



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 09:34 am BST

PDB ID : 2G88
Title : MSRECA-dATP COMPLEX
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Deposited on : 2006-03-02
Resolution : 3.20 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 ⓘ symbol.

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

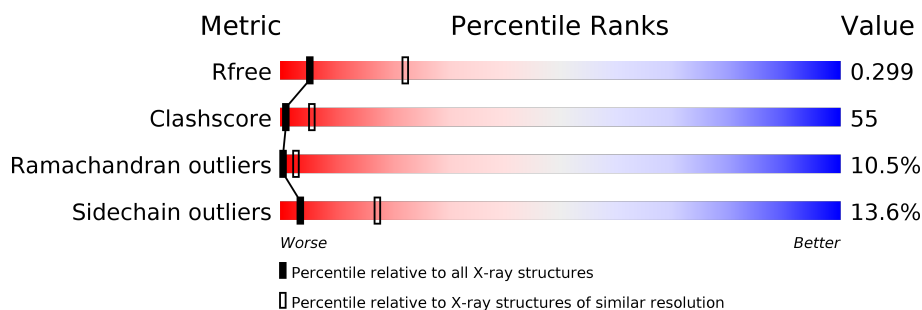
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	349	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2581 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.

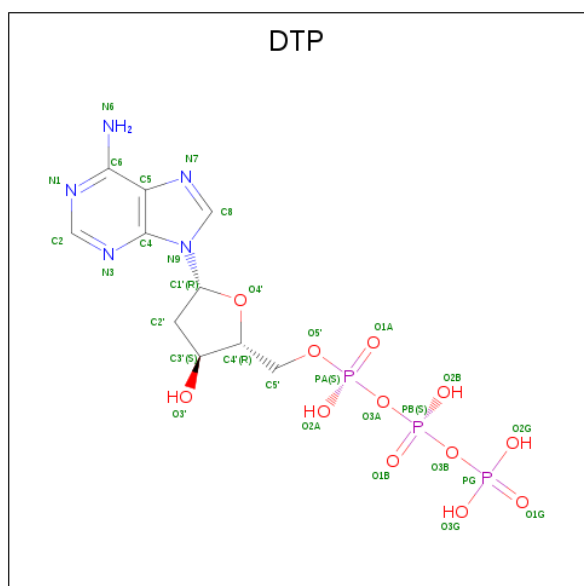
- Molecule 1 is a protein called Protein recA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2399	1504	421	468	6			

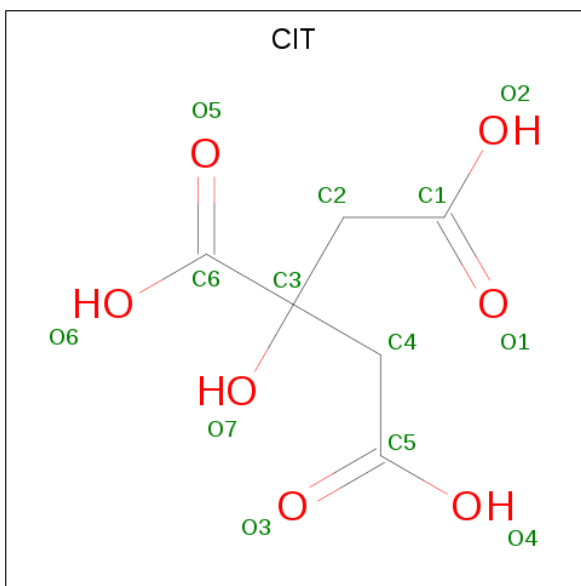
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).



- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	108	Total	O	0	0
			108	108		

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	108.21 Å 108.21 Å 72.97 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.40 – 3.20 25.37 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.3 (25.40-3.20) 96.4 (25.37-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 3.17 Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.237 , 0.309 0.228 , 0.299	Depositor DCC
R_{free} test set	829 reflections (10.59%)	wwPDB-VP
Wilson B-factor (Å ²)	60.6	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 14.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.440 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2581	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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, DTP, CIT

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	0.60	3/2427 (0.1%)	1.16	24/3284 (0.7%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282	GLU	CB-CG	6.70	1.64	1.52
1	A	282	GLU	CG-CD	5.36	1.59	1.51
1	A	245	ARG	CB-CG	5.05	1.66	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	SER	N-CA-C	-11.37	80.31	111.00
1	A	245	ARG	CA-CB-CG	10.70	136.93	113.40
1	A	245	ARG	N-CA-CB	10.62	129.72	110.60
1	A	345	ALA	N-CA-C	9.05	135.43	111.00
1	A	292	TRP	N-CA-C	8.98	135.25	111.00
1	A	343	LEU	N-CA-C	8.31	133.43	111.00
1	A	344	PRO	N-CA-C	7.90	132.65	112.10
1	A	333	ALA	N-CA-C	7.82	132.12	111.00
1	A	340	ASP	N-CA-C	7.77	131.98	111.00
1	A	168	LEU	N-CA-C	7.08	130.13	111.00
1	A	345	ALA	C-N-CD	7.06	143.22	128.40
1	A	245	ARG	CB-CG-CD	6.63	128.84	111.60
1	A	329	LEU	N-CA-C	-6.33	93.90	111.00
1	A	213	GLY	N-CA-C	-6.32	97.30	113.10
1	A	349	PHE	N-CA-C	-6.26	94.09	111.00
1	A	287	ARG	N-CA-C	6.23	127.81	111.00
1	A	337	ALA	N-CA-C	6.11	127.50	111.00
1	A	346	PRO	N-CA-C	-6.00	96.51	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	ASP	N-CA-C	-5.80	95.33	111.00
1	A	334	VAL	N-CA-C	5.68	126.34	111.00
1	A	197	LEU	N-CA-C	5.64	126.23	111.00
1	A	289	SER	N-CA-C	5.52	125.91	111.00
1	A	13	GLU	CA-CB-CG	5.41	125.30	113.40
1	A	349	PHE	N-CA-CB	5.02	119.64	110.60

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	2399	0	2356	263	0
2	A	1	0	0	0	0
3	A	60	0	24	16	0
4	A	13	0	4	4	0
5	A	108	0	0	5	0
All	All	2581	0	2384	265	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 55.

All (265) 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:291:SER:HB3	1:A:302:GLN:HG3	1.27	1.12
1:A:326:LYS:HG2	1:A:331:ILE:HD12	1.36	1.07
1:A:330:GLY:O	1:A:331:ILE:HG13	1.54	1.07
1:A:286:ILE:HD11	1:A:321:ILE:HD13	1.44	0.97
1:A:279:MET:CE	3:A:833:DTP:H2'1	1.97	0.95
1:A:289:SER:HA	1:A:292:TRP:O	1.65	0.95
1:A:5:ALA:HB1	1:A:6:PRO:CD	2.00	0.91
1:A:237:THR:O	1:A:238:ASP:CG	2.11	0.88
1:A:291:SER:CB	1:A:302:GLN:HG3	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ALA:O	1:A:135:VAL:HG23	1.74	0.87
1:A:78:ALA:O	1:A:82:VAL:HG23	1.75	0.85
1:A:130:ILE:O	1:A:134:LEU:HB2	1.76	0.85
1:A:64:ILE:HG23	1:A:223:VAL:HB	1.60	0.82
1:A:3:GLN:O	1:A:4:GLN:HG3	1.80	0.81
1:A:2:ALA:O	1:A:5:ALA:HB3	1.80	0.81
1:A:335:VAL:HG13	1:A:336:THR:N	1.96	0.81
1:A:157:ILE:HG13	1:A:157:ILE:O	1.79	0.81
1:A:323:LYS:NZ	1:A:335:VAL:HG11	1.95	0.80
1:A:329:LEU:O	1:A:330:GLY:O	2.00	0.79
1:A:127:ALA:O	1:A:131:ALA:HB2	1.84	0.78
1:A:330:GLY:O	1:A:331:ILE:CG1	2.31	0.77
1:A:125:GLU:CD	1:A:154:ARG:H	1.87	0.76
1:A:5:ALA:CB	1:A:6:PRO:CD	2.64	0.75
1:A:95:ILE:HG21	1:A:127:ALA:HB1	1.69	0.75
1:A:335:VAL:CG1	1:A:336:THR:N	2.49	0.74
1:A:136:ARG:HH21	1:A:179:LYS:HG2	1.53	0.74
1:A:73:GLY:O	1:A:77:VAL:HG23	1.89	0.73
1:A:136:ARG:NH2	1:A:179:LYS:HG2	2.03	0.73
1:A:335:VAL:CG1	1:A:336:THR:H	2.01	0.73
1:A:265:LEU:HB2	1:A:268:GLN:HB2	1.71	0.72
1:A:245:ARG:HB3	1:A:261:GLU:HG3	1.72	0.72
1:A:5:ALA:HB1	1:A:6:PRO:HD3	1.72	0.71
1:A:25:LYS:N	4:A:1322:CIT:O5	2.23	0.71
1:A:237:THR:O	1:A:238:ASP:OD1	2.09	0.70
1:A:5:ALA:HB1	1:A:6:PRO:HD2	1.74	0.69
1:A:279:MET:SD	3:A:833:DTP:H2'1	2.32	0.69
1:A:105:TYR:O	1:A:109:LEU:HG	1.93	0.69
1:A:184:LEU:HD23	1:A:189:THR:HB	1.75	0.69
1:A:314:ASN:O	1:A:317:VAL:HG12	1.93	0.69
1:A:76:THR:HG22	1:A:77:VAL:N	2.09	0.68
1:A:283:HIS:CE1	3:A:833:DTP:O3'	2.46	0.68
1:A:39:ILE:H	1:A:39:ILE:HD12	1.59	0.68
1:A:51:VAL:HG12	1:A:331:ILE:HD11	1.76	0.67
1:A:344:PRO:O	1:A:345:ALA:HB2	1.93	0.67
1:A:102:ASP:HB3	3:A:832:DTP:HN62	1.59	0.67
1:A:323:LYS:HZ2	1:A:335:VAL:CG1	2.07	0.66
1:A:4:GLN:HG2	5:A:504:HOH:O	1.96	0.66
1:A:327:GLU:OE2	1:A:335:VAL:HG13	1.95	0.66
1:A:171:ARG:O	1:A:175:GLN:HG3	1.96	0.66
1:A:91:ILE:HB	1:A:140:LEU:HA	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:PHE:CE1	1:A:325:ILE:HG12	2.31	0.65
1:A:285:PHE:CD1	1:A:325:ILE:HG12	2.32	0.65
1:A:305:GLU:O	1:A:308:ARG:HB3	1.97	0.65
1:A:215:LYS:HG3	1:A:215:LYS:O	1.96	0.65
1:A:323:LYS:HZ2	1:A:335:VAL:HG11	1.61	0.64
1:A:44:THR:CB	1:A:49:LEU:HD23	2.28	0.63
1:A:286:ILE:HD11	1:A:321:ILE:CD1	2.26	0.62
1:A:102:ASP:HB3	3:A:832:DTP:N6	2.15	0.62
1:A:96:ASP:HB3	1:A:120:GLN:HG2	1.82	0.62
1:A:272:ARG:O	1:A:275:SER:HB2	2.00	0.62
1:A:345:ALA:C	1:A:346:PRO:O	2.34	0.62
1:A:283:HIS:CE1	1:A:329:LEU:HD21	2.35	0.62
1:A:71:SER:H	3:A:832:DTP:PG	2.22	0.62
1:A:3:GLN:C	1:A:4:GLN:HG3	2.19	0.61
1:A:289:SER:CA	1:A:292:TRP:O	2.45	0.61
1:A:23:PHE:HB2	1:A:27:SER:OG	2.00	0.61
1:A:323:LYS:CE	1:A:335:VAL:HG11	2.30	0.60
1:A:345:ALA:CB	5:A:499:HOH:O	2.49	0.60
1:A:64:ILE:HG23	1:A:223:VAL:CB	2.31	0.60
1:A:327:GLU:OE2	1:A:336:THR:HA	2.02	0.60
1:A:32:GLY:O	1:A:346:PRO:HD3	2.01	0.60
1:A:53:LEU:HD21	1:A:225:LEU:HD21	1.84	0.59
1:A:136:ARG:NH1	1:A:183:ALA:HB2	2.17	0.59
1:A:24:GLY:HA3	4:A:1322:CIT:O6	2.03	0.59
1:A:264:ILE:HG12	1:A:270:ILE:HG12	1.83	0.59
1:A:168:LEU:O	1:A:172:LEU:HG	2.03	0.59
1:A:3:GLN:O	1:A:4:GLN:CG	2.50	0.59
1:A:321:ILE:O	1:A:325:ILE:HG13	2.03	0.58
1:A:227:VAL:HG22	1:A:246:VAL:HG22	1.85	0.58
1:A:337:ALA:HA	5:A:404:HOH:O	2.03	0.58
1:A:287:ARG:HG2	1:A:287:ARG:HH11	1.66	0.58
1:A:125:GLU:OE2	1:A:154:ARG:N	2.36	0.58
1:A:230:ILE:HD11	1:A:245:ARG:N	2.19	0.58
1:A:14:LEU:O	1:A:17:ALA:HB3	2.03	0.57
1:A:63:VAL:HG13	1:A:221:ALA:HA	1.86	0.57
1:A:197:LEU:O	1:A:198:ARG:CB	2.53	0.57
1:A:276:LEU:H	1:A:276:LEU:HD22	1.69	0.57
1:A:327:GLU:HG3	1:A:336:THR:CB	2.35	0.57
1:A:254:SER:OG	1:A:255:PRO:HD2	2.05	0.57
1:A:279:MET:HE1	3:A:833:DTP:H2'1	1.83	0.57
1:A:108:LYS:NZ	1:A:108:LYS:HB3	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:VAL:HG23	5:A:456:HOH:O	2.05	0.57
1:A:47:ILE:CG2	1:A:279:MET:HG2	2.35	0.56
1:A:76:THR:HG21	1:A:270:ILE:HG13	1.87	0.56
1:A:307:ALA:O	1:A:311:LEU:HD13	2.04	0.56
1:A:2:ALA:O	1:A:5:ALA:CB	2.53	0.56
1:A:75:THR:O	1:A:79:LEU:N	2.34	0.56
1:A:102:ASP:CB	3:A:832:DTP:HN62	2.19	0.56
1:A:127:ALA:HB3	1:A:151:LEU:HD12	1.88	0.56
1:A:64:ILE:CD1	1:A:223:VAL:HB	2.35	0.56
1:A:48:SER:OG	3:A:833:DTP:H8	2.06	0.56
1:A:180:MET:HG2	1:A:184:LEU:HD11	1.88	0.55
1:A:33:GLU:HG2	1:A:34:GLU:H	1.71	0.55
1:A:66:ILE:HG22	1:A:74:LYS:HG2	1.88	0.55
1:A:70:GLU:HG3	3:A:832:DTP:O3G	2.07	0.55
1:A:47:ILE:HD11	1:A:326:LYS:HG3	1.89	0.55
1:A:76:THR:CG2	1:A:270:ILE:HG13	2.37	0.55
1:A:47:ILE:O	1:A:50:ASP:HB2	2.07	0.55
1:A:121:PRO:HG3	1:A:127:ALA:HB2	1.89	0.55
1:A:147:SER:O	1:A:151:LEU:CD2	2.54	0.55
1:A:96:ASP:O	1:A:121:PRO:HD2	2.07	0.55
1:A:5:ALA:CB	1:A:6:PRO:HD2	2.35	0.55
1:A:74:LYS:HB2	3:A:832:DTP:O2B	2.07	0.55
1:A:92:ALA:O	1:A:116:LEU:HD23	2.07	0.55
1:A:140:LEU:HD22	1:A:140:LEU:H	1.71	0.54
1:A:327:GLU:HG3	1:A:336:THR:CA	2.37	0.54
1:A:279:MET:HE3	3:A:833:DTP:H2'1	1.85	0.54
1:A:140:LEU:HD22	1:A:140:LEU:N	2.21	0.54
1:A:153:PRO:HG3	1:A:172:LEU:CD1	2.37	0.54
1:A:335:VAL:HG12	1:A:336:THR:H	1.70	0.54
1:A:93:ALA:HB3	1:A:143:ILE:HG13	1.88	0.54
1:A:212:THR:O	1:A:212:THR:HG22	2.07	0.54
1:A:153:PRO:CA	1:A:172:LEU:HD11	2.38	0.54
1:A:94:PHE:HE2	1:A:146:ASP:HB2	1.72	0.54
1:A:180:MET:HG2	1:A:184:LEU:CD1	2.38	0.53
1:A:330:GLY:O	1:A:331:ILE:CB	2.56	0.53
1:A:8:ARG:HB3	1:A:10:LYS:HE3	1.90	0.53
1:A:91:ILE:HD12	1:A:139:ALA:O	2.08	0.53
1:A:64:ILE:HD12	1:A:223:VAL:HB	1.91	0.53
1:A:33:GLU:HG2	1:A:34:GLU:N	2.23	0.53
1:A:323:LYS:NZ	1:A:335:VAL:CG1	2.64	0.52
1:A:153:PRO:CB	1:A:172:LEU:HD11	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:TYR:HA	1:A:195:ASN:O	2.09	0.52
1:A:224:ARG:HB2	1:A:250:LYS:HB3	1.90	0.52
1:A:132:ASP:O	1:A:135:VAL:N	2.40	0.52
1:A:142:ILE:HA	1:A:190:THR:O	2.09	0.52
1:A:175:GLN:O	1:A:178:ARG:N	2.30	0.51
1:A:44:THR:HB	1:A:49:LEU:HD23	1.92	0.51
1:A:132:ASP:HB2	1:A:180:MET:HE2	1.92	0.51
1:A:148:VAL:HG12	1:A:148:VAL:O	2.09	0.51
1:A:125:GLU:OE2	1:A:153:PRO:HA	2.11	0.51
1:A:214:GLY:C	1:A:216:ALA:H	2.14	0.50
1:A:323:LYS:HE3	1:A:335:VAL:HG11	1.94	0.50
1:A:76:THR:O	1:A:77:VAL:C	2.49	0.50
1:A:153:PRO:HG3	1:A:172:LEU:HD11	1.92	0.50
1:A:276:LEU:N	1:A:276:LEU:HD22	2.27	0.50
1:A:340:ASP:O	1:A:341:ASP:CB	2.60	0.50
1:A:148:VAL:HB	1:A:195:ASN:OD1	2.12	0.50
1:A:67:TYR:OH	1:A:226:ASP:HB2	2.12	0.50
1:A:67:TYR:CZ	1:A:226:ASP:HB2	2.47	0.50
1:A:178:ARG:HH11	1:A:178:ARG:HG2	1.77	0.49
1:A:281:VAL:C	1:A:283:HIS:H	2.14	0.49
1:A:140:LEU:CD2	1:A:140:LEU:H	2.25	0.49
1:A:308:ARG:O	1:A:312:LEU:HG	2.11	0.49
4:A:1322:CIT:O7	4:A:1322:CIT:O4	2.26	0.49
1:A:276:LEU:O	1:A:280:GLY:N	2.45	0.49
1:A:70:GLU:HA	3:A:832:DTP:O2G	2.11	0.49
1:A:293:PHE:HE2	1:A:304:LYS:N	2.10	0.49
1:A:39:ILE:CD1	1:A:39:ILE:H	2.21	0.49
1:A:94:PHE:CE1	1:A:101:LEU:HD13	2.48	0.49
1:A:47:ILE:HG21	1:A:279:MET:HG2	1.94	0.49
1:A:344:PRO:O	1:A:345:ALA:CB	2.59	0.49
1:A:62:ARG:HH21	1:A:62:ARG:HG3	1.78	0.49
1:A:240:VAL:O	1:A:266:TYR:HD2	1.95	0.49
1:A:40:SER:HB2	1:A:60:ARG:HD2	1.94	0.49
1:A:61:GLY:HA2	1:A:184:LEU:O	2.12	0.49
1:A:60:ARG:HA	1:A:190:THR:HG22	1.94	0.48
1:A:75:THR:O	1:A:78:ALA:HB3	2.13	0.48
1:A:142:ILE:HG23	1:A:142:ILE:O	2.12	0.48
1:A:335:VAL:O	1:A:337:ALA:N	2.47	0.48
1:A:276:LEU:CD2	1:A:276:LEU:H	2.26	0.48
1:A:125:GLU:OE2	1:A:125:GLU:N	2.46	0.47
1:A:345:ALA:HB3	5:A:499:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LEU:CD2	1:A:271:SER:HB2	2.45	0.47
1:A:46:SER:O	1:A:47:ILE:C	2.53	0.47
1:A:327:GLU:CG	1:A:336:THR:HA	2.44	0.47
1:A:74:LYS:N	3:A:832:DTP:O2B	2.48	0.47
1:A:263:ASP:HB2	1:A:271:SER:HB3	1.97	0.47
1:A:125:GLU:OE1	1:A:154:ARG:N	2.46	0.47
1:A:329:LEU:C	1:A:330:GLY:O	2.53	0.47
1:A:283:HIS:ND1	3:A:833:DTP:O3'	2.48	0.47
1:A:153:PRO:HG2	1:A:168:LEU:CB	2.45	0.47
1:A:49:LEU:HD13	1:A:246:VAL:HG11	1.97	0.47
1:A:153:PRO:HA	1:A:172:LEU:HD11	1.98	0.46
1:A:70:GLU:HG3	1:A:71:SER:H	1.81	0.46
1:A:128:LEU:O	1:A:131:ALA:HB3	2.16	0.46
1:A:347:VAL:O	1:A:348:ASP:CB	2.63	0.46
1:A:345:ALA:O	1:A:346:PRO:C	2.47	0.46
1:A:145:ILE:HD12	1:A:145:ILE:N	2.31	0.46
1:A:136:ARG:HH21	1:A:179:LYS:CG	2.25	0.46
1:A:19:ILE:HG21	1:A:28:VAL:CG2	2.46	0.46
1:A:327:GLU:HG3	1:A:336:THR:HA	1.98	0.46
1:A:148:VAL:HG13	1:A:173:MET:SD	2.56	0.45
1:A:153:PRO:CG	1:A:172:LEU:HD11	2.46	0.45
1:A:180:MET:C	1:A:182:GLY:N	2.70	0.45
1:A:31:LEU:O	1:A:255:PRO:CB	2.65	0.45
1:A:84:ASN:O	1:A:85:ALA:C	2.55	0.45
1:A:156:GLU:C	1:A:158:GLU:H	2.18	0.45
1:A:74:LYS:NZ	1:A:74:LYS:HB2	2.31	0.45
1:A:254:SER:O	1:A:255:PRO:C	2.54	0.45
1:A:230:ILE:HD12	1:A:243:ARG:CG	2.47	0.45
1:A:323:LYS:HZ1	1:A:335:VAL:HG21	1.81	0.45
1:A:47:ILE:HG23	1:A:279:MET:HG2	1.99	0.45
1:A:64:ILE:HG23	1:A:223:VAL:CG1	2.48	0.44
1:A:281:VAL:HG23	1:A:282:GLU:N	2.30	0.44
1:A:333:ALA:HB1	1:A:334:VAL:HG23	1.99	0.44
1:A:265:LEU:HD22	1:A:265:LEU:N	2.32	0.44
1:A:122:ASP:O	1:A:123:THR:HG23	2.16	0.44
1:A:240:VAL:C	1:A:266:TYR:HD2	2.20	0.44
1:A:175:GLN:O	1:A:177:LEU:N	2.50	0.44
1:A:327:GLU:CD	1:A:336:THR:HA	2.38	0.44
1:A:136:ARG:HG2	1:A:136:ARG:HH11	1.82	0.44
1:A:226:ASP:O	1:A:246:VAL:HA	2.18	0.44
1:A:230:ILE:HD12	1:A:243:ARG:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:VAL:HG13	1:A:248:VAL:O	2.18	0.43
1:A:224:ARG:HD3	1:A:250:LYS:HD3	2.00	0.43
1:A:121:PRO:CG	1:A:127:ALA:HB2	2.48	0.43
1:A:3:GLN:O	1:A:4:GLN:CB	2.66	0.43
1:A:70:GLU:HG3	1:A:71:SER:N	2.32	0.43
1:A:60:ARG:HH12	1:A:141:ASP:CG	2.21	0.43
1:A:152:VAL:HA	1:A:153:PRO:HD3	1.81	0.43
1:A:153:PRO:O	1:A:154:ARG:C	2.56	0.43
1:A:327:GLU:OE2	1:A:335:VAL:CG1	2.64	0.43
1:A:226:ASP:C	1:A:226:ASP:OD2	2.57	0.43
1:A:98:GLU:CG	1:A:147:SER:HB2	2.49	0.43
1:A:264:ILE:HA	1:A:270:ILE:HA	2.00	0.43
1:A:147:SER:O	1:A:151:LEU:HD21	2.19	0.43
1:A:49:LEU:CD1	1:A:246:VAL:HG11	2.49	0.43
1:A:285:PHE:CE1	1:A:325:ILE:HA	2.54	0.43
1:A:293:PHE:O	1:A:300:LEU:HB2	2.18	0.43
1:A:75:THR:O	1:A:76:THR:C	2.57	0.43
1:A:278:ASP:O	1:A:282:GLU:HB2	2.20	0.42
1:A:333:ALA:HB1	1:A:334:VAL:H	1.23	0.42
1:A:67:TYR:CD1	1:A:67:TYR:C	2.91	0.42
1:A:294:THR:HA	1:A:299:GLN:HA	2.00	0.42
1:A:253:VAL:HG12	1:A:253:VAL:O	2.18	0.42
1:A:23:PHE:CB	1:A:27:SER:OG	2.66	0.42
1:A:265:LEU:O	1:A:266:TYR:C	2.57	0.42
3:A:833:DTP:N3	3:A:833:DTP:H5'1	2.34	0.42
1:A:148:VAL:HA	1:A:151:LEU:HD23	2.01	0.42
1:A:289:SER:CB	1:A:293:PHE:CD1	3.03	0.42
1:A:102:ASP:HA	1:A:103:PRO:HD2	1.80	0.42
1:A:52:ALA:HB2	1:A:260:ALA:HB2	2.01	0.42
1:A:24:GLY:HA3	4:A:1322:CIT:C6	2.50	0.42
1:A:256:PRO:HG2	1:A:257:PHE:CD2	2.55	0.41
1:A:53:LEU:HD13	1:A:58:LEU:HD23	2.02	0.41
1:A:59:PRO:HB2	1:A:62:ARG:HD3	2.02	0.41
1:A:177:LEU:CD2	1:A:217:LEU:HA	2.50	0.41
1:A:42:ILE:HD11	1:A:190:THR:HG21	2.03	0.41
1:A:287:ARG:HG2	1:A:287:ARG:NH1	2.34	0.41
1:A:265:LEU:CB	1:A:268:GLN:HB2	2.45	0.41
1:A:175:GLN:O	1:A:176:ALA:C	2.59	0.41
1:A:262:PHE:CE1	1:A:270:ILE:HG12	2.56	0.41
1:A:317:VAL:HG13	1:A:318:ALA:N	2.35	0.41
1:A:326:LYS:HE2	1:A:331:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ALA:C	1:A:82:VAL:HG23	2.41	0.41
1:A:15:ALA:O	1:A:18:GLN:N	2.54	0.41
1:A:157:ILE:CG1	1:A:157:ILE:O	2.61	0.41
1:A:288:LYS:HB3	1:A:289:SER:H	1.43	0.40
1:A:338:GLU:O	1:A:339:ALA:HB2	2.21	0.40
1:A:47:ILE:CG2	1:A:48:SER:N	2.85	0.40
1:A:64:ILE:HD13	1:A:223:VAL:HB	2.03	0.40
1:A:74:LYS:O	1:A:75:THR:C	2.58	0.40
1:A:132:ASP:HA	1:A:135:VAL:HB	2.04	0.40
1:A:31:LEU:O	1:A:255:PRO:HB3	2.22	0.40

There are no symmetry-related clashes.

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	325/349 (93%)	233 (72%)	58 (18%)	34 (10%)	0 3

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ALA
1	A	4	GLN
1	A	5	ALA
1	A	168	LEU
1	A	197	LEU
1	A	235	ASP
1	A	238	ASP
1	A	292	TRP
1	A	330	GLY
1	A	331	ILE
1	A	336	THR

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Mol	Chain	Res	Type
1	A	344	PRO
1	A	6	PRO
1	A	140	LEU
1	A	175	GLN
1	A	176	ALA
1	A	212	THR
1	A	233	LEU
1	A	288	LYS
1	A	335	VAL
1	A	338	GLU
1	A	339	ALA
1	A	341	ASP
1	A	345	ALA
1	A	348	ASP
1	A	9	GLU
1	A	141	ASP
1	A	340	ASP
1	A	343	LEU
1	A	15	ALA
1	A	147	SER
1	A	103	PRO
1	A	342	VAL
1	A	256	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	235/275 (86%)	203 (86%)	32 (14%)	3 17

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	PRO
1	A	7	ASP
1	A	8	ARG

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Mol	Chain	Res	Type
1	A	10	LYS
1	A	22	ASN
1	A	25	LYS
1	A	34	GLU
1	A	39	ILE
1	A	62	ARG
1	A	63	VAL
1	A	76	THR
1	A	94	PHE
1	A	116	LEU
1	A	132	ASP
1	A	134	LEU
1	A	141	ASP
1	A	147	SER
1	A	157	ILE
1	A	171	ARG
1	A	190	THR
1	A	212	THR
1	A	235	ASP
1	A	243	ARG
1	A	245	ARG
1	A	261	GLU
1	A	283	HIS
1	A	288	LYS
1	A	291	SER
1	A	300	LEU
1	A	335	VAL
1	A	340	ASP
1	A	349	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	283	HIS
1	A	302	GLN
1	A	314	ASN

5.3.3 RNA ⓘ

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 4 ligands modelled in this entry, 1 is 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
3	DTP	A	832	-	26,32,32	2.79	10 (38%)	30,50,50	1.55	6 (20%)
4	CIT	A	1322	-	3,12,12	4.96	2 (66%)	3,17,17	3.77	3 (100%)
3	DTP	A	833	2	26,32,32	1.99	9 (34%)	30,50,50	2.19	8 (26%)

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
3	DTP	A	832	-	-	5/18/34/34	0/3/3/3
4	CIT	A	1322	-	-	3/6/16/16	-
3	DTP	A	833	2	-	5/18/34/34	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	832	DTP	C2-N3	8.09	1.45	1.32
4	A	1322	CIT	O7-C3	-7.54	1.31	1.43
3	A	832	DTP	C4-N3	6.27	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	832	DTP	PG-O2G	-4.01	1.39	1.54
4	A	1322	CIT	C2-C3	-3.98	1.49	1.54
3	A	832	DTP	C1'-N9	3.97	1.61	1.49
3	A	833	DTP	C8-N7	-3.72	1.28	1.34
3	A	833	DTP	PA-O5'	-3.64	1.44	1.59
3	A	833	DTP	PG-O2G	-3.59	1.41	1.54
3	A	832	DTP	PA-O5'	-3.49	1.45	1.59
3	A	833	DTP	C2-N3	3.46	1.37	1.32
3	A	832	DTP	PB-O2B	-3.41	1.39	1.55
3	A	833	DTP	C2'-C3'	-3.28	1.44	1.52
3	A	832	DTP	C5-N7	-3.02	1.28	1.39
3	A	833	DTP	PB-O2B	-2.99	1.41	1.55
3	A	832	DTP	C2-N1	2.84	1.39	1.33
3	A	833	DTP	C4-N3	2.63	1.39	1.35
3	A	833	DTP	O3'-C3'	-2.41	1.38	1.43
3	A	832	DTP	C5'-C4'	2.41	1.59	1.51
3	A	832	DTP	O3'-C3'	-2.33	1.38	1.43
3	A	833	DTP	PA-O2A	-2.10	1.45	1.55

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	833	DTP	C2'-C1'-N9	-7.42	97.16	114.27
4	A	1322	CIT	C3-C2-C1	5.10	123.14	114.98
3	A	832	DTP	C4-C5-N7	4.25	113.83	109.40
3	A	833	DTP	O5'-C5'-C4'	3.74	121.86	108.99
3	A	833	DTP	O5'-PA-O1A	-3.59	95.02	109.07
3	A	833	DTP	PB-O3B-PG	3.48	144.75	132.83
3	A	832	DTP	O4'-C4'-C5'	3.34	120.37	109.37
4	A	1322	CIT	C3-C4-C5	-3.14	109.95	114.98
4	A	1322	CIT	C4-C3-C2	-2.59	102.40	109.33
3	A	832	DTP	C2'-C3'-C4'	2.52	108.01	102.76
3	A	832	DTP	O5'-C5'-C4'	2.49	117.58	108.99
3	A	833	DTP	O2G-PG-O1G	-2.36	101.46	110.68
3	A	832	DTP	C2'-C1'-N9	2.32	119.63	114.27
3	A	833	DTP	C4-C5-N7	2.31	111.80	109.40
3	A	833	DTP	O4'-C4'-C5'	-2.23	102.03	109.37
3	A	832	DTP	C4'-O4'-C1'	2.19	114.74	109.45
3	A	833	DTP	C3'-C2'-C1'	2.05	107.66	102.54

There are no chirality outliers.

All (13) torsion outliers are listed below:

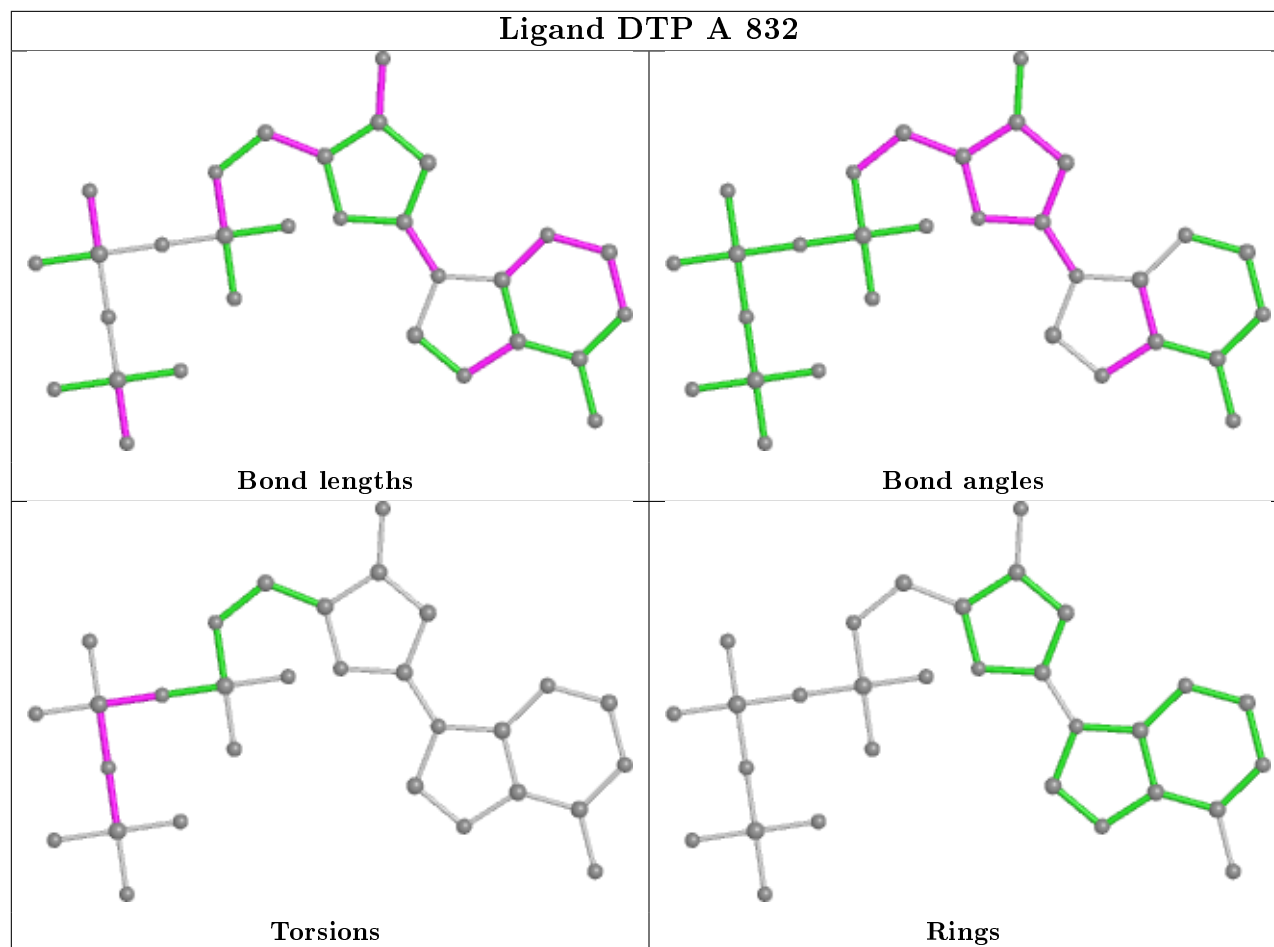
Mol	Chain	Res	Type	Atoms
4	A	1322	CIT	C6-C3-C4-C5
3	A	833	DTP	PB-O3B-PG-O3G
3	A	833	DTP	O4'-C4'-C5'-O5'
3	A	832	DTP	PB-O3B-PG-O1G
3	A	833	DTP	PB-O3B-PG-O1G
3	A	832	DTP	PG-O3B-PB-O1B
3	A	832	DTP	PA-O3A-PB-O1B
3	A	833	DTP	PG-O3B-PB-O1B
3	A	832	DTP	PB-O3B-PG-O3G
3	A	832	DTP	PA-O3A-PB-O2B
3	A	833	DTP	PB-O3A-PA-O2A
4	A	1322	CIT	O7-C3-C4-C5
4	A	1322	CIT	C2-C3-C4-C5

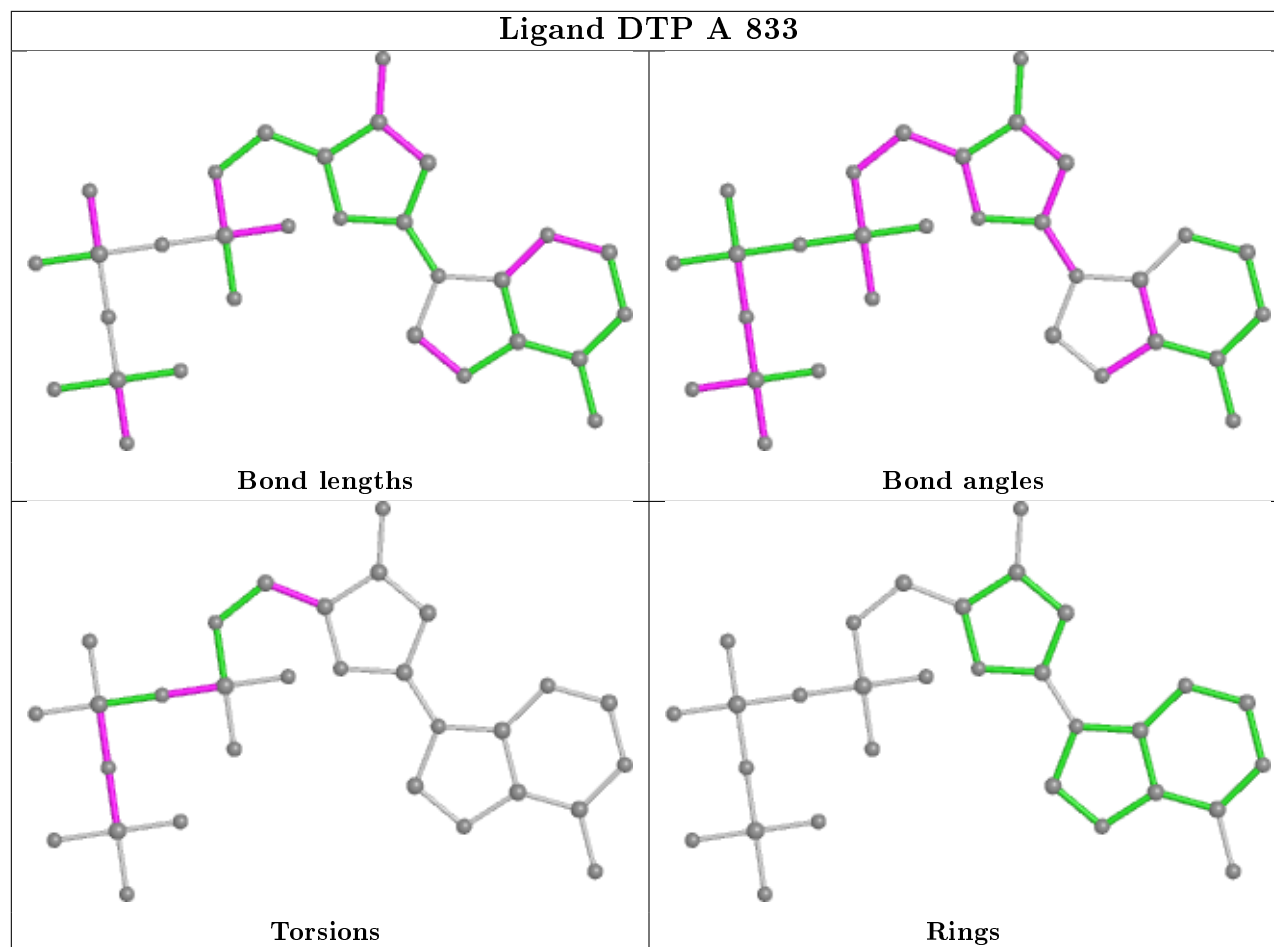
There are no ring outliers.

3 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	832	DTP	8	0
4	A	1322	CIT	4	0
3	A	833	DTP	8	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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

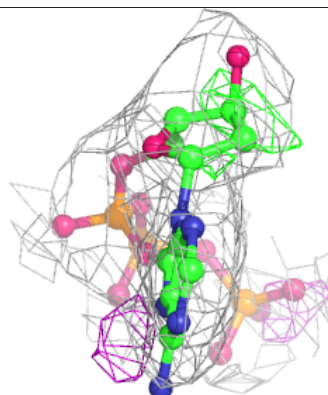
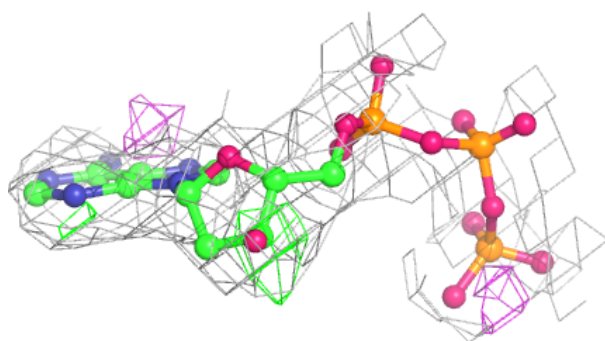
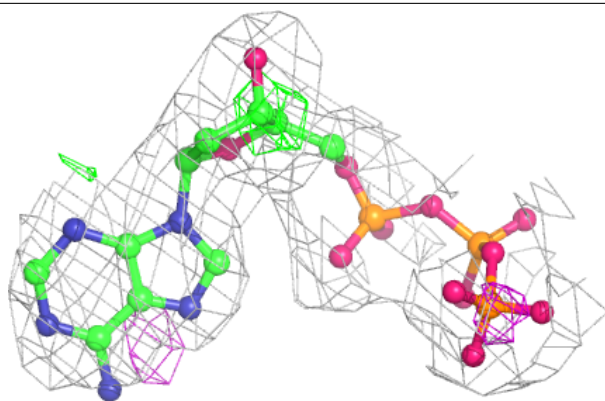
6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

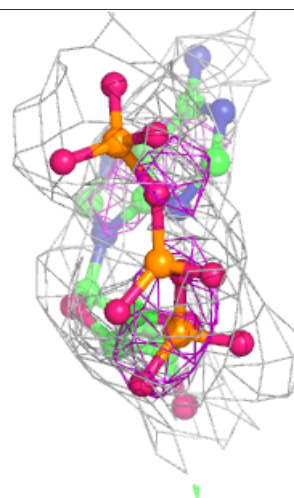
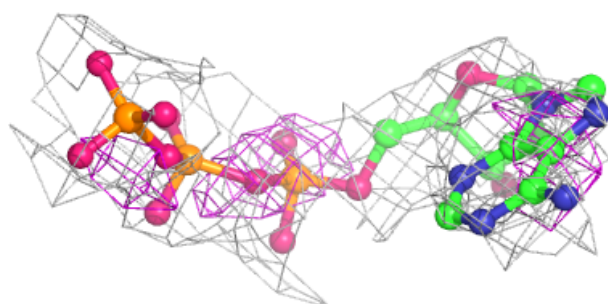
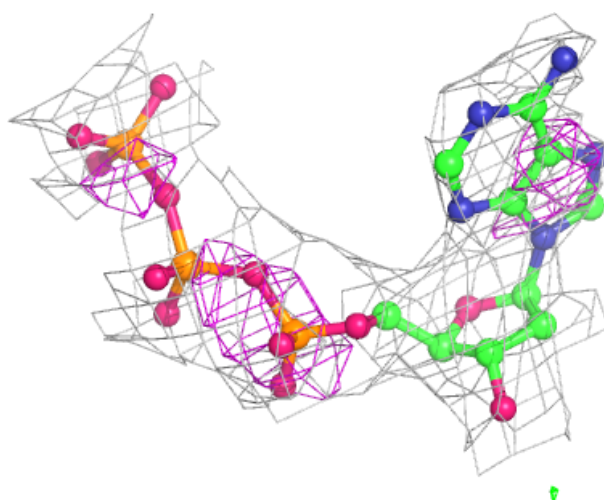
Electron density around DTP A 832:

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



Electron density around DTP A 833:

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



6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.