



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2016 – 02:16 AM EDT

PDB ID : 5DDY  
Title : Binary complex of human Polymerase lambda with dCTP  
Authors : Liu, M.S.; Tsai, M.D.  
Deposited on : 2014-08-15  
Resolution : 3.36 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](mailto: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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0122  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

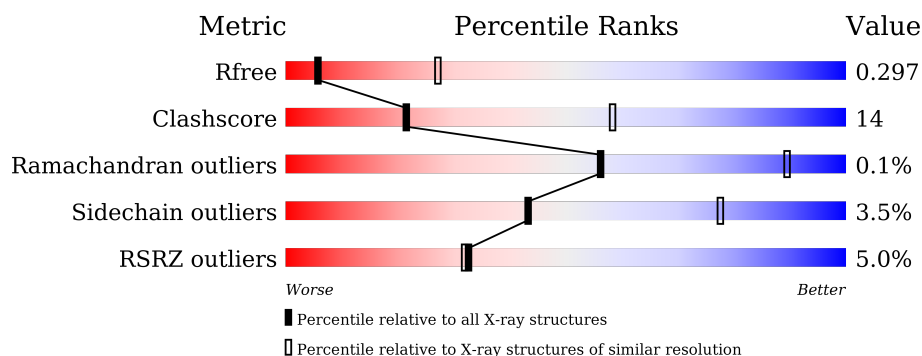
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.36 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	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

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  $\geq 3$ , 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	335	<div> <div>4%</div> <div>77%</div> <div>21%</div> <div>.</div> </div>
1	C	335	<div> <div>%</div> <div>78%</div> <div>19%</div> <div>..</div> </div>
1	E	335	<div> <div>7%</div> <div>56%</div> <div>15%</div> <div>.</div> <div>27%</div> </div>
1	G	335	<div> <div>4%</div> <div>45%</div> <div>26%</div> <div>.</div> <div>27%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9076 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 lambda.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2554	1604	466	472	12			
1	C	327	Total	C	N	O	S	0	0	0
			2553	1600	468	473	12			
1	E	244	Total	C	N	O	S	0	0	0
			1921	1202	355	354	10			
1	G	244	Total	C	N	O	S	0	0	0
			1921	1202	355	354	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	MET	-	expression tag	UNP Q9UGP5
C	241	MET	-	expression tag	UNP Q9UGP5
E	241	MET	-	expression tag	UNP Q9UGP5
G	241	MET	-	expression tag	UNP Q9UGP5

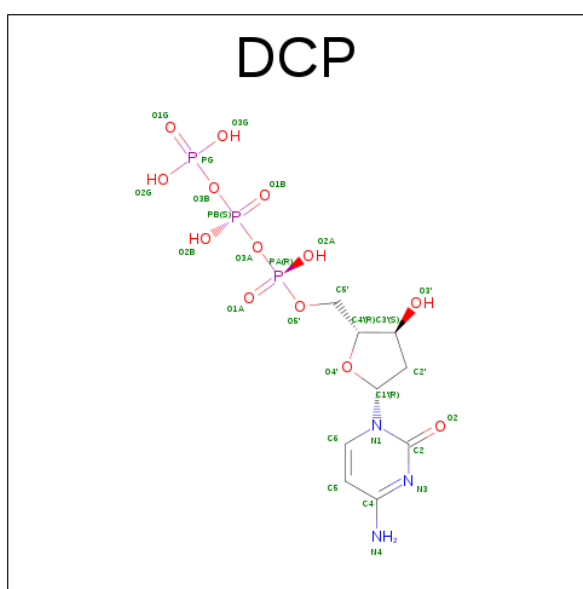
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	2	Total Mn 2 2	0	0
3	A	2	Total Mn 2 2	0	0
3	C	2	Total Mn 2 2	0	0
3	E	2	Total Mn 2 2	0	0

- Molecule 4 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula:  $\text{C}_9\text{H}_{16}\text{N}_3\text{O}_{13}\text{P}_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 28	C 9	N 3	O 13	P 3	0	0
4	C	1	Total 28	C 9	N 3	O 13	P 3	0	0
4	E	1	Total 28	C 9	N 3	O 13	P 3	0	0
4	G	1	Total 28	C 9	N 3	O 13	P 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total O 2 2	0	0

*Continued on next page...*

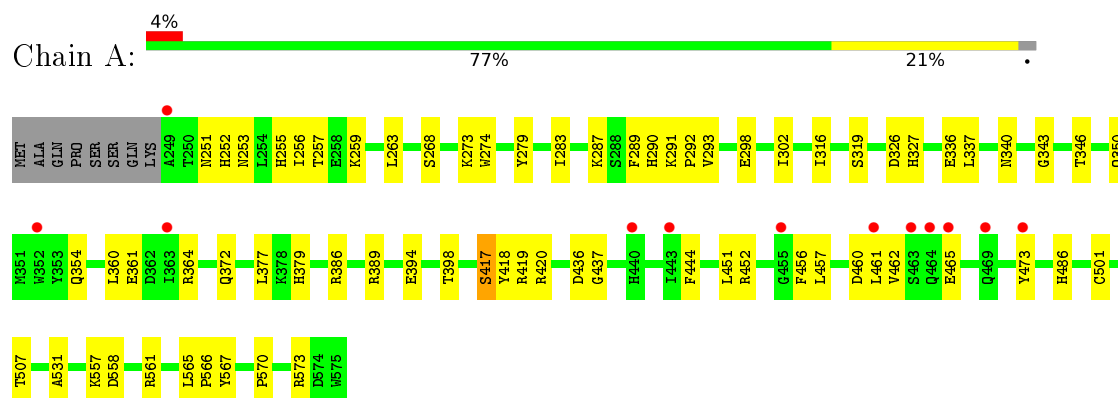
*Continued from previous page...*

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

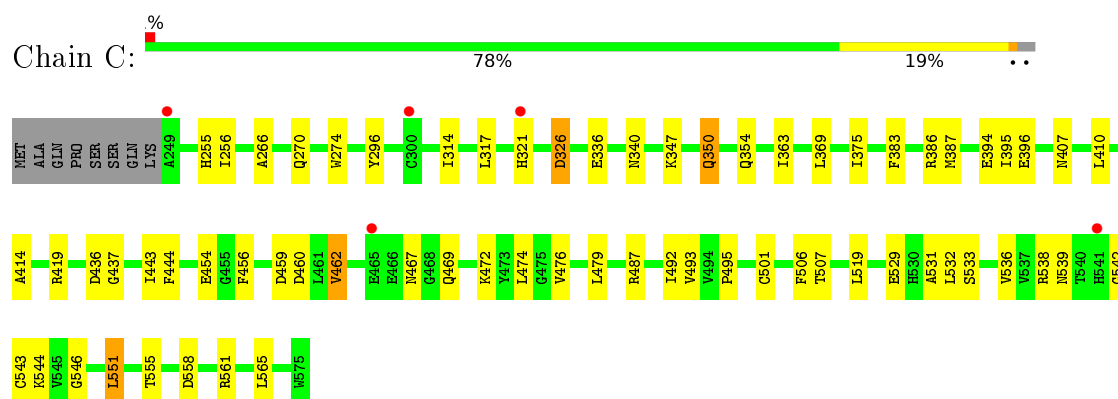
### 3 Residue-property plots [i](#)

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.

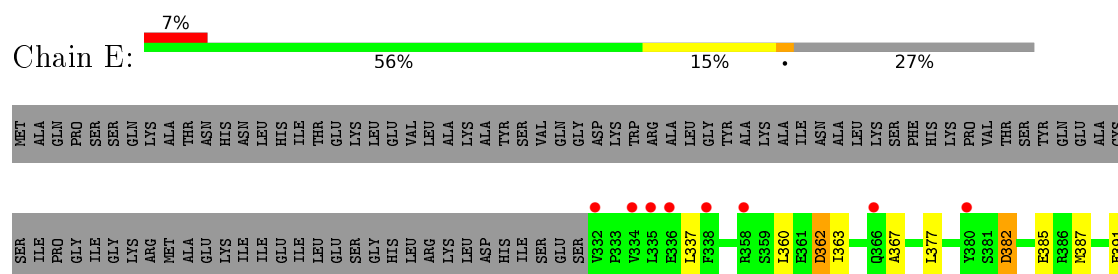
#### • Molecule 1: DNA polymerase lambda

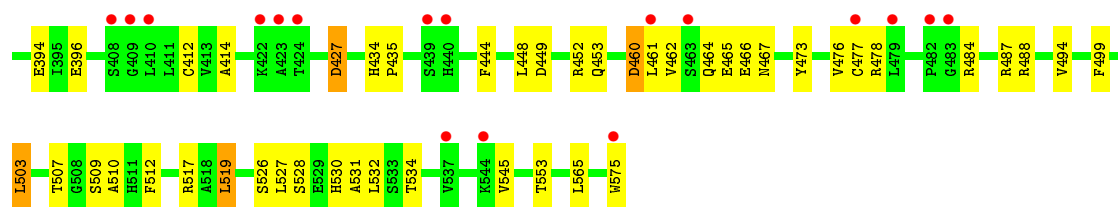


#### • Molecule 1: DNA polymerase lambda

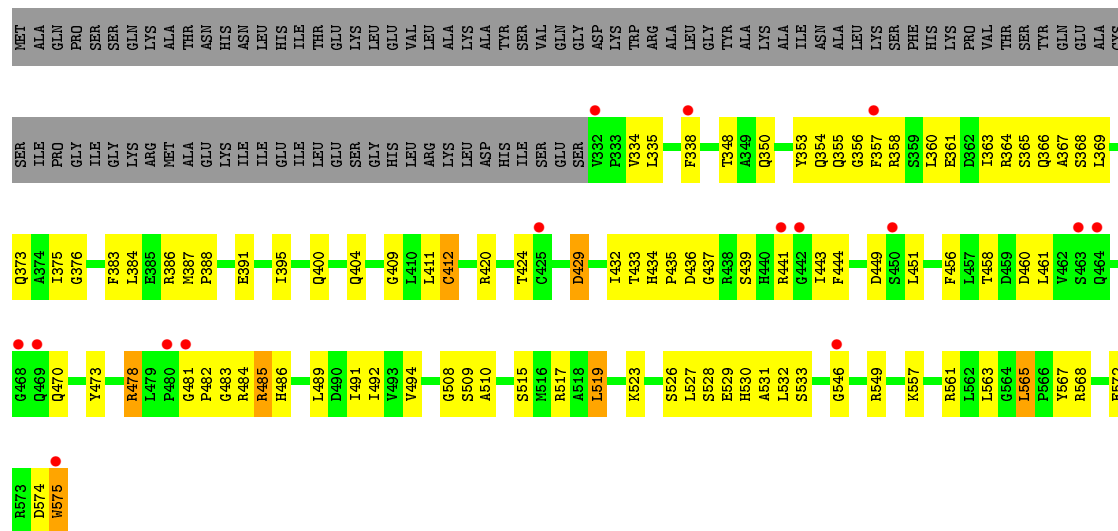


#### • Molecule 1: DNA polymerase lambda





• Molecule 1: DNA polymerase lambda



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	206.01Å 206.01Å 114.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.66 – 3.36 29.66 – 3.36	Depositor EDS
% Data completeness (in resolution range)	90.8 (29.66-3.36) 89.5 (29.66-3.36)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 3.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.262 , 0.297 0.261 , 0.297	Depositor DCC
$R_{free}$ test set	1800 reflections (5.68%)	DCC
Wilson B-factor (Å <sup>2</sup> )	119.3	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 77.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 35395 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9076	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 75.25 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.3091e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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: MG, MN, DCP

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	0.21	0/2606	0.38	0/3519
1	C	0.27	0/2606	0.42	0/3520
1	E	0.22	0/1961	0.41	0/2649
1	G	0.27	0/1961	0.46	0/2649
All	All	0.24	0/9134	0.41	0/12337

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	2554	0	2542	60	0
1	C	2553	0	2524	50	1
1	E	1921	0	1905	44	0
1	G	1921	0	1904	103	1
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	0	0
3	A	2	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2	0	0	0	0
3	E	2	0	0	0	0
3	G	2	0	0	0	0
4	A	28	0	12	3	0
4	C	28	0	12	2	0
4	E	28	0	12	0	0
4	G	28	0	12	4	0
5	A	2	0	0	0	0
5	C	1	0	0	0	0
All	All	9076	0	8923	254	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (254) 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:G:412:CYS:CB	1:G:432:ILE:HD13	1.45	1.46
1:G:412:CYS:CA	1:G:432:ILE:HD13	1.57	1.35
1:G:411:LEU:O	1:G:432:ILE:HD12	1.27	1.28
1:G:411:LEU:C	1:G:432:ILE:CD1	2.19	1.10
1:G:412:CYS:CA	1:G:432:ILE:CD1	2.29	1.09
1:G:412:CYS:HB3	1:G:432:ILE:HD13	1.37	1.06
1:G:366:GLN:N	1:G:366:GLN:OE1	1.90	1.04
1:G:411:LEU:C	1:G:432:ILE:HD12	1.78	1.02
1:G:412:CYS:N	1:G:432:ILE:CD1	2.24	1.00
1:A:290:HIS:CD2	1:A:291:LYS:HG2	1.96	1.00
1:G:353:TYR:O	1:G:358:ARG:NH1	1.96	0.98
1:A:255:HIS:CE1	1:A:256:ILE:HG13	1.99	0.98
1:G:412:CYS:CB	1:G:432:ILE:CD1	2.41	0.98
1:G:434:HIS:CE1	1:G:436:ASP:HB2	1.99	0.97
1:G:411:LEU:O	1:G:432:ILE:CD1	2.13	0.93
1:A:279:TYR:O	1:A:283:ILE:HG13	1.67	0.92
1:G:360:LEU:HD12	1:G:361:GLU:N	1.83	0.92
1:C:539:ASN:OD1	1:C:542:GLY:N	2.07	0.88
1:E:460:ASP:HB3	1:E:473:TYR:HE1	1.36	0.88
1:A:251:ASN:HD21	1:A:257:THR:HG21	1.40	0.86
1:E:526:SER:O	1:E:532:LEU:HD12	1.77	0.84
1:A:379:HIS:CE1	1:A:486:HIS:CD2	2.65	0.84
1:G:412:CYS:HA	1:G:432:ILE:HD13	1.60	0.83
1:G:363:ILE:O	1:G:367:ALA:HB3	1.78	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:528:SER:OG	1:G:531:ALA:O	1.95	0.83
1:E:461:LEU:HD22	1:E:462:VAL:HG23	1.61	0.83
1:A:253:ASN:OD1	1:A:292:PRO:HA	1.80	0.81
1:G:360:LEU:HD13	1:G:364:ARG:NH1	1.95	0.81
1:G:526:SER:O	1:G:532:LEU:HD12	1.81	0.80
1:G:360:LEU:HD13	1:G:364:ARG:HH12	1.44	0.80
1:G:412:CYS:HA	1:G:432:ILE:CD1	2.09	0.80
1:A:253:ASN:O	1:A:257:THR:HG23	1.82	0.80
1:G:411:LEU:C	1:G:432:ILE:HD11	2.01	0.80
1:A:255:HIS:ND1	1:A:256:ILE:HG13	1.96	0.80
1:E:528:SER:OG	1:E:531:ALA:O	2.01	0.79
1:A:379:HIS:CE1	1:A:486:HIS:CG	2.71	0.78
1:G:409:GLY:O	1:G:435:PRO:CD	2.31	0.78
1:C:533:SER:HA	1:C:551:LEU:CD2	2.13	0.78
1:C:539:ASN:OD1	1:C:543:CYS:N	2.17	0.78
1:G:338:PHE:CZ	1:G:363:ILE:HD11	2.20	0.77
1:C:539:ASN:ND2	1:C:543:CYS:HB2	2.00	0.76
1:G:412:CYS:SG	1:G:432:ILE:HD13	2.26	0.76
1:G:409:GLY:O	1:G:435:PRO:HD3	1.86	0.75
1:G:434:HIS:HE1	1:G:436:ASP:HB2	1.48	0.75
1:A:364:ARG:HB2	1:A:377:LEU:HD21	1.68	0.75
1:C:551:LEU:N	1:C:551:LEU:HD22	2.01	0.75
1:E:461:LEU:O	1:E:461:LEU:HD23	1.87	0.74
1:C:532:LEU:O	1:C:551:LEU:HD23	1.88	0.74
1:E:467:ASN:O	1:E:530:HIS:NE2	2.20	0.73
1:A:379:HIS:HE1	1:A:486:HIS:CD2	2.06	0.72
1:A:379:HIS:HE1	1:A:486:HIS:NE2	1.88	0.72
1:E:460:ASP:HB3	1:E:473:TYR:CE1	2.23	0.70
1:A:379:HIS:ND1	1:A:486:HIS:CG	2.60	0.70
1:A:253:ASN:HD21	1:A:293:VAL:HG23	1.56	0.69
1:C:533:SER:HA	1:C:551:LEU:HD22	1.75	0.69
1:G:420:ARG:HH21	1:G:508:GLY:HA3	1.59	0.68
1:C:462:VAL:HG21	1:C:474:LEU:HB2	1.75	0.68
1:G:441:ARG:HD2	1:G:441:ARG:C	2.15	0.67
1:G:412:CYS:HB3	1:G:432:ILE:CD1	2.20	0.67
1:G:412:CYS:N	1:G:432:ILE:HD13	1.98	0.67
1:A:263:LEU:HD11	1:A:336:GLU:HG3	1.76	0.66
1:G:412:CYS:SG	1:G:432:ILE:CD1	2.84	0.66
1:A:291:LYS:HE2	1:A:298:GLU:OE2	1.96	0.66
1:A:274:TRP:HB2	1:C:274:TRP:HB2	1.77	0.66
1:C:336:GLU:O	1:C:340:ASN:ND2	2.30	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:HIS:HE1	1:A:486:HIS:CE1	2.15	0.65
1:G:517:ARG:HG2	1:G:527:LEU:HB3	1.79	0.64
1:A:290:HIS:NE2	1:A:291:LYS:HG2	2.11	0.64
1:G:338:PHE:CE1	1:G:363:ILE:HD11	2.32	0.64
1:E:427:ASP:HB2	1:E:488:ARG:HG3	1.80	0.64
1:A:251:ASN:ND2	1:A:257:THR:HG21	2.12	0.63
1:G:557:LYS:HG3	1:G:567:TYR:CD1	2.32	0.63
1:A:420:ARG:NH1	4:A:603:DCP:O1B	2.28	0.63
1:A:462:VAL:HG11	1:A:465:GLU:HG3	1.81	0.63
1:A:558:ASP:OD1	1:A:561:ARG:NH1	2.31	0.63
1:G:433:THR:OG1	1:G:494:VAL:O	2.14	0.63
1:C:462:VAL:HG11	1:C:474:LEU:H	1.63	0.62
1:G:350:GLN:O	1:G:354:GLN:HG2	1.97	0.62
1:A:364:ARG:HB2	1:A:377:LEU:CD2	2.29	0.62
1:A:372:GLN:HG3	1:A:461:LEU:HD11	1.82	0.61
1:G:355:GLN:OE1	1:G:357:PHE:HE2	1.84	0.61
1:C:407:ASN:HB3	1:C:410:LEU:HG	1.82	0.61
1:A:379:HIS:CE1	1:A:486:HIS:CE1	2.89	0.61
1:C:467:ASN:ND2	1:C:529:GLU:OE2	2.34	0.60
1:E:478:ARG:NH1	1:E:484:ARG:O	2.34	0.60
1:G:420:ARG:NH2	4:G:603:DCP:O3'	2.34	0.60
1:G:368:SER:O	1:G:369:LEU:HD23	2.02	0.60
1:C:386:ARG:NH2	4:C:603:DCP:O3G	2.30	0.60
1:G:375:ILE:HD12	1:G:461:LEU:HD23	1.84	0.60
1:G:420:ARG:HH21	1:G:509:SER:HA	1.66	0.60
1:A:289:PHE:CE1	1:A:302:ILE:HG12	2.37	0.59
1:E:385:GLU:O	1:E:487:ARG:NH1	2.36	0.59
1:A:394:GLU:O	1:A:398:THR:OG1	2.19	0.59
1:C:536:VAL:HG13	1:C:546:GLY:O	2.02	0.59
1:A:337:LEU:HD11	1:A:360:LEU:HD11	1.85	0.59
1:A:451:LEU:HB3	1:A:457:LEU:HD13	1.85	0.58
1:E:461:LEU:C	1:E:461:LEU:HD23	2.22	0.58
1:G:433:THR:HG23	1:G:494:VAL:O	2.03	0.58
1:C:419:ARG:HH11	1:C:507:THR:HG21	1.68	0.58
1:E:466:GLU:HA	1:E:466:GLU:OE1	2.04	0.58
1:C:296:TYR:HB2	1:C:314:ILE:HD11	1.84	0.57
1:G:353:TYR:CG	1:G:358:ARG:NH1	2.73	0.57
1:G:353:TYR:CD1	1:G:358:ARG:NH1	2.73	0.56
1:G:557:LYS:HA	1:G:567:TYR:CE1	2.40	0.56
1:C:532:LEU:O	1:C:551:LEU:CD2	2.54	0.56
1:C:256:ILE:HG12	1:C:317:LEU:HD21	1.86	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:519:LEU:HD11	1:G:515:SER:HA	1.87	0.56
1:G:434:HIS:CD2	1:G:439:SER:HB2	2.41	0.56
1:C:395:ILE:HG23	1:C:456:PHE:HZ	1.72	0.55
1:C:395:ILE:HG12	1:C:479:LEU:HD21	1.89	0.55
1:A:354:GLN:HB3	1:G:561:ARG:CZ	2.37	0.55
1:A:386:ARG:NH2	4:A:603:DCP:O3G	2.39	0.54
1:G:458:THR:HG21	1:G:486:HIS:CD2	2.41	0.54
1:A:361:GLU:OE1	1:A:364:ARG:NH2	2.40	0.54
1:G:523:LYS:NZ	1:G:563:LEU:O	2.32	0.54
1:G:434:HIS:ND1	1:G:436:ASP:HB2	2.22	0.54
1:G:483:GLY:N	1:G:484:ARG:HA	2.22	0.54
1:G:473:TYR:HB3	1:G:491:ILE:HB	1.88	0.54
1:A:251:ASN:HD21	1:A:257:THR:CG2	2.18	0.54
1:E:362:ASP:OD2	1:E:362:ASP:N	2.41	0.53
1:G:519:LEU:HD22	1:G:565:LEU:HD21	1.89	0.53
1:A:570:PRO:HA	1:A:573:ARG:HG2	1.91	0.53
1:C:472:LYS:HG3	1:C:492:ILE:HG13	1.91	0.53
1:G:433:THR:CG2	1:G:494:VAL:O	2.56	0.53
1:C:436:ASP:OD1	1:C:437:GLY:N	2.43	0.52
1:E:509:SER:OG	1:E:510:ALA:N	2.43	0.52
1:E:462:VAL:HG11	1:E:465:GLU:HG3	1.91	0.52
1:A:451:LEU:HD22	1:A:456:PHE:HD2	1.74	0.52
1:C:444:PHE:HB2	1:C:493:VAL:HG21	1.90	0.52
1:E:534:THR:HG21	1:E:545:VAL:HG23	1.91	0.51
1:A:289:PHE:HE1	1:A:302:ILE:HG12	1.76	0.51
1:C:396:GLU:HG3	1:C:414:ALA:HB2	1.91	0.51
1:C:551:LEU:CD2	1:C:551:LEU:N	2.73	0.51
1:G:568:ARG:NH1	1:G:572:GLU:O	2.44	0.51
1:E:394:GLU:OE1	1:E:484:ARG:NH2	2.44	0.50
1:G:354:GLN:HA	1:G:354:GLN:OE1	2.12	0.50
1:G:356:GLY:HA2	1:G:358:ARG:CZ	2.41	0.50
1:G:420:ARG:NH2	4:G:603:DCP:O1B	2.44	0.50
1:A:252:HIS:ND1	1:A:289:PHE:O	2.45	0.50
1:C:469:GLN:CD	1:C:469:GLN:H	2.15	0.50
1:G:529:GLU:HG2	1:G:530:HIS:H	1.76	0.50
1:E:464:GLN:HG2	1:E:465:GLU:N	2.26	0.50
1:G:400:GLN:O	1:G:404:GLN:HG2	2.12	0.49
1:G:334:VAL:HG13	1:G:335:LEU:HD12	1.93	0.49
1:G:365:SER:HB2	1:G:366:GLN:OE1	2.12	0.49
1:A:419:ARG:NH1	1:A:507:THR:OG1	2.45	0.49
1:A:350:GLN:O	1:A:354:GLN:HG2	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:467:ASN:OD1	1:E:530:HIS:CE1	2.66	0.49
1:E:476:VAL:HA	1:E:488:ARG:HA	1.94	0.49
1:C:539:ASN:ND2	1:C:543:CYS:CB	2.73	0.49
1:G:360:LEU:HD12	1:G:360:LEU:C	2.32	0.49
1:A:460:ASP:OD1	1:A:473:TYR:OH	2.21	0.48
1:G:470:GLN:HG3	1:G:530:HIS:HD2	1.78	0.48
1:E:460:ASP:CB	1:E:473:TYR:HE1	2.17	0.48
1:G:444:PHE:CZ	1:G:473:TYR:HB2	2.49	0.48
1:C:506:PHE:O	4:C:603:DCP:H4'	2.14	0.48
1:E:449:ASP:O	1:E:453:GLN:HG2	2.14	0.48
1:G:429:ASP:OD2	1:G:429:ASP:N	2.46	0.48
1:G:434:HIS:ND1	1:G:437:GLY:N	2.60	0.48
1:G:434:HIS:CE1	1:G:436:ASP:CB	2.85	0.47
1:E:363:ILE:HA	1:E:367:ALA:HB3	1.95	0.47
1:A:565:LEU:HD23	1:A:566:PRO:HD2	1.97	0.47
1:A:417:SER:OG	4:A:603:DCP:O3G	2.29	0.47
1:G:412:CYS:N	1:G:432:ILE:HD11	2.17	0.47
1:G:412:CYS:HA	1:G:432:ILE:HD12	1.84	0.47
1:G:451:LEU:HB3	1:G:456:PHE:HD2	1.80	0.47
1:C:555:THR:OG1	1:C:558:ASP:OD2	2.19	0.47
1:A:268:SER:O	1:A:273:LYS:NZ	2.42	0.47
1:C:255:HIS:CD2	1:C:255:HIS:H	2.33	0.47
1:C:539:ASN:HD21	1:C:543:CYS:CB	2.28	0.46
1:E:337:LEU:HD11	1:E:360:LEU:HD11	1.97	0.46
1:E:448:LEU:HD12	1:E:449:ASP:N	2.30	0.46
1:C:533:SER:CA	1:C:551:LEU:CD2	2.90	0.46
1:C:419:ARG:NH1	1:C:507:THR:HG21	2.29	0.46
1:A:389:ARG:NH1	1:A:418:TYR:O	2.35	0.46
1:A:255:HIS:CE1	1:A:256:ILE:CG1	2.86	0.46
1:E:461:LEU:CD2	1:E:462:VAL:HG23	2.40	0.46
1:E:519:LEU:HD23	1:E:565:LEU:HD11	1.98	0.46
1:G:368:SER:C	1:G:369:LEU:HD23	2.35	0.46
1:G:420:ARG:NH1	4:G:603:DCP:O1B	2.45	0.46
1:A:283:ILE:O	1:A:287:LYS:HG3	2.16	0.45
1:C:387:MET:HE2	1:C:487:ARG:HD2	1.98	0.45
1:G:458:THR:HG23	1:G:478:ARG:HB3	1.97	0.45
1:A:326:ASP:HB3	1:A:327:HIS:H	1.53	0.45
1:C:363:ILE:HG22	1:C:369:LEU:HD21	1.97	0.45
1:G:420:ARG:NH2	1:G:508:GLY:HA3	2.30	0.45
4:G:603:DCP:O5'	4:G:603:DCP:H6	2.17	0.45
1:G:338:PHE:CE1	1:G:363:ILE:CD1	3.00	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:529:GLU:HG2	1:G:530:HIS:N	2.32	0.45
1:A:436:ASP:OD1	1:A:437:GLY:N	2.50	0.45
1:G:482:PRO:C	1:G:484:ARG:HA	2.38	0.45
1:G:485:ARG:HG3	1:G:486:HIS:H	1.81	0.45
1:C:266:ALA:O	1:C:270:GLN:HG2	2.17	0.45
1:E:434:HIS:HA	1:E:435:PRO:HD2	1.82	0.45
1:G:420:ARG:NH2	1:G:509:SER:HA	2.32	0.45
1:A:444:PHE:CZ	1:A:473:TYR:HB2	2.52	0.44
1:E:575:TRP:HA	1:G:575:TRP:CH2	2.53	0.44
1:G:456:PHE:O	1:G:478:ARG:N	2.41	0.44
1:G:509:SER:OG	1:G:510:ALA:N	2.49	0.44
1:E:387:MET:HE3	1:E:391:GLU:HG2	1.99	0.44
1:G:441:ARG:O	1:G:441:ARG:HD2	2.17	0.44
1:A:379:HIS:CE1	1:A:486:HIS:ND1	2.85	0.44
1:A:343:GLY:HA3	1:A:372:GLN:HG2	1.99	0.44
1:C:375:ILE:HD12	1:C:459:ASP:HB3	2.00	0.44
1:E:509:SER:H	1:E:512:PHE:HB3	1.82	0.44
1:A:501:CYS:SG	1:A:531:ALA:HA	2.58	0.44
1:G:443:ILE:HD12	1:G:444:PHE:N	2.33	0.44
1:G:348:THR:HG21	1:G:373:GLN:HE22	1.83	0.43
1:G:376:GLY:HA2	1:G:383:PHE:HE2	1.83	0.43
1:G:386:ARG:HG2	1:G:424:THR:HB	2.00	0.43
1:G:481:GLY:HA2	1:G:483:GLY:N	2.33	0.43
1:C:383:PHE:HZ	1:C:476:VAL:HG22	1.84	0.43
1:C:551:LEU:H	1:C:551:LEU:HD22	1.79	0.43
1:E:461:LEU:C	1:E:461:LEU:CD2	2.86	0.43
1:E:382:ASP:N	1:E:382:ASP:OD1	2.51	0.43
1:A:259:LYS:HD3	1:A:316:ILE:CG2	2.47	0.43
1:E:517:ARG:HG2	1:E:527:LEU:HB3	2.01	0.43
1:G:391:GLU:O	1:G:395:ILE:HG13	2.18	0.43
1:A:372:GLN:NE2	1:A:461:LEU:HD21	2.34	0.43
1:E:444:PHE:O	1:E:448:LEU:HG	2.18	0.42
1:G:533:SER:HB2	1:G:549:ARG:O	2.19	0.42
1:G:509:SER:HB2	1:G:574:ASP:HA	2.00	0.42
1:A:336:GLU:O	1:A:340:ASN:ND2	2.37	0.42
1:E:460:ASP:N	1:E:460:ASP:OD1	2.52	0.42
1:G:529:GLU:CG	1:G:530:HIS:N	2.83	0.42
1:A:263:LEU:HD12	1:A:263:LEU:HA	1.85	0.42
1:C:350:GLN:O	1:C:354:GLN:HG2	2.19	0.42
1:E:396:GLU:HG3	1:E:414:ALA:HB2	2.02	0.42
1:C:539:ASN:CG	1:C:543:CYS:H	2.20	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:477:CYS:N	1:E:487:ARG:O	2.53	0.42
1:A:452:ARG:NH2	1:A:460:ASP:OD2	2.46	0.42
1:C:326:ASP:OD1	1:C:326:ASP:N	2.51	0.42
1:A:557:LYS:HG2	1:A:567:TYR:CD1	2.55	0.42
1:C:469:GLN:HG3	1:C:495:PRO:HG2	2.02	0.41
1:C:539:ASN:HD21	1:C:543:CYS:HB2	1.81	0.41
1:C:538:ARG:NE	1:C:544:LYS:HG2	2.36	0.41
1:E:519:LEU:HD22	1:E:565:LEU:HD21	2.03	0.41
1:G:434:HIS:HB3	1:G:437:GLY:HA2	2.02	0.41
1:G:470:GLN:NE2	1:G:530:HIS:HA	2.35	0.41
1:C:410:LEU:HD11	1:C:443:ILE:HG21	2.01	0.41
1:G:451:LEU:O	1:G:456:PHE:HB3	2.21	0.41
1:A:319:SER:HB2	1:A:346:THR:HG21	2.03	0.41
1:G:458:THR:HG21	1:G:486:HIS:NE2	2.36	0.41
1:G:557:LYS:HA	1:G:567:TYR:CD1	2.56	0.41
1:E:499:PHE:O	1:E:503:LEU:HB2	2.21	0.41
1:G:360:LEU:HD12	1:G:361:GLU:CA	2.50	0.40
1:C:519:LEU:HD13	1:C:565:LEU:HD11	2.02	0.40
1:C:501:CYS:SG	1:C:531:ALA:HA	2.62	0.40
1:E:503:LEU:O	1:E:507:THR:OG1	2.34	0.40
1:E:444:PHE:HZ	1:E:473:TYR:HB2	1.86	0.40
1:G:485:ARG:HG3	1:G:486:HIS:N	2.36	0.40
1:C:538:ARG:HH21	1:C:544:LYS:HD3	1.87	0.40
1:E:448:LEU:O	1:E:452:ARG:HG3	2.20	0.40
1:G:546:GLY:HA2	1:G:549:ARG:HG2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:561:ARG:NE	1:G:355:GLN:NE2[3_454]	1.88	0.32

## 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	325/335 (97%)	319 (98%)	6 (2%)	0	100	100
1	C	325/335 (97%)	323 (99%)	2 (1%)	0	100	100
1	E	242/335 (72%)	237 (98%)	5 (2%)	0	100	100
1	G	242/335 (72%)	237 (98%)	4 (2%)	1 (0%)	39	78
All	All	1134/1340 (85%)	1116 (98%)	17 (2%)	1 (0%)	56	89

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	388	PRO

### 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	270/281 (96%)	269 (100%)	1 (0%)	93	97
1	C	269/281 (96%)	260 (97%)	9 (3%)	45	79
1	E	205/281 (73%)	195 (95%)	10 (5%)	31	69
1	G	205/281 (73%)	192 (94%)	13 (6%)	22	61
All	All	949/1124 (84%)	916 (96%)	33 (4%)	43	77

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	417	SER
1	C	321	HIS
1	C	326	ASP
1	C	347	LYS
1	C	350	GLN
1	C	394	GLU
1	C	454	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	460	ASP
1	C	462	VAL
1	C	551	LEU
1	E	362	ASP
1	E	377	LEU
1	E	382	ASP
1	E	412	CYS
1	E	427	ASP
1	E	460	ASP
1	E	494	VAL
1	E	503	LEU
1	E	519	LEU
1	E	553	THR
1	G	384	LEU
1	G	387	MET
1	G	412	CYS
1	G	429	ASP
1	G	449	ASP
1	G	460	ASP
1	G	478	ARG
1	G	485	ARG
1	G	489	LEU
1	G	492	ILE
1	G	519	LEU
1	G	565	LEU
1	G	575	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	379	HIS
1	A	434	HIS
1	C	404	GLN
1	C	407	ASN
1	G	530	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 12 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	DCP	A	603	2	22,29,29	2.05	5 (22%)	28,45,45	1.59	2 (7%)
4	DCP	C	603	3,2	22,29,29	2.05	5 (22%)	28,45,45	1.53	2 (7%)
4	DCP	E	603	2	22,29,29	2.05	5 (22%)	28,45,45	1.77	3 (10%)
4	DCP	G	603	2	22,29,29	2.07	5 (22%)	28,45,45	1.55	3 (10%)

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	DCP	A	603	2	-	0/18/34/34	0/2/2/2
4	DCP	C	603	3,2	-	0/18/34/34	0/2/2/2
4	DCP	E	603	2	-	0/18/34/34	0/2/2/2
4	DCP	G	603	2	-	0/18/34/34	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	DCP	O4'-C4'	-2.58	1.39	1.45
4	G	603	DCP	O4'-C4'	-2.56	1.39	1.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	603	DCP	O4'-C4'	-2.56	1.39	1.45
4	E	603	DCP	O4'-C4'	-2.47	1.39	1.45
4	A	603	DCP	C4-N4	3.16	1.44	1.35
4	C	603	DCP	C4-N4	3.17	1.44	1.35
4	E	603	DCP	C4-N4	3.19	1.44	1.35
4	G	603	DCP	C4-N4	3.25	1.44	1.35
4	C	603	DCP	C2-N3	3.74	1.46	1.38
4	A	603	DCP	C2-N3	3.81	1.46	1.38
4	E	603	DCP	C2-N3	3.82	1.46	1.38
4	G	603	DCP	C2-N3	3.83	1.46	1.38
4	A	603	DCP	C6-N1	4.14	1.41	1.35
4	C	603	DCP	C6-N1	4.19	1.41	1.35
4	E	603	DCP	C6-N1	4.33	1.41	1.35
4	G	603	DCP	C6-N1	4.39	1.41	1.35
4	C	603	DCP	C5-C4	5.45	1.53	1.41
4	A	603	DCP	C5-C4	5.49	1.53	1.41
4	E	603	DCP	C5-C4	5.51	1.53	1.41
4	G	603	DCP	C5-C4	5.52	1.53	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	603	DCP	O3G-PG-O1G	-3.17	100.28	110.63
4	G	603	DCP	O3G-PG-O1G	-2.44	102.65	110.63
4	A	603	DCP	O4'-C1'-N1	3.63	114.06	107.71
4	C	603	DCP	O4'-C1'-N1	3.69	114.16	107.71
4	E	603	DCP	O4'-C1'-N1	4.33	115.28	107.71
4	G	603	DCP	C6-C5-C4	4.33	119.13	117.44
4	G	603	DCP	O4'-C1'-N1	4.37	115.36	107.71
4	C	603	DCP	C6-C5-C4	5.43	119.56	117.44
4	A	603	DCP	C6-C5-C4	5.89	119.75	117.44
4	E	603	DCP	C6-C5-C4	5.97	119.77	117.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	DCP	3	0
4	C	603	DCP	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	603	DCP	4	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	327/335 (97%)	0.09	12 (3%) 45 45	97, 130, 192, 264	0
1	C	327/335 (97%)	0.04	5 (1%) 76 77	94, 127, 182, 247	0
1	E	244/335 (72%)	0.57	25 (10%) 9 9	98, 169, 221, 269	0
1	G	244/335 (72%)	0.49	15 (6%) 25 25	99, 164, 212, 272	0
All	All	1142/1340 (85%)	0.26	57 (4%) 32 32	94, 141, 206, 272	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	332	VAL	7.1
1	A	249	ALA	5.8
1	G	463	SER	4.5
1	G	338	PHE	4.0
1	G	481	GLY	3.7
1	E	482	PRO	3.7
1	E	463	SER	3.6
1	E	366	GLN	3.6
1	C	249	ALA	3.6
1	G	469	GLN	3.4
1	G	332	VAL	3.4
1	E	358	ARG	3.3
1	C	321	HIS	3.3
1	E	422	LYS	3.1
1	E	575	TRP	3.1
1	E	335	LEU	3.0
1	E	439	SER	3.0
1	E	334	VAL	2.9
1	A	352	TRP	2.9
1	E	410	LEU	2.9
1	E	477	CYS	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	425	CYS	2.8
1	G	357	PHE	2.7
1	G	441	ARG	2.7
1	G	546	GLY	2.7
1	E	338	PHE	2.6
1	A	461	LEU	2.6
1	A	440	HIS	2.6
1	A	363	ILE	2.6
1	E	409	GLY	2.5
1	A	463	SER	2.5
1	E	461	LEU	2.5
1	G	575	TRP	2.5
1	G	464	GLN	2.5
1	A	473	TYR	2.5
1	C	465	GLU	2.4
1	A	455	GLY	2.4
1	E	440	HIS	2.3
1	G	468	GLY	2.3
1	G	480	PRO	2.3
1	E	424	THR	2.3
1	E	423	ALA	2.3
1	G	442	GLY	2.3
1	A	443	ILE	2.2
1	A	465	GLU	2.2
1	E	380	TYR	2.2
1	C	300	CYS	2.2
1	A	469	GLN	2.2
1	G	450	SER	2.2
1	E	336	GLU	2.2
1	E	408	SER	2.2
1	E	544	LYS	2.1
1	E	537	VAL	2.1
1	E	483	GLY	2.1
1	E	479	LEU	2.1
1	A	464	GLN	2.0
1	C	541	HIS	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 [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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	MG	C	601	1/1	0.86	0.26	0.13	108,108,108,108	0
4	DCP	A	603	28/28	0.92	0.25	0.08	96,110,122,126	0
4	DCP	C	603	28/28	0.94	0.21	-0.19	97,111,123,133	0
4	DCP	G	603	28/28	0.91	0.23	-0.30	124,150,172,175	0
3	MN	A	604	1/1	0.93	0.22	-0.48	176,176,176,176	0
2	MG	G	601	1/1	0.98	0.20	-0.54	162,162,162,162	0
4	DCP	E	603	28/28	0.91	0.24	-0.55	129,142,177,185	0
3	MN	G	604	1/1	0.77	0.18	-0.84	211,211,211,211	0
2	MG	E	601	1/1	0.90	0.32	-	159,159,159,159	0
3	MN	C	602	1/1	0.94	0.09	-	218,218,218,218	0
3	MN	A	602	1/1	0.92	0.31	-	214,214,214,214	0
2	MG	A	601	1/1	0.98	0.34	-	112,112,112,112	0
3	MN	G	602	1/1	0.94	0.34	-	230,230,230,230	0
3	MN	E	604	1/1	0.59	0.16	-	224,224,224,224	0
3	MN	C	604	1/1	0.85	0.23	-	195,195,195,195	0
3	MN	E	602	1/1	0.95	0.27	-	247,247,247,247	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.