



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2024 – 05:11 AM EST

PDB ID : 3SI8
Title : Human DNA polymerase eta - DNA ternary complex with the 5'T of a CPD in the active site (TT2)
Authors : Biertumpfel, C.; Zhao, Y.; Kondo, Y.; Ramon-Maiques, S.; Gregory, M.; Lee, J.Y.; Masutani, C.; Lehmann, A.R.; Hanaoka, F.; Yang, W.
Deposited on : 2011-06-17
Resolution : 2.15 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 types of validation reports are described at

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

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 : 2.36
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) : 2.36

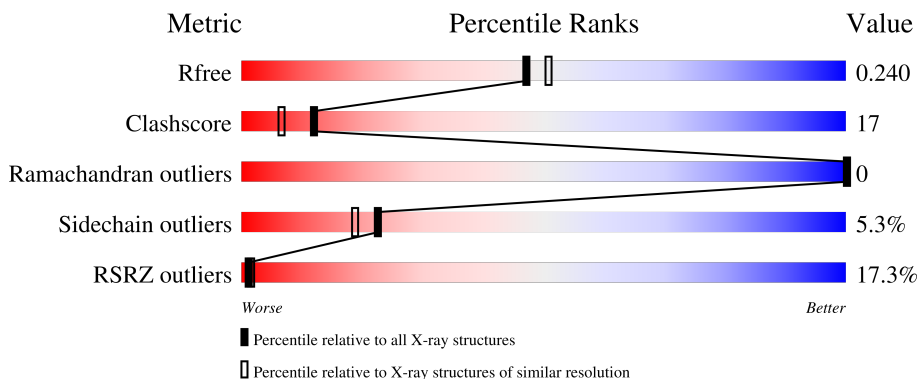
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	435	
2	T	12	
3	P	9	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	434	-	-	-	X
5	GOL	A	435	-	-	-	X
5	GOL	A	436	-	-	-	X
5	GOL	A	441	-	-	X	X
6	3D1	A	438	-	-	-	X

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 3972 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 DNA polymerase eta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	422	3309	2077	596	613	23	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q9Y253
A	-1	PRO	-	expression tag	UNP Q9Y253
A	0	HIS	-	expression tag	UNP Q9Y253

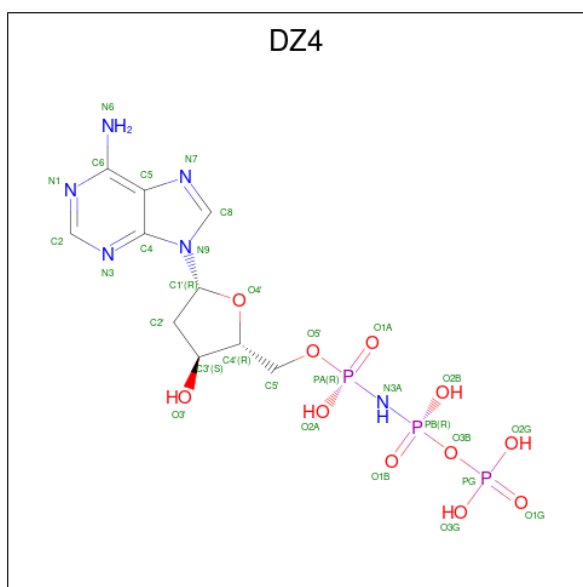
- Molecule 2 is a DNA chain called DNA (5'-D(*TP*A*AP*CP*(TTD)P*AP*TP*GP*AP*CP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	T	10	221	107	40	64	10	0	0	0

- Molecule 3 is a DNA chain called DNA (5'-D(*TP*GP*CP*GP*TP*CP*AP*TP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	P	9	181	88	32	53	8	0	0	0

- Molecule 4 is 2'-deoxy-5'-O-[(R)-hydroxy{[(R)-hydroxy(phosphonooxy)phosphoryl]amino}phosphoryl]adenosine (three-letter code: DZ4) (formula: C₁₀H₁₇N₆O₁₁P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	30	10	6	11	3	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



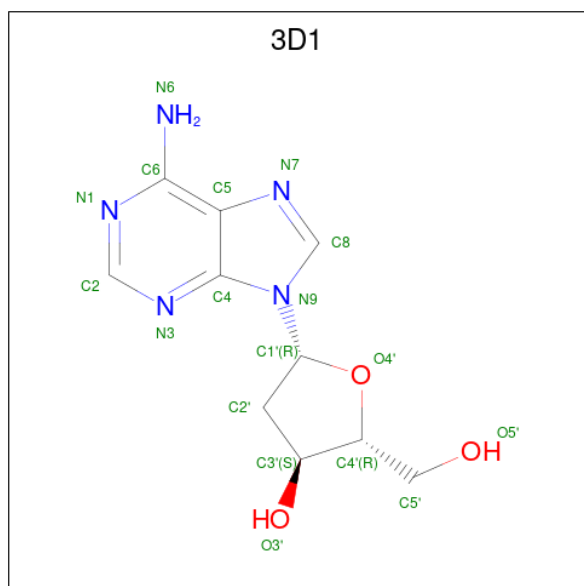
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	6	3	3	0	0
5	A	1	6	3	3	0	0
5	A	1	6	3	3	0	0

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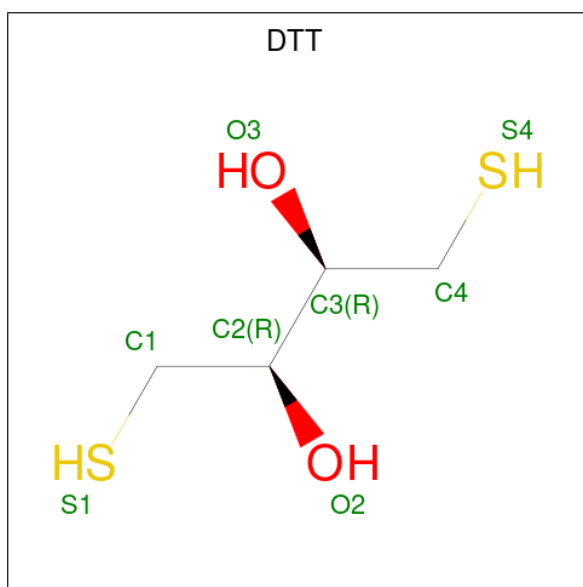
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is (2R,3S,5R)-5-(6-amino-9H-purin-9-yl)-tetrahydro-2-(hydroxymethyl)furan-3-ol (three-letter code: 3D1) (formula: C₁₀H₁₃N₅O₃).



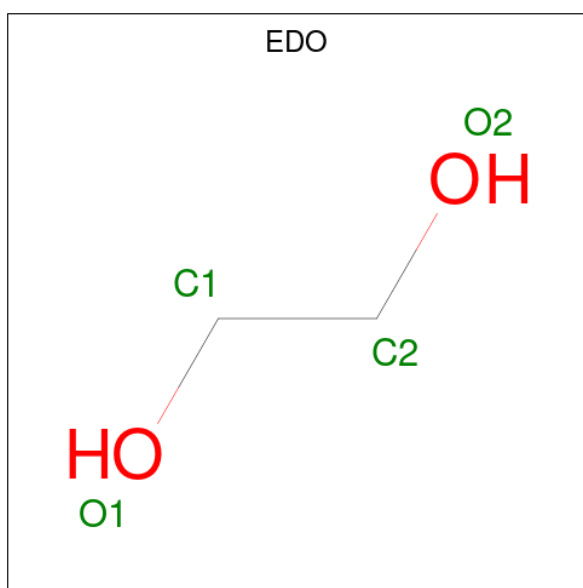
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			18	10	5	3		

- Molecule 7 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: C₄H₁₀O₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
7	A	1	Total	C	O	S	0	0
			8	4	2	2		
7	A	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
8	A	1	Total	C	O		0	0
			4	2	2			
8	A	1	Total	C	O		0	0
			4	2	2			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 10 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total Co 1 1	0	0

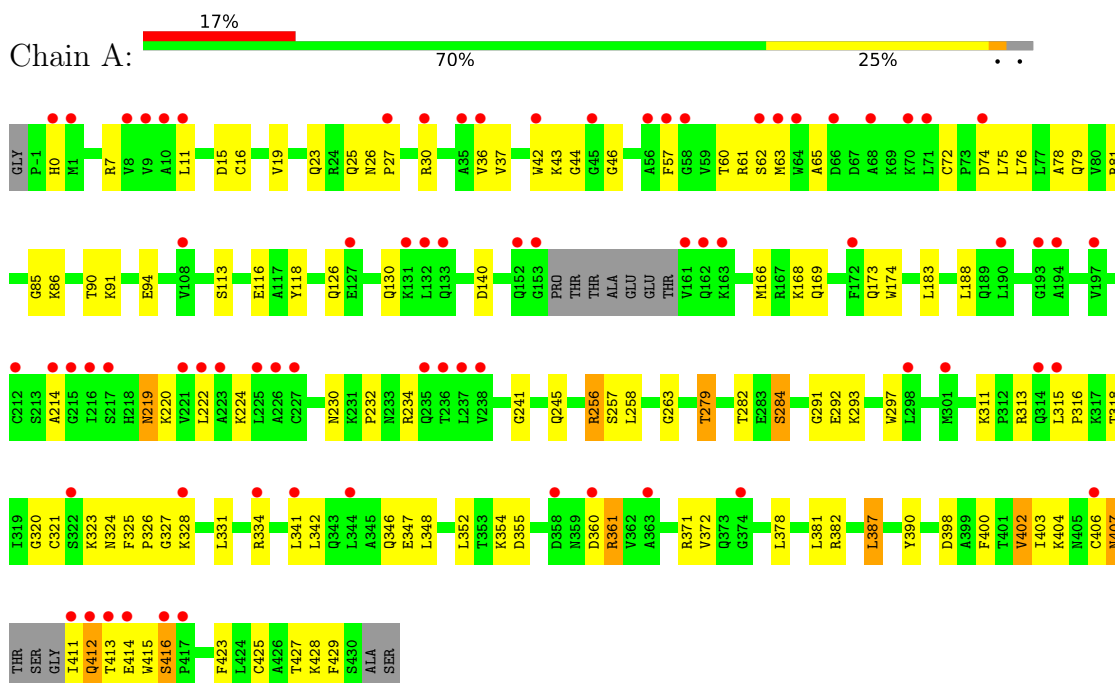
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	112	Total O 112 112	0	0
11	T	7	Total O 7 7	0	0
11	P	7	Total O 7 7	0	0

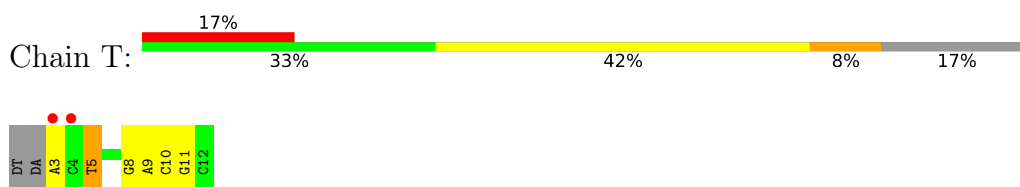
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

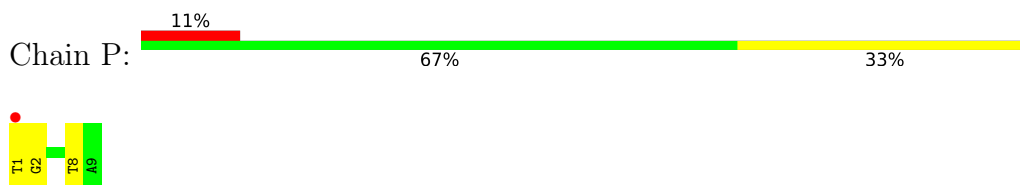
- Molecule 1: DNA polymerase eta



- Molecule 2: DNA (5'-D(*TP*A*AP*CP*(TTD)P*AP*TP*GP*AP*CP*GP*C)-3')



- Molecule 3: DNA (5'-D(*TP*GP*CP*GP*TP*CP*AP*TP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.24Å 80.26Å 139.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.28 – 2.15 26.28 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.6 (26.28-2.15) 98.7 (26.28-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.15Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.258 0.229 , 0.240	Depositor DCC
R_{free} test set	2896 reflections (7.65%)	wwPDB-VP
Wilson B-factor (Å ²)	49.4	Xtrriage
Anisotropy	0.632	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 67.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3972	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% 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: GOL, DTT, 3D1, EDO, MG, DZ4, TTD, CO

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	0.37	0/3366	0.63	0/4542
2	T	0.40	0/202	0.84	0/307
3	P	0.36	0/202	0.70	0/310
All	All	0.37	0/3770	0.65	0/5159

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3309	0	3338	124	0
2	T	221	0	126	12	0
3	P	181	0	103	2	0
4	A	30	0	12	0	0
5	A	48	0	62	13	0
6	A	18	0	12	3	0
7	A	16	0	20	5	0
8	A	20	0	30	1	0
9	A	2	0	0	0	0
10	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	112	0	0	11	0
11	P	7	0	0	0	0
11	T	7	0	0	1	0
All	All	3972	0	3703	130	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 17.

All (130) 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:27:PRO:HA	1:A:30:ARG:HE	1.19	1.03
1:A:25:GLN:HE22	1:A:91:LYS:HD2	1.33	0.90
1:A:284:SER:HB3	5:A:435:GOL:H31	1.53	0.89
1:A:168:LYS:HZ3	5:A:441:GOL:H31	1.40	0.86
1:A:168:LYS:NZ	5:A:441:GOL:H31	1.90	0.84
1:A:292:GLU:H	7:A:443:DTT:H12	1.43	0.83
1:A:27:PRO:HG3	1:A:30:ARG:HH21	1.46	0.79
1:A:326:PRO:HB2	2:T:3:DA:H3'	1.65	0.79
1:A:25:GLN:NE2	1:A:91:LYS:HD2	1.97	0.78
1:A:168:LYS:HZ1	5:A:441:GOL:H11	1.48	0.78
1:A:342:LEU:O	1:A:346:GLN:HG3	1.85	0.77
1:A:27:PRO:HA	1:A:30:ARG:NE	2.00	0.76
1:A:27:PRO:HG3	1:A:30:ARG:NH2	2.02	0.74
1:A:326:PRO:HB2	2:T:3:DA:C3'	2.18	0.73
1:A:241:GLY:HA2	5:A:434:GOL:H11	1.70	0.73
1:A:60:THR:O	1:A:63:MET:HG2	1.89	0.73
1:A:354:LYS:HE2	11:A:550:HOH:O	1.89	0.72
1:A:361:ARG:HD3	1:A:429:PHE:CD1	2.25	0.71
1:A:219:ASN:ND2	1:A:222:LEU:H	1.89	0.70
1:A:323:LYS:HE3	11:A:482:HOH:O	1.91	0.70
1:A:292:GLU:N	7:A:443:DTT:H12	2.07	0.70
1:A:334:ARG:HH22	1:A:404:LYS:CE	2.05	0.69
1:A:90:THR:O	1:A:94:GLU:HG3	1.94	0.68
1:A:19:VAL:O	1:A:23:GLN:HG3	1.94	0.67
1:A:25:GLN:HE22	1:A:91:LYS:CD	2.05	0.67
1:A:334:ARG:HH22	1:A:404:LYS:NZ	1.94	0.65
1:A:326:PRO:HB2	2:T:3:DA:C2'	2.27	0.65
1:A:74:ASP:O	1:A:76:LEU:HD12	1.97	0.65
1:A:323:LYS:HG2	1:A:325:PHE:CZ	2.34	0.62
1:A:352:LEU:HB3	1:A:390:TYR:CE1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ARG:O	1:A:62:SER:HB3	2.00	0.61
1:A:113:SER:OG	1:A:116:GLU:HG2	2.01	0.61
1:A:284:SER:HB3	5:A:435:GOL:C3	2.29	0.61
2:T:5:TTD:H2'	2:T:5:TTD:O5R	2.01	0.60
1:A:86:LYS:HB2	11:T:86:HOH:O	2.03	0.58
5:A:442:GOL:H11	8:A:447:EDO:O1	2.03	0.57
1:A:324:ASN:OD1	1:A:371:ARG:NH2	2.35	0.57
1:A:341:LEU:HD11	1:A:403:ILE:HD11	1.87	0.56
1:A:85:GLY:O	1:A:323:LYS:NZ	2.38	0.56
1:A:297:TRP:CD1	6:A:438:3D1:H2'1	2.41	0.55
1:A:411:ILE:HG13	1:A:413:THR:HG22	1.87	0.55
1:A:126:GLN:NE2	1:A:126:GLN:HA	2.21	0.55
1:A:360:ASP:O	1:A:360:ASP:OD1	2.24	0.55
1:A:36:VAL:HA	1:A:78:ALA:O	2.06	0.55
1:A:15:ASP:O	1:A:16:CYS:C	2.45	0.54
1:A:411:ILE:O	1:A:412:GLN:HB2	2.06	0.54
1:A:230:ASN:O	1:A:234:ARG:HB2	2.08	0.54
1:A:311:LYS:HE3	11:A:485:HOH:O	2.07	0.53
1:A:313:ARG:NH2	2:T:9:DA:OP1	2.42	0.53
1:A:371:ARG:NH1	1:A:378:LEU:O	2.41	0.53
1:A:411:ILE:N	1:A:414:GLU:O	2.42	0.53
1:A:257:SER:N	3:P:8:DT:OP1	2.42	0.53
1:A:37:VAL:HA	1:A:46:GLY:O	2.09	0.52
1:A:320:GLY:HA2	1:A:348:LEU:HD11	1.90	0.52
2:T:10:DC:H2''	2:T:11:DG:C8	2.45	0.52
1:A:174:TRP:HZ3	7:A:444:DTT:S4	2.33	0.52
1:A:11:LEU:HD22	1:A:224:LYS:HA	1.90	0.51
1:A:355:ASP:OD2	1:A:361:ARG:HD2	2.10	0.51
1:A:37:VAL:HG23	1:A:79:GLN:HG3	1.91	0.51
1:A:219:ASN:HD21	1:A:222:LEU:H	1.58	0.51
1:A:411:ILE:O	1:A:412:GLN:CB	2.59	0.51
1:A:279:THR:HG22	11:A:505:HOH:O	2.11	0.51
1:A:168:LYS:HZ1	5:A:441:GOL:H31	1.74	0.50
1:A:25:GLN:OE1	1:A:91:LYS:HD2	2.12	0.50
1:A:327:GLY:HA3	2:T:3:DA:H5'	1.94	0.50
1:A:423:PHE:CE1	1:A:425:CYS:HB2	2.46	0.50
1:A:423:PHE:CZ	1:A:425:CYS:HB2	2.47	0.50
1:A:293:LYS:HE3	6:A:438:3D1:O4'	2.10	0.50
1:A:11:LEU:CD2	1:A:224:LYS:HA	2.42	0.50
1:A:387:LEU:C	1:A:387:LEU:HD12	2.33	0.49
1:A:411:ILE:CG2	1:A:416:SER:OG	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:TRP:O	1:A:43:LYS:HB2	2.12	0.49
1:A:398:ASP:O	1:A:402:VAL:HG13	2.11	0.49
1:A:25:GLN:CD	1:A:91:LYS:HD2	2.32	0.49
1:A:140:ASP:OD2	5:A:441:GOL:O3	2.30	0.49
1:A:130:GLN:NE2	11:A:528:HOH:O	2.45	0.48
1:A:25:GLN:HE22	1:A:91:LYS:CG	2.27	0.48
1:A:174:TRP:HZ3	7:A:444:DTT:HS2	1.58	0.48
1:A:297:TRP:HD1	6:A:438:3D1:H2'1	1.77	0.48
1:A:411:ILE:HG13	1:A:411:ILE:O	2.13	0.47
1:A:166:MET:HA	1:A:166:MET:HE2	1.96	0.47
1:A:407:ASN:N	11:A:500:HOH:O	2.43	0.47
2:T:5:TTD:H2'	2:T:5:TTD:O4R	2.14	0.46
1:A:7:ARG:HD3	11:A:465:HOH:O	2.15	0.46
1:A:72:CYS:O	1:A:75:LEU:HB2	2.14	0.46
1:A:334:ARG:HH22	1:A:404:LYS:HE3	1.77	0.46
1:A:361:ARG:HD3	1:A:429:PHE:HD1	1.77	0.46
1:A:11:LEU:O	1:A:214:ALA:HA	2.16	0.45
1:A:318:THR:HG22	1:A:427:THR:OG1	2.15	0.45
1:A:355:ASP:OD2	1:A:361:ARG:CD	2.65	0.45
1:A:355:ASP:OD2	1:A:361:ARG:NE	2.50	0.45
1:A:328:LYS:NZ	11:A:546:HOH:O	2.50	0.45
1:A:245:GLN:HB2	11:A:456:HOH:O	2.17	0.45
1:A:428:LYS:HE2	1:A:428:LYS:HB3	1.74	0.45
2:T:5:TTD:O4R	2:T:5:TTD:H1'	2.16	0.45
1:A:315:LEU:HB2	11:A:481:HOH:O	2.17	0.45
1:A:282:THR:HB	5:A:435:GOL:H2	1.99	0.44
1:A:44:GLY:HA3	1:A:65:ALA:HB3	2.00	0.44
1:A:11:LEU:HD21	5:A:437:GOL:H12	1.99	0.44
1:A:11:LEU:HD13	1:A:118:TYR:CE2	2.53	0.44
1:A:37:VAL:HG11	1:A:65:ALA:HB2	2.00	0.44
1:A:258:LEU:O	1:A:263:GLY:HA3	2.18	0.44
1:A:57:PHE:CB	1:A:72:CYS:HB2	2.48	0.43
1:A:118:TYR:CD2	1:A:220:LYS:HG2	2.53	0.43
1:A:355:ASP:CG	1:A:361:ARG:HE	2.20	0.43
1:A:256:ARG:HE	1:A:257:SER:HB3	1.84	0.43
1:A:411:ILE:HG23	1:A:416:SER:HB3	2.01	0.43
1:A:406:CYS:O	1:A:407:ASN:CB	2.66	0.43
1:A:404:LYS:HE2	11:A:514:HOH:O	2.18	0.43
1:A:126:GLN:HA	1:A:126:GLN:HE21	1.84	0.42
1:A:26:ASN:OD1	1:A:26:ASN:C	2.57	0.42
1:A:407:ASN:N	1:A:407:ASN:OD1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:1:DT:H2'	3:P:2:DG:C8	2.54	0.42
1:A:168:LYS:HZ1	5:A:441:GOL:C1	2.26	0.42
1:A:326:PRO:CB	2:T:3:DA:H3'	2.45	0.42
1:A:168:LYS:NZ	5:A:441:GOL:C3	2.74	0.42
1:A:74:ASP:O	1:A:76:LEU:CD1	2.68	0.42
1:A:291:GLY:HA2	7:A:443:DTT:H12	2.01	0.41
1:A:326:PRO:HB2	2:T:3:DA:H2'	1.98	0.41
1:A:334:ARG:HG2	1:A:400:PHE:HZ	1.84	0.41
1:A:86:LYS:HE3	1:A:321:CYS:HB2	2.03	0.41
1:A:381:LEU:C	1:A:381:LEU:HD12	2.41	0.41
1:A:86:LYS:HD3	1:A:347:GLU:OE1	2.20	0.41
1:A:316:PRO:HA	2:T:8:DG:OP1	2.21	0.41
1:A:219:ASN:C	1:A:219:ASN:HD22	2.23	0.40
1:A:411:ILE:HG13	1:A:413:THR:CG2	2.51	0.40
1:A:169:GLN:O	1:A:173:GLN:HG3	2.21	0.40
1:A:406:CYS:O	1:A:407:ASN:HB2	2.21	0.40
1:A:318:THR:HG22	1:A:427:THR:HG1	1.87	0.40
1:A:334:ARG:HH11	1:A:334:ARG:HG3	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	416/435 (96%)	406 (98%)	10 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	360/372 (97%)	341 (95%)	19 (5%)	22	19

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	81	ARG
1	A	183	LEU
1	A	188	LEU
1	A	219	ASN
1	A	232	PRO
1	A	256	ARG
1	A	279	THR
1	A	284	SER
1	A	331	LEU
1	A	361	ARG
1	A	372	VAL
1	A	382	ARG
1	A	387	LEU
1	A	402	VAL
1	A	407	ASN
1	A	412	GLN
1	A	415	TRP
1	A	416	SER

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

Mol	Chain	Res	Type
1	A	126	GLN
1	A	169	GLN
1	A	219	ASN
1	A	287	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TTD	T	5	2	42,45,46	1.33	4 (9%)	62,74,77	3.32	21 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TTD	T	5	2	-	11/22/109/110	0/5/6/6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	5	TTD	C1R-N1T	4.36	1.51	1.45
2	T	5	TTD	C5T-C6T	3.83	1.59	1.55
2	T	5	TTD	C5-C4	-3.79	1.44	1.51
2	T	5	TTD	C5T-C4T	-3.18	1.45	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	5	TTD	C5T-C4T-N3T	11.83	126.37	116.06
2	T	5	TTD	C5-C6-N1	8.63	127.71	115.61
2	T	5	TTD	O4R-C1R-N1T	6.94	116.88	108.65
2	T	5	TTD	C5-C4-N3	6.84	122.02	116.06
2	T	5	TTD	C5T-C6T-N1T	-6.78	106.12	115.61
2	T	5	TTD	O4T-C4T-C5T	-6.66	117.56	122.88
2	T	5	TTD	C4T-N3T-C2T	-6.06	117.35	126.67
2	T	5	TTD	C5T-C6T-C6	-5.47	80.31	89.28
2	T	5	TTD	C5T-C5-C6	-5.02	82.13	88.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	5	TTD	C5M-C5T-C4T	4.50	115.98	108.22
2	T	5	TTD	C5T-C5-C4	4.46	127.90	113.21
2	T	5	TTD	O4-C4-C5	-4.45	119.32	122.88
2	T	5	TTD	C5-C5T-C6T	4.37	93.82	88.38
2	T	5	TTD	C5-C6-C6T	4.07	95.97	89.28
2	T	5	TTD	C5-C5T-C4T	-3.62	101.27	113.21
2	T	5	TTD	N3-C2-N1	3.54	120.37	116.69
2	T	5	TTD	C6T-C6-N1	-3.53	104.08	118.20
2	T	5	TTD	N3T-C2T-N1T	3.41	120.23	116.69
2	T	5	TTD	O4T-C4T-N3T	-2.78	116.07	120.50
2	T	5	TTD	O2-C2-N1	-2.65	119.38	123.49
2	T	5	TTD	C6-C5-C4	-2.18	108.28	114.50

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	5	TTD	C5R-O5R-PB-O5P
2	T	5	TTD	C5R-O5R-PB-O4P
2	T	5	TTD	C4'-C5R-O5R-PB
2	T	5	TTD	C2'-C1'-N1-C6
2	T	5	TTD	C5R-O5R-PB-O3R
2	T	5	TTD	C2'-C1'-N1-C2
2	T	5	TTD	O4'-C1'-N1-C6
2	T	5	TTD	O4'-C1'-N1-C2
2	T	5	TTD	O4'-C4R-C5'-O5'
2	T	5	TTD	C3R-C4R-C5'-O5'
2	T	5	TTD	C2R-C1R-N1T-C2T

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	5	TTD	3	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 3 are monoatomic - leaving 17 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
5	GOL	A	442	-	5,5,5	1.33	1 (20%)	5,5,5	0.67	0
5	GOL	A	439	-	5,5,5	0.33	0	5,5,5	0.32	0
4	DZ4	A	433	9	29,32,32	4.86	12 (41%)	33,50,50	1.99	10 (30%)
5	GOL	A	437	-	5,5,5	0.24	0	5,5,5	0.27	0
5	GOL	A	441	-	5,5,5	0.23	0	5,5,5	0.28	0
5	GOL	A	436	-	5,5,5	0.33	0	5,5,5	0.30	0
7	DTT	A	444	-	7,7,7	1.20	1 (14%)	4,8,8	1.46	1 (25%)
8	EDO	A	449	-	3,3,3	0.44	0	2,2,2	0.33	0
8	EDO	A	447	-	3,3,3	0.44	0	2,2,2	0.39	0
8	EDO	A	445	-	3,3,3	0.46	0	2,2,2	0.35	0
8	EDO	A	448	-	3,3,3	0.63	0	2,2,2	0.15	0
6	3D1	A	438	-	18,20,20	1.72	3 (16%)	17,29,29	2.23	6 (35%)
5	GOL	A	434	-	5,5,5	0.28	0	5,5,5	0.29	0
5	GOL	A	440	-	5,5,5	1.45	1 (20%)	5,5,5	0.78	0
7	DTT	A	443	-	7,7,7	1.56	2 (28%)	4,8,8	1.37	1 (25%)
5	GOL	A	435	-	5,5,5	0.37	0	5,5,5	0.18	0
8	EDO	A	446	-	3,3,3	0.44	0	2,2,2	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	442	-	-	0/4/4/4	-
5	GOL	A	439	-	-	0/4/4/4	-
4	DZ4	A	433	9	-	5/15/34/34	0/3/3/3
5	GOL	A	437	-	-	0/4/4/4	-
5	GOL	A	441	-	-	0/4/4/4	-
5	GOL	A	436	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	DTT	A	444	-	-	0/8/8/8	-
8	EDO	A	449	-	-	0/1/1/1	-
8	EDO	A	447	-	-	1/1/1/1	-
8	EDO	A	445	-	-	1/1/1/1	-
8	EDO	A	448	-	-	1/1/1/1	-
6	3D1	A	438	-	-	2/2/18/18	0/3/3/3
5	GOL	A	434	-	-	0/4/4/4	-
5	GOL	A	440	-	-	0/4/4/4	-
7	DTT	A	443	-	-	0/8/8/8	-
5	GOL	A	435	-	-	0/4/4/4	-
8	EDO	A	446	-	-	0/1/1/1	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	433	DZ4	PB-O1B	-13.01	1.25	1.46
4	A	433	DZ4	PA-O1A	-11.99	1.27	1.46
4	A	433	DZ4	PB-O2B	-11.63	1.25	1.56
4	A	433	DZ4	PA-O2A	-6.92	1.38	1.56
4	A	433	DZ4	PG-O1G	-5.77	1.31	1.50
4	A	433	DZ4	PG-O2G	-5.52	1.33	1.54
4	A	433	DZ4	O3'-C3'	-5.37	1.32	1.43
4	A	433	DZ4	PB-O3B	-5.19	1.52	1.59
4	A	433	DZ4	PG-O3G	-5.06	1.35	1.54
6	A	438	3D1	O3'-C3'	-4.68	1.33	1.43
4	A	433	DZ4	O4'-C1'	-3.42	1.34	1.42
6	A	438	3D1	O4'-C1'	-3.40	1.34	1.42
6	A	438	3D1	O4'-C4'	-3.18	1.37	1.45
4	A	433	DZ4	O4'-C4'	-3.10	1.38	1.45
5	A	440	GOL	O2-C2	-3.03	1.34	1.43
5	A	442	GOL	O2-C2	-2.94	1.34	1.43
7	A	443	DTT	O3-C3	2.59	1.48	1.43
7	A	443	DTT	O2-C2	2.55	1.48	1.43
7	A	444	DTT	O3-C3	2.26	1.48	1.43
4	A	433	DZ4	C8-N7	-2.13	1.30	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	438	3D1	N3-C2-N1	-5.07	120.76	128.68
4	A	433	DZ4	O2A-PA-O1A	4.74	119.86	109.92
4	A	433	DZ4	N3-C2-N1	-4.63	121.44	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	438	3D1	O4'-C4'-C5'	3.99	117.84	109.21
4	A	433	DZ4	O1B-PB-N3A	-3.83	106.14	111.77
4	A	433	DZ4	O5'-C5'-C4'	3.10	119.65	108.99
4	A	433	DZ4	C2'-C1'-N9	-2.74	107.95	114.27
4	A	433	DZ4	O4'-C4'-C3'	2.65	111.86	105.67
4	A	433	DZ4	O3'-C3'-C2'	2.47	119.72	110.90
6	A	438	3D1	O4'-C4'-C3'	2.36	111.18	105.67
4	A	433	DZ4	C3'-C2'-C1'	2.30	108.30	102.54
6	A	438	3D1	C2-N1-C6	2.24	122.59	118.75
7	A	444	DTT	C3-C4-S4	-2.18	108.14	114.47
4	A	433	DZ4	C2-N1-C6	2.07	122.29	118.75
6	A	438	3D1	O5'-C5'-C4'	2.06	118.37	111.29
6	A	438	3D1	C3'-C2'-C1'	2.06	107.69	102.54
7	A	443	DTT	C3-C4-S4	-2.04	108.52	114.47
4	A	433	DZ4	O2A-PA-O5'	-2.01	101.30	106.75

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	433	DZ4	PB-N3A-PA-O1A
6	A	438	3D1	O4'-C4'-C5'-O5'
6	A	438	3D1	C3'-C4'-C5'-O5'
8	A	448	EDO	O1-C1-C2-O2
8	A	447	EDO	O1-C1-C2-O2
4	A	433	DZ4	PB-O3B-PG-O1G
8	A	445	EDO	O1-C1-C2-O2
4	A	433	DZ4	PB-N3A-PA-O5'
4	A	433	DZ4	PB-O3B-PG-O2G
4	A	433	DZ4	PB-O3B-PG-O3G

There are no ring outliers.

9 monomers are involved in 21 short contacts:

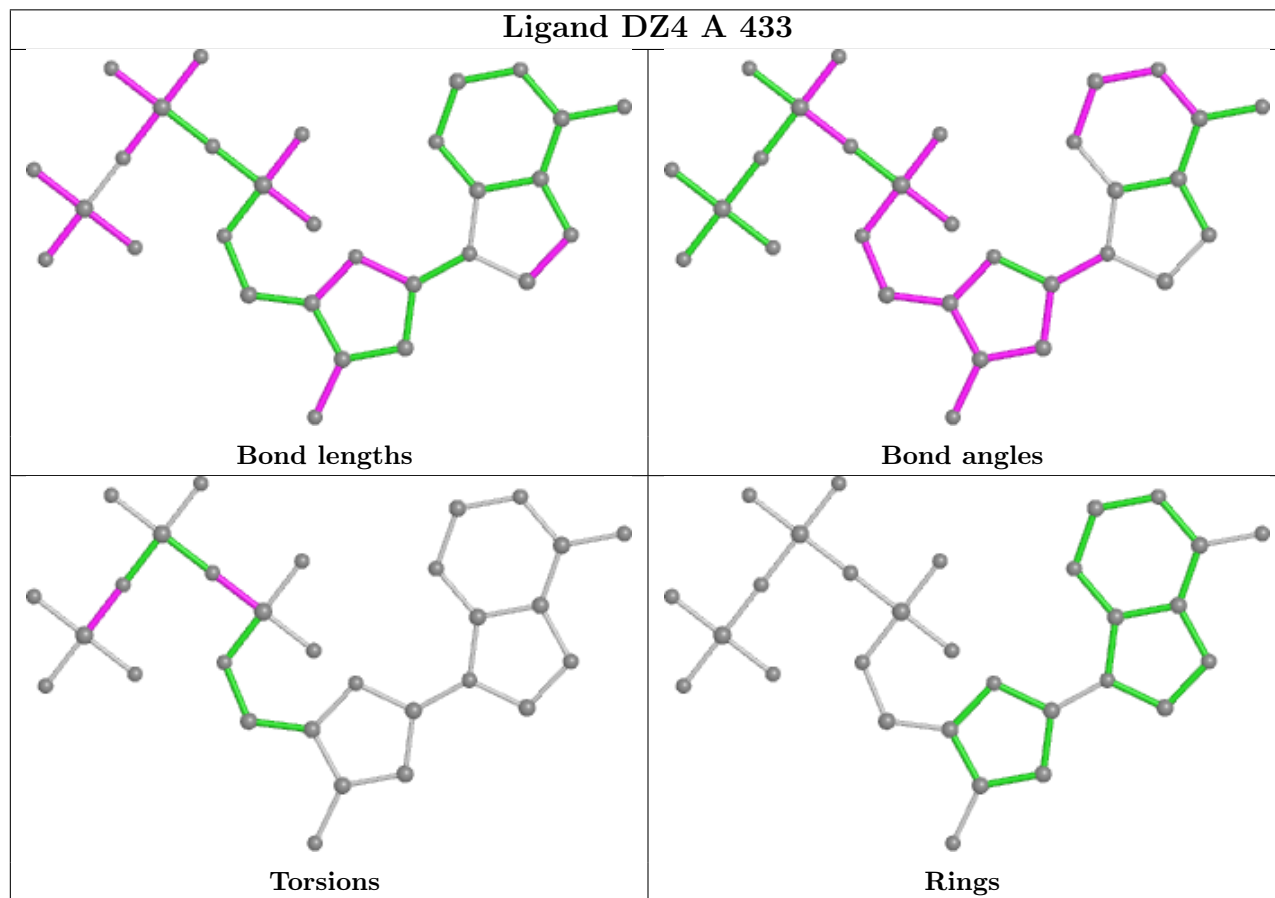
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	442	GOL	1	0
5	A	437	GOL	1	0
5	A	441	GOL	7	0
7	A	444	DTT	2	0
8	A	447	EDO	1	0
6	A	438	3D1	3	0

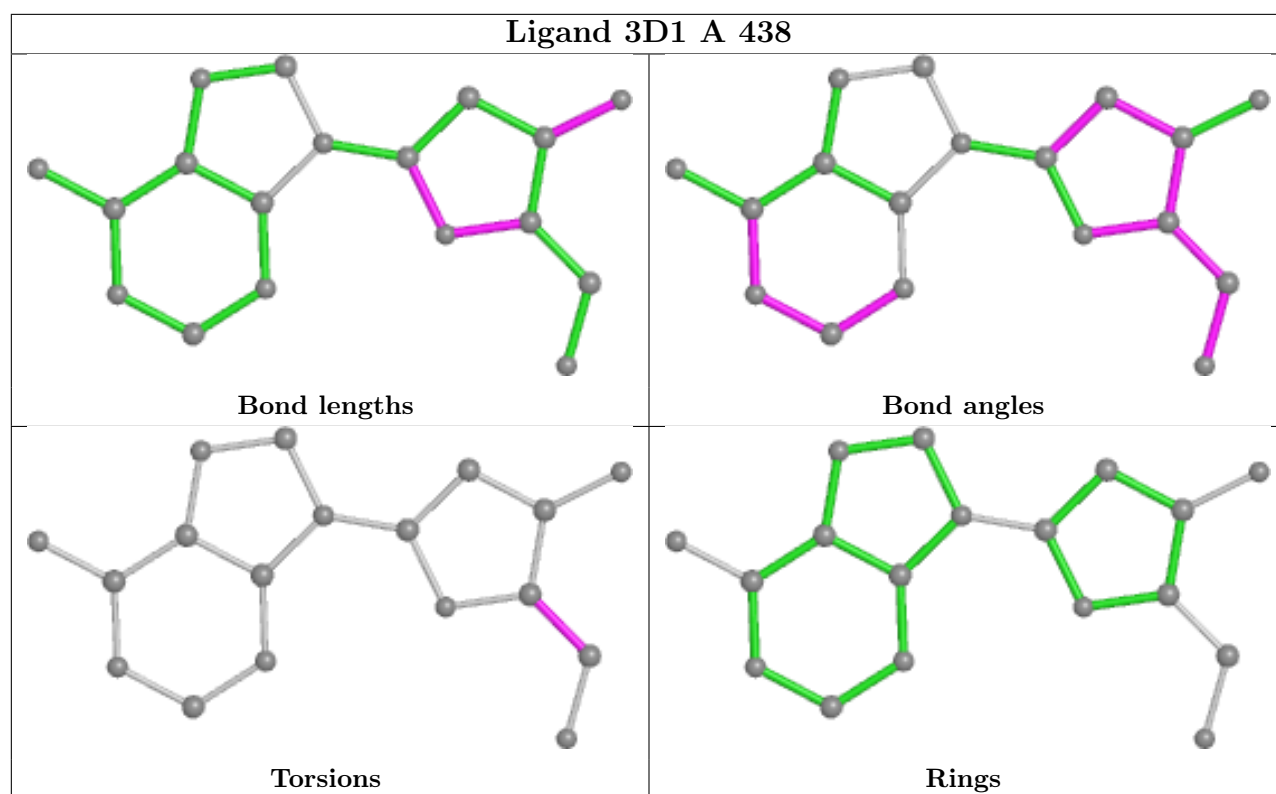
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	434	GOL	1	0
7	A	443	DTT	3	0
5	A	435	GOL	3	0

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	422/435 (97%)	0.91	73 (17%) 1 1	40, 60, 101, 111	0
2	T	9/12 (75%)	1.55	2 (22%) 0 0	65, 75, 127, 132	0
3	P	9/9 (100%)	0.22	1 (11%) 5 7	51, 60, 92, 116	0
All	All	440/456 (96%)	0.91	76 (17%) 1 1	40, 61, 102, 132	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	T	3	DA	7.6
1	A	161	VAL	7.3
1	A	42	TRP	6.5
1	A	216	ILE	5.4
1	A	153	GLY	5.4
1	A	315	LEU	4.8
1	A	190	LEU	4.7
1	A	133	GLN	4.4
1	A	132	LEU	4.3
1	A	217	SER	4.3
1	A	152	GLN	4.3
2	T	4	DC	4.2
1	A	71	LEU	4.2
1	A	328	LYS	4.1
1	A	108	VAL	4.0
1	A	417	PRO	4.0
1	A	413	THR	4.0
1	A	222	LEU	3.8
1	A	45	GLY	3.8
1	A	214	ALA	3.7
1	A	162	GLN	3.7
1	A	62	SER	3.7
1	A	411	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	412	GLN	3.6
1	A	74	ASP	3.5
1	A	9	VAL	3.4
1	A	238	VAL	3.4
1	A	237	LEU	3.3
1	A	68	ALA	3.3
1	A	223	ALA	3.2
3	P	1	DT	3.2
1	A	374	GLY	3.2
1	A	58	GLY	3.2
1	A	314	GLN	3.2
1	A	197	VAL	3.1
1	A	194	ALA	3.0
1	A	221	VAL	3.0
1	A	358	ASP	3.0
1	A	10	ALA	3.0
1	A	172	PHE	3.0
1	A	11	LEU	2.9
1	A	0	HIS	2.9
1	A	36	VAL	2.8
1	A	416	SER	2.8
1	A	27	PRO	2.8
1	A	236	THR	2.8
1	A	63	MET	2.8
1	A	215	GLY	2.8
1	A	414	GLU	2.8
1	A	363	ALA	2.7
1	A	163	LYS	2.6
1	A	57	PHE	2.6
1	A	227	CYS	2.6
1	A	70	LYS	2.6
1	A	226	ALA	2.6
1	A	30	ARG	2.5
1	A	131	LYS	2.5
1	A	341	LEU	2.5
1	A	225	LEU	2.3
1	A	360	ASP	2.3
1	A	193	GLY	2.3
1	A	344	LEU	2.3
1	A	1	MET	2.3
1	A	406	CYS	2.3
1	A	8	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	235	GLN	2.2
1	A	334	ARG	2.2
1	A	127	GLU	2.2
1	A	322	SER	2.2
1	A	56	ALA	2.1
1	A	66	ASP	2.1
1	A	212	CYS	2.1
1	A	35	ALA	2.1
1	A	298	LEU	2.0
1	A	301	MET	2.0
1	A	64	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 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(Å ²)	Q<0.9
2	TTD	T	5	40/41	0.86	0.16	68,75,112,113	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 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.

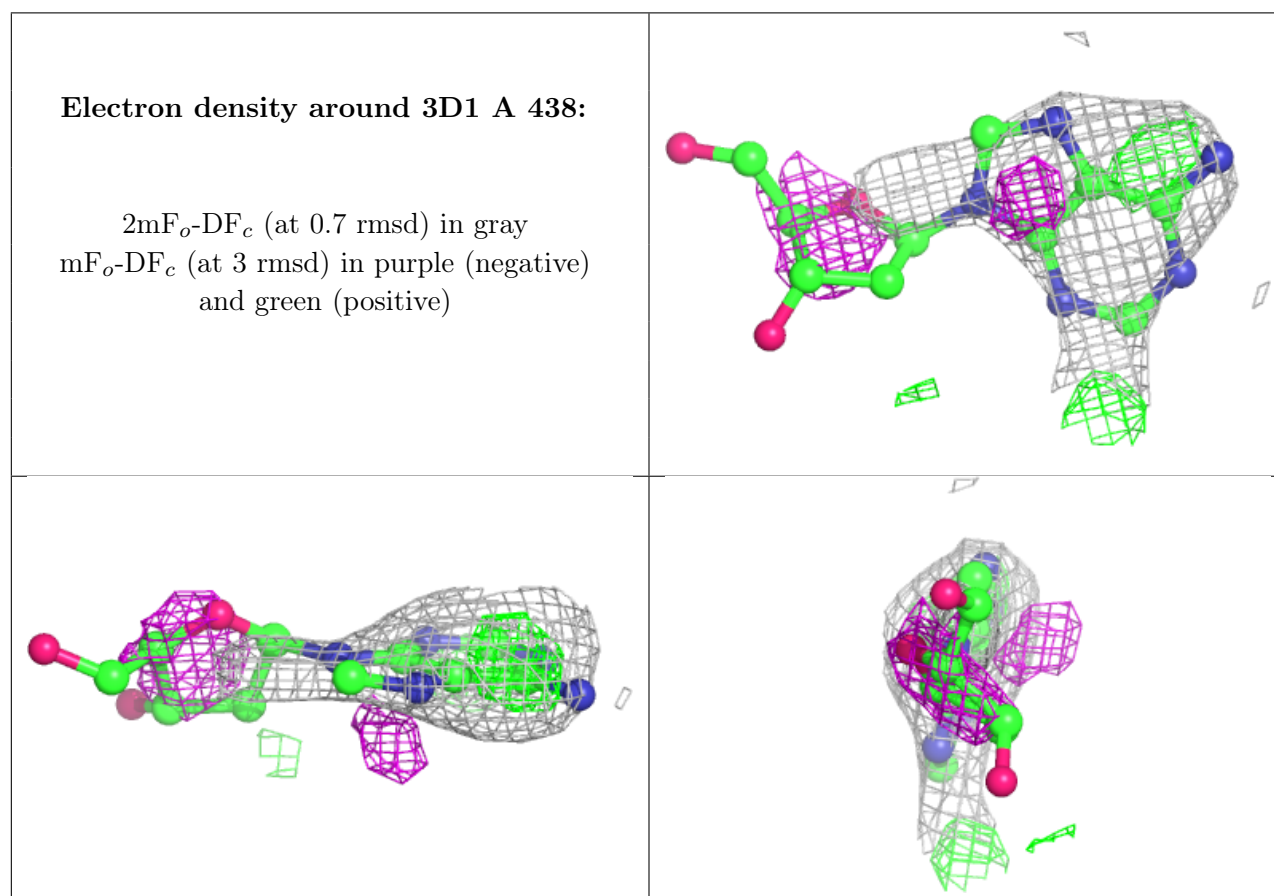
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	A	435	6/6	0.30	0.75	109,110,110,110	0
6	3D1	A	438	18/18	0.43	0.59	98,101,106,107	0
7	DTT	A	444	8/8	0.55	0.40	110,111,113,117	0
5	GOL	A	436	6/6	0.57	0.46	99,99,100,100	0
8	EDO	A	448	4/4	0.61	0.31	80,82,82,83	0
5	GOL	A	434	6/6	0.65	0.56	108,108,108,109	0

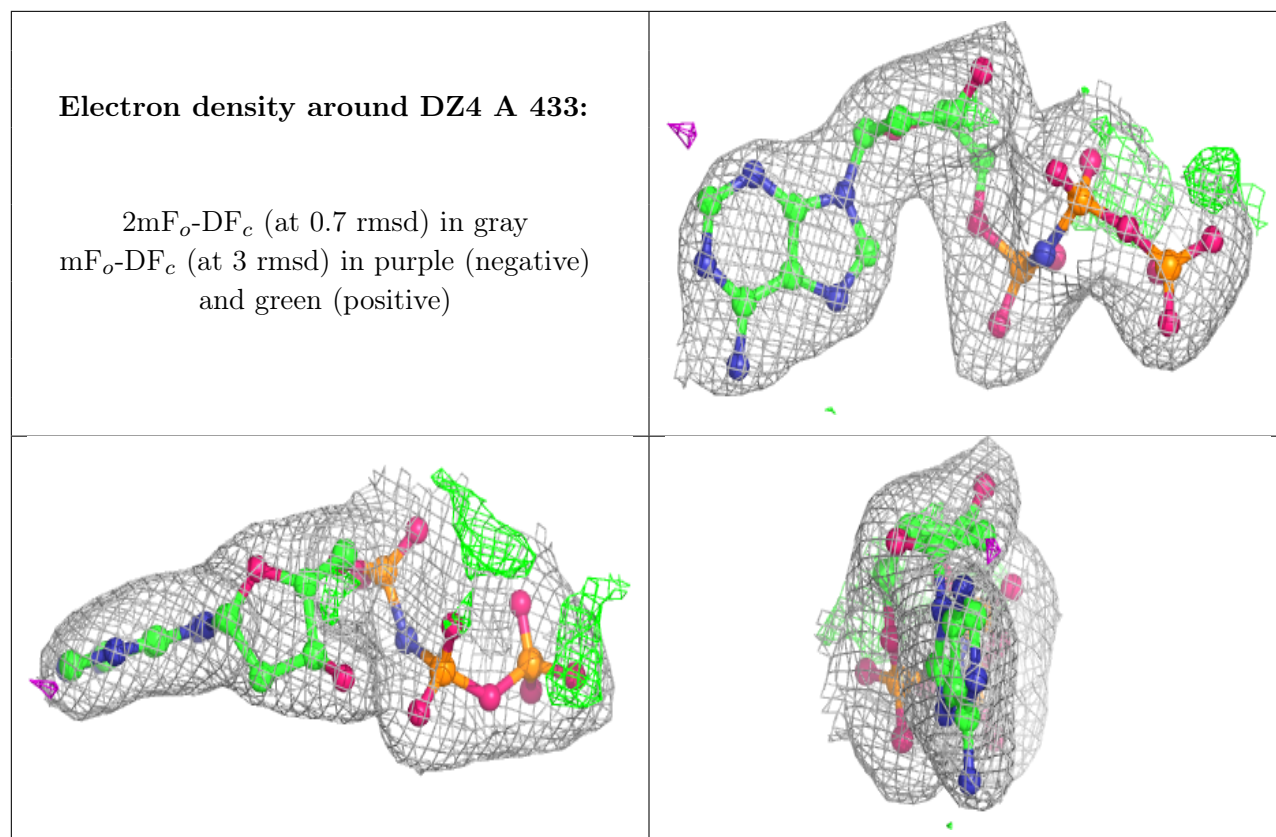
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	A	441	6/6	0.72	0.42	96,96,97,98	0
5	GOL	A	440	6/6	0.73	0.28	99,100,101,101	0
5	GOL	A	442	6/6	0.84	0.32	104,105,106,107	0
7	DTT	A	443	8/8	0.84	0.21	101,102,104,108	0
8	EDO	A	447	4/4	0.85	0.13	86,86,87,88	0
5	GOL	A	437	6/6	0.85	0.28	76,77,77,78	0
8	EDO	A	449	4/4	0.85	0.18	94,94,94,96	0
8	EDO	A	445	4/4	0.89	0.19	89,89,89,90	0
8	EDO	A	446	4/4	0.92	0.19	72,73,73,78	0
5	GOL	A	439	6/6	0.94	0.11	54,57,62,63	0
4	DZ4	A	433	30/30	0.97	0.12	41,51,54,57	0
9	MG	A	450	1/1	0.97	0.19	40,40,40,40	0
9	MG	A	451	1/1	0.98	0.11	40,40,40,40	0
10	CO	A	452	1/1	0.99	0.14	43,43,43,43	0

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





6.5 Other polymers [i](#)

There are no such residues in this entry.