PA-O3A-PB-O2B
2	B	1601	TTP	PG-O3B-PB-O2B
2	A	1601	TTP	PG-O3B-PB-O1B

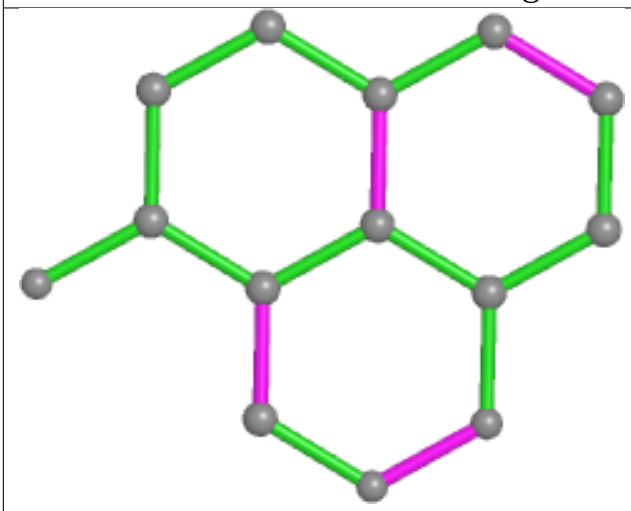
There are no ring outliers.

2 monomers are involved in 3 short contacts:

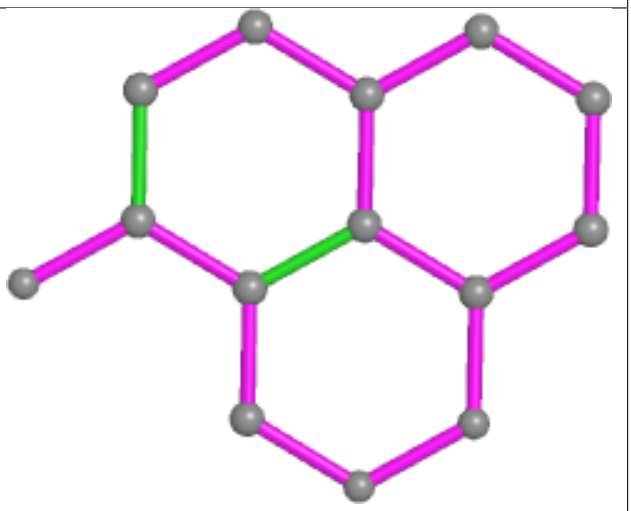
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1603	7LL	2	0
2	B	1601	TTP	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

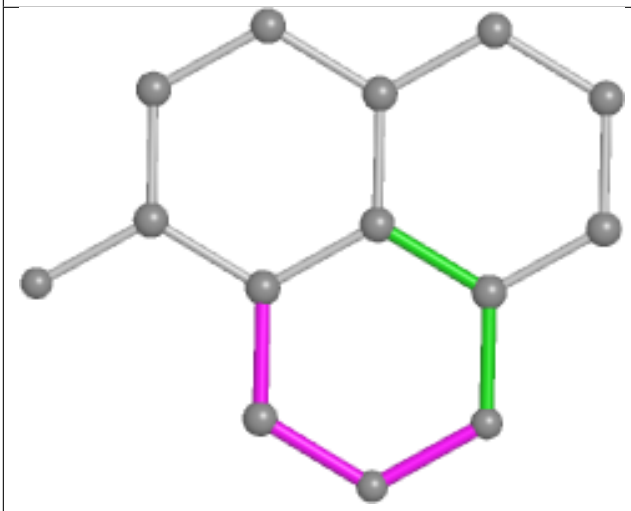
Ligand 7LL B 1603



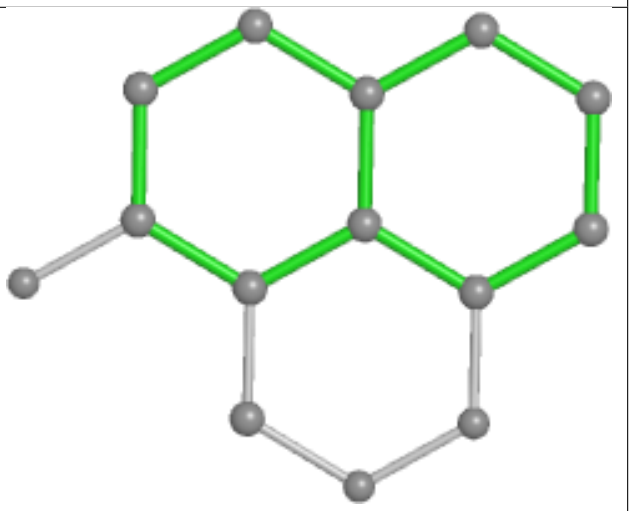
Bond lengths



Bond angles

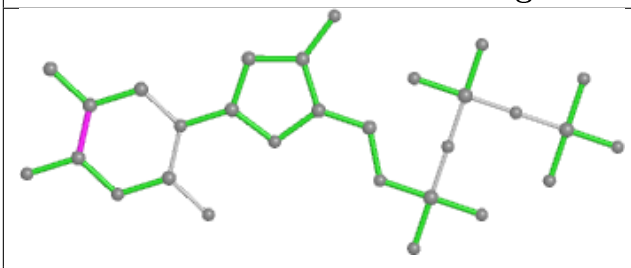


Torsions

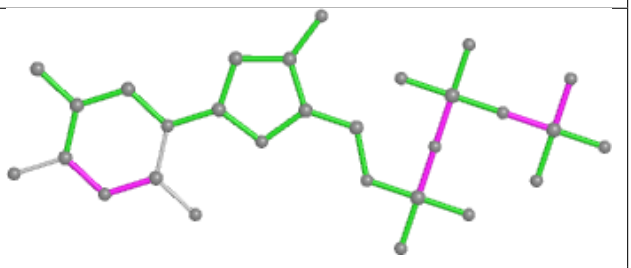


Rings

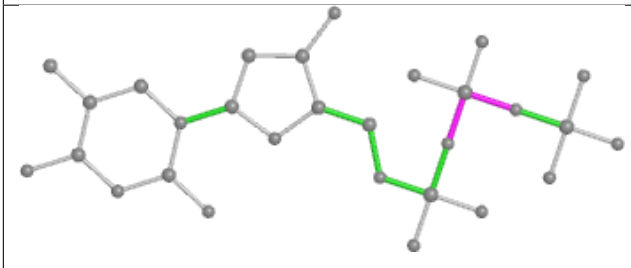
Ligand TTP B 1601



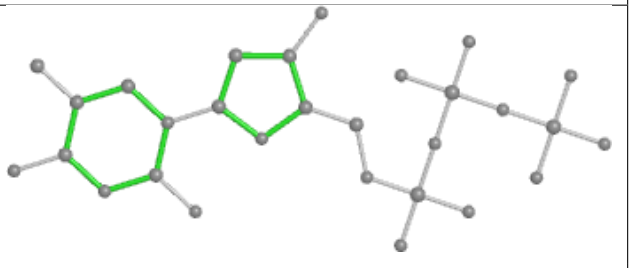
Bond lengths



Bond angles

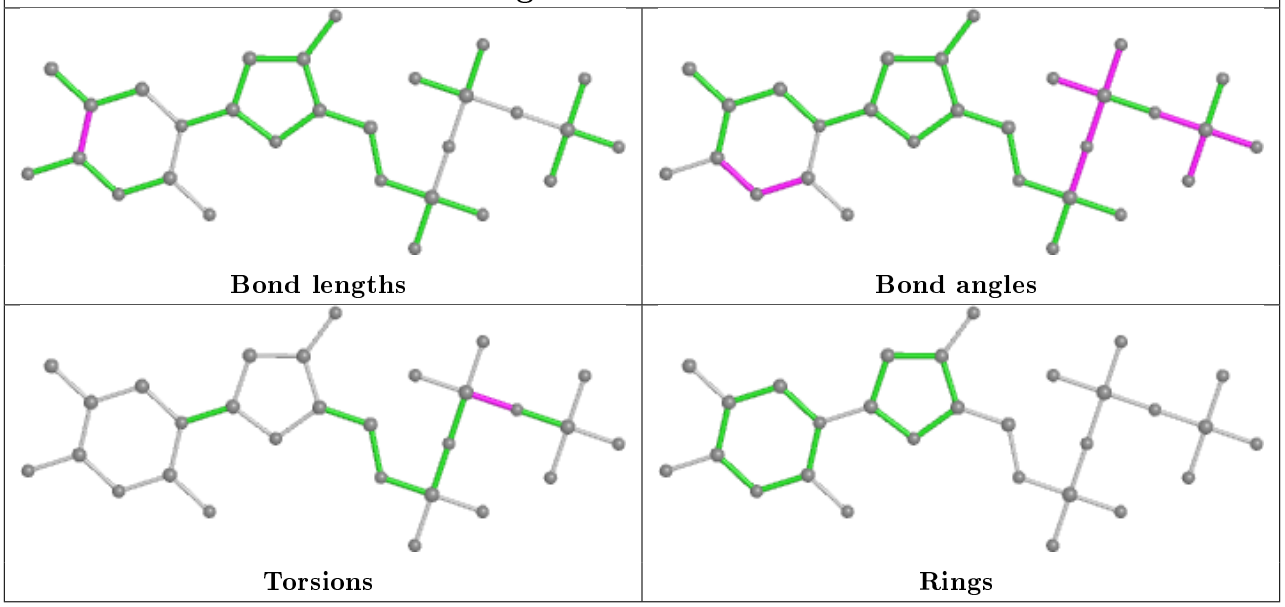


Torsions



Rings

Ligand TTP A 1601



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, 95^{th} 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	720/792 (90%)	-0.04	12 (1%)	70	67	36, 50, 86, 141	0
1	B	731/792 (92%)	0.04	13 (1%)	68	65	40, 55, 85, 123	0
All	All	1451/1584 (91%)	0.00	25 (1%)	70	67	36, 52, 86, 141	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	16	ASP	5.2
1	A	53	THR	4.8
1	B	108	HIS	3.8
1	A	108	HIS	3.5
1	B	632	GLY	3.5
1	B	631	SER	3.2
1	B	317	ASN	3.2
1	B	107	PRO	3.1
1	B	314	LEU	2.7
1	B	629	VAL	2.6
1	A	15	PHE	2.6
1	B	485	TYR	2.5
1	B	212	ARG	2.5
1	B	118	LYS	2.5
1	B	402	THR	2.4
1	B	48	TYR	2.4
1	A	13	VAL	2.4
1	A	160	ASN	2.3
1	A	47	LEU	2.2
1	A	14	MET	2.2
1	A	46	GLY	2.2
1	B	105	ILE	2.2
1	A	326	ARG	2.2
1	A	261	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	52	THR	2.1

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)

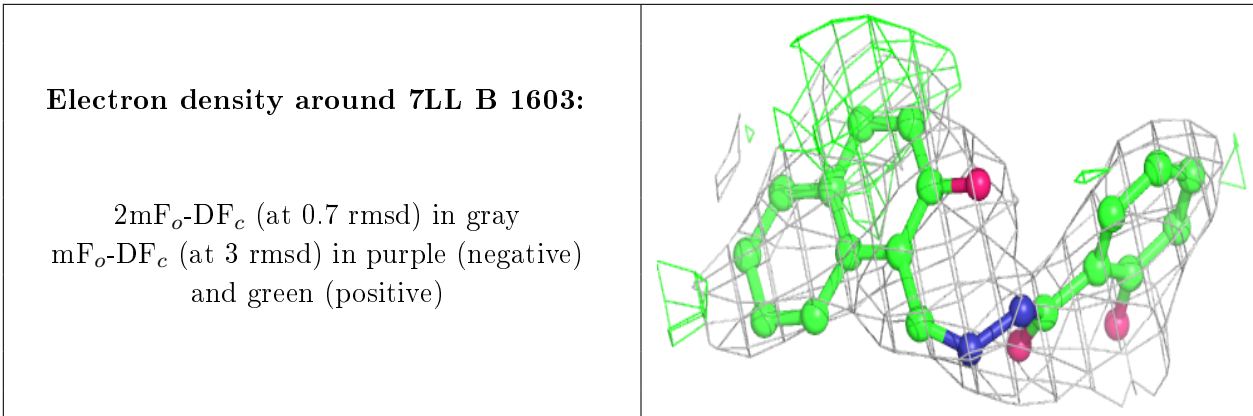
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	7LL	B	1603	23/23	0.81	0.26	58,86,98,105	0
2	TTP	B	1601	29/29	0.96	0.15	45,56,77,94	0
2	TTP	A	1601	29/29	0.98	0.14	43,49,72,80	0
3	MG	A	1602	1/1	0.98	0.11	46,46,46,46	0
3	MG	B	1602	1/1	0.98	0.12	45,45,45,45	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.

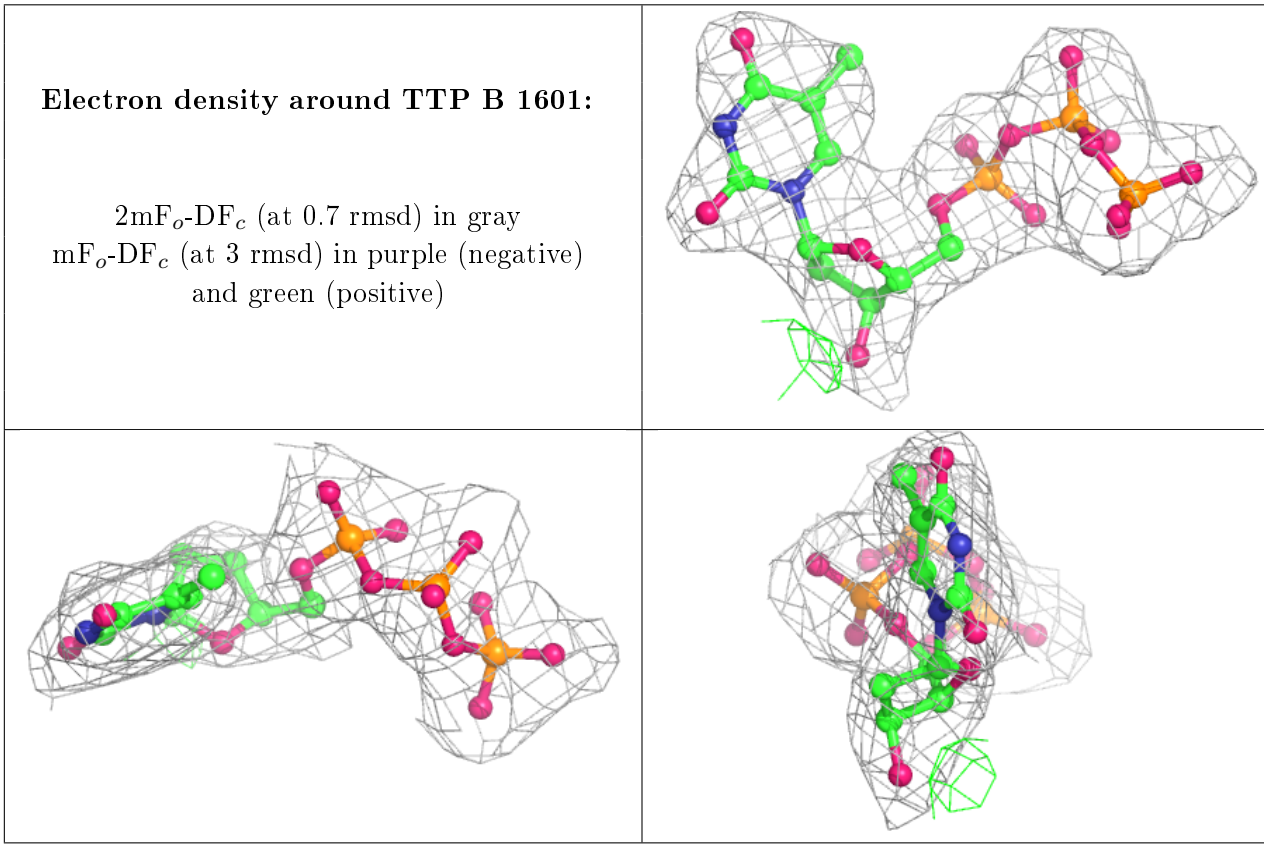
Electron density around 7LL B 1603:

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



Electron density around TTP B 1601:

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



Electron density around TTP A 1601:

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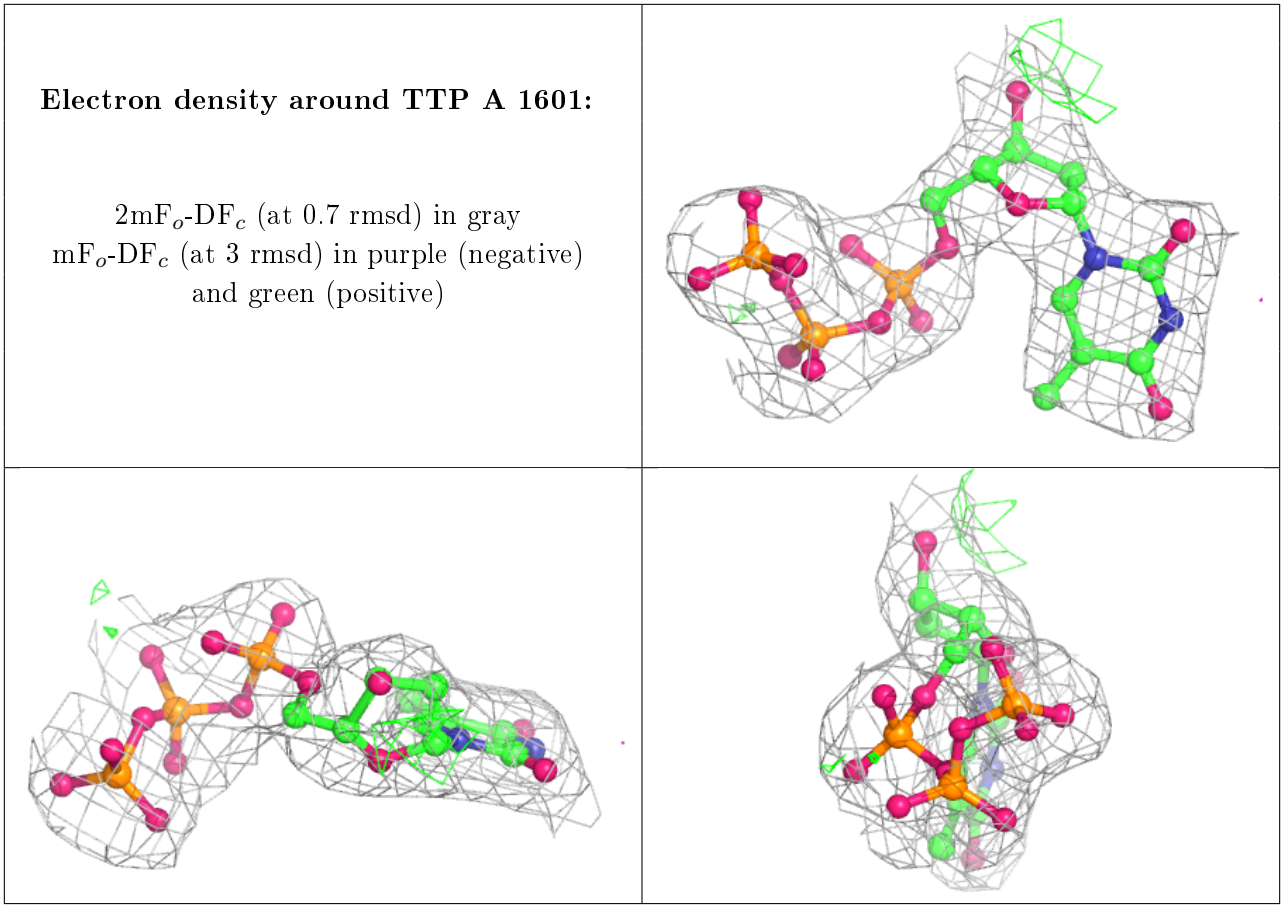
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.