



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:21 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 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

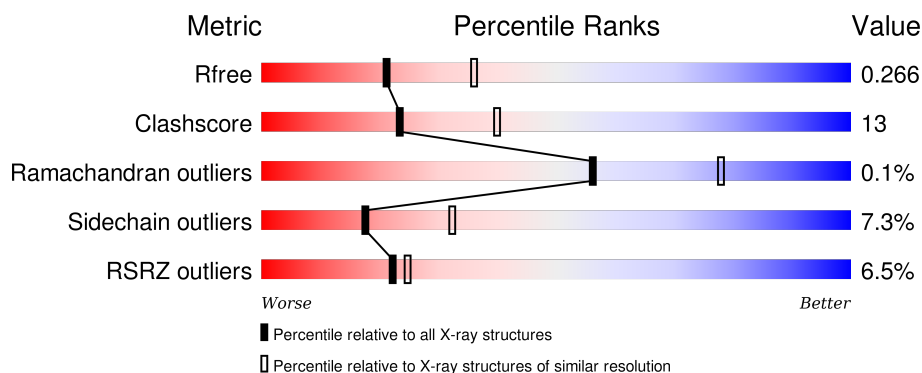
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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. 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	536	<div> <div>10%</div> <div>68%</div> <div>24%</div> <div>5%</div> </div>
1	B	536	<div> <div>2%</div> <div>69%</div> <div>23%</div> <div>5%</div> </div>
2	O	17	<div> <div>6%</div> <div>18%</div> <div>41%</div> <div>24%</div> <div>18%</div> </div>
2	S	17	<div> <div>12%</div> <div>18%</div> <div>41%</div> <div>12%</div> <div>29%</div> </div>
3	P	9	<div> <div>11%</div> <div>22%</div> <div>67%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
3	T	9	 A horizontal bar chart showing the quality of chain T. The bar is divided into three segments: a red segment at the beginning labeled '11%', a green segment in the middle labeled '33%', and a yellow segment at the end labeled '67%'. The segments are stacked horizontally, with the red segment starting from the left, followed by the green segment, and then the yellow segment.

2 Entry composition

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
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			

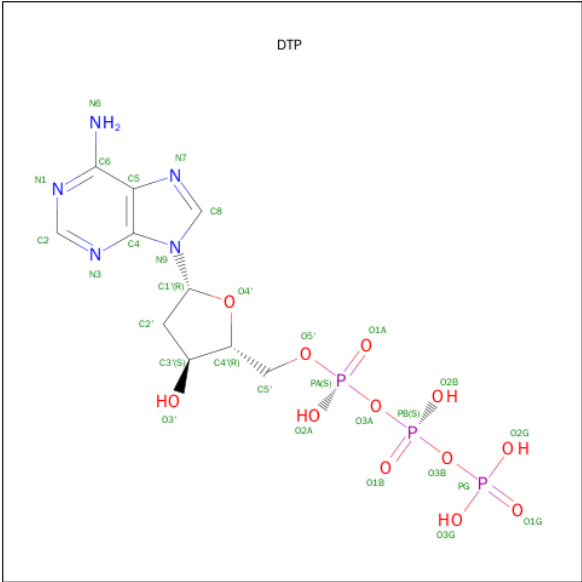
- Molecule 2 is a DNA chain called 5'-D(*TP*CP*TP*TP*CP*TP*GP*TP*GP*CP *TP*C P*AP*CP*CP*AP*CP)-3'.

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).

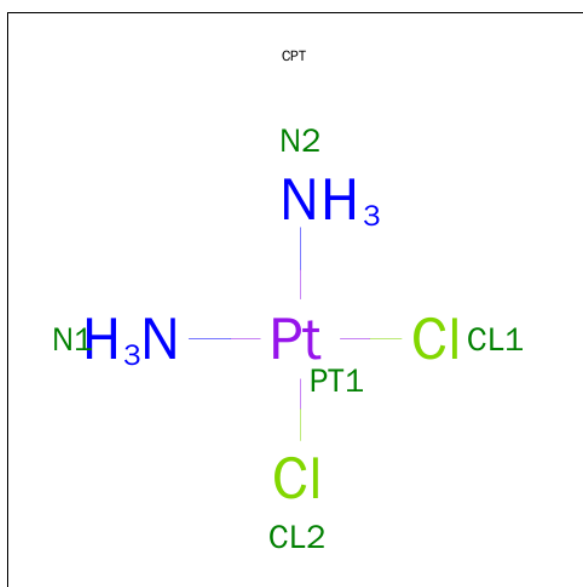


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
4	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- 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		

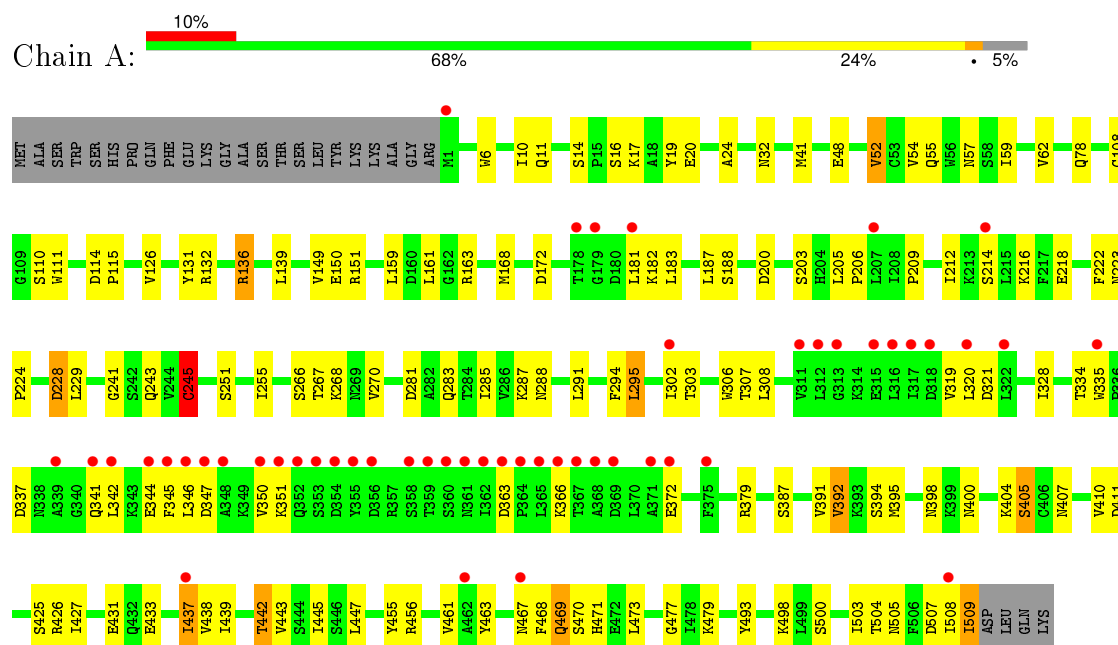
- Molecule 7 is water.

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		

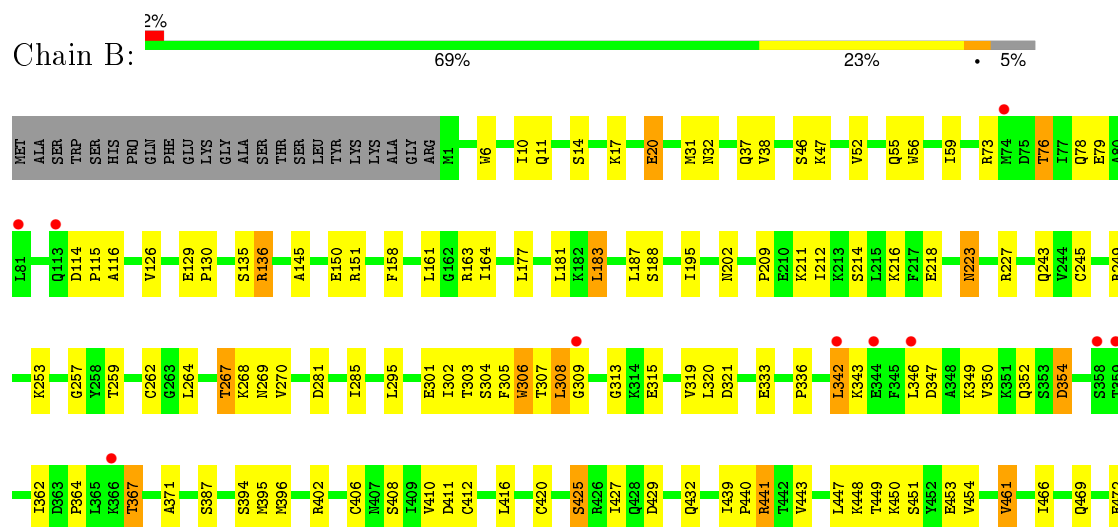
3 Residue-property plots

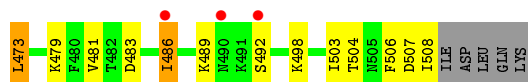
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

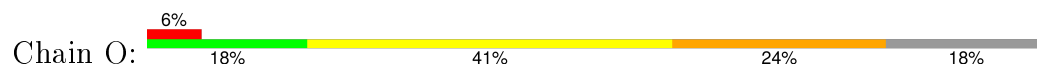


• Molecule 1: DNA POLYMERASE ETA

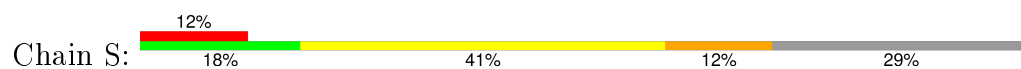




● Molecule 2: 5'-D(*TP*CP*TP*TP*CP*TP*GP*TP*GP*CP *TP*CP*AP*CP*CP*AP*CP)-3',



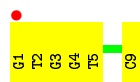
● Molecule 2: 5'-D(*TP*CP*TP*TP*CP*TP*GP*TP*GP*CP *TP*CP*AP*CP*CP*AP*CP)-3',



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



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



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 , 0.266	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)	0.33 , 36.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	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 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	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

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 13.

All (234) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 [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%)	52	75
1	B	508/536 (95%)	486 (96%)	22 (4%)	0	100	100
All	All	1015/1072 (95%)	976 (96%)	38 (4%)	1 (0%)	56	78

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%)	18	33
1	B	453/478 (95%)	420 (93%)	33 (7%)	17	32
All	All	896/956 (94%)	831 (93%)	65 (7%)	17	32

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

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Mol	Chain	Res	Type
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
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
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 [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 carbohydrates 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	A	1510	5	24,32,32	1.21	2 (8%)	32,50,50	1.81	3 (9%)
4	DTP	B	1511	5	24,32,32	1.08	1 (4%)	32,50,50	1.85	4 (12%)
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	-	0/18/34/34	0/3/3/3
4	DTP	B	1511	5	-	0/18/34/34	0/3/3/3
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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1510	DTP	C2-N3	2.17	1.36	1.32
4	A	1510	DTP	C5-C4	2.87	1.47	1.40
4	B	1511	DTP	C5-C4	2.94	1.47	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1511	DTP	N3-C2-N1	-6.62	123.82	128.89
4	A	1510	DTP	N3-C2-N1	-6.20	124.15	128.89
4	B	1511	DTP	C2'-C1'-N9	-4.98	102.06	114.16
4	A	1510	DTP	C4-C5-N7	-3.85	105.94	109.48
4	A	1510	DTP	C2'-C1'-N9	-3.59	105.42	114.16
4	B	1511	DTP	O2G-PG-O1G	2.13	117.44	110.58
4	B	1511	DTP	O3G-PG-O2G	3.27	119.82	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

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

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	509/536 (94%)	0.56	51 (10%) 9 10	21, 38, 84, 105	0
1	B	508/536 (94%)	0.33	13 (2%) 59 63	16, 36, 60, 72	0
2	O	14/17 (82%)	0.91	1 (7%) 19 21	40, 53, 68, 85	0
2	S	12/17 (70%)	0.65	2 (16%) 2 2	43, 63, 74, 83	0
3	P	9/9 (100%)	0.33	1 (11%) 7 7	39, 45, 56, 57	0
3	T	9/9 (100%)	0.65	1 (11%) 7 7	40, 50, 56, 56	0
All	All	1061/1124 (94%)	0.46	69 (6%) 22 25	16, 38, 75, 105	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	364	PRO	7.2
1	A	359	THR	6.3
1	A	365	LEU	5.7
1	B	358	SER	5.6
1	A	355	TYR	4.8
1	A	367	THR	4.8
1	A	350	VAL	4.7
1	A	342	LEU	4.5
1	A	346	LEU	4.3
1	A	354	ASP	4.1
1	A	508	ILE	4.1
1	A	362	ILE	4.1
1	A	335	TRP	3.9
1	A	315	GLU	3.8
1	A	351	LYS	3.7
1	A	356	ASP	3.6
1	A	352	GLN	3.5
1	A	361	ASN	3.4
1	B	486	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	348	ALA	3.4
1	A	363	ASP	3.3
1	A	366	LYS	3.3
2	S	1	DT	3.3
1	A	358	SER	3.2
1	A	312	LEU	3.2
1	A	368	ALA	3.1
1	B	490	ASN	3.1
1	A	316	LEU	3.1
1	A	318	ASP	3.0
1	A	467	ASN	3.0
1	A	371	ALA	2.9
1	A	369	ASP	2.9
1	A	345	PHE	2.9
1	A	360	SER	2.8
2	S	0	DG	2.8
1	B	74	MET	2.8
1	A	178	THR	2.8
1	B	359	THR	2.8
1	A	462	ALA	2.8
1	A	311	VAL	2.7
1	B	346	LEU	2.7
1	B	113	GLN	2.7
1	A	372	GLU	2.7
2	O	-2	DC	2.6
1	A	341	GLN	2.6
3	T	1	DG	2.6
1	A	313	GLY	2.6
1	A	181	LEU	2.6
1	A	320	LEU	2.5
1	B	344	GLU	2.5
1	B	309	GLY	2.5
1	A	339	ALA	2.4
1	B	492	SER	2.4
1	A	344	GLU	2.4
1	B	366	LYS	2.4
1	A	1	MET	2.4
1	A	207	LEU	2.3
1	B	342	LEU	2.3
1	A	375	PHE	2.2
1	A	317	ILE	2.2
1	A	322	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	347	ASP	2.1
1	A	214	SER	2.1
1	B	81	LEU	2.1
1	A	302	ILE	2.1
1	A	437	ILE	2.0
3	P	6	DG	2.0
1	A	179	GLY	2.0
1	A	353	SER	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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	DTP	B	1511	30/30	0.98	0.13	-0.99	21,26,35,36	0
4	DTP	A	1510	30/30	0.98	0.15	-1.27	19,24,27,29	0
5	CA	A	1511	1/1	0.97	0.16	-1.94	24,24,24,24	0
5	CA	B	1510	1/1	0.99	0.10	-4.48	24,24,24,24	0
6	CPT	S	1014	3/5	0.99	0.07	-	62,62,64,68	0
5	CA	A	1513	1/1	0.73	0.10	-	88,88,88,88	0
6	CPT	O	1014	3/5	1.00	0.10	-	45,45,51,55	0
5	CA	B	1513	1/1	0.91	0.15	-	64,64,64,64	0
5	CA	B	1514	1/1	0.83	0.11	-	67,67,67,67	0
5	CA	B	1512	1/1	0.55	0.30	-	59,59,59,59	1
5	CA	A	1514	1/1	0.80	0.09	-	74,74,74,74	0
5	CA	A	1512	1/1	0.82	0.17	-	57,57,57,57	0
5	CA	B	1515	1/1	0.86	0.19	-	48,48,48,48	0
5	CA	B	1509	1/1	0.97	0.15	-	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.