Full wwPDB X-ray Structure Validation Report (i)

Aug 26, 2026 – 04:16 am BST

PDB ID	:	2WTF / pdb_00002wtf
Title	:	DNA polymerase eta in complex with the cis-diammineplatinum (II) 1,3- GTG intrastrand cross-link
Authors	:	Reissner, T.; Schneider, S.; Ziv, O.; Schorr, S.; Livneh, Z.; Carell, T.
Deposited on	:	2009-09-16
Resolution	:	2.50 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

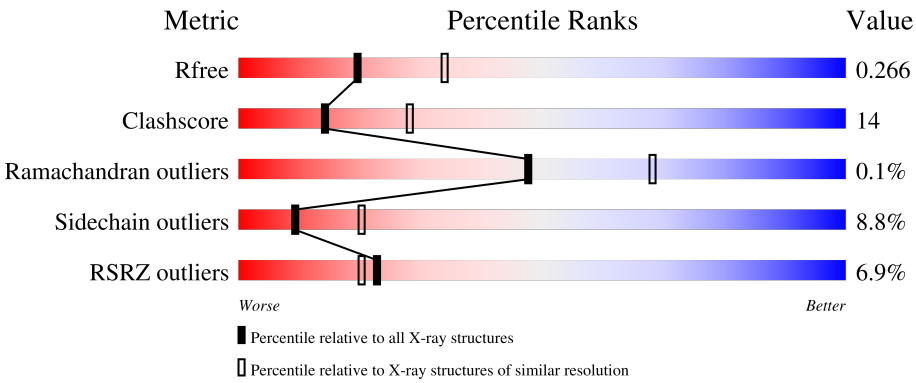
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 <=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	536	8%, 67%, 24%, • 5%
1	B	536	6%, 66%, 25%, • 5%
2	O	17	6%, 47%, 35%, 18%
2	S	17	47%, 18%, 6%, 29%
3	P	9	11%, 67%, 33%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	T	9	44% 56%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9100 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	509	3992	2544	669	755	24	0	0	0
1	B	508	4034	2570	680	760	24	0	2	0

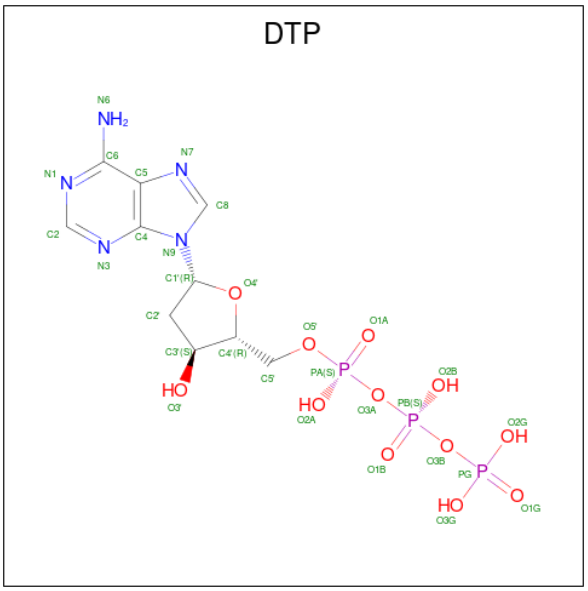
- Molecule 2 is a DNA chain called 5'-D(*TP*CP*TP*TP*CP*TP*GP*TP*GP*CP *TP*CP*AP*CP*CP*AP*CP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	O	14	267	129	44	81	13	0	0	0
2	S	12	241	115	41	73	12	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	P	9	185	89	37	51	8	0	0	0
3	T	9	185	89	37	51	8	0	0	0

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$)

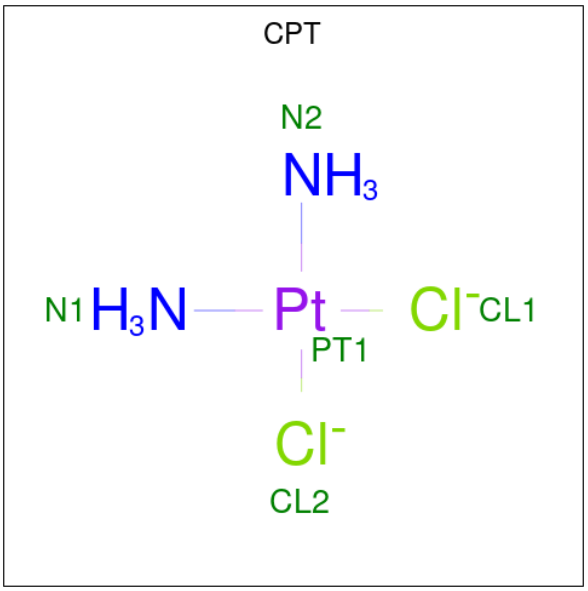


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	30	10	5	12	3	0	0
			Total	C	N	O	P		
4	B	1	30	10	5	12	3	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	A	4	4	4	0	0
			Total	Ca		
5	B	6	6	6	0	0

- Molecule 6 is Cisplatin (CCD ID: CPT) (formula: $Cl_2H_6N_2Pt$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Pt		
6	O	1	3	2	1	0	0
			Total	N	Pt		
6	S	1	3	2	1	0	0

- Molecule 7 is water.

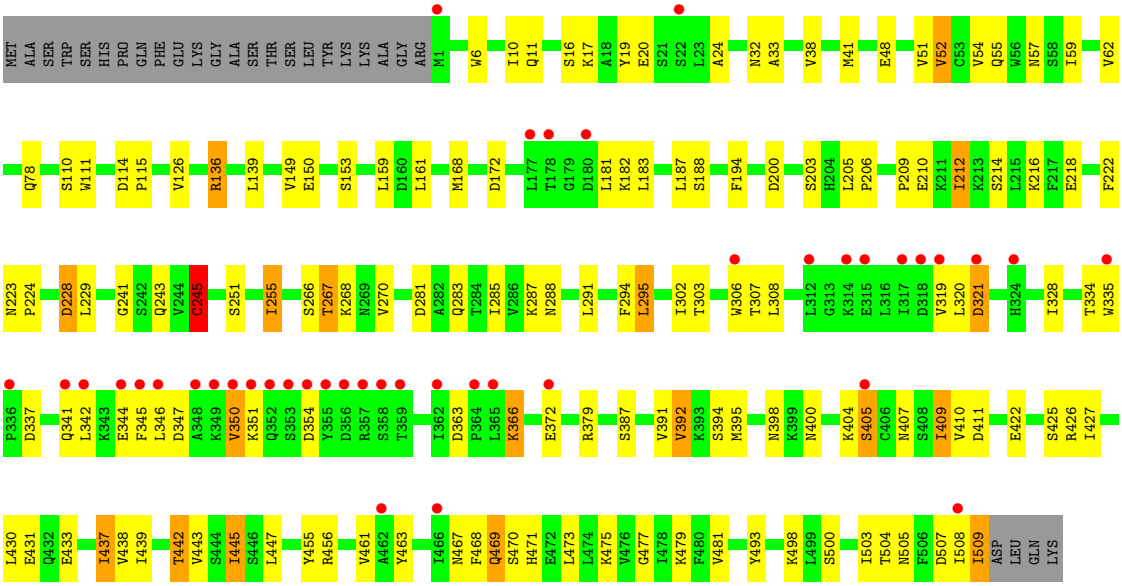
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	52	52	52	0	0
			Total	O		
7	B	67	67	67	0	0
			Total	O		
7	O	1	1	1	0	0

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.

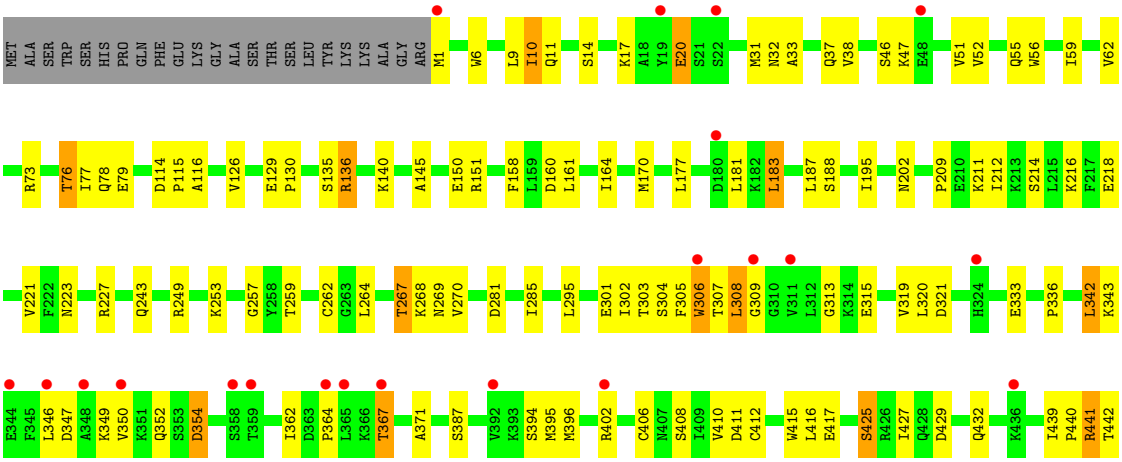
• Molecule 1: DNA POLYMERASE ETA

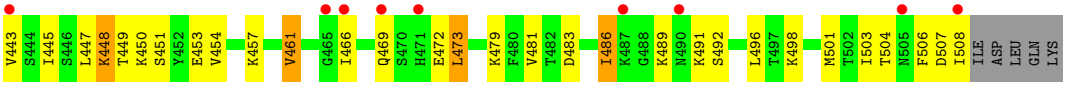
Chain A:



• Molecule 1: DNA POLYMERASE ETA

Chain B:



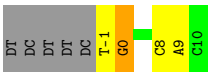


• Molecule 2: 5'-D(*TP*CP*TP*TP*CP*TP*GP*TP*GP*CP *TP*CP*AP*CP*CP*AP*CP)-3'

Chain O:

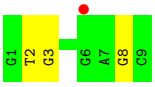
• Molecule 2: 5'-D(*TP*CP*TP*TP*CP*TP*GP*TP*GP*CP *TP*CP*AP*CP*CP*AP*CP)-3'

Chain S:



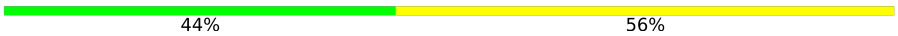
• Molecule 3: 5'-D(*GP*TP*GP*GP*TP*GP*AP*GP*CP)-3'

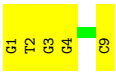
Chain P:



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

Chain T:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	103.24Å 103.24Å 292.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 2.50 48.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.00-2.50) 98.5 (48.00-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.66 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.227 , 0.269 0.230 , 0.266	Depositor DCC
R_{free} test set	2793 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	42.1	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 33.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9100	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, DTP, CPT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	1.02	3/4068 (0.1%)	1.00	5/5489 (0.1%)
1	B	1.08	3/4118 (0.1%)	1.00	2/5555 (0.0%)
2	O	0.64	0/296	1.32	1/451 (0.2%)
2	S	0.60	0/268	1.26	1/410 (0.2%)
3	P	0.65	0/208	1.40	1/321 (0.3%)
3	T	0.58	0/208	0.97	0/321
All	All	1.01	6/9166 (0.1%)	1.03	10/12547 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	470	SER	CA-CB	-12.86	1.33	1.53
1	A	372	GLU	CA-CB	-10.47	1.37	1.53
1	B	10	ILE	CA-CB	5.64	1.61	1.54
1	A	153	SER	C-O	-5.62	1.18	1.24
1	B	415	TRP	C-O	-5.17	1.18	1.24
1	B	221	VAL	CA-CB	-5.05	1.48	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	350	VAL	N-CA-C	7.39	118.16	110.62
3	P	8	DG	O4'-C1'-N9	7.09	119.04	108.40
1	B	417	GLU	N-CA-C	-6.41	104.21	111.07
1	A	350	VAL	CB-CA-C	-5.99	104.05	112.14
1	A	372	GLU	N-CA-CB	5.56	118.07	110.01
2	O	-1	DT	O5'-C5'-C4'	-5.39	102.71	110.80
1	B	442	THR	N-CA-C	5.20	117.88	109.40
2	S	0	DG	O3'-P-O5'	-5.08	96.38	104.00
1	A	245	CYS	N-CA-C	5.07	116.81	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	409	ILE	CB-CA-C	-5.06	105.31	112.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3992	0	3993	114	0
1	B	4034	0	4070	121	0
2	O	267	0	152	6	0
2	S	241	0	136	5	0
3	P	185	0	98	3	0
3	T	185	0	98	3	0
4	A	30	0	12	1	0
4	B	30	0	12	2	0
5	A	4	0	0	0	0
5	B	6	0	0	0	0
6	O	3	0	0	0	0
6	S	3	0	0	1	0
7	A	52	0	0	1	0
7	B	67	0	0	2	0
7	O	1	0	0	0	0
All	All	9100	0	8571	249	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 14.

All (249) 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:347:ASP:O	1:A:350:VAL:HG22	1.38	1.23
1:B:443:VAL:HG21	1:B:473:LEU:HD21	1.28	1.13
1:B:508:ILE:HG13	1:B:508:ILE:O	1.46	1.11
1:B:52:VAL:CG2	1:B:59:ILE:HG23	1.84	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LEU:O	1:A:350:VAL:HG13	1.54	1.07
1:B:443:VAL:HG21	1:B:473:LEU:CD2	1.86	1.06
1:B:76:THR:HG22	1:B:79:GLU:H	1.19	1.01
1:B:443:VAL:HG22	1:B:503:ILE:HG22	1.46	0.93
1:A:442:THR:HG21	1:A:505:ASN:HD22	1.34	0.89
1:B:32:ASN:HD21	1:B:281:ASP:H	1.22	0.87
1:B:443:VAL:CG2	1:B:473:LEU:HD21	2.05	0.86
1:B:76:THR:CG2	1:B:79:GLU:H	1.89	0.85
1:A:183:LEU:HD22	1:A:187:LEU:HD12	1.57	0.85
1:A:32:ASN:HD21	1:A:281:ASP:H	1.25	0.84
1:A:442:THR:CG2	1:A:505:ASN:HD22	1.93	0.81
1:B:507:ASP:O	1:B:508:ILE:CG2	2.30	0.80
2:S:8:DC:H2"	2:S:9:DA:OP2	1.80	0.79
1:A:439:ILE:HG12	1:A:468:PHE:HB2	1.67	0.77
1:B:333:GLU:O	1:B:336:PRO:HG3	1.85	0.77
1:B:395:MET:HE1	1:B:427:ILE:HD13	1.68	0.75
1:B:52:VAL:HG21	1:B:59:ILE:HG23	1.68	0.75
1:A:11:GLN:HE21	1:A:17:LYS:HB3	1.49	0.75
1:A:55:GLN:HE21	1:A:126:VAL:HG11	1.52	0.75
1:A:442:THR:HG21	1:A:505:ASN:ND2	2.02	0.75
1:A:229:LEU:O	1:A:287:LYS:NZ	2.20	0.74
1:B:507:ASP:O	1:B:508:ILE:HG22	1.87	0.74
1:A:350:VAL:HG23	1:A:351:LYS:HG3	1.70	0.73
1:B:343:LYS:HG3	1:B:367:THR:HG23	1.71	0.73
1:A:17:LYS:HG2	1:A:20:GLU:OE1	1.88	0.73
1:A:222:PHE:CD2	1:A:222:PHE:O	2.42	0.73
1:B:267:THR:HG22	1:B:270:VAL:H	1.55	0.72
1:B:52:VAL:CG2	1:B:59:ILE:CG2	2.65	0.72
1:A:183:LEU:HD22	1:A:187:LEU:CD1	2.19	0.71
1:A:456:ARG:HH12	3:P:3:DG:P	2.15	0.69
1:A:347:ASP:O	1:A:350:VAL:CG2	2.30	0.69
1:B:302:ILE:HD12	1:B:305:PHE:CD1	2.27	0.68
1:A:445:ILE:HD12	1:A:477:GLY:HA2	1.76	0.68
1:B:267:THR:HG21	7:B:2059:HOH:O	1.93	0.68
1:B:52:VAL:HG21	1:B:59:ILE:CG2	2.24	0.67
1:B:76:THR:HG22	1:B:79:GLU:N	2.02	0.67
1:B:269[B]:ASN:ND2	1:B:305:PHE:CD2	2.62	0.67
1:B:52:VAL:HG23	1:B:59:ILE:HG23	1.74	0.66
2:O:3:DC:H2'	2:O:4:DT:H71	1.77	0.66
1:A:400:ASN:ND2	1:A:498:LYS:HD2	2.10	0.66
1:B:17:LYS:NZ	1:B:20:GLU:HG2	2.10	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:ASP:C	1:B:508:ILE:HG23	2.21	0.66
1:B:1:MET:HE2	1:B:1:MET:HA	1.77	0.65
1:B:448:LYS:HG2	1:B:454:VAL:HG22	1.75	0.65
1:B:59:ILE:O	1:B:73:ARG:HG3	1.97	0.64
1:A:350:VAL:CG2	1:A:351:LYS:HG3	2.28	0.64
1:A:509:ILE:HD12	1:A:509:ILE:C	2.21	0.64
1:A:394:SER:HB3	1:A:504:THR:HG22	1.80	0.64
1:A:431:GLU:OE2	1:A:437:ILE:HD13	1.98	0.64
1:A:350:VAL:HG23	1:A:351:LYS:N	2.12	0.63
1:B:181:LEU:HD21	1:B:211:LYS:HG2	1.80	0.63
1:A:218:GLU:O	1:A:285:ILE:HD11	1.99	0.63
1:A:57:ASN:ND2	1:A:110:SER:OG	2.32	0.63
1:A:302:ILE:CD1	1:A:308:LEU:HD23	2.28	0.62
1:A:442:THR:HG23	1:A:505:ASN:HB2	1.82	0.62
1:A:302:ILE:HD11	1:A:308:LEU:HD23	1.81	0.62
1:A:442:THR:CG2	1:A:505:ASN:ND2	2.63	0.62
1:A:320:LEU:HD23	1:A:335:TRP:CH2	2.35	0.61
1:A:427:ILE:HG23	1:A:438:VAL:HG23	1.82	0.61
1:A:32:ASN:ND2	1:A:281:ASP:H	1.96	0.61
1:B:135:SER:OG	1:B:151[B]:ARG:NH2	2.34	0.61
1:B:55:GLN:HG3	1:B:126:VAL:HG21	1.81	0.61
1:B:37:GLN:NE2	1:B:47:LYS:HE3	2.15	0.61
1:B:443:VAL:HG21	1:B:473:LEU:HD23	1.82	0.60
1:B:302:ILE:HD12	1:B:305:PHE:HD1	1.64	0.60
1:A:391:VAL:CG2	1:A:508:ILE:HD11	2.31	0.60
1:A:400:ASN:HD21	1:A:498:LYS:HD2	1.65	0.60
1:B:223:ASN:HD21	1:B:227:ARG:H	1.48	0.60
1:B:315:GLU:OE1	1:B:362:ILE:HD12	2.01	0.59
1:B:306:TRP:C	1:B:307:THR:HG23	2.26	0.59
1:B:507:ASP:C	1:B:508:ILE:CG2	2.74	0.59
1:A:344:GLU:OE2	1:A:344:GLU:HA	2.03	0.59
1:B:343:LYS:NZ	1:B:347:ASP:OD2	2.28	0.59
1:A:439:ILE:HG12	1:A:468:PHE:CB	2.33	0.58
1:B:114:ASP:OD1	1:B:116:ALA:N	2.35	0.58
1:A:149:VAL:HG22	1:A:159:LEU:CD2	2.34	0.58
1:A:55:GLN:HG3	1:A:126:VAL:HG21	1.86	0.57
2:S:-1:DT:O2	6:S:1014:CPT:N2	2.37	0.57
1:B:55:GLN:HG2	1:B:56:TRP:CD1	2.40	0.57
1:A:55:GLN:CG	1:A:126:VAL:HG21	2.35	0.56
1:B:306:TRP:O	1:B:307:THR:HG23	2.05	0.56
1:A:78:GLN:HE22	1:A:111:TRP:HA	1.69	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ASN:HD22	1:A:291:LEU:HD11	1.70	0.56
1:A:342:LEU:O	1:A:342:LEU:HD23	2.05	0.56
1:A:345:PHE:C	1:A:345:PHE:CD2	2.83	0.56
1:B:507:ASP:O	1:B:508:ILE:HG23	2.02	0.56
1:B:412:CYS:HB3	1:B:481:VAL:HG21	1.87	0.56
4:B:1511:DTP:O5'	4:B:1511:DTP:H8	2.04	0.56
2:O:2:DG:H2"	2:O:3:DC:OP1	2.05	0.56
1:A:319:VAL:O	1:A:319:VAL:CG1	2.54	0.55
1:B:136:ARG:NH1	1:B:429:ASP:OD1	2.40	0.55
1:A:136:ARG:NH2	1:A:433:GLU:HG3	2.20	0.55
2:S:-1:DT:C2'	2:S:0:DG:H5'	2.36	0.55
1:A:437:ILE:HD11	1:B:202:ASN:ND2	2.21	0.55
1:A:52:VAL:HG22	1:A:59:ILE:HG23	1.89	0.54
1:B:145:ALA:O	1:B:164:ILE:HD11	2.06	0.54
1:A:55:GLN:NE2	1:A:126:VAL:HG11	2.21	0.54
4:A:1510:DTP:O5'	4:A:1510:DTP:H8	2.08	0.53
1:A:181:LEU:HD12	1:A:182:LYS:H	1.72	0.53
1:B:17:LYS:HZ2	1:B:20:GLU:HG2	1.73	0.53
1:A:404:LYS:HB3	1:A:407:ASN:ND2	2.23	0.53
1:A:54:VAL:HG21	1:A:111:TRP:CZ3	2.44	0.53
1:B:183:LEU:HD22	1:B:187:LEU:HD12	1.90	0.53
2:O:0:DG:C2'	2:O:2:DG:OP1	2.56	0.53
1:B:253:LYS:O	1:B:257:GLY:HA2	2.09	0.52
1:B:319:VAL:O	1:B:349:LYS:HG2	2.08	0.52
1:A:216:LYS:O	1:A:243:GLN:NE2	2.39	0.52
1:A:363:ASP:OD2	1:A:366:LYS:HG3	2.10	0.52
1:B:303:THR:O	1:B:309:GLY:HA2	2.09	0.52
1:B:306:TRP:HA	1:B:306:TRP:CE3	2.45	0.52
1:B:440:PRO:HG3	1:B:503:ILE:HD12	1.91	0.52
1:B:269[B]:ASN:HD21	1:B:305:PHE:HD2	1.51	0.52
1:A:222:PHE:O	1:A:222:PHE:HD2	1.90	0.52
1:A:319:VAL:O	1:A:319:VAL:HG12	2.09	0.51
1:B:479:LYS:HE2	1:B:483:ASP:OD1	2.10	0.51
1:A:150:GLU:OE2	1:A:268:LYS:NZ	2.44	0.51
1:A:200:ASP:HB3	1:A:203:SER:OG	2.10	0.51
1:B:508:ILE:O	1:B:508:ILE:CG1	2.30	0.51
1:A:350:VAL:CG2	1:A:351:LYS:N	2.73	0.51
1:A:306:TRP:O	1:A:307:THR:OG1	2.27	0.50
1:B:306:TRP:HA	1:B:306:TRP:HE3	1.74	0.50
3:T:3:DG:H4'	3:T:4:DG:OP1	2.10	0.50
1:B:489:LYS:O	1:B:489:LYS:HD3	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:MET:CE	1:A:503:ILE:HD11	2.41	0.50
1:A:149:VAL:HG22	1:A:159:LEU:HD22	1.94	0.50
1:A:335:TRP:HD1	1:A:341:GLN:HG3	1.75	0.50
1:A:447:LEU:CD1	1:A:455:TYR:HB2	2.42	0.50
1:B:32:ASN:ND2	1:B:281:ASP:H	2.01	0.49
1:B:308:LEU:O	1:B:313:GLY:HA3	2.12	0.49
1:B:302:ILE:HD12	1:B:305:PHE:CE1	2.47	0.49
1:B:76:THR:HG23	1:B:78:GLN:N	2.28	0.49
3:T:1:DG:H2"	3:T:2:DT:OP2	2.12	0.49
1:A:426:ARG:NH2	2:O:5:DC:OP1	2.37	0.49
1:A:222:PHE:CE2	1:A:294:PHE:HA	2.48	0.48
1:A:447:LEU:HD11	1:A:455:TYR:HB2	1.95	0.48
1:B:301:GLU:O	1:B:304:SER:HB2	2.12	0.48
1:B:394:SER:CB	1:B:504:THR:HG22	2.43	0.48
1:A:6:TRP:O	1:A:10:ILE:HG12	2.13	0.48
1:A:24:ALA:O	1:A:266:SER:HA	2.13	0.48
1:B:136:ARG:HH12	1:B:429:ASP:CG	2.21	0.48
2:O:0:DG:H2"	2:O:2:DG:OP1	2.14	0.48
1:A:438:VAL:HG23	1:A:438:VAL:O	2.13	0.48
1:B:443:VAL:CG2	1:B:503:ILE:HG22	2.32	0.47
1:A:445:ILE:CD1	1:A:477:GLY:HA2	2.42	0.47
1:B:47:LYS:HE2	1:B:259:THR:HG23	1.97	0.47
1:B:223:ASN:ND2	1:B:227:ARG:H	2.10	0.47
1:A:334:THR:HB	1:A:335:TRP:CE3	2.49	0.47
2:S:-1:DT:H2"	2:S:0:DG:H5'	1.96	0.47
1:A:223:ASN:O	1:A:224:PRO:C	2.56	0.47
1:A:52:VAL:HG13	1:A:54:VAL:CG1	2.45	0.47
1:B:439:ILE:HG23	1:B:439:ILE:O	2.14	0.47
1:B:17:LYS:HZ3	1:B:20:GLU:HG2	1.79	0.47
1:B:209:PRO:O	1:B:212:ILE:HG22	2.14	0.47
4:B:1511:DTP:H1'	3:T:9:DC:H2'	1.96	0.47
1:A:57:ASN:HD21	1:A:110:SER:CB	2.27	0.47
1:B:76:THR:HG22	1:B:79:GLU:HG3	1.97	0.47
1:B:347:ASP:OD1	1:B:367:THR:HG21	2.15	0.47
1:A:391:VAL:CG2	1:A:508:ILE:CD1	2.93	0.47
1:A:255:ILE:N	1:A:255:ILE:HD13	2.29	0.47
1:A:439:ILE:CG2	1:A:463:TYR:CE2	2.98	0.46
1:B:449:THR:HG23	1:B:453:GLU:O	2.15	0.46
1:B:11:GLN:HE22	1:B:20:GLU:HG2	1.80	0.46
1:B:346:LEU:O	1:B:350:VAL:HG22	2.16	0.46
1:B:249:ARG:HD2	1:B:262:CYS:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:ILE:O	1:B:364:PRO:HD3	2.16	0.46
1:A:136:ARG:HH21	1:A:139:LEU:HD22	1.79	0.46
1:A:150:GLU:HG3	1:A:387:SER:O	2.16	0.46
1:B:320:LEU:O	1:B:321:ASP:C	2.58	0.45
1:A:509:ILE:HD12	1:A:509:ILE:O	2.16	0.45
1:B:114:ASP:OD1	1:B:114:ASP:C	2.60	0.45
1:B:469:GLN:HB2	1:B:472:GLU:HG2	1.98	0.45
1:B:506:PHE:O	1:B:507:ASP:HB2	2.16	0.45
1:B:150:GLU:HG3	1:B:387:SER:O	2.17	0.45
1:B:416:LEU:HD22	1:B:501:MET:HE3	1.99	0.45
1:A:168:MET:HA	1:A:172:ASP:HB2	1.98	0.45
1:A:456:ARG:NH1	3:P:3:DG:OP1	2.48	0.45
1:A:267:THR:HG22	1:A:270:VAL:H	1.81	0.45
1:B:129:GLU:OE2	1:B:425:SER:HB2	2.17	0.45
1:B:483:ASP:O	1:B:486:ILE:HB	2.17	0.45
1:A:395:MET:HE2	1:A:503:ILE:HD11	1.97	0.44
1:B:181:LEU:CD2	1:B:211:LYS:HG2	2.47	0.44
1:B:150:GLU:HB3	1:B:158:PHE:HB2	1.99	0.44
1:B:450:LYS:HB3	1:B:492:SER:O	2.17	0.44
1:A:6:TRP:HA	1:A:205:LEU:HD21	2.00	0.44
1:A:114:ASP:HA	1:A:115:PRO:HD3	1.89	0.44
1:B:394:SER:HB3	1:B:504:THR:HG22	1.98	0.44
1:A:442:THR:CG2	1:A:505:ASN:HB2	2.47	0.44
1:A:405:SER:O	1:A:411:ASP:OD1	2.36	0.43
1:B:11:GLN:HE21	1:B:17:LYS:HB3	1.83	0.43
2:S:8:DC:C2'	2:S:9:DA:OP2	2.55	0.43
1:A:398:ASN:OD1	1:A:500:SER:HB3	2.18	0.43
1:B:412:CYS:O	1:B:416:LEU:HG	2.19	0.43
1:B:160:ASP:OD1	1:B:160:ASP:C	2.61	0.43
1:A:218:GLU:O	1:A:283:GLN:NE2	2.52	0.43
1:A:55:GLN:HE21	1:A:126:VAL:HG21	1.83	0.43
1:A:392:VAL:O	1:A:392:VAL:CG1	2.64	0.43
1:A:354:ASP:OD1	1:A:354:ASP:C	2.61	0.43
1:A:57:ASN:ND2	1:A:110:SER:CB	2.82	0.43
1:A:394:SER:CB	1:A:504:THR:HG22	2.48	0.43
1:B:32:ASN:O	1:B:33:ALA:C	2.59	0.43
1:B:195:ILE:HD12	1:B:195:ILE:HA	1.93	0.43
1:A:59:ILE:HG21	1:A:62:VAL:HG22	2.01	0.42
1:A:469:GLN:HB3	1:A:471:HIS:CE1	2.53	0.42
1:B:343:LYS:CG	1:B:367:THR:HG23	2.45	0.42
1:B:136:ARG:HD3	1:B:432:GLN:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:LEU:HD13	1:B:371:ALA:HA	2.01	0.42
1:B:268:LYS:HG3	7:B:2060:HOH:O	2.19	0.42
3:P:2:DT:H2"	3:P:3:DG:N7	2.34	0.42
1:A:205:LEU:HB3	1:A:206:PRO:HD2	2.02	0.42
1:B:9:LEU:HD21	1:B:170:MET:HE2	2.00	0.42
1:A:241:GLY:O	1:A:245:CYS:HB2	2.20	0.42
1:B:129:GLU:N	1:B:130:PRO:CD	2.83	0.42
1:B:216:LYS:O	1:B:243:GLN:NE2	2.45	0.42
1:B:395:MET:CE	1:B:427:ILE:HD13	2.44	0.42
1:B:406:CYS:HA	1:B:411:ASP:HB3	2.00	0.42
1:B:441:ARG:O	1:B:461:VAL:CG1	2.68	0.42
1:B:447:LEU:HA	1:B:498:LYS:O	2.20	0.42
1:A:55:GLN:NE2	1:A:126:VAL:HG21	2.35	0.42
1:B:457:LYS:NZ	1:B:483:ASP:OD1	2.52	0.42
1:B:352:GLN:HG3	1:B:354:ASP:HB2	2.00	0.42
1:B:441:ARG:O	1:B:461:VAL:HG12	2.20	0.42
1:A:52:VAL:HG22	1:A:59:ILE:CG2	2.50	0.41
1:A:209:PRO:O	1:A:210:GLU:C	2.62	0.41
1:A:212:ILE:HD12	1:A:212:ILE:HA	1.90	0.41
1:A:391:VAL:HG23	1:A:508:ILE:HD11	2.03	0.41
1:B:491:LYS:O	1:B:492:SER:C	2.63	0.41
1:B:269[B]:ASN:ND2	1:B:305:PHE:CE2	2.76	0.41
1:A:228:ASP:O	1:A:287:LYS:NZ	2.52	0.41
1:A:307:THR:O	1:A:308:LEU:HD12	2.21	0.41
1:B:218:GLU:O	1:B:285:ILE:HD11	2.21	0.41
1:A:194:PHE:O	1:B:140:LYS:NZ	2.49	0.41
1:A:222:PHE:CD2	1:A:222:PHE:C	2.99	0.41
1:B:114:ASP:HA	1:B:115:PRO:HD2	1.84	0.41
1:A:320:LEU:O	1:A:321:ASP:C	2.63	0.41
1:B:6:TRP:O	1:B:10:ILE:HG12	2.20	0.41
1:B:76:THR:HG23	1:B:78:GLN:H	1.86	0.41
1:B:269[A]:ASN:ND2	1:B:269[A]:ASN:H	2.17	0.41
1:A:19:TYR:CE1	1:A:20:GLU:HG3	2.56	0.40
1:B:11:GLN:HE22	1:B:20:GLU:CG	2.34	0.40
1:A:209:PRO:HG3	7:A:2030:HOH:O	2.20	0.40
1:A:295:LEU:HB3	1:A:328:ILE:HG21	2.03	0.40
1:B:269[B]:ASN:ND2	1:B:305:PHE:HD2	2.14	0.40
2:O:3:DC:H2"	2:O:4:DT:H5'	2.02	0.40
1:B:136:ARG:NH1	1:B:429:ASP:CG	2.79	0.40
1:A:32:ASN:O	1:A:33:ALA:C	2.65	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	507/536 (95%)	490 (97%)	16 (3%)	1 (0%)	43 63
1	B	508/536 (95%)	486 (96%)	22 (4%)	0	100 100
All	All	1015/1072 (95%)	976 (96%)	38 (4%)	1 (0%)	48 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	493	TYR

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	443/478 (93%)	401 (90%)	42 (10%)	8 17
1	B	453/478 (95%)	416 (92%)	37 (8%)	10 23
All	All	896/956 (94%)	817 (91%)	79 (9%)	9 20

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	38	VAL
1	A	41	MET
1	A	48	GLU
1	A	51	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	52	VAL
1	A	136	ARG
1	A	161	LEU
1	A	188	SER
1	A	212	ILE
1	A	214	SER
1	A	228	ASP
1	A	245	CYS
1	A	251	SER
1	A	255	ILE
1	A	267	THR
1	A	295	LEU
1	A	303	THR
1	A	321	ASP
1	A	337	ASP
1	A	366	LYS
1	A	379	ARG
1	A	392	VAL
1	A	405	SER
1	A	409	ILE
1	A	410	VAL
1	A	422	GLU
1	A	425	SER
1	A	430	LEU
1	A	437	ILE
1	A	442	THR
1	A	443	VAL
1	A	445	ILE
1	A	461	VAL
1	A	467	ASN
1	A	469	GLN
1	A	473	LEU
1	A	475	LYS
1	A	479	LYS
1	A	481	VAL
1	A	507	ASP
1	A	509	ILE
1	B	14	SER
1	B	20	GLU
1	B	31	MET
1	B	38	VAL
1	B	46	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	51	VAL
1	B	62	VAL
1	B	76	THR
1	B	77	ILE
1	B	136	ARG
1	B	161	LEU
1	B	177	LEU
1	B	183	LEU
1	B	188	SER
1	B	214	SER
1	B	264	LEU
1	B	267	THR
1	B	295	LEU
1	B	306	TRP
1	B	308	LEU
1	B	342	LEU
1	B	354	ASP
1	B	367	THR
1	B	396	MET
1	B	402	ARG
1	B	408	SER
1	B	410	VAL
1	B	425	SER
1	B	441	ARG
1	B	445	ILE
1	B	448	LYS
1	B	451	SER
1	B	461	VAL
1	B	466	ILE
1	B	473	LEU
1	B	486	ILE
1	B	496	LEU

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

Mol	Chain	Res	Type
1	A	11	GLN
1	A	32	ASN
1	A	55	GLN
1	A	57	ASN
1	A	78	GLN
1	A	113	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	269	ASN
1	A	283	GLN
1	A	288	ASN
1	A	330	HIS
1	A	361	ASN
1	A	400	ASN
1	A	469	GLN
1	A	505	ASN
1	B	11	GLN
1	B	32	ASN
1	B	105	HIS
1	B	124	HIS
1	B	198	ASN
1	B	202	ASN
1	B	223	ASN
1	B	288	ASN
1	B	361	ASN
1	B	400	ASN
1	B	469	GLN
1	B	505	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	DTP	B	1511	5	28,32,32	1.38	3 (10%)	42,50,50	1.96	7 (16%)
4	DTP	A	1510	5	28,32,32	1.60	6 (21%)	42,50,50	2.07	10 (23%)
6	CPT	S	1014	2	0,2,4	-	-	-		
6	CPT	O	1014	2	0,2,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DTP	B	1511	5	-	4/22/34/34	0/3/3/3
4	DTP	A	1510	5	-	2/22/34/34	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1511	DTP	C5-C4	4.35	1.47	1.39
4	A	1510	DTP	C5-C4	4.26	1.47	1.39
4	A	1510	DTP	C5-C6	3.29	1.50	1.41
4	A	1510	DTP	C8-N7	3.23	1.37	1.31
4	B	1511	DTP	C5-C6	2.49	1.48	1.41
4	A	1510	DTP	C4-N9	-2.38	1.32	1.37
4	B	1511	DTP	C5-N7	-2.37	1.34	1.39
4	A	1510	DTP	C5-N7	-2.37	1.34	1.39
4	A	1510	DTP	C8-N9	-2.16	1.33	1.37

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1510	DTP	C5-C4-N3	-6.78	117.91	126.75
4	B	1511	DTP	C5-C4-N3	-5.96	118.97	126.75
4	B	1511	DTP	C2'-C1'-N9	-5.21	102.06	114.28
4	B	1511	DTP	N3-C4-N9	5.00	135.32	127.08
4	A	1510	DTP	N3-C4-N9	4.61	134.68	127.08
4	A	1510	DTP	C2-N3-C4	4.15	121.55	111.75
4	B	1511	DTP	C2-N3-C4	3.89	120.93	111.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1510	DTP	C4-C5-N7	-3.84	105.94	110.62
4	A	1510	DTP	C2'-C1'-N9	-3.78	105.42	114.28
4	B	1511	DTP	O3G-PG-O2G	3.19	119.82	107.64
4	B	1511	DTP	N3-C2-N1	-3.06	123.82	128.60
4	A	1510	DTP	N3-C2-N1	-2.85	124.15	128.60
4	A	1510	DTP	C5-N7-C8	2.59	107.19	103.51
4	A	1510	DTP	C4-N9-C8	2.52	108.45	105.73
4	A	1510	DTP	N9-C8-N7	-2.14	110.98	113.91
4	B	1511	DTP	C4-C5-N7	-2.06	108.11	110.62
4	A	1510	DTP	C6-C5-N7	2.06	135.85	132.02

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1511	DTP	PB-O3B-PG-O2G
4	B	1511	DTP	PB-O3B-PG-O1G
4	A	1510	DTP	PB-O3B-PG-O3G
4	B	1511	DTP	PB-O3B-PG-O3G
4	A	1510	DTP	O4'-C1'-N9-C8
4	B	1511	DTP	PA-O3A-PB-O1B

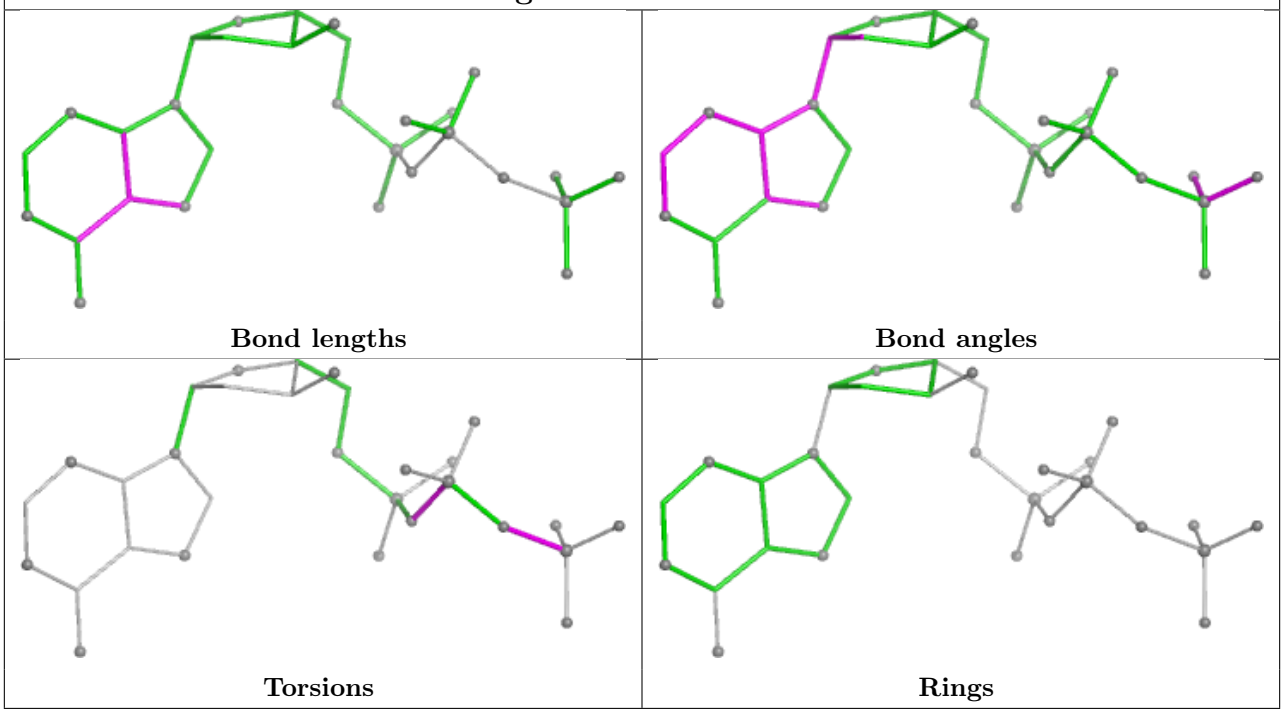
There are no ring outliers.

3 monomers are involved in 4 short contacts:

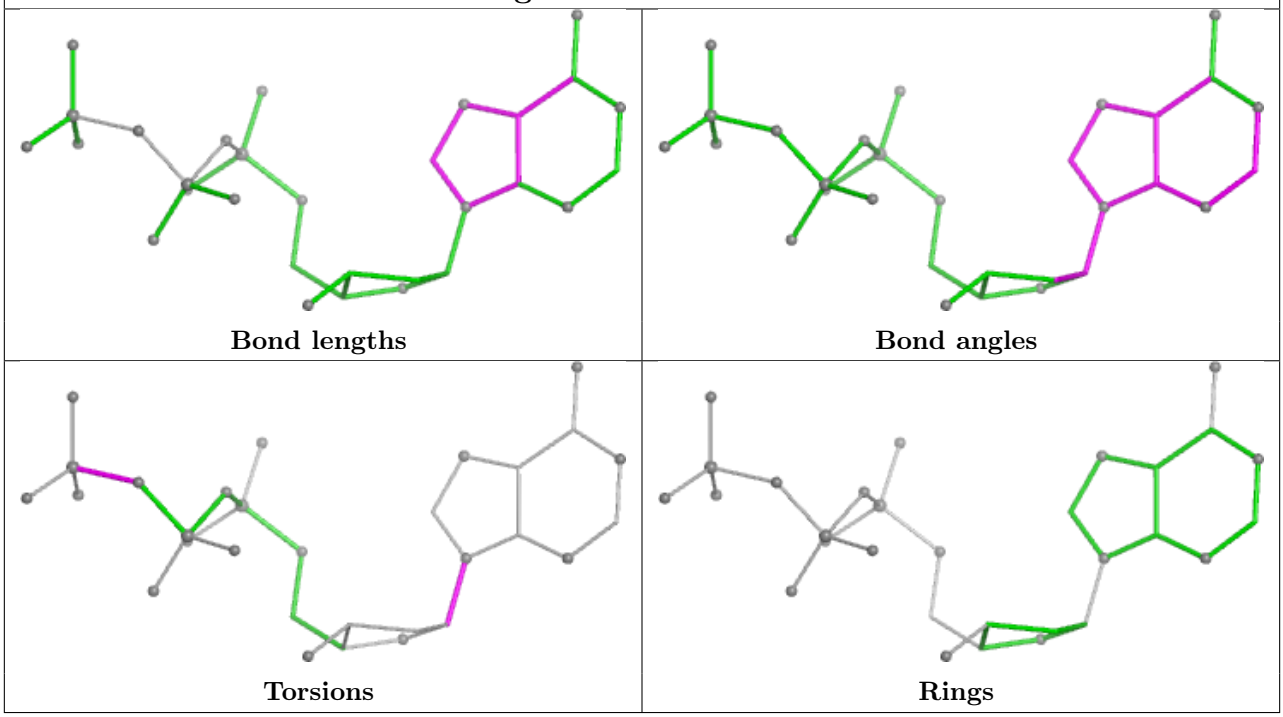
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1511	DTP	2	0
4	A	1510	DTP	1	0
6	S	1014	CPT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand DTP B 1511



Ligand DTP A 1510



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	O	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	O	-6:DT	O3'	-2:DC	P	11.97

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	509/536 (94%)	0.46	41 (8%) 18 15	21, 38, 84, 105	0
1	B	508/536 (94%)	0.32	30 (5%) 28 24	16, 36, 60, 72	2 (0%)
2	O	14/17 (82%)	0.97	1 (7%) 22 19	39, 52, 66, 85	0
2	S	12/17 (70%)	0.79	0 100 100	43, 62, 74, 83	0
3	P	9/9 (100%)	0.55	1 (11%) 10 8	39, 45, 55, 56	0
3	T	9/9 (100%)	0.58	0 100 100	40, 50, 55, 56	0
All	All	1061/1124 (94%)	0.40	73 (6%) 23 20	16, 38, 75, 105	2 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	357	ARG	6.5
1	B	508	ILE	4.9
1	A	348	ALA	4.6
1	A	462	ALA	4.0
1	B	466	ILE	3.9
1	B	306	TRP	3.9
1	B	358	SER	3.8
1	A	362	ILE	3.7
1	A	405	SER	3.6
1	A	364	PRO	3.5
1	A	346	LEU	3.3
1	A	351	LYS	3.2
1	A	466	ILE	3.2
1	A	354	ASP	3.1
1	A	352	GLN	3.0
1	A	324	HIS	3.0
1	B	490	ASN	3.0
1	A	319	VAL	2.9
1	B	22	SER	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	365	LEU	2.9
1	A	1	MET	2.9
1	A	355	TYR	2.9
1	A	345	PHE	2.8
1	A	306	TRP	2.8
1	A	358	SER	2.8
1	B	309	GLY	2.7
1	A	353	SER	2.7
1	A	341	GLN	2.7
1	A	350	VAL	2.6
1	A	356	ASP	2.6
1	B	344	GLU	2.6
1	A	178	THR	2.6
1	B	487	LYS	2.6
1	A	349	LYS	2.5
1	B	367	THR	2.5
1	A	177	LEU	2.5
1	A	508	ILE	2.4
1	A	372	GLU	2.4
2	O	-2	DC	2.4
1	B	402	ARG	2.4
3	P	6	DG	2.4
1	B	392	VAL	2.4
1	A	22	SER	2.4
1	A	342	LEU	2.4
1	B	469	GLN	2.4
1	B	350	VAL	2.4
1	A	321	ASP	2.3
1	B	311	VAL	2.3
1	A	359	THR	2.3
1	A	335	TRP	2.3
1	B	346	LEU	2.3
1	A	318	ASP	2.3
1	B	364	PRO	2.3
1	B	465	GLY	2.2
1	B	365	LEU	2.2
1	B	436	LYS	2.2
1	B	180	ASP	2.2
1	A	315	GLU	2.2
1	A	312	LEU	2.2
1	A	180	ASP	2.2
1	B	471	HIS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	359	THR	2.2
1	A	317	ILE	2.2
1	A	314	LYS	2.2
1	A	344	GLU	2.1
1	B	1	MET	2.1
1	B	348	ALA	2.1
1	B	19	TYR	2.1
1	A	336	PRO	2.1
1	B	443	VAL	2.0
1	B	48	GLU	2.0
1	B	505	ASN	2.0
1	B	324	HIS	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	CA	B	1512	1/1	0.67	0.17	59,59,59,59	1
5	CA	B	1514	1/1	0.81	0.16	67,67,67,67	0
5	CA	B	1513	1/1	0.83	0.17	64,64,64,64	0
5	CA	A	1513	1/1	0.84	0.12	88,88,88,88	0
5	CA	B	1515	1/1	0.86	0.14	48,48,48,48	0
5	CA	A	1512	1/1	0.87	0.10	57,57,57,57	0
5	CA	A	1514	1/1	0.88	0.16	74,74,74,74	0
4	DTP	A	1510	30/30	0.98	0.05	19,24,27,29	0
5	CA	B	1509	1/1	0.98	0.06	41,41,41,41	0
4	DTP	B	1511	30/30	0.98	0.05	21,26,35,36	0
6	CPT	S	1014	3/5	0.99	0.06	62,62,64,68	0

Continued on next page...

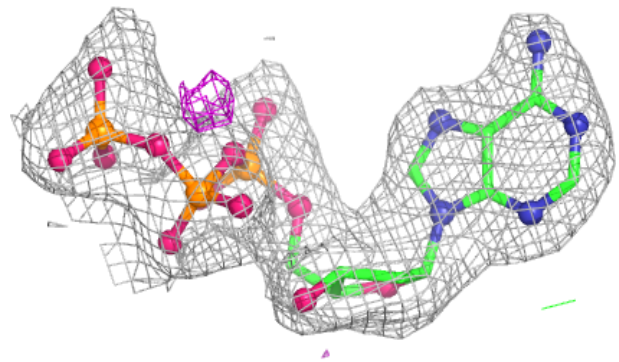
Continued from previous page...

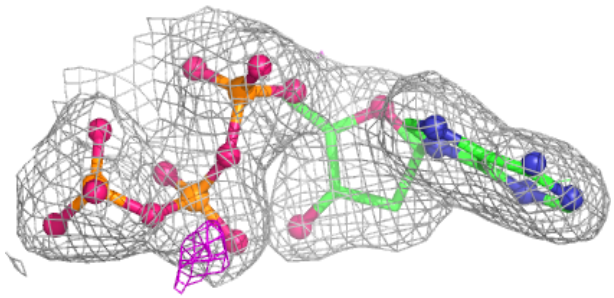
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CA	B	1510	1/1	1.00	0.02	24,24,24,24	0
6	CPT	O	1014	3/5	1.00	0.06	45,45,51,55	0
5	CA	A	1511	1/1	1.00	0.01	24,24,24,24	0

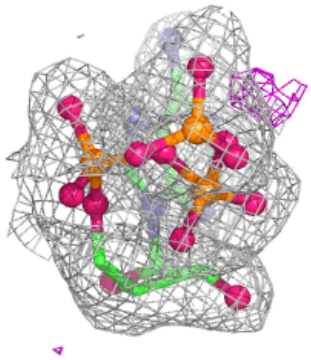
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DTP A 1510:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

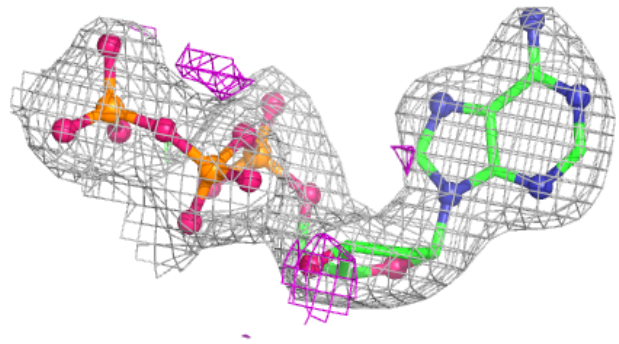


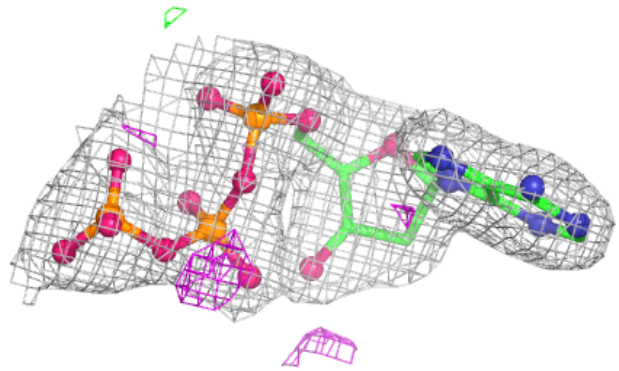


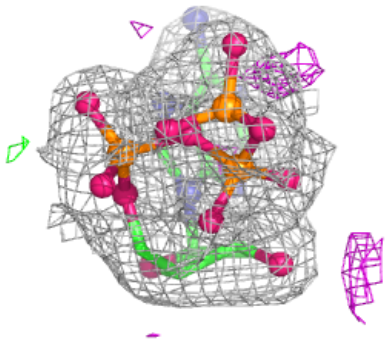


Electron density around DTP B 1511:

$2mF_o$-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)

There are no such residues in this entry.