



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:33 AM GMT

PDB ID : 2WTF
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

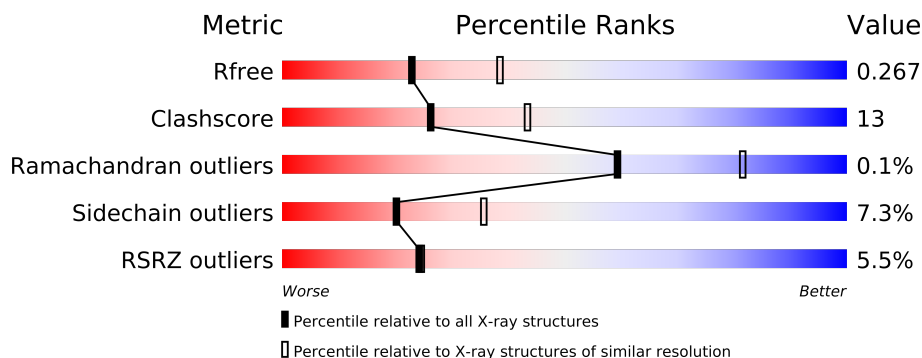
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	536	
1	B	536	
2	O	17	
2	S	17	
3	P	9	
3	T	9	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	CA	B	1509	-	X
5	CA	B	1512	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9100 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	509	Total	C	N	O	S	0	0	0
			3992	2544	669	755	24			
1	B	508	Total	C	N	O	S	0	2	0
			4034	2570	680	760	24			

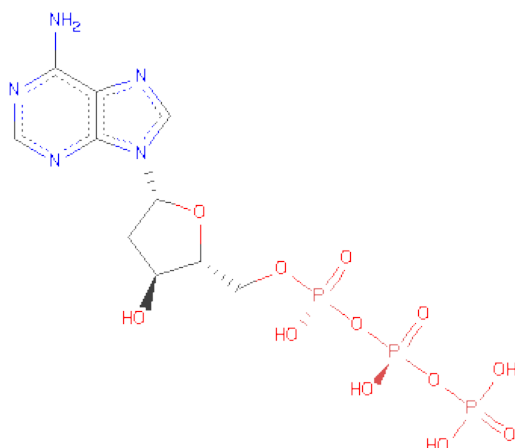
- Molecule 2 is a DNA chain called 5'-D(*TP*CP*TP*TP*CP*TP*GP*TP*GP*CP*TP*CP*AP*CP*CP*AP*CP)-3'.

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

- 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
3	P	9	Total	C	N	O	P	0	0	0
			185	89	37	51	8			
3	T	9	Total	C	N	O	P	0	0	0
			185	89	37	51	8			

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃).

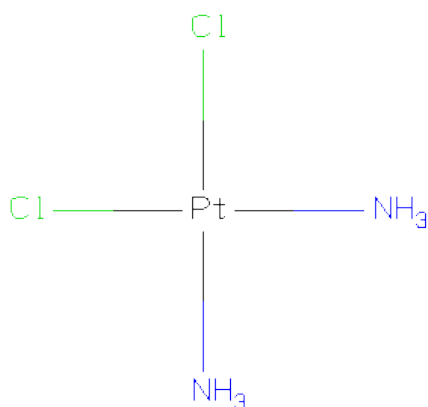


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
4	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is CISPLATIN (three-letter code: CPT) (formula: Cl₂H₆N₂Pt).



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

- Molecule 7 is water.

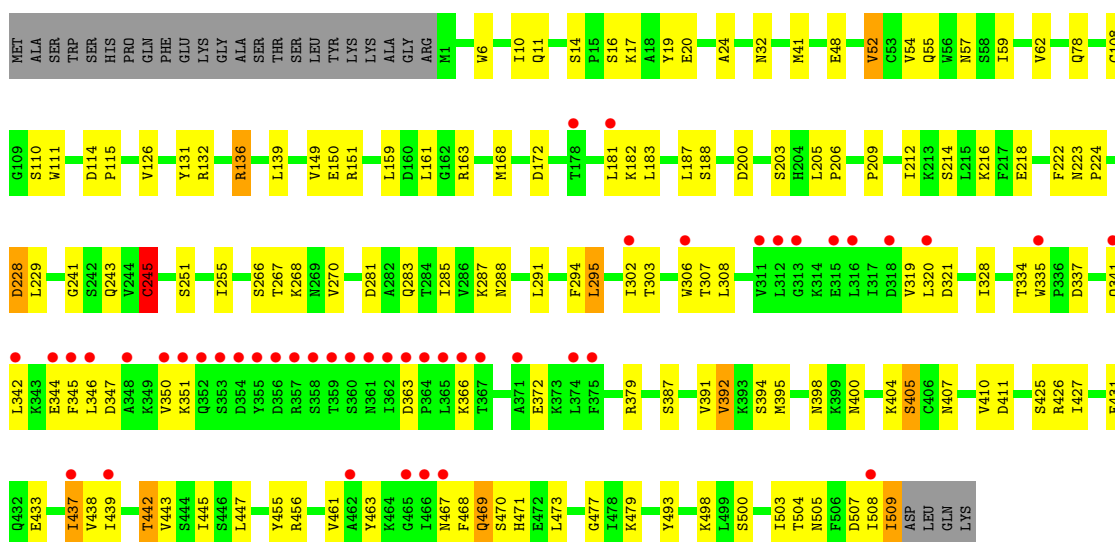
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	52	Total	O	0	0
			52	52		
7	B	67	Total	O	0	0
			67	67		
7	O	1	Total	O	0	0
			1	1		

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 errors 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.

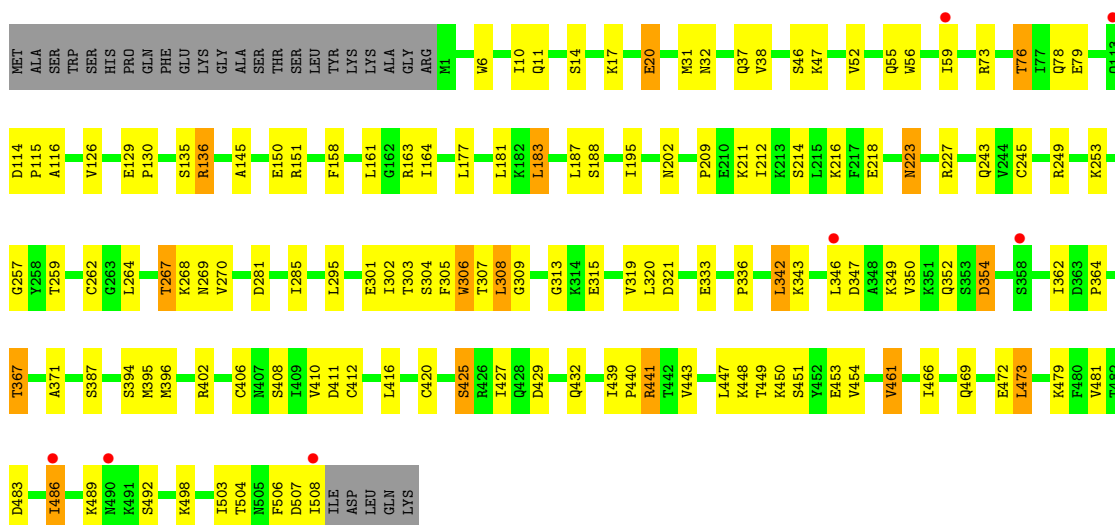
• Molecule 1: DNA POLYMERASE ETA

Chain A:



• Molecule 1: DNA POLYMERASE ETA

Chain B:



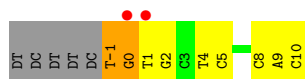
- Molecule 2: 5'-D(*TP*CP*TP*TP*CP*TP*GP*TP*GP*CP*TP*CP*AP*CP*CP*AP*CP)-3',

Chain O: 



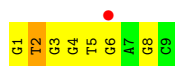
- Molecule 2: 5'-D(*TP*CP*TP*TP*CP*TP*GP*TP*GP*CP*TP*CP*AP*CP*CP*AP*CP)-3',

Chain S: 



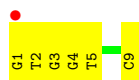
- Molecule 3: 5'-D(*GP*TP*GP*GP*TP*GP*AP*GP*CP)-3'

Chain P: 



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

Chain T: 



4 Data and refinement statistics

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 46.17 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.00-2.50) 98.5 (46.17-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.66 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.227 , 0.269 0.230 , 0.267	Depositor DCC
R_{free} test set	2793 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 20.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 54999 reflections	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.*

¹Intensities estimated from amplitudes.

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	0.82	5/4068 (0.1%)	0.78	3/5489 (0.1%)
1	B	0.87	2/4118 (0.0%)	0.78	0/5555
2	O	1.37	1/296 (0.3%)	2.00	14/451 (3.1%)
2	S	1.26	1/268 (0.4%)	1.84	10/410 (2.4%)
3	P	1.45	0/208	2.35	11/321 (3.4%)
3	T	1.16	0/208	1.54	1/321 (0.3%)
All	All	0.91	9/9166 (0.1%)	0.99	39/12547 (0.3%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	470	SER	CA-CB	-13.07	1.33	1.52
1	B	245	CYS	CB-SG	-8.54	1.67	1.82
1	B	420	CYS	CB-SG	-8.14	1.68	1.82
1	A	372	GLU	CA-CB	-7.65	1.37	1.53
1	A	245	CYS	CB-SG	-6.14	1.71	1.82
1	A	108	CYS	CB-SG	-5.65	1.72	1.81
2	O	-6	DT	C3'-O3'	5.50	1.51	1.44
1	A	131	TYR	CD1-CE1	-5.34	1.31	1.39
2	S	5	DC	C3'-O3'	-5.03	1.37	1.44

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	8	DG	O4'-C1'-N9	15.77	119.04	108.00
3	P	6	DG	O4'-C1'-N9	10.39	115.27	108.00
3	P	1	DG	O4'-C4'-C3'	-10.20	99.88	106.00
3	P	4	DG	N1-C6-O6	-10.08	113.85	119.90
2	S	2	DG	O4'-C1'-N9	-9.61	101.27	108.00
2	O	-1	DT	C5-C4-O4	-9.43	118.30	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	2	DT	C5-C4-O4	-9.16	118.49	124.90
2	O	-1	DT	N3-C4-O4	8.50	125.00	119.90
3	P	1	DG	O4'-C1'-N9	-8.26	102.22	108.00
2	O	4	DT	C4-C5-C7	7.96	123.77	119.00
2	S	10	DC	N3-C4-N4	-7.45	112.79	118.00
2	O	3	DC	C1'-O4'-C4'	-7.30	102.80	110.10
2	S	-1	DT	N3-C2-O2	-7.25	117.95	122.30
2	S	10	DC	C5-C4-N4	7.11	125.18	120.20
3	P	2	DT	N3-C4-O4	6.45	123.77	119.90
1	A	132	ARG	NE-CZ-NH2	-6.32	117.14	120.30
3	P	4	DG	P-O3'-C3'	6.23	127.18	119.70
2	S	0	DG	P-O3'-C3'	6.23	127.17	119.70
3	T	5	DT	C4-C5-C7	6.20	122.72	119.00
2	S	10	DC	N3-C2-O2	-6.12	117.61	121.90
2	O	7	DC	N3-C2-O2	-6.11	117.62	121.90
2	S	1	DT	P-O3'-C3'	6.09	127.00	119.70
1	A	132	ARG	NE-CZ-NH1	5.97	123.29	120.30
2	S	2	DG	N1-C6-O6	-5.92	116.35	119.90
2	O	4	DT	N3-C4-O4	5.82	123.39	119.90
2	O	6	DA	O4'-C1'-N9	-5.77	103.96	108.00
3	P	4	DG	C5-C6-O6	5.68	132.01	128.60
2	O	4	DT	C6-C5-C7	-5.62	119.53	122.90
2	S	4	DT	C1'-O4'-C4'	-5.58	104.52	110.10
1	A	151	ARG	NE-CZ-NH2	-5.43	117.58	120.30
2	O	8	DC	C2-N3-C4	5.40	122.60	119.90
2	S	-1	DT	N1-C2-O2	5.33	127.37	123.10
2	O	10	DC	O4'-C4'-C3'	-5.32	102.37	104.50
3	P	4	DG	C5-C6-N1	5.27	114.13	111.50
2	O	7	DC	N1-C2-O2	5.26	122.06	118.90
3	P	5	DT	O4'-C1'-N1	5.14	111.60	108.00
2	O	0	DG	C6-C5-N7	5.09	133.45	130.40
2	O	6	DA	P-O3'-C3'	5.04	125.75	119.70
2	O	2	DG	C5-C6-N1	5.03	114.02	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3992	0	3993	108	0
1	B	4034	0	4070	112	0
2	O	267	0	152	5	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	234	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (234) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:O	1:A:222:PHE:CD2	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:B:267:THR:HG21	7:B:2059:HOH:O	1.93	0.68
1:A:445:ILE:HD12	1:A:477:GLY:HA2	1.76	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
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
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: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:427:ILE:HG23	1:A:438:VAL:HG23	1.82	0.61
1:A:320:LEU:HD23	1:A:335:TRP:CH2	2.35	0.61
1:B:507:ASP:C	1:B:508:ILE:HG23	2.21	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:395:MET:HE1	1:B:427:ILE:HD13	1.83	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:A:509:ILE:C	1:A:509:ILE:HD12	2.21	0.59
1:B:343:LYS:NZ	1:B:347:ASP:OD2	2.28	0.59
1:A:344:GLU:HA	1:A:344:GLU:OE2	2.03	0.59
1:A:439:ILE:HG12	1:A:468:PHE:CB	2.33	0.58
1:B:507:ASP:O	1:B:508:ILE:HG23	2.02	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:342:LEU:O	1:A:342:LEU:HD23	2.05	0.56
1:A:288:ASN:HD22	1:A:291:LEU:HD11	1.70	0.56
1:A:78:GLN:HE22	1:A:111:TRP:HA	1.69	0.56
1:B:412:CYS:HB3	1:B:481:VAL:HG21	1.87	0.56
4:B:1511:DTP:H8	4:B:1511:DTP:O5'	2.04	0.56
2:O:2:DG:H2''	2:O:3:DC:OP1	2.05	0.56
1:A:319:VAL:CG1	1:A:319:VAL:O	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:B:306:TRP:C	1:B:307:THR:HG23	2.26	0.55
1:A:437:ILE:HD11	1:B:202:ASN:ND2	2.21	0.55
1:B:507:ASP:C	1:B:508:ILE:CG2	2.74	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:B:17:LYS:HZ2	1:B:20:GLU:HG2	1.73	0.53
1:A:181:LEU:HD12	1:A:182:LYS:H	1.72	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:O:0:DG:C2'	2:O:2:DG:OP1	2.56	0.53
1:B:183:LEU:HD22	1:B:187:LEU:HD12	1.90	0.53
1:B:319:VAL:O	1:B:349:LYS:HG2	2.08	0.52
1:B:253:LYS:O	1:B:257:GLY:HA2	2.09	0.52
1:A:216:LYS:O	1:A:243:GLN:NE2	2.39	0.52
1:B:440:PRO:HG3	1:B:503:ILE:HD12	1.91	0.52
1:B:306:TRP:CE3	1:B:306:TRP:HA	2.45	0.52
1:B:303:THR:O	1:B:309:GLY:HA2	2.09	0.52
1:A:363:ASP:OD2	1:A:366:LYS:HG3	2.10	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:345:PHE:CD2	1:A:345:PHE:C	2.83	0.52
1:A:319:VAL:HG12	1:A:319:VAL:O	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:B:508:ILE:O	1:B:508:ILE:CG1	2.30	0.51
1:A:200:ASP:HB3	1:A:203:SER:OG	2.10	0.51
1:A:350:VAL:CG2	1:A:351:LYS:N	2.73	0.51
1:B:306:TRP:HE3	1:B:306:TRP:HA	1.74	0.50
3:T:3:DG:H4'	3:T:4:DG:OP1	2.10	0.50
1:B:489:LYS:HD3	1:B:489:LYS:O	2.11	0.50
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:24:ALA:O	1:A:266:SER:HA	2.13	0.48
1:A:6:TRP:O	1:A:10:ILE:HG12	2.13	0.48
2:O:0:DG:H2''	2:O:2:DG:OP1	2.14	0.48
1:A:395:MET:HE2	1:A:503:ILE:HD11	1.95	0.48
1:B:395:MET:CE	1:B:427:ILE:HD13	2.44	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:439:ILE:O	1:B:439:ILE:HG23	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:52:VAL:HG13	1:A:54:VAL:CG1	2.45	0.47
1:B:17:LYS:HZ3	1:B:20:GLU:HG2	1.79	0.47
4:B:1511:DTP:H1'	3:T:9:DC:H2'	1.96	0.47
1:B:209:PRO:O	1:B:212:ILE:HG22	2.14	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:57:ASN:HD21	1:A:110:SER:CB	2.27	0.47
1:A:391:VAL:CG2	1:A:508:ILE:CD1	2.93	0.47
1:A:255:ILE:HD13	1:A:255:ILE:N	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:362:ILE:O	1:B:364:PRO:HD3	2.16	0.46
1:B:249:ARG:HD2	1:B:262:CYS:HB2	1.98	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:A:306:TRP:O	1:A:307:THR:OG1	2.27	0.45
1:A:509:ILE:O	1:A:509:ILE:HD12	2.16	0.45
1:B:506:PHE:O	1:B:507:ASP:HB2	2.16	0.45
1:B:469:GLN:HB2	1:B:472:GLU:HG2	1.98	0.45
1:B:150:GLU:HG3	1:B:387:SER:O	2.17	0.45
1:A:456:ARG:NH1	3:P:3:DG:OP1	2.48	0.45
1:A:168:MET:HA	1:A:172:ASP:HB2	1.98	0.45
1:B:483:ASP:O	1:B:486:ILE:HB	2.17	0.45
1:B:129:GLU:OE2	1:B:425:SER:HB2	2.17	0.45
1:A:267:THR:HG22	1:A:270:VAL:H	1.81	0.45
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:B:394:SER:HB3	1:B:504:THR:HG22	1.98	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:A:442:THR:CG2	1:A:505:ASN:HB2	2.47	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:S:8:DC:C2'	2:S:9:DA:OP2	2.55	0.43
1:B:11:GLN:HE21	1:B:17:LYS:HB3	1.83	0.43
1:A:405:SER:O	1:A:411:ASP:OD1	2.36	0.43
1:B:412:CYS:O	1:B:416:LEU:HG	2.19	0.43
1:B:136:ARG:HH12	1:B:429:ASP:CG	2.21	0.43
1:A:398:ASN:OD1	1:A:500:SER:HB3	2.18	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:CG1	1:A:392:VAL:O	2.64	0.43
1:A:394:SER:CB	1:A:504:THR:HG22	2.48	0.43
1:A:57:ASN:ND2	1:A:110:SER:CB	2.82	0.43
1:B:195:ILE:HA	1:B:195:ILE:HD12	1.93	0.43
1:B:343:LYS:CG	1:B:367:THR:HG23	2.45	0.42
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:269[A]:ASN:ND2	1:B:269[A]:ASN:H	2.17	0.42
1:B:136:ARG:HD3	1:B:432:GLN:HB3	2.01	0.42
1:A:223:ASN:O	1:A:224:PRO:C	2.56	0.42
1:B:342:LEU:HD13	1:B:371:ALA:HA	2.01	0.42
3:P:2:DT:H2"	3:P:3:DG:N7	2.34	0.42
1:B:268:LYS:HG3	7:B:2060:HOH:O	2.19	0.42
1:A:205:LEU:HB3	1:A:206:PRO:HD2	2.02	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:A:241:GLY:O	1:A:245:CYS:HB2	2.20	0.42
1:B:406:CYS:HA	1:B:411:ASP:HB3	2.00	0.42
1:B:447:LEU:HA	1:B:498:LYS:O	2.20	0.42
1:B:441:ARG:O	1:B:461:VAL:CG1	2.68	0.42
1:A:55:GLN:NE2	1:A:126:VAL:HG21	2.35	0.42
1:B:441:ARG:O	1:B:461:VAL:HG12	2.20	0.42
1:B:352:GLN:HG3	1:B:354:ASP:HB2	2.00	0.42
1:A:52:VAL:HG22	1:A:59:ILE:CG2	2.50	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: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:B:114:ASP:HA	1:B:115:PRO:HD2	1.84	0.41
1:B:76:THR:HG23	1:B:78:GLN:H	1.86	0.41
1:B:6:TRP:O	1:B:10:ILE:HG12	2.20	0.41
1:B:320:LEU:O	1:B:321:ASP:C	2.58	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:269[B]:ASN:ND2	1:B:305:PHE:HD2	2.14	0.40
1:B:114:ASP:C	1:B:114:ASP:OD1	2.60	0.40
2:O:3:DC:H2''	2:O:4:DT:H5'	2.02	0.40
1:A:295:LEU:HB3	1:A:328:ILE:HG21	2.03	0.40
1:A:209:PRO:HG3	7:A:2030:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	507/536 (95%)	490 (97%)	16 (3%)	1 (0%)	56	79
1	B	508/536 (95%)	486 (96%)	22 (4%)	0	100	100
All	All	1015/1072 (95%)	976 (96%)	38 (4%)	1 (0%)	59	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	493	TYR

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	443/478 (93%)	411 (93%)	32 (7%)	21	36
1	B	453/478 (95%)	420 (93%)	33 (7%)	20	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	896/956 (94%)	831 (93%)	65 (7%)	20	36

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

Mol	Chain	Res	Type
1	A	14	SER
1	A	16	SER
1	A	41	MET
1	A	48	GLU
1	A	52	VAL
1	A	136	ARG
1	A	161	LEU
1	A	163	ARG
1	A	188	SER
1	A	214	SER
1	A	228	ASP
1	A	245	CYS
1	A	251	SER
1	A	295	LEU
1	A	303	THR
1	A	321	ASP
1	A	337	ASP
1	A	379	ARG
1	A	392	VAL
1	A	405	SER
1	A	410	VAL
1	A	425	SER
1	A	437	ILE
1	A	442	THR
1	A	443	VAL
1	A	461	VAL
1	A	467	ASN
1	A	469	GLN
1	A	473	LEU
1	A	479	LYS
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

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Mol	Chain	Res	Type
1	B	76	THR
1	B	136	ARG
1	B	161	LEU
1	B	163	ARG
1	B	177	LEU
1	B	183	LEU
1	B	188	SER
1	B	214	SER
1	B	223	ASN
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	451	SER
1	B	461	VAL
1	B	466	ILE
1	B	473	LEU
1	B	486	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) 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	202	ASN
1	A	288	ASN
1	A	330	HIS
1	A	400	ASN
1	A	469	GLN

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Mol	Chain	Res	Type
1	A	505	ASN
1	B	11	GLN
1	B	32	ASN
1	B	57	ASN
1	B	124	HIS
1	B	202	ASN
1	B	223	ASN
1	B	288	ASN
1	B	400	ASN
1	B	505	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 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	A	1510	5	32,32,32	1.32	3 (9%)	50,50,50	1.79	8 (16%)
4	DTP	B	1511	5	32,32,32	1.23	3 (9%)	50,50,50	1.72	8 (16%)
6	CPT	O	1014	2	0,2,4	0.00	-	0,1,6	0.00	-
6	CPT	S	1014	2	0,2,4	0.00	-	0,1,6	0.00	-

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	A	1510	5	-	0/20/34/34	0/1/3/3
4	DTP	B	1511	5	-	0/20/34/34	0/1/3/3
6	CPT	O	1014	2	-	0/0/0/0	0/0/0/0
6	CPT	S	1014	2	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1510	DTP	C4-N9	-3.67	1.32	1.37
4	B	1511	DTP	C4-N9	-3.05	1.33	1.37
4	B	1511	DTP	C5-C4	2.94	1.47	1.40
4	A	1510	DTP	C5-C4	2.87	1.47	1.40
4	B	1511	DTP	PA-O3A	2.27	1.64	1.59
4	A	1510	DTP	C8-N9	-2.00	1.33	1.36

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1511	DTP	N3-C2-N1	-5.84	123.82	128.71
4	B	1511	DTP	N3-C4-N9	5.48	135.32	125.43
4	A	1510	DTP	N3-C2-N1	-5.45	124.15	128.71
4	A	1510	DTP	N3-C4-N9	5.12	134.68	125.43
4	B	1511	DTP	C2'-C1'-N9	-4.63	102.06	114.08
4	A	1510	DTP	C4-C5-N7	-4.18	105.94	109.52
4	A	1510	DTP	C5-C4-N3	-3.58	117.91	125.70
4	A	1510	DTP	C2'-C1'-N9	-3.33	105.42	114.08
4	A	1510	DTP	O3A-PB-O3B	-3.24	95.07	101.66
4	B	1511	DTP	O3G-PG-O2G	3.14	119.82	107.61
4	B	1511	DTP	C5-C4-N3	-3.09	118.97	125.70
4	A	1510	DTP	C2-N3-C4	2.65	121.55	114.01
4	B	1511	DTP	C2-N3-C4	2.43	120.93	114.01
4	B	1511	DTP	O2G-PG-O1G	2.14	117.44	110.44
4	A	1510	DTP	C8-N9-C4	2.04	108.45	106.90
4	B	1511	DTP	O3A-PB-O3B	2.04	105.81	101.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.44	46 (9%) 10 9	21, 38, 84, 105	0
1	B	508/536 (94%)	0.18	7 (1%) 72 74	16, 36, 60, 72	0
2	O	14/17 (82%)	0.80	1 (7%) 16 15	40, 53, 68, 85	0
2	S	12/17 (70%)	0.52	2 (16%) 2 2	43, 63, 74, 83	0
3	P	9/9 (100%)	0.28	1 (11%) 6 6	39, 45, 56, 57	0
3	T	9/9 (100%)	0.54	1 (11%) 6 6	40, 50, 56, 56	0
All	All	1061/1124 (94%)	0.32	58 (5%) 24 24	16, 38, 75, 105	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	364	PRO	6.3
1	A	355	TYR	5.5
1	A	359	THR	5.3
1	A	365	LEU	5.0
1	A	356	ASP	4.7
1	A	342	LEU	4.6
1	B	358	SER	4.5
1	A	335	TRP	4.4
1	A	346	LEU	4.0
1	A	508	ILE	3.9
1	A	354	ASP	3.8
1	A	350	VAL	3.8
1	A	352	GLN	3.7
1	A	351	LYS	3.7
1	A	467	ASN	3.5
1	A	362	ILE	3.5
1	A	345	PHE	3.4
1	A	462	ALA	3.3
1	B	486	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	367	THR	3.2
1	A	466	ILE	3.2
1	B	490	ASN	3.2
1	A	358	SER	3.1
1	A	361	ASN	3.0
1	A	312	LEU	3.0
1	A	316	LEU	2.9
1	A	366	LYS	2.8
1	A	363	ASP	2.7
2	S	1	DT	2.7
1	A	341	GLN	2.7
1	A	178	THR	2.7
1	A	348	ALA	2.7
1	A	311	VAL	2.7
1	A	315	GLU	2.6
1	A	437	ILE	2.5
1	A	371	ALA	2.5
1	A	306	TRP	2.5
1	A	357	ARG	2.4
1	A	465	GLY	2.4
1	A	353	SER	2.4
1	A	344	GLU	2.4
1	A	181	LEU	2.4
1	A	302	ILE	2.3
2	O	-2	DC	2.3
3	T	1	DG	2.3
1	A	375	PHE	2.3
1	A	313	GLY	2.3
1	B	346	LEU	2.2
1	A	374	LEU	2.2
1	A	318	ASP	2.2
1	B	113	GLN	2.2
1	B	508	ILE	2.1
1	A	320	LEU	2.1
3	P	6	DG	2.1
1	A	439	ILE	2.1
1	A	360	SER	2.1
1	B	59	ILE	2.0
2	S	0	DG	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	CA	B	1512	1/1	0.28	3.80	59,59,59,59	1
5	CA	B	1509	1/1	0.15	2.35	41,41,41,41	0
5	CA	B	1515	1/1	0.20	0.28	48,48,48,48	0
5	CA	A	1511	1/1	0.16	-0.20	24,24,24,24	0
5	CA	B	1513	1/1	0.12	-0.65	64,64,64,64	0
4	DTP	A	1510	30/30	0.14	-1.03	19,24,27,29	0
4	DTP	B	1511	30/30	0.12	-1.08	21,26,35,36	0
6	CPT	S	1014	3/5	0.06	-1.83	62,62,64,68	0
5	CA	A	1514	1/1	0.09	-2.40	74,74,74,74	0
5	CA	B	1514	1/1	0.10	-2.42	67,67,67,67	0
5	CA	A	1512	1/1	0.12	-3.04	57,57,57,57	0
5	CA	B	1510	1/1	0.09	-3.15	24,24,24,24	0
5	CA	A	1513	1/1	0.08	-3.97	88,88,88,88	0
6	CPT	O	1014	3/5	0.08	-4.44	45,45,51,55	0

6.5 Other polymers ⓘ

There are no such residues in this entry.