



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:47 AM UTC

PDB ID : 2PFQ / pdb_00002pfq
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

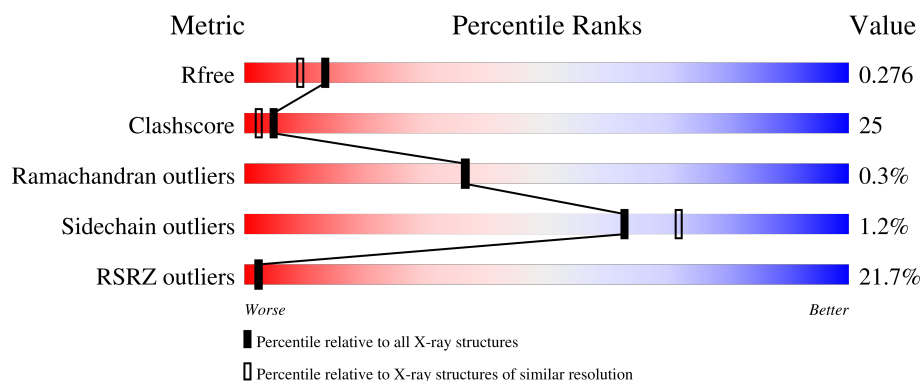
1 Overall quality at a glance

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 (CCD ID: MG) (formula: Mg).

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

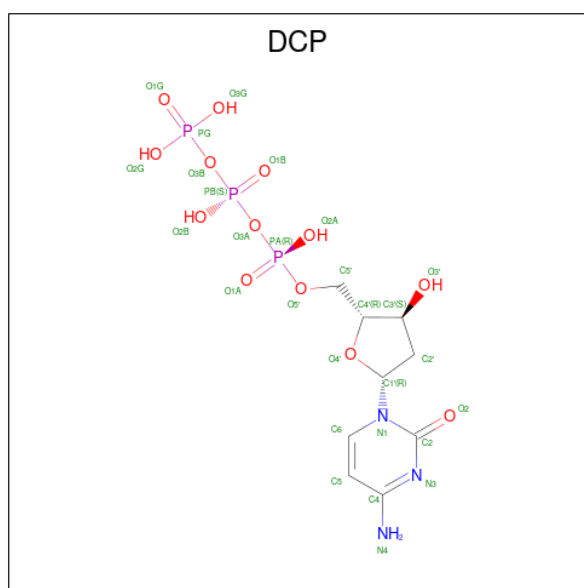
- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 7 is MANGANESE (II) ION (CCD ID: 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 (CCD ID: 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 (CCD ID: 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 [i](#)

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

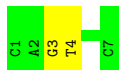
- Molecule 1: Template

Chain T: 

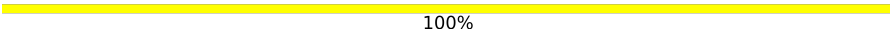


- Molecule 2: Primer

Chain P: 



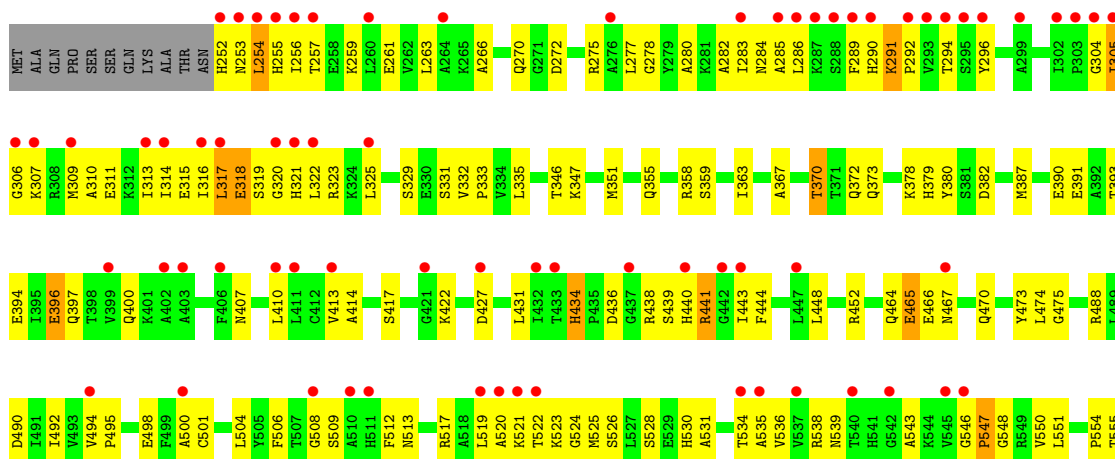
- Molecule 3: Downstream Primer

Chain D: 



- Molecule 4: DNA polymerase lambda

Chain A: 



E556	K557	D558	V559	F560	R561	L562	L563	G564	L565	P566	Y567	R568	E569	P570	A571	E572	R573	D574	W575
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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 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	85.9 (50.00-2.10) 85.8 (50.00-2.10)	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 0.247 , 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)	0.32 , 71.7	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	0.92	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

5.1 Standard geometry

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

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	0.26	0/252	0.69	0/388
2	P	0.31	0/175	0.59	0/267
3	D	0.46	0/92	0.59	0/138
4	A	0.47	3/2619 (0.1%)	0.92	13/3546 (0.4%)
All	All	0.45	3/3138 (0.1%)	0.88	13/4339 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	289	PHE	C-N	5.70	1.41	1.33
4	A	317	LEU	CA-C	-5.46	1.45	1.52
4	A	318	GLU	N-CA	-5.24	1.40	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	291	LYS	CA-C-N	6.65	126.61	119.76
4	A	291	LYS	C-N-CA	6.65	126.61	119.76
4	A	317	LEU	O-C-N	6.58	129.09	122.12
4	A	441	ARG	N-CA-C	6.27	118.81	109.59
4	A	317	LEU	CA-C-O	5.89	126.99	120.63
4	A	254	LEU	N-CA-C	5.86	118.50	110.24
4	A	289	PHE	CA-C-N	5.83	128.36	120.38
4	A	289	PHE	C-N-CA	5.83	128.36	120.38
4	A	396	GLU	N-CA-C	-5.52	105.17	111.07
4	A	291	LYS	O-C-N	5.38	127.50	121.32
4	A	434	HIS	CA-C-N	5.25	125.57	119.47
4	A	434	HIS	C-N-CA	5.25	125.57	119.47
4	A	370	THR	N-CA-C	-5.13	103.63	110.55

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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
3	D	83	0	45	7	0
4	A	2565	0	2471	145	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	13	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	148	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 (148) 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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:466:GLU:H	4:A:466:GLU:CD	2.05	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
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: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:329:SER:C	4:A:331:SER:H	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:282:ALA:CB	4:A:309:MET:HE3	2.41	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:528:SER:C	4:A:530:HIS:H	2.21	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:528:SER:C	4:A:530:HIS:N	2.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:254:LEU:C	4:A:256:ILE:N	2.73	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
4:A:443:ILE:O	4:A:444:PHE:C	2.58	0.45
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:474:LEU:HD22	4:A:490[B]:ASP:CG	2.42	0.44
4:A:546:GLY:O	4:A:547:PRO:O	2.36	0.44
4:A:436:ASP:OD2	4:A:436:ASP:C	2.60	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: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:431:LEU:C	4:A:431:LEU:HD23	2.43	0.43
4:A:522:THR:C	4:A:524:GLY:H	2.27	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:329:SER:C	4:A:331:SER:N	2.77	0.42
4:A:379:HIS:O	4:A:380:TYR:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:254:LEU:C	4:A:256:ILE:H	2.28	0.41
4:A:285:ALA:HB3	4:A:305:ILE:HD11	2.01	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: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
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: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%)	36	36

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%)	65 74

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

Mol	Chain	Res	Type
4	A	305	ILE
4	A	465	GLU
4	A	506	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	253	ASN
4	A	321	HIS
4	A	464	GLN
4	A	471	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
9	PPV	A	1439[A]	7	6,8,8	1.27	0	12,13,13	1.11	2 (16%)
8	DCP	A	1438[B]	6,5	28,29,29	3.02	3 (10%)	41,45,45	0.80	1 (2%)

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
9	PPV	A	1439[A]	7	-	0/6/6/6	-
8	DCP	A	1438[B]	6,5	-	3/22/34/34	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1438[B]	DCP	PB-O3B	-9.26	1.49	1.59
8	A	1438[B]	DCP	PA-O3A	-8.91	1.49	1.59
8	A	1438[B]	DCP	PB-O3A	-8.80	1.50	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1438[B]	DCP	O2G-PG-O1G	2.22	119.48	110.83
9	A	1439[A]	PPV	O12-P2-O22	2.20	119.41	110.83
9	A	1439[A]	PPV	O21-P1-O31	2.16	119.23	110.83

There are no chirality outliers.

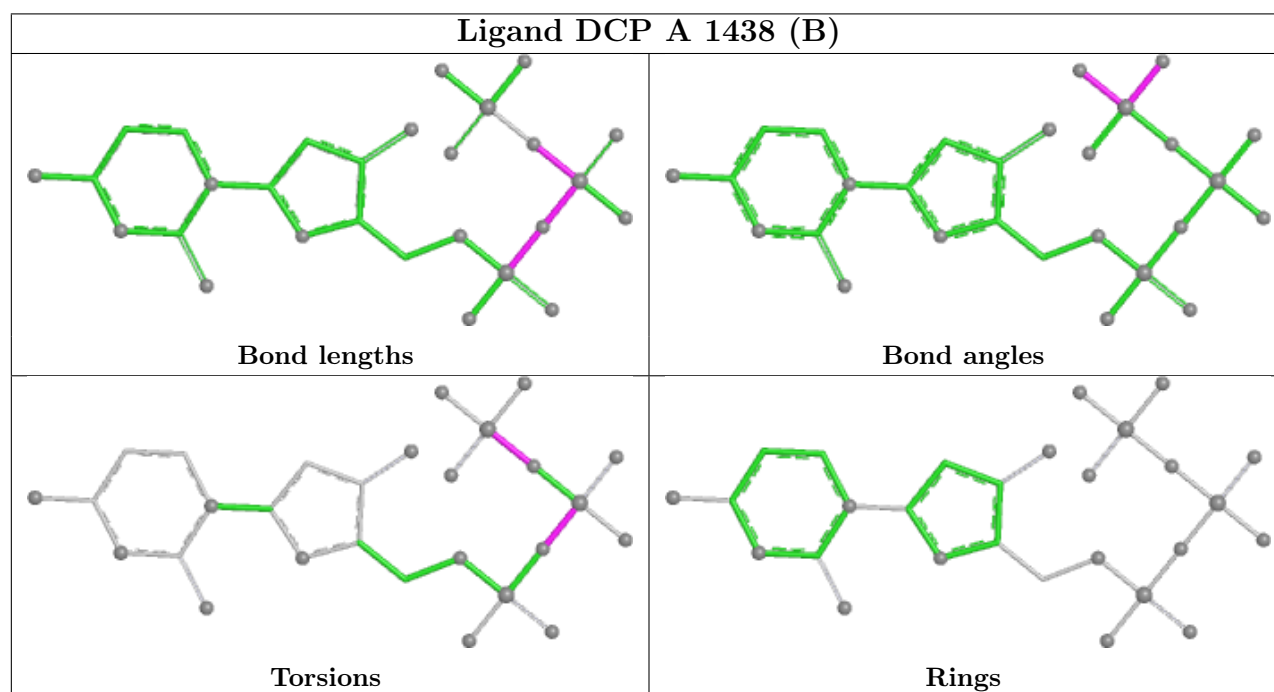
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1438[B]	DCP	PB-O3B-PG-O3G
8	A	1438[B]	DCP	PA-O3A-PB-O1B
8	A	1438[B]	DCP	PA-O3A-PB-O2B

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
1	T	11/11 (100%)	-0.31	0	100	100	26, 31, 42, 48	0
2	P	7/7 (100%)	-0.78	0	100	100	12, 21, 25, 26	2 (28%)
3	D	4/4 (100%)	0.35	0	100	100	45, 47, 51, 54	0
4	A	324/335 (96%)	1.16	75 (23%)	2	2	10, 47, 96, 110	8 (2%)
All	All	346/357 (96%)	1.07	75 (21%)	2	2	10, 46, 94, 110	10 (2%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	286	LEU	5.7
4	A	289	PHE	5.2
4	A	299	ALA	4.3
4	A	256	ILE	4.1
4	A	296	TYR	4.0
4	A	500	ALA	3.9
4	A	511[A]	HIS	3.8
4	A	305	ILE	3.7
4	A	294	THR	3.7
4	A	535	ALA	3.7
4	A	293	VAL	3.7
4	A	253	ASN	3.6
4	A	292	PRO	3.5
4	A	314	ILE	3.5
4	A	303	PRO	3.5
4	A	254	LEU	3.4
4	A	317	LEU	3.4
4	A	304	GLY	3.3
4	A	545	VAL	3.2
4	A	252	HIS	3.2
4	A	537	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
4	A	316	ILE	3.1
4	A	290	HIS	3.1
4	A	575	TRP	3.1
4	A	320	GLY	3.1
4	A	309	MET	3.0
4	A	411	LEU	3.0
4	A	283	ILE	3.0
4	A	406	PHE	2.9
4	A	285	ALA	2.8
4	A	295	SER	2.8
4	A	302	ILE	2.8
4	A	447	LEU	2.8
4	A	403	ALA	2.7
4	A	440[A]	HIS	2.7
4	A	546	GLY	2.7
4	A	264	ALA	2.7
4	A	443	ILE	2.6
4	A	306	GLY	2.6
4	A	567	TYR	2.6
4	A	437	GLY	2.6
4	A	260	LEU	2.6
4	A	410	LEU	2.6
4	A	399	VAL	2.5
4	A	257	THR	2.5
4	A	322	LEU	2.5
4	A	467	ASN	2.5
4	A	313	ILE	2.5
4	A	307	LYS	2.4
4	A	321	HIS	2.4
4	A	520	ALA	2.4
4	A	432	ILE	2.3
4	A	519	LEU	2.3
4	A	427[A]	ASP	2.3
4	A	288	SER	2.3
4	A	540	THR	2.3
4	A	325	LEU	2.3
4	A	542	GLY	2.3
4	A	276	ALA	2.3
4	A	522	THR	2.2
4	A	534	THR	2.2
4	A	413	VAL	2.2
4	A	571	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
4	A	255	HIS	2.2
4	A	442	GLY	2.1
4	A	508	GLY	2.1
4	A	566	PRO	2.1
4	A	494	VAL	2.1
4	A	421	GLY	2.1
4	A	287	LYS	2.1
4	A	402	ALA	2.1
4	A	562	LEU	2.0
4	A	433	THR	2.0
4	A	521	LYS	2.0
4	A	510	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

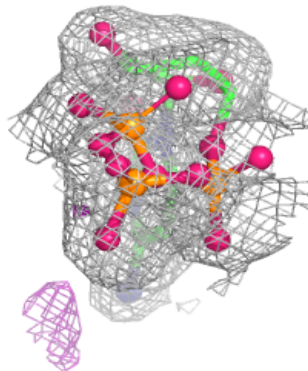
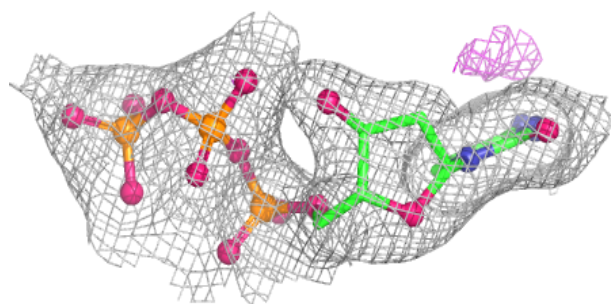
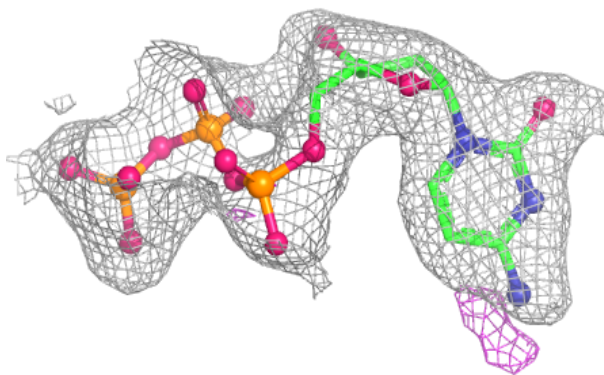
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	PPV	A	1439[A]	9/9	0.92	0.09	49,53,54,54	9
7	MN	A	1297[A]	1/1	0.94	0.05	42,42,42,42	1
8	DCP	A	1438[B]	28/28	0.95	0.07	26,29,30,31	28
6	NA	A	1295[B]	1/1	0.97	0.05	30,30,30,30	1
7	MN	A	1296[A]	1/1	0.98	0.04	45,45,45,45	1
5	MG	A	1294[B]	1/1	0.99	0.04	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.