



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 05:46 AM EDT

PDB ID : 2PFQ
Title : Manganese promotes catalysis in a DNA polymerase lambda-DNA crystal
Authors : Garcia-Diaz, M.; Bebenek, K.; Krahn, J.M.; Pedersen, L.C.; Kunkel, T.A.
Deposited on : 2007-04-05
Resolution : 2.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

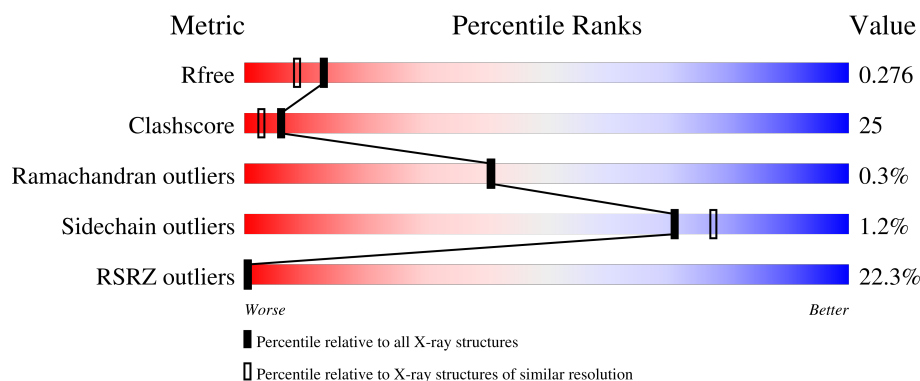
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	T	11	
2	P	7	
3	D	4	
4	A	335	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 3302 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 DNA chain called Template.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	11	Total	C	N	O	P	0	0	0
			225	107	43	65	10			

- Molecule 2 is a DNA chain called Primer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	P	0	2	0
			157	76	29	45	7			

- Molecule 3 is a DNA chain called Downstream Primer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	4	Total	C	N	O	P	0	0	0
			83	38	16	25	4			

- Molecule 4 is a protein called DNA polymerase lambda.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	324	Total	C	N	O	S	0	8	0
			2565	1603	472	479	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	MET	-	initiating methionine	UNP Q9UGP5
A	543	ALA	CYS	engineered mutation	UNP Q9UGP5

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	1
			1	1		

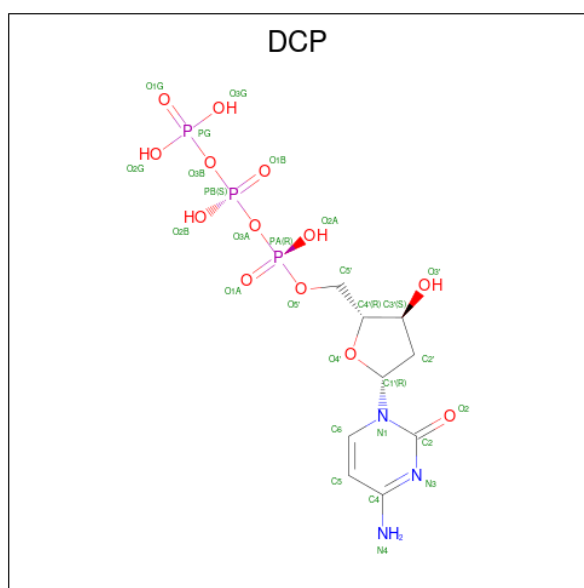
- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Na	0	1
			2	2		

- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Mn	0	2
			2	2		

- Molecule 8 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: C₉H₁₆N₃O₁₃P₃).



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

- Molecule 9 is PYROPHOSPHATE (three-letter code: PPV) (formula: H₄O₇P₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	P	0	1
			9	7	2		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	T	32	Total	O	0	0
			32	32		
10	P	26	Total	O	0	0
			26	26		
10	D	6	Total	O	0	0
			6	6		
10	A	166	Total	O	0	0
			166	166		

3 Residue-property plots

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

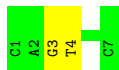
- Molecule 1: Template

Chain T: 




- Molecule 2: Primer

Chain P: 



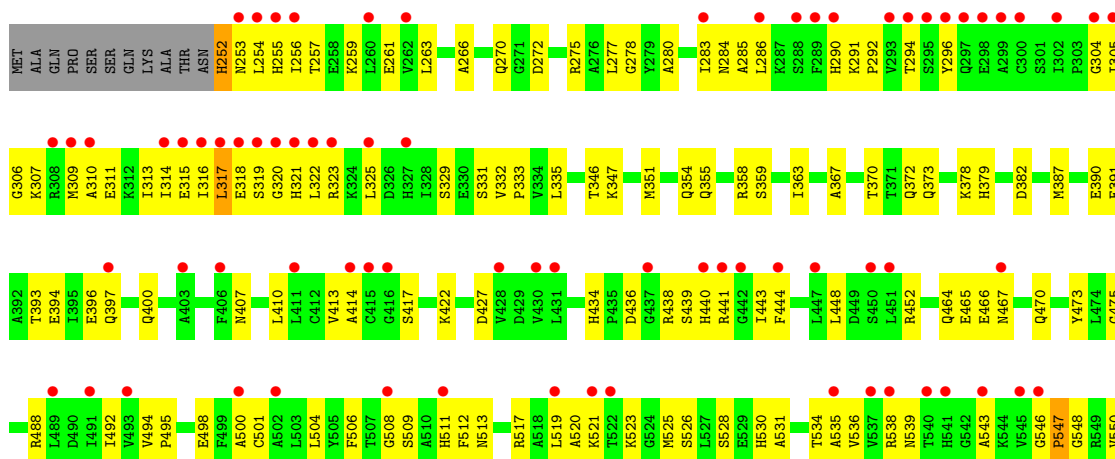
- Molecule 3: Downstream Primer

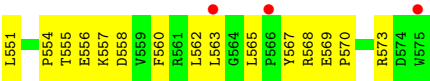
Chain D: 



- Molecule 4: DNA polymerase lambda

Chain A: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.09Å 63.48Å 139.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 36.02 – 2.10	Depositor EDS
% Data completeness (in resolution range)	85.9 (50.00-2.10) 85.7 (36.02-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.256 , 0.287 0.246 , 0.276	Depositor DCC
R_{free} test set	1276 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 64.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3302	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, DCP, PPV, MG, MN

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	T	0.37	0/252	0.86	0/388
2	P	0.47	0/175	0.73	0/267
3	D	0.97	1/92 (1.1%)	0.80	0/138
4	A	0.35	0/2619	0.58	1/3546 (0.0%)
All	All	0.39	1/3138 (0.0%)	0.63	1/4339 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	DG	OP3-P	-7.40	1.52	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	317	LEU	CA-C-N	-6.06	103.88	117.20

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	T	225	0	125	3	0
2	P	157	0	90	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	83	0	45	7	0
4	A	2565	0	2471	141	0
5	A	1	0	0	0	0
6	A	2	0	0	0	0
7	A	2	0	0	0	0
8	A	28	0	11	0	0
9	A	9	0	0	0	0
10	A	166	0	0	15	0
10	D	6	0	0	1	0
10	P	26	0	0	0	0
10	T	32	0	0	2	0
All	All	3302	0	2742	144	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 25.

All (144) 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)
4:A:511[B]:HIS:HE1	10:A:1565:HOH:O	1.16	1.22
4:A:314:ILE:HG22	4:A:318:GLU:OE1	1.53	1.09
3:D:1:DG:H1'	4:A:278:GLY:HA3	1.53	0.88
4:A:314:ILE:O	4:A:318:GLU:HB3	1.80	0.82
4:A:539:ASN:HD21	4:A:543:ALA:HB3	1.45	0.79
4:A:539:ASN:ND2	4:A:543:ALA:HB3	2.02	0.75
4:A:511[B]:HIS:CE1	10:A:1565:HOH:O	2.01	0.75
4:A:256:ILE:HG13	4:A:316:ILE:HD12	1.70	0.74
4:A:314:ILE:CG2	4:A:318:GLU:OE1	2.35	0.72
4:A:520:ALA:HB2	4:A:563:LEU:HD21	1.72	0.72
4:A:316:ILE:HD11	4:A:322:LEU:HD22	1.73	0.69
4:A:396:GLU:HG3	4:A:414:ALA:HB2	1.75	0.68
4:A:519:LEU:HD11	4:A:523:LYS:HE3	1.76	0.68
4:A:296:TYR:CD1	4:A:314:ILE:HD11	2.27	0.68
4:A:254:LEU:CB	4:A:256:ILE:HG22	2.24	0.67
4:A:332:VAL:HB	4:A:333:PRO:HD3	1.79	0.65
4:A:448:LEU:O	4:A:452:ARG:HG3	1.96	0.65
4:A:370:THR:OG1	4:A:373:GLN:HG3	1.97	0.64
4:A:314:ILE:O	4:A:318:GLU:CB	2.45	0.64
4:A:440[A]:HIS:NE2	4:A:495:PRO:HB3	2.12	0.64
4:A:256:ILE:CD1	4:A:313:ILE:HG23	2.28	0.64
4:A:305:ILE:HD12	4:A:305:ILE:N	2.13	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:448:LEU:HB3	4:A:452:ARG:NH1	2.13	0.63
3:D:2:DC:H5'	4:A:306:GLY:H	1.65	0.62
4:A:351:MET:O	4:A:355:GLN:HG3	1.99	0.61
4:A:316:ILE:O	4:A:320:GLY:N	2.34	0.61
4:A:466:GLU:H	4:A:466:GLU:CD	2.05	0.59
4:A:252:HIS:ND1	4:A:292:PRO:HG3	2.16	0.59
4:A:256:ILE:HD11	4:A:313:ILE:HG12	1.86	0.58
4:A:272:ASP:OD1	4:A:275:ARG:HB3	2.04	0.58
4:A:464:GLN:HE21	4:A:467:ASN:HB3	1.68	0.58
10:T:26:HOH:O	4:A:372:GLN:HG3	2.03	0.58
3:D:1:DG:C1'	4:A:278:GLY:HA3	2.31	0.57
4:A:252:HIS:CE1	4:A:254:LEU:CB	2.88	0.57
4:A:513:ASN:O	4:A:517:ARG:HG3	2.05	0.57
4:A:554:PRO:HB2	10:A:1581:HOH:O	2.06	0.56
4:A:438:ARG:O	4:A:441:ARG:HG3	2.05	0.55
4:A:443:ILE:HG13	4:A:444:PHE:N	2.21	0.55
4:A:331:SER:O	4:A:335:LEU:HG	2.06	0.55
4:A:504:LEU:HD12	10:A:1447:HOH:O	2.06	0.55
4:A:315:GLU:O	4:A:319:SER:CB	2.55	0.55
4:A:252:HIS:CG	4:A:292:PRO:HG3	2.42	0.55
4:A:387:MET:HB2	4:A:391:GLU:OE1	2.07	0.55
3:D:2:DC:OP1	4:A:309:MET:HB2	2.07	0.54
4:A:346:THR:HG22	10:A:1459:HOH:O	2.05	0.54
4:A:440[B]:HIS:NE2	4:A:495:PRO:HB3	2.21	0.54
4:A:534:THR:O	4:A:535:ALA:HB3	2.07	0.54
4:A:567:TYR:CD2	4:A:568:ARG:N	2.75	0.54
4:A:256:ILE:HD11	4:A:313:ILE:HA	1.90	0.54
4:A:257:THR:HG22	4:A:286:LEU:HD12	1.90	0.53
4:A:261:GLU:HG3	4:A:283:ILE:HD13	1.90	0.53
1:T:7:DT:H5'	4:A:528:SER:HB2	1.90	0.53
4:A:557:LYS:NZ	4:A:557:LYS:HB2	2.24	0.53
4:A:501:CYS:SG	4:A:531:ALA:HA	2.49	0.53
4:A:253:ASN:O	4:A:253:ASN:ND2	2.42	0.53
4:A:329:SER:C	4:A:331:SER:H	2.11	0.52
4:A:256:ILE:HD12	4:A:313:ILE:HG23	1.90	0.52
4:A:567:TYR:HD2	4:A:568:ARG:H	1.57	0.52
4:A:393:THR:O	4:A:397:GLN:HG2	2.10	0.51
4:A:440[B]:HIS:HD2	10:A:1508:HOH:O	1.93	0.51
4:A:427[A]:ASP:HB3	10:A:1530:HOH:O	2.08	0.51
4:A:554:PRO:HD2	10:A:1581:HOH:O	2.10	0.51
1:T:6:DG:OP1	4:A:521:LYS:HD3	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:464:GLN:HG3	4:A:466:GLU:OE2	2.10	0.51
4:A:436:ASP:O	4:A:438:ARG:HG2	2.10	0.51
4:A:448:LEU:HB3	4:A:452:ARG:HH12	1.75	0.51
4:A:307:LYS:O	4:A:311:GLU:HG3	2.11	0.50
4:A:417:SER:HB2	4:A:422:LYS:HG3	1.93	0.50
4:A:555:THR:HA	10:A:1529:HOH:O	2.11	0.50
4:A:531:ALA:HB1	4:A:550:VAL:HG13	1.94	0.50
2:P:4:DT:P	4:A:347:LYS:HB2	2.52	0.49
4:A:315:GLU:HG2	4:A:321:HIS:O	2.12	0.49
4:A:488:ARG:HB3	4:A:488:ARG:NH1	2.28	0.49
4:A:556:GLU:O	4:A:560:PHE:HD1	1.95	0.49
4:A:498:GLU:HB3	4:A:530:HIS:O	2.13	0.48
4:A:277:LEU:O	4:A:280:ALA:HB3	2.13	0.48
4:A:285:ALA:CB	4:A:305:ILE:HD11	2.43	0.48
4:A:294:THR:HG22	4:A:317:LEU:HD21	1.95	0.48
4:A:396:GLU:OE2	4:A:400:GLN:NE2	2.44	0.48
4:A:570:PRO:HA	4:A:573:ARG:HD2	1.96	0.48
4:A:413:VAL:HG12	4:A:414:ALA:N	2.29	0.47
4:A:296:TYR:HB2	4:A:314:ILE:HD11	1.97	0.47
4:A:534:THR:HG21	4:A:551:LEU:HD21	1.95	0.47
3:D:2:DC:H4'	4:A:304:GLY:O	2.14	0.47
4:A:255:HIS:O	4:A:259:LYS:HG3	2.15	0.47
4:A:427[B]:ASP:HB3	10:A:1530:HOH:O	2.13	0.47
4:A:315:GLU:O	4:A:319:SER:HB2	2.15	0.47
4:A:322:LEU:HD23	4:A:325:LEU:HG	1.97	0.47
4:A:520:ALA:HB1	4:A:525:MET:HB2	1.96	0.47
1:T:2:DG:H5'	10:T:12:HOH:O	2.14	0.47
4:A:464:GLN:O	4:A:470:GLN:HB2	2.15	0.47
4:A:523:LYS:O	4:A:525:MET:HG3	2.15	0.47
4:A:440[B]:HIS:CD2	4:A:495:PRO:HA	2.50	0.46
4:A:569:GLU:O	4:A:573:ARG:HG3	2.16	0.46
4:A:315:GLU:OE1	4:A:323:ARG:HG3	2.15	0.46
4:A:259:LYS:HB3	4:A:325:LEU:HD11	1.97	0.46
4:A:560:PHE:HB3	4:A:565:LEU:O	2.16	0.46
4:A:500:ALA:HB3	10:A:1448:HOH:O	2.14	0.46
10:D:207:HOH:O	4:A:278:GLY:HA2	2.15	0.46
4:A:359:SER:O	4:A:363:ILE:HG12	2.16	0.46
4:A:263:LEU:O	4:A:266:ALA:HB3	2.16	0.46
4:A:257:THR:HG22	4:A:286:LEU:CD1	2.46	0.45
3:D:3:DC:H2''	3:D:4:DG:C8	2.51	0.45
4:A:296:TYR:CG	4:A:314:ILE:HD11	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:558:ASP:O	4:A:562:LEU:HG	2.16	0.45
4:A:284:ASN:ND2	10:A:1565:HOH:O	2.50	0.45
4:A:310:ALA:HA	4:A:313:ILE:HD12	1.99	0.45
4:A:310:ALA:O	4:A:314:ILE:HG13	2.17	0.45
4:A:528:SER:C	4:A:530:HIS:H	2.21	0.44
4:A:546:GLY:O	4:A:547:PRO:O	2.36	0.44
4:A:379:HIS:HB3	4:A:382:ASP:HB2	2.00	0.44
4:A:519:LEU:HD23	4:A:565:LEU:HD11	2.00	0.44
4:A:528:SER:C	4:A:530:HIS:N	2.71	0.44
4:A:390:GLU:O	4:A:394:GLU:HG3	2.18	0.43
4:A:434:HIS:CD2	4:A:439:SER:HB2	2.54	0.43
4:A:256:ILE:HG23	4:A:257:THR:N	2.34	0.43
4:A:538:ARG:HA	4:A:543:ALA:O	2.19	0.43
4:A:526:SER:HB2	4:A:538:ARG:NH2	2.34	0.43
4:A:509:SER:O	4:A:512:PHE:HB3	2.19	0.43
4:A:526:SER:CB	4:A:536:VAL:HG21	2.49	0.43
2:P:3:DG:H2''	2:P:4:DT:O5'	2.20	0.42
4:A:290:HIS:ND1	4:A:291:LYS:N	2.68	0.42
4:A:508:GLY:HA3	4:A:509:SER:HA	1.90	0.42
4:A:494:VAL:HG12	10:A:1496:HOH:O	2.18	0.42
4:A:315:GLU:O	4:A:319:SER:OG	2.36	0.42
4:A:492:ILE:O	4:A:492:ILE:HG13	2.19	0.41
4:A:285:ALA:HB3	4:A:305:ILE:HD11	2.01	0.41
4:A:521:LYS:HZ2	4:A:538:ARG:HE	1.68	0.41
4:A:378:LYS:NZ	10:A:1543:HOH:O	2.52	0.41
4:A:266:ALA:O	4:A:270[B]:GLN:HG3	2.20	0.41
4:A:547:PRO:HB2	4:A:548:GLY:H	1.74	0.41
4:A:254:LEU:C	4:A:256:ILE:N	2.73	0.41
4:A:259:LYS:O	4:A:325:LEU:HD21	2.21	0.41
4:A:358:ARG:HH11	4:A:358:ARG:HG2	1.85	0.41
4:A:390:GLU:HA	10:A:1468:HOH:O	2.20	0.41
4:A:557:LYS:HB2	4:A:557:LYS:HZ2	1.84	0.41
3:D:2:DC:H5''	4:A:306:GLY:N	2.32	0.40
4:A:407:ASN:HB3	4:A:410:LEU:HG	2.03	0.40
4:A:570:PRO:HA	4:A:573:ARG:CD	2.51	0.40
4:A:443:ILE:O	4:A:444:PHE:C	2.58	0.40
4:A:473:TYR:CZ	4:A:475:GLY:HA3	2.56	0.40
4:A:363:ILE:O	4:A:367:ALA:HB3	2.21	0.40
4:A:440[A]:HIS:H	4:A:440[A]:HIS:HD1	1.70	0.40
4:A:448:LEU:HD13	4:A:465:GLU:OE2	2.22	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	
4	A	330/335 (98%)	300 (91%)	29 (9%)	1 (0%)	41	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	547	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	263/280 (94%)	260 (99%)	3 (1%)	73	79

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	252	HIS
4	A	354	GLN
4	A	506	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	252	HIS
4	A	253	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A	464	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 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	$\# Z > 2$
8	DCP	A	1438[B]	6,5	23,29,29	0.90	0	30,45,45	1.22	3 (10%)
9	PPV	A	1439[A]	7	6,8,8	1.24	0	13,13,13	1.31	3 (23%)

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
8	DCP	A	1438[B]	6,5	-	3/19/34/34	0/2/2/2
9	PPV	A	1439[A]	7	-	0/6/6/6	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1438[B]	DCP	C2-N3-C4	3.74	120.13	116.34
8	A	1438[B]	DCP	PB-O3B-PG	-3.32	121.42	132.83
9	A	1439[A]	PPV	P2-OPP-P1	-2.76	123.37	132.83
8	A	1438[B]	DCP	O2G-PG-O1G	2.25	119.48	110.68
9	A	1439[A]	PPV	O12-P2-O22	2.23	119.41	110.68
9	A	1439[A]	PPV	O21-P1-O31	2.18	119.23	110.68

There are no chirality outliers.

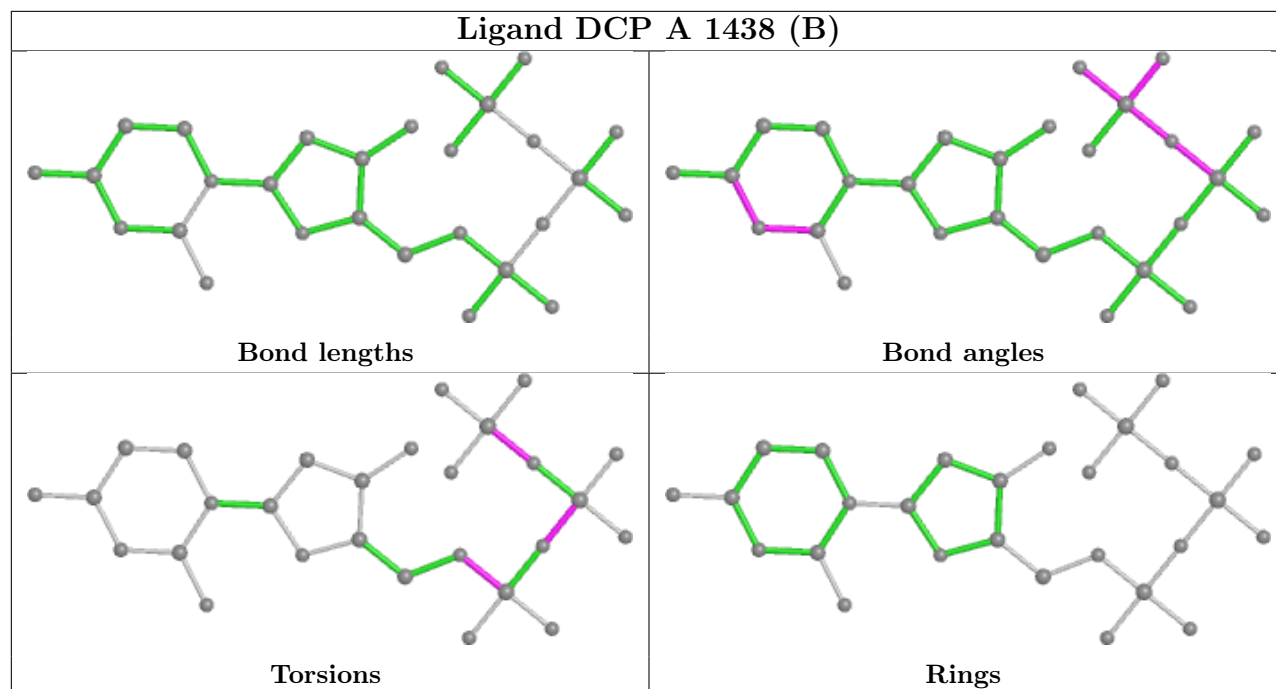
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1438[B]	DCP	PB-O3B-PG-O3G
8	A	1438[B]	DCP	C5'-O5'-PA-O3A
8	A	1438[B]	DCP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9
1	T	11/11 (100%)	0.16	0	100100	26, 31, 42, 48	0
2	P	7/7 (100%)	0.30	0	100100	19, 23, 26, 31	1 (14%)
3	D	4/4 (100%)	0.40	0	100100	45, 47, 51, 54	0
4	A	324/335 (96%)	1.29	77 (23%)	00	15, 47, 96, 110	1 (0%)
All	All	346/357 (96%)	1.22	77 (22%)	00	15, 46, 94, 110	2 (0%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	316	ILE	8.1
4	A	545	VAL	7.1
4	A	319	SER	6.5
4	A	290	HIS	6.0
4	A	296	TYR	5.7
4	A	286	LEU	5.7
4	A	314	ILE	5.4
4	A	289	PHE	5.4
4	A	320	GLY	5.3
4	A	317	LEU	5.1
4	A	318	GLU	4.9
4	A	256	ILE	4.9
4	A	295	SER	4.6
4	A	253	ASN	4.3
4	A	288	SER	4.1
4	A	299	ALA	4.0
4	A	535	ALA	4.0
4	A	500	ALA	3.8
4	A	543	ALA	3.8
4	A	491	ILE	3.6
4	A	321	HIS	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	A	302	ILE	3.5
4	A	255	HIS	3.5
4	A	309	MET	3.4
4	A	283	ILE	3.3
4	A	415	CYS	3.1
4	A	327	HIS	3.1
4	A	441	ARG	3.1
4	A	511[A]	HIS	3.1
4	A	305	ILE	3.0
4	A	467	ASN	3.0
4	A	522	THR	3.0
4	A	537	VAL	2.9
4	A	294	THR	2.9
4	A	310	ALA	2.8
4	A	300	CYS	2.8
4	A	566	PRO	2.8
4	A	254	LEU	2.7
4	A	489	LEU	2.7
4	A	521	LYS	2.7
4	A	411	LEU	2.6
4	A	260	LEU	2.5
4	A	403	ALA	2.5
4	A	575	TRP	2.5
4	A	298	GLU	2.5
4	A	540	THR	2.5
4	A	406	PHE	2.5
4	A	450	SER	2.4
4	A	308	ARG	2.4
4	A	323	ARG	2.3
4	A	325	LEU	2.3
4	A	437	GLY	2.3
4	A	322	LEU	2.3
4	A	431	LEU	2.3
4	A	493	VAL	2.3
4	A	397	GLN	2.3
4	A	447	LEU	2.3
4	A	538	ARG	2.3
4	A	519	LEU	2.2
4	A	440[A]	HIS	2.2
4	A	414	ALA	2.2
4	A	508	GLY	2.2
4	A	546	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	A	428	VAL	2.2
4	A	541	HIS	2.2
4	A	297	GLN	2.1
4	A	442	GLY	2.1
4	A	293	VAL	2.1
4	A	315	GLU	2.1
4	A	444	PHE	2.1
4	A	304	GLY	2.1
4	A	563	LEU	2.1
4	A	430	VAL	2.1
4	A	502	ALA	2.1
4	A	416	GLY	2.1
4	A	262	VAL	2.0
4	A	451	LEU	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

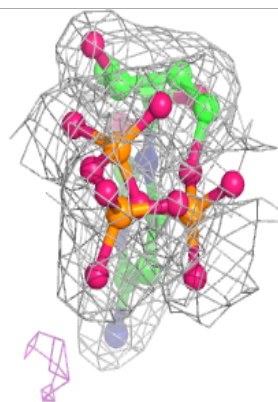
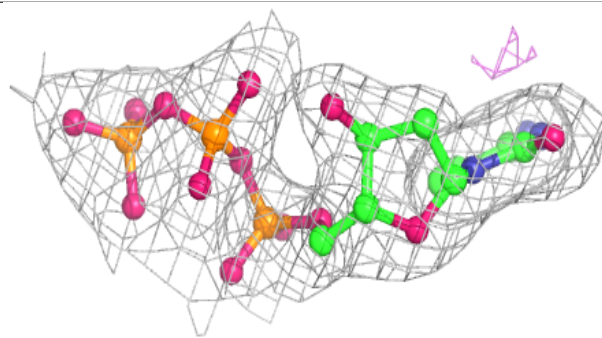
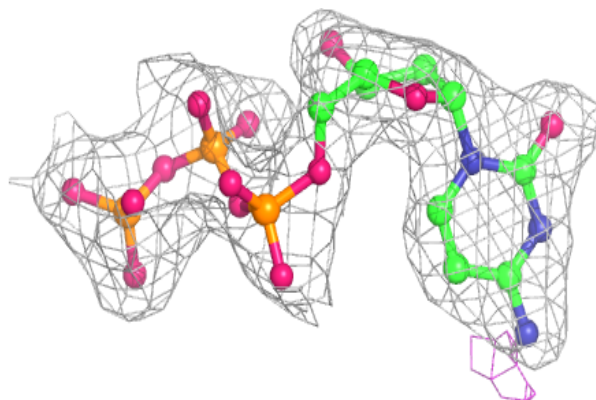
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NA	A	1295[B]	1/1	0.90	0.08	30,30,30,30	1
7	MN	A	1297[A]	1/1	0.90	0.08	42,42,42,42	1
8	DCP	A	1438[B]	28/28	0.92	0.17	26,29,30,31	28
9	PPV	A	1439[A]	9/9	0.94	0.14	49,53,54,54	9
7	MN	A	1296[A]	1/1	0.96	0.09	45,45,45,45	1
5	MG	A	1294[B]	1/1	0.96	0.10	38,38,38,38	1
6	NA	A	1	1/1	0.99	0.09	15,15,15,15	0

The following is a graphical depiction of the model fit to experimental electron density of all

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

Electron density around DCP A 1438 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.