



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:03 am BST

PDB ID : 1XJF
Title : Structural mechanism of allosteric substrate specificity in a ribonucleotide reductase: dATP complex
Authors : Larsson, K.-M.; Jordan, A.; Eliasson, R.; Reichard, P.; Logan, D.T.; Nordlund, P.
Deposited on : 2004-09-23
Resolution : 2.40 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

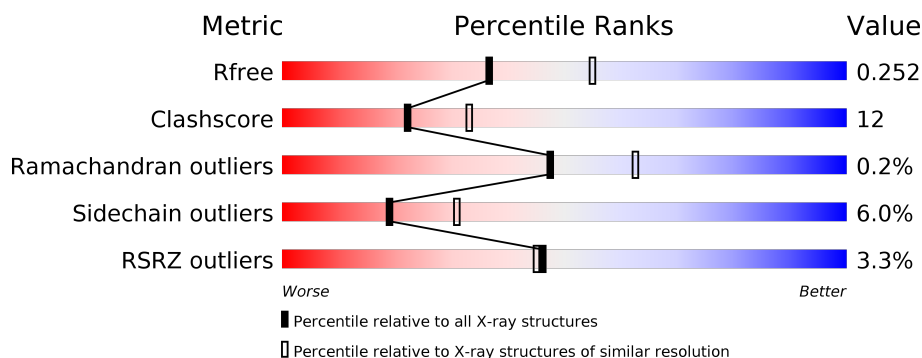
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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 $\leq 5\%$. 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	644	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div>• •</div> </div> </div>
1	B	644	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div>• 5%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10194 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 ribonucleotide reductase, B12-dependent.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	619	Total	C	N	O	S	0	0	0
			4974	3190	843	921	20			
1	B	611	Total	C	N	O	S	0	0	0
			4904	3142	836	906	20			

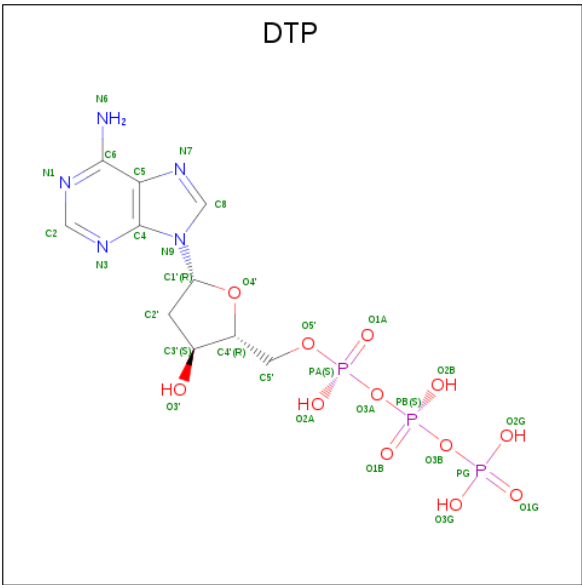
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	205	SER	TYR	SEE REMARK 999	UNP O33839
B	205	SER	TYR	SEE REMARK 999	UNP O33839

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

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

- Molecule 3 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

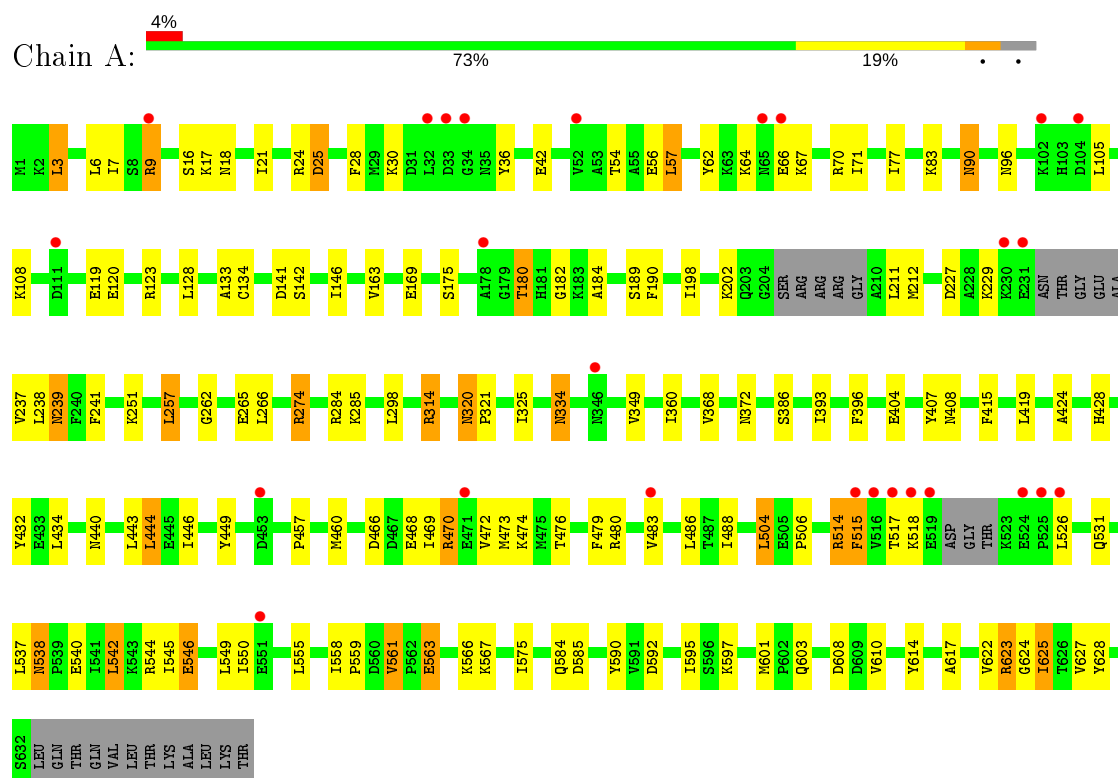
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	121	Total	O	0	0
			121	121		
4	B	133	Total	O	0	0
			133	133		

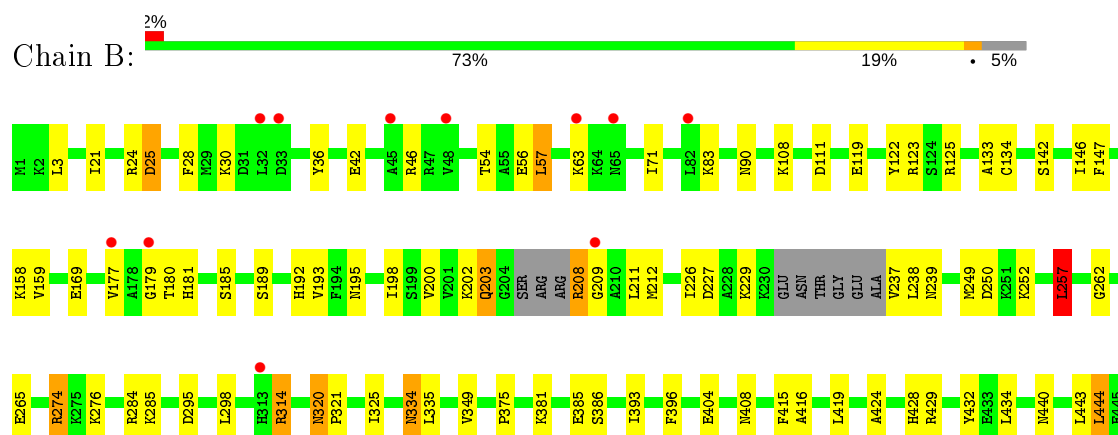
3 Residue-property plots

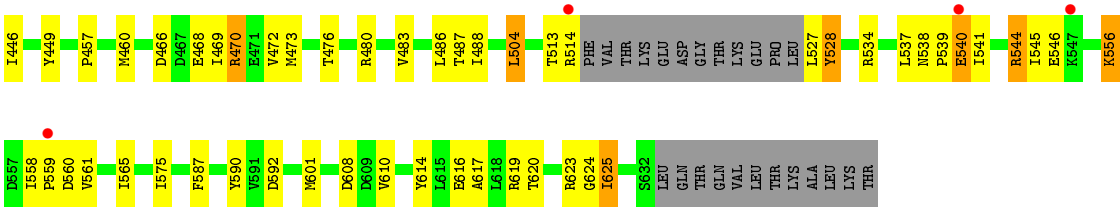
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: ribonucleotide reductase, B12-dependent



- Molecule 1: ribonucleotide reductase, B12-dependent





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	116.30Å 123.76Å 107.03Å 90.00° 103.82° 90.00°	Depositor
Resolution (Å)	22.88 – 2.40 22.89 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (22.88-2.40) 99.8 (22.89-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.208 , 0.260 0.205 , 0.252	Depositor DCC
R_{free} test set	4050 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10194	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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

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	0.77	0/5072	0.81	2/6845 (0.0%)
1	B	0.73	0/5000	0.80	3/6747 (0.0%)
All	All	0.75	0/10072	0.80	5/13592 (0.0%)

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	623	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	B	625	ILE	CG1-CB-CG2	-6.47	97.17	111.40
1	A	623	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	B	295	ASP	CB-CG-OD1	5.54	123.28	118.30
1	B	257	LEU	CA-CB-CG	5.07	126.96	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	PHE	Peptide

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	4974	0	5026	118	0
1	B	4904	0	4955	122	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	30	0	12	6	0
3	B	30	0	12	3	0
4	A	121	0	0	5	0
4	B	133	0	0	5	0
All	All	10194	0	10005	233	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 (233) 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:237:VAL:HG12	1:B:238:LEU:H	1.17	1.08
1:A:237:VAL:HG12	1:A:238:LEU:H	1.20	1.05
1:A:128:LEU:HD11	1:B:179:GLY:HA2	1.43	0.98
1:B:514:ARG:H	1:B:527:LEU:HD12	1.28	0.96
1:A:428:HIS:HD2	1:A:480:ARG:HH22	1.00	0.95
1:B:470:ARG:HG3	1:B:470:ARG:HH11	1.29	0.93
1:A:466:ASP:HB3	1:A:470:ARG:HH12	1.33	0.93
1:A:563:GLU:HA	1:A:563:GLU:OE1	1.68	0.91
1:B:466:ASP:HB3	1:B:470:ARG:HH12	1.35	0.90
1:A:96:ASN:OD1	1:B:181:HIS:HE1	1.58	0.87
1:B:177:VAL:HB	1:B:180:THR:HG22	1.55	0.86
1:A:428:HIS:CD2	1:A:480:ARG:HH22	1.91	0.86
1:A:449:TYR:HE1	1:A:473:MET:HE1	1.41	0.85
1:B:428:HIS:HD2	1:B:480:ARG:HH22	1.22	0.85
1:B:449:TYR:HE1	1:B:473:MET:HE1	1.42	0.84
1:B:449:TYR:HE1	1:B:473:MET:CE	1.92	0.82
1:A:470:ARG:HH11	1:A:470:ARG:HG3	1.44	0.82
1:B:90:ASN:OD1	4:B:1050:HOH:O	1.99	0.81
1:B:90:ASN:OD1	4:B:1046:HOH:O	2.00	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ASN:HD21	1:A:133:ALA:HB2	1.47	0.80
1:B:470:ARG:CG	1:B:470:ARG:HH11	1.96	0.78
1:B:314:ARG:HH11	1:B:314:ARG:HG2	1.49	0.78
1:A:428:HIS:HD2	1:A:480:ARG:NH2	1.80	0.77
1:A:449:TYR:HE1	1:A:473:MET:CE	1.96	0.77
1:A:320:ASN:H	1:A:320:ASN:HD22	1.31	0.76
1:A:470:ARG:HH11	1:A:470:ARG:CG	1.99	0.75
1:A:601:MET:HE3	1:A:610:VAL:HG22	1.68	0.75
1:B:428:HIS:CD2	1:B:480:ARG:HH22	2.05	0.75
1:B:208:ARG:HB2	1:B:208:ARG:HH11	1.52	0.74
1:B:457:PRO:HD3	1:B:473:MET:CE	2.18	0.73
1:B:624:GLY:O	1:B:625:ILE:HD12	1.89	0.73
1:B:320:ASN:H	1:B:320:ASN:HD22	1.33	0.72
1:B:514:ARG:N	1:B:527:LEU:HD12	2.03	0.72
1:B:90:ASN:HD21	1:B:133:ALA:HB2	1.54	0.71
1:B:601:MET:HE3	1:B:610:VAL:HG22	1.71	0.71
1:B:514:ARG:H	1:B:527:LEU:CD1	2.02	0.71
1:B:538:ASN:O	1:B:541:ILE:HG22	1.91	0.71
1:B:334:ASN:HD22	1:B:334:ASN:C	1.94	0.71
1:B:237:VAL:HG12	1:B:238:LEU:N	2.00	0.70
1:A:229:LYS:HD3	1:A:238:LEU:O	1.91	0.70
1:A:62:TYR:CE2	1:A:70:ARG:HD2	2.26	0.70
1:B:592:ASP:O	1:B:623:ARG:NH2	2.25	0.69
1:B:177:VAL:HB	1:B:180:THR:CG2	2.21	0.69
1:B:237:VAL:CG1	1:B:238:LEU:H	1.97	0.69
1:B:46:ARG:HD2	4:B:1059:HOH:O	1.91	0.69
1:B:470:ARG:NH1	1:B:470:ARG:HG3	1.98	0.69
1:A:617:ALA:HB1	1:A:625:ILE:HD13	1.73	0.68
1:A:237:VAL:CG1	1:A:238:LEU:H	2.01	0.67
1:A:408:ASN:HB3	1:A:575:ILE:HG23	1.76	0.67
1:B:257:LEU:HD22	1:B:262:GLY:HA3	1.76	0.67
1:B:212:MET:HB2	1:B:321:PRO:HA	1.76	0.67
1:A:21:ILE:O	1:A:25:ASP:HB2	1.95	0.67
1:A:470:ARG:NH1	1:A:470:ARG:HG3	2.07	0.67
1:B:457:PRO:HD3	1:B:473:MET:HE2	1.77	0.67
1:A:601:MET:CE	1:A:610:VAL:HG22	2.26	0.65
1:B:428:HIS:HD2	1:B:480:ARG:NH2	1.94	0.65
1:A:449:TYR:CE1	1:A:473:MET:CE	2.80	0.65
1:A:180:THR:HG21	3:A:1002:DTP:HN61	1.60	0.65
1:A:538:ASN:HB3	1:A:540:GLU:HB3	1.79	0.65
1:B:449:TYR:CE1	1:B:473:MET:CE	2.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ARG:NH2	1:A:608:ASP:OD1	2.29	0.64
1:A:128:LEU:CD1	1:B:179:GLY:HA2	2.25	0.64
1:B:440:ASN:ND2	1:B:444:LEU:HD12	2.13	0.63
1:B:539:PRO:O	1:B:540:GLU:HB2	1.97	0.63
1:B:449:TYR:CE1	1:B:473:MET:HE1	2.31	0.63
1:A:237:VAL:HG12	1:A:238:LEU:N	2.04	0.63
1:B:198:ILE:HD12	1:B:211:LEU:HD21	1.80	0.63
1:B:320:ASN:HD21	1:B:325:ILE:H	1.47	0.62
1:B:527:LEU:HB3	1:B:528:TYR:HB2	1.82	0.62
1:A:320:ASN:H	1:A:320:ASN:ND2	1.99	0.61
1:B:527:LEU:HD13	1:B:528:TYR:CD1	2.36	0.60
1:A:457:PRO:HD3	1:A:473:MET:CE	2.32	0.60
1:A:617:ALA:CB	1:A:625:ILE:HD13	2.32	0.60
1:B:159:VAL:HG21	1:B:375:PRO:HG3	1.83	0.60
1:B:527:LEU:HB3	1:B:528:TYR:CB	2.32	0.60
1:A:449:TYR:CE1	1:A:473:MET:HE1	2.31	0.59
1:A:96:ASN:OD1	1:B:181:HIS:CE1	2.48	0.59
1:B:601:MET:CE	1:B:610:VAL:HG22	2.33	0.58
1:B:320:ASN:H	1:B:320:ASN:ND2	2.01	0.58
1:A:624:GLY:O	1:A:625:ILE:HD12	2.03	0.58
1:B:469:ILE:O	1:B:473:MET:HG2	2.03	0.58
1:B:408:ASN:HB3	1:B:575:ILE:HG23	1.86	0.57
3:B:1001:DTP:O5'	3:B:1001:DTP:H8	2.04	0.57
1:A:251:LYS:NZ	1:A:622:VAL:O	2.37	0.57
1:A:617:ALA:HB1	1:A:625:ILE:CD1	2.35	0.57
1:A:257:LEU:HD22	1:A:262:GLY:HA3	1.87	0.56
1:B:320:ASN:ND2	1:B:325:ILE:H	2.03	0.56
1:A:141:ASP:O	3:A:1002:DTP:H5'2	2.06	0.56
1:B:21:ILE:O	1:B:25:ASP:HB2	2.06	0.56
1:B:527:LEU:HD13	1:B:528:TYR:HD1	1.70	0.56
1:B:119:GLU:HB3	1:B:123:ARG:HH22	1.71	0.56
1:B:177:VAL:CB	1:B:180:THR:HG22	2.33	0.56
1:A:265:GLU:OE2	1:A:274:ARG:NH1	2.39	0.55
1:A:128:LEU:HD11	1:B:179:GLY:CA	2.27	0.55
1:A:545:ILE:HG13	1:A:546:GLU:N	2.22	0.55
1:A:488:ILE:HG21	1:A:504:LEU:HG	1.88	0.55
1:A:119:GLU:HB3	1:A:123:ARG:HH22	1.72	0.55
1:A:212:MET:HB2	1:A:321:PRO:HA	1.87	0.55
1:A:227:ASP:OD2	1:A:285:LYS:NZ	2.38	0.55
1:B:147:PHE:CE1	1:B:193:VAL:HG11	2.42	0.55
1:B:298:LEU:HD11	1:B:614:TYR:CD1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:THR:HA	1:B:527:LEU:HB2	1.88	0.54
1:A:198:ILE:HG13	1:A:211:LEU:HD11	1.89	0.54
1:A:314:ARG:HG2	1:A:314:ARG:HH11	1.72	0.54
1:A:424:ALA:HA	1:A:486:LEU:HD11	1.90	0.54
1:A:515:PHE:HD2	1:A:515:PHE:H	1.56	0.54
1:A:601:MET:HE2	1:A:627:VAL:HB	1.88	0.54
1:B:616:GLU:O	1:B:620:THR:HG23	2.08	0.54
1:B:185:SER:OG	3:B:1001:DTP:H2	2.08	0.53
1:B:189:SER:HA	1:B:192:HIS:HD2	1.73	0.53
1:A:457:PRO:HD3	1:A:473:MET:HE2	1.91	0.53
1:A:6:LEU:O	1:A:9:ARG:HB3	2.08	0.53
1:B:386:SER:HB3	1:B:483:VAL:HG11	1.91	0.52
1:A:320:ASN:HD21	1:A:325:ILE:H	1.55	0.52
1:A:239:ASN:HD22	1:A:239:ASN:H	1.56	0.52
1:A:472:VAL:O	1:A:476:THR:HG23	2.09	0.52
1:B:284:ARG:NH2	1:B:608:ASP:OD1	2.33	0.52
1:B:457:PRO:HD3	1:B:473:MET:HE1	1.91	0.51
1:B:227:ASP:OD2	1:B:285:LYS:NZ	2.39	0.51
1:B:488:ILE:HG21	1:B:504:LEU:HG	1.93	0.50
1:B:527:LEU:CB	1:B:528:TYR:HB2	2.41	0.50
1:A:56:GLU:HB2	1:A:71:ILE:HG12	1.93	0.50
1:B:198:ILE:CD1	1:B:211:LEU:HD21	2.41	0.50
1:B:544:ARG:HH22	1:B:560:ASP:HB2	1.77	0.50
1:A:537:LEU:HD23	1:A:542:LEU:HG	1.93	0.50
1:B:119:GLU:HB3	1:B:123:ARG:NH2	2.26	0.50
1:A:592:ASP:O	1:A:623:ARG:NH2	2.45	0.50
1:B:229:LYS:HD3	1:B:238:LEU:O	2.12	0.50
1:B:504:LEU:HD12	4:B:1028:HOH:O	2.11	0.49
3:A:1002:DTP:O1A	3:A:1002:DTP:O2B	2.31	0.49
1:A:77:ILE:HG13	1:A:360:ILE:HD13	1.94	0.49
1:A:393:ILE:HD12	1:A:396:PHE:HB2	1.93	0.49
1:A:334:ASN:HD22	1:A:334:ASN:C	2.16	0.49
1:A:542:LEU:O	1:A:546:GLU:HB2	2.13	0.49
1:A:180:THR:HG23	1:B:158:LYS:O	2.12	0.48
1:A:3:LEU:O	1:A:7:ILE:HG13	2.12	0.48
1:B:537:LEU:HD13	1:B:565:ILE:HG21	1.95	0.48
1:A:189:SER:HB3	4:A:1077:HOH:O	2.14	0.48
1:B:142:SER:O	1:B:146:ILE:HG13	2.14	0.48
1:B:314:ARG:HH11	1:B:314:ARG:CG	2.24	0.48
1:B:56:GLU:HB2	1:B:71:ILE:HG12	1.95	0.48
1:A:180:THR:HG21	3:A:1002:DTP:N6	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:GLN:HE22	1:B:209:GLY:N	2.11	0.47
1:A:237:VAL:CG1	1:A:238:LEU:N	2.73	0.47
1:A:407:TYR:CZ	1:A:506:PRO:HD3	2.48	0.47
1:B:334:ASN:ND2	1:B:334:ASN:C	2.66	0.47
1:A:468:GLU:O	1:A:472:VAL:HG23	2.14	0.47
1:A:432:TYR:HA	1:A:479:PHE:O	2.13	0.47
1:A:617:ALA:CB	1:A:625:ILE:CD1	2.91	0.47
1:A:320:ASN:ND2	1:A:325:ILE:H	2.11	0.47
1:A:349:VAL:HG21	1:A:415:PHE:HZ	1.79	0.47
1:B:460:MET:HG2	1:B:590:TYR:CE1	2.50	0.47
1:A:119:GLU:HB3	1:A:123:ARG:NH2	2.29	0.47
1:A:18:ASN:HD21	1:A:514:ARG:HH21	1.63	0.47
1:B:428:HIS:CD2	1:B:480:ARG:HH12	2.33	0.47
1:A:57:LEU:HD13	1:A:71:ILE:HD11	1.97	0.46
1:A:558:ILE:O	1:A:566:LYS:NZ	2.44	0.46
1:B:393:ILE:HD12	1:B:396:PHE:HB2	1.97	0.46
1:B:274:ARG:HH11	1:B:274:ARG:HB2	1.80	0.46
1:A:440:ASN:ND2	1:A:444:LEU:HD12	2.30	0.46
1:A:474:LYS:HA	4:A:1075:HOH:O	2.15	0.46
1:B:617:ALA:HB1	1:B:625:ILE:HD13	1.98	0.46
1:A:469:ILE:O	1:A:473:MET:HG2	2.16	0.46
1:B:237:VAL:CG1	1:B:238:LEU:N	2.70	0.46
1:A:16:SER:OG	1:A:18:ASN:HB2	2.16	0.45
1:A:202:LYS:NZ	4:A:1079:HOH:O	2.49	0.45
1:B:424:ALA:HA	1:B:486:LEU:HD11	1.97	0.45
1:A:561:VAL:HG22	1:A:566:LYS:HG3	1.98	0.45
1:A:386:SER:HB3	1:A:483:VAL:HG11	1.97	0.45
1:A:184:ALA:HA	3:A:1002:DTP:N3	2.32	0.45
1:A:190:PHE:CE1	1:B:200:VAL:HG13	2.52	0.45
1:B:449:TYR:CE1	1:B:473:MET:HE3	2.49	0.44
1:A:18:ASN:ND2	1:A:514:ARG:HH21	2.14	0.44
1:B:226:ILE:HG21	1:B:285:LYS:HG2	2.00	0.44
1:A:77:ILE:CG1	1:A:360:ILE:HD13	2.47	0.44
1:A:42:GLU:HG3	1:A:83:LYS:HE3	2.00	0.44
1:B:349:VAL:HG21	1:B:415:PHE:HZ	1.81	0.44
1:A:190:PHE:CE1	1:B:200:VAL:CG1	3.01	0.44
1:A:180:THR:HB	1:A:182:GLY:H	1.83	0.44
1:B:265:GLU:OE2	1:B:274:ARG:NH1	2.51	0.44
1:B:443:LEU:HD22	1:B:446:ILE:HD11	1.99	0.44
1:A:24:ARG:HA	1:A:28:PHE:CD2	2.53	0.44
1:B:335:LEU:HD22	1:B:487:THR:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:MET:HG2	1:A:590:TYR:CE1	2.53	0.43
1:A:628:TYR:HD2	4:A:1051:HOH:O	2.00	0.43
1:B:54:THR:O	1:B:57:LEU:HB2	2.18	0.43
1:A:488:ILE:HD12	1:A:595:ILE:HD12	2.01	0.43
1:B:30:LYS:HE2	1:B:36:TYR:CE1	2.53	0.43
1:B:556:LYS:HE3	1:B:556:LYS:HB3	1.71	0.43
1:A:30:LYS:HE2	1:A:36:TYR:CZ	2.53	0.43
1:A:66:GLU:O	1:A:67:LYS:C	2.57	0.43
1:B:314:ARG:NH1	1:B:314:ARG:HG2	2.27	0.43
1:B:142:SER:HA	3:B:1001:DTP:H5'2	2.01	0.43
1:B:30:LYS:HE2	1:B:36:TYR:CZ	2.53	0.43
1:B:250:ASP:OD1	1:B:252:LYS:HB2	2.19	0.43
1:A:320:ASN:ND2	1:A:320:ASN:N	2.67	0.43
1:B:24:ARG:HA	1:B:28:PHE:CD2	2.53	0.43
1:B:472:VAL:O	1:B:476:THR:HG23	2.18	0.43
1:A:549:LEU:HD13	1:A:555:LEU:HD23	2.01	0.43
1:A:190:PHE:CD1	1:B:200:VAL:CG1	3.02	0.43
1:B:57:LEU:HD13	1:B:71:ILE:HD11	2.01	0.42
1:A:105:LEU:HD11	1:A:120:GLU:HG2	2.02	0.42
1:B:545:ILE:HG13	1:B:546:GLU:N	2.34	0.42
1:A:30:LYS:HE2	1:A:36:TYR:CE1	2.54	0.42
1:A:531:GLN:HB3	4:A:1103:HOH:O	2.18	0.42
1:A:584:GLN:HB2	1:A:597:LYS:HG2	2.01	0.42
1:B:265:GLU:OE1	1:B:276:LYS:HE2	2.19	0.42
1:A:558:ILE:HA	1:A:559:PRO:HD3	1.78	0.42
1:B:457:PRO:CD	1:B:473:MET:CE	2.96	0.42
1:B:468:GLU:O	1:B:472:VAL:HG23	2.20	0.42
1:A:449:TYR:CE1	1:A:473:MET:HE3	2.53	0.41
1:A:142:SER:O	1:A:146:ILE:HG13	2.20	0.41
1:A:54:THR:O	1:A:57:LEU:HB2	2.20	0.41
1:A:298:LEU:HD11	1:A:614:TYR:CD1	2.56	0.41
1:A:443:LEU:HD22	1:A:446:ILE:HD11	2.02	0.41
1:A:266:LEU:O	1:A:274:ARG:HA	2.21	0.41
1:A:603:GLN:HE21	1:A:603:GLN:HB2	1.64	0.41
1:B:239:ASN:H	1:B:239:ASN:HD22	1.69	0.41
1:B:195:ASN:HD21	1:B:239:ASN:ND2	2.18	0.41
1:B:320:ASN:ND2	1:B:320:ASN:N	2.68	0.41
1:B:416:ALA:HB1	1:B:587:PHE:CE2	2.56	0.41
1:A:18:ASN:HD21	1:A:514:ARG:NH2	2.18	0.40
1:A:542:LEU:HD22	1:A:546:GLU:HB2	2.03	0.40
1:A:142:SER:HA	3:A:1002:DTP:H5'2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:LYS:O	1:B:385:GLU:HG3	2.22	0.40
1:B:429:ARG:O	1:B:432:TYR:HB3	2.21	0.40
1:B:558:ILE:HA	1:B:559:PRO:HD2	1.84	0.40
1:A:368:VAL:O	1:A:372:ASN:HB2	2.20	0.40
1:B:42:GLU:HG3	1:B:83:LYS:HE3	2.04	0.40
1:B:468:GLU:HG3	4:B:1043:HOH:O	2.21	0.40
1:B:208:ARG:NH1	1:B:208:ARG:HB2	2.30	0.40
1:A:17:LYS:O	1:A:21:ILE:HG12	2.22	0.40
1:B:122:TYR:O	1:B:125:ARG:HD3	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:B:111:ASP:OD1	1:B:619:ARG:NH2[4_354]	2.09	0.11

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	611/644 (95%)	581 (95%)	30 (5%)	0	100	100
1	B	603/644 (94%)	573 (95%)	28 (5%)	2 (0%)	41	55
All	All	1214/1288 (94%)	1154 (95%)	58 (5%)	2 (0%)	47	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	63	LYS
1	B	540	GLU

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	546/566 (96%)	507 (93%)	39 (7%)	14	23
1	B	537/566 (95%)	511 (95%)	26 (5%)	25	41
All	All	1083/1132 (96%)	1018 (94%)	65 (6%)	19	31

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	9	ARG
1	A	25	ASP
1	A	57	LEU
1	A	64	LYS
1	A	90	ASN
1	A	108	LYS
1	A	134	CYS
1	A	163	VAL
1	A	169	GLU
1	A	175	SER
1	A	180	THR
1	A	239	ASN
1	A	257	LEU
1	A	274	ARG
1	A	314	ARG
1	A	320	ASN
1	A	334	ASN
1	A	404	GLU
1	A	419	LEU
1	A	434	LEU
1	A	444	LEU
1	A	470	ARG
1	A	504	LEU
1	A	514	ARG
1	A	515	PHE
1	A	517	THR

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Mol	Chain	Res	Type
1	A	518	LYS
1	A	526	LEU
1	A	538	ASN
1	A	542	LEU
1	A	544	ARG
1	A	546	GLU
1	A	550	ILE
1	A	561	VAL
1	A	563	GLU
1	A	567	LYS
1	A	585	ASP
1	A	625	ILE
1	B	3	LEU
1	B	25	ASP
1	B	57	LEU
1	B	108	LYS
1	B	134	CYS
1	B	169	GLU
1	B	202	LYS
1	B	203	GLN
1	B	208	ARG
1	B	249	MET
1	B	257	LEU
1	B	274	ARG
1	B	314	ARG
1	B	320	ASN
1	B	334	ASN
1	B	404	GLU
1	B	419	LEU
1	B	434	LEU
1	B	444	LEU
1	B	470	ARG
1	B	504	LEU
1	B	528	TYR
1	B	534	ARG
1	B	544	ARG
1	B	556	LYS
1	B	561	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	90	ASN
1	A	203	GLN
1	A	239	ASN
1	A	289	ASN
1	A	320	ASN
1	A	334	ASN
1	A	345	ASN
1	A	428	HIS
1	A	584	GLN
1	A	603	GLN
1	A	612	ASN
1	A	621	ASN
1	B	90	ASN
1	B	181	HIS
1	B	192	HIS
1	B	239	ASN
1	B	289	ASN
1	B	320	ASN
1	B	334	ASN
1	B	345	ASN
1	B	428	HIS
1	B	496	ASN
1	B	584	GLN
1	B	603	GLN
1	B	612	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

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	1002	2	26,32,32	1.57	4 (15%)	30,50,50	1.47	4 (13%)
3	DTP	B	1001	2	26,32,32	1.58	4 (15%)	30,50,50	1.95	6 (20%)

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	1002	2	-	8/18/34/34	0/3/3/3
3	DTP	B	1001	2	-	7/18/34/34	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	DTP	PG-O1G	5.20	1.67	1.50
3	B	1001	DTP	PG-O1G	4.49	1.65	1.50
3	B	1001	DTP	O4'-C1'	3.77	1.50	1.42
3	A	1002	DTP	PG-O2G	3.01	1.66	1.54
3	B	1001	DTP	PG-O2G	2.96	1.66	1.54
3	A	1002	DTP	O4'-C1'	2.63	1.48	1.42
3	B	1001	DTP	C6-C5	-2.16	1.35	1.43
3	A	1002	DTP	C2-N3	2.14	1.35	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	DTP	PA-O3A-PB	-5.88	112.66	132.83
3	B	1001	DTP	N3-C2-N1	-4.72	121.30	128.68
3	B	1001	DTP	PB-O3B-PG	-4.67	116.79	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	DTP	N3-C2-N1	-3.97	122.47	128.68
3	A	1002	DTP	PB-O3B-PG	-3.82	119.73	132.83
3	A	1002	DTP	PA-O3A-PB	-3.37	121.28	132.83
3	B	1001	DTP	C5-C6-N6	-2.43	116.66	120.35
3	B	1001	DTP	N6-C6-N1	2.26	123.26	118.57
3	B	1001	DTP	O4'-C4'-C5'	2.19	116.59	109.37
3	A	1002	DTP	O3G-PG-O3B	2.03	111.44	104.64

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	DTP	C5'-O5'-PA-O1A
3	B	1001	DTP	C5'-O5'-PA-O1A
3	B	1001	DTP	C5'-O5'-PA-O2A
3	B	1001	DTP	O4'-C4'-C5'-O5'
3	B	1001	DTP	C3'-C4'-C5'-O5'
3	A	1002	DTP	O4'-C4'-C5'-O5'
3	A	1002	DTP	C5'-O5'-PA-O3A
3	A	1002	DTP	PG-O3B-PB-O2B
3	A	1002	DTP	C5'-O5'-PA-O2A
3	A	1002	DTP	C3'-C4'-C5'-O5'
3	A	1002	DTP	PG-O3B-PB-O1B
3	B	1001	DTP	PA-O3A-PB-O2B
3	B	1001	DTP	C5'-O5'-PA-O3A
3	A	1002	DTP	PA-O3A-PB-O2B
3	B	1001	DTP	PG-O3B-PB-O2B

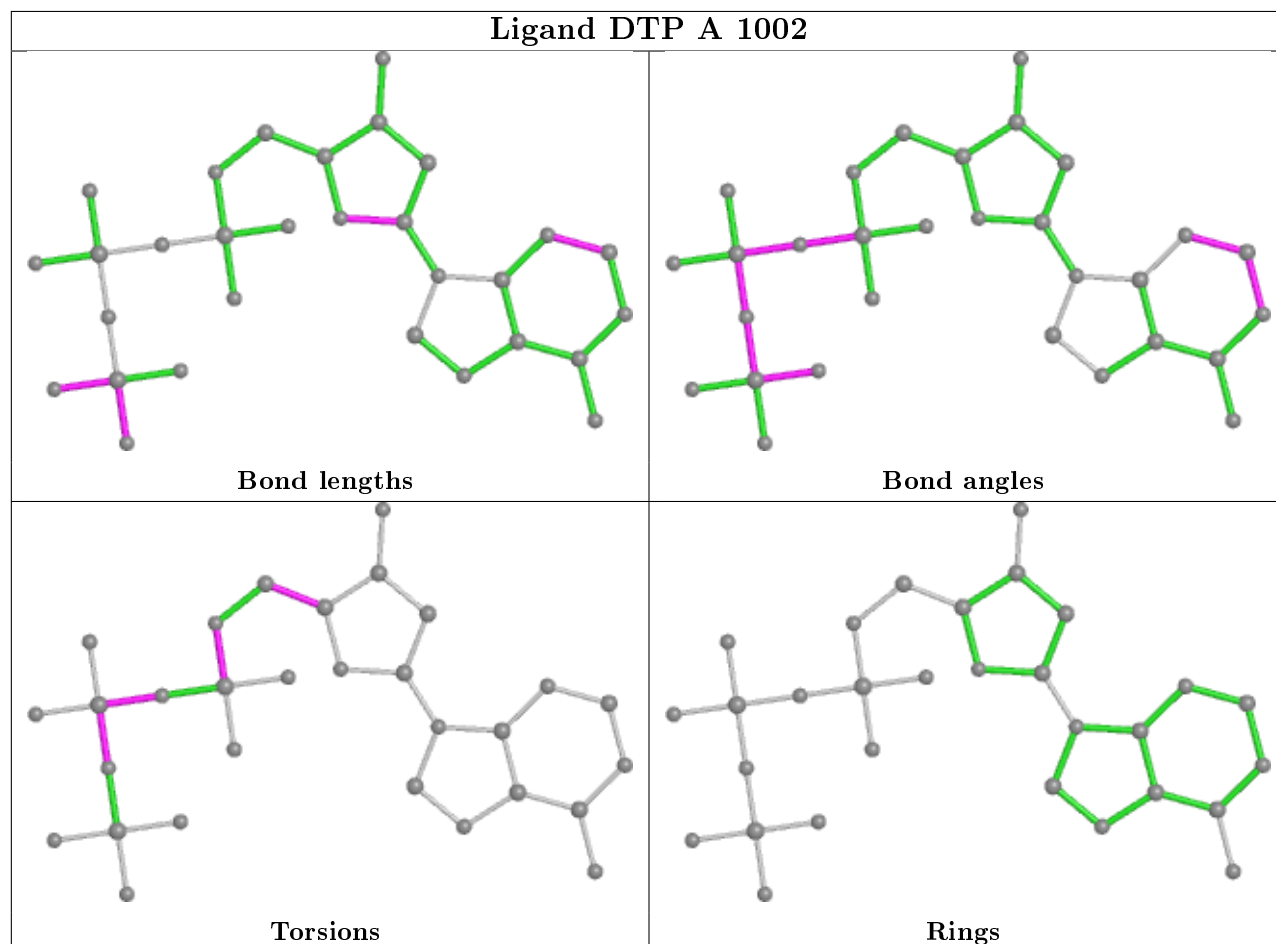
There are no ring outliers.

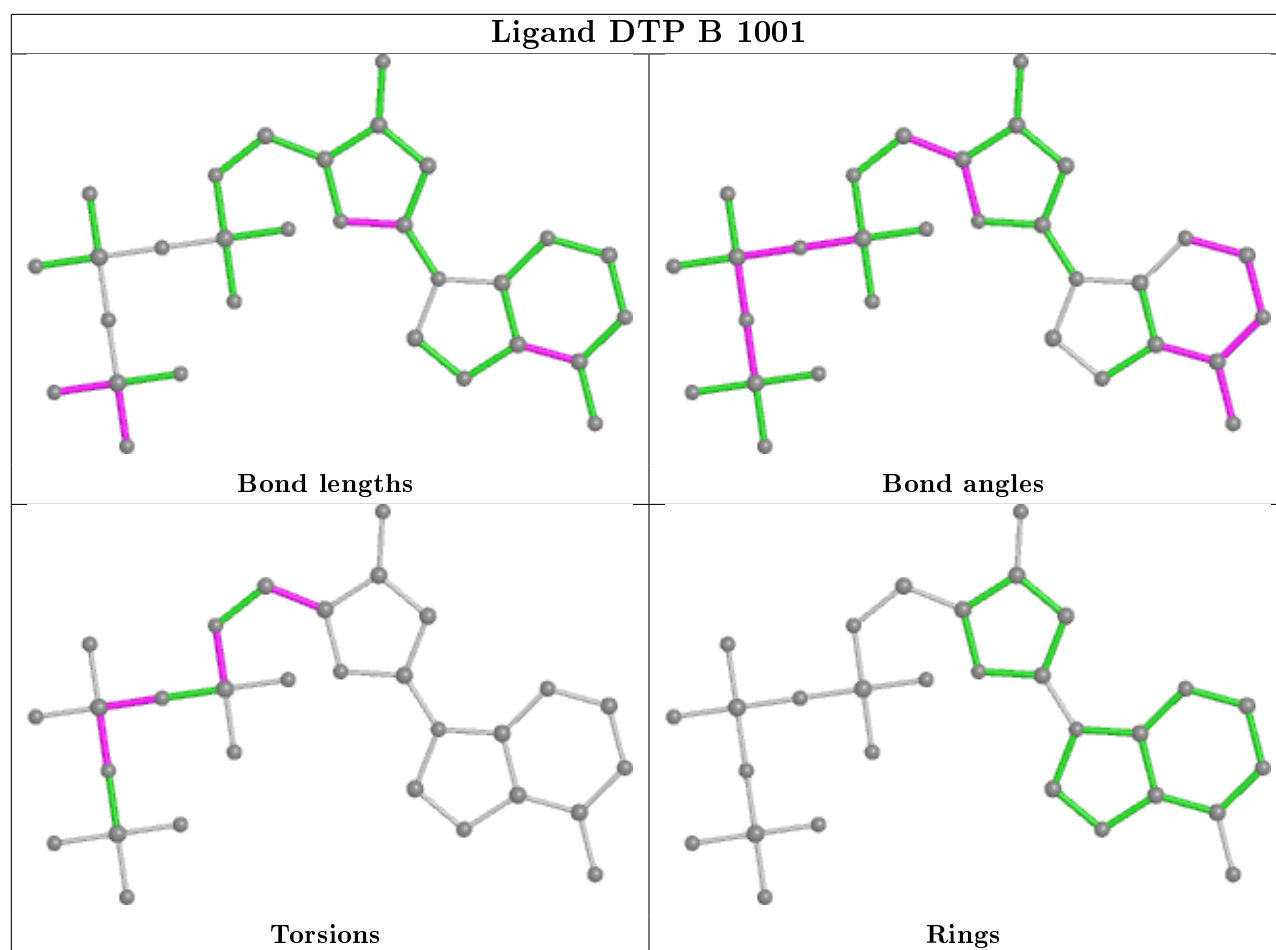
2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	DTP	6	0
3	B	1001	DTP	3	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, 95th 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	619/644 (96%)	-0.10	26 (4%) 36 35	27, 43, 74, 107	0
1	B	611/644 (94%)	-0.13	15 (2%) 57 55	28, 43, 70, 85	0
All	All	1230/1288 (95%)	-0.11	41 (3%) 46 45	27, 43, 72, 107	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	515	PHE	7.1
1	A	516	VAL	6.5
1	A	517	THR	5.4
1	A	518	LYS	4.0
1	A	65	ASN	3.8
1	A	178	ALA	3.5
1	A	519	GLU	3.5
1	A	104	ASP	3.4
1	A	231	GLU	3.4
1	A	33	ASP	3.4
1	B	65	ASN	3.2
1	A	524	GLU	3.2
1	A	526	LEU	3.1
1	B	48	VAL	3.1
1	B	45	ALA	3.0
1	B	540	GLU	2.9
1	B	179	GLY	2.8
1	A	525	PRO	2.8
1	A	111	ASP	2.8
1	A	66	GLU	2.6
1	B	559	PRO	2.6
1	B	209	GLY	2.6
1	A	9	ARG	2.5
1	A	34	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	32	LEU	2.5
1	A	32	LEU	2.5
1	A	346	ASN	2.4
1	B	313	HIS	2.3
1	A	471	GLU	2.2
1	B	514	ARG	2.2
1	A	483	VAL	2.2
1	A	453	ASP	2.2
1	A	52	VAL	2.1
1	A	551	GLU	2.1
1	B	63	LYS	2.1
1	B	82	LEU	2.1
1	A	102	LYS	2.1
1	A	230	LYS	2.1
1	B	177	VAL	2.0
1	B	547	LYS	2.0
1	B	33	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th 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.

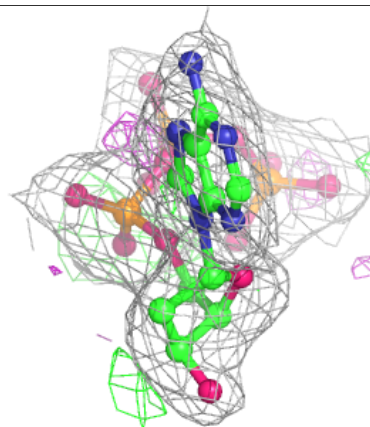
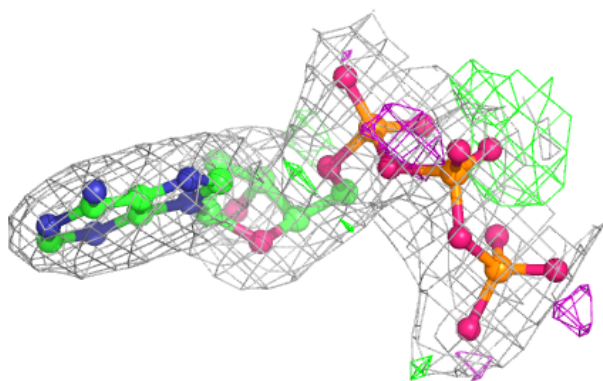
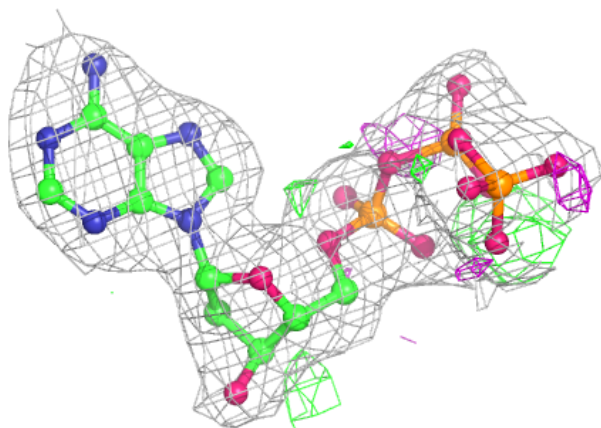
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	DTP	A	1002	30/30	0.92	0.12	32,37,67,69	0
3	DTP	B	1001	30/30	0.93	0.12	30,39,68,69	0
2	MG	B	1003	1/1	0.96	0.15	48,48,48,48	0
2	MG	A	1004	1/1	0.97	0.19	50,50,50,50	0

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.

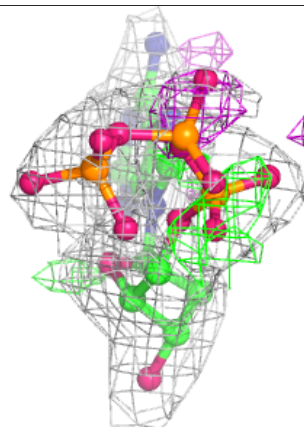
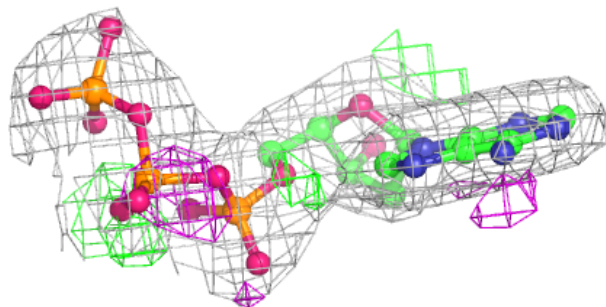
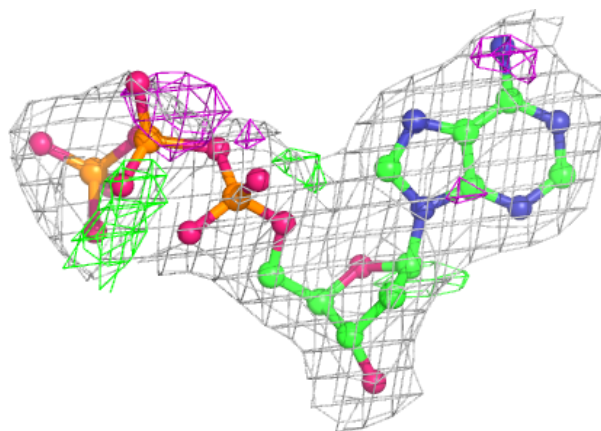
Electron density around DTP A 1002:

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



Electron density around DTP B 1001:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.