



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:43 AM UTC

PDB ID : 4DQI / pdb_00004dqi
Title : Ternary complex of Bacillus DNA Polymerase I Large Fragment, DNA duplex, and dCTP (paired with dG of template)
Authors : Wang, W.; Beese, L.S.
Deposited on : 2012-02-15
Resolution : 1.69 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:

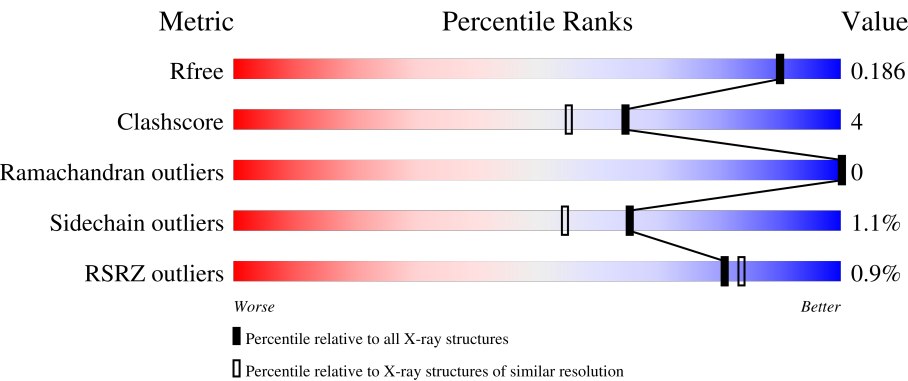
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.69 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	A	592	% 90%7% .
1	D	592	% 90%7% ..
2	B	9	78%11%11%
2	E	9	67%22%11%
3	C	13	92%8%

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Mol	Chain	Length	Quality of chain
3	F	13	85% 8% 8%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 22370 atoms, of which 10238 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 I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	579	Total	C	H	N	O	S	20	16	0
			9534	3001	4810	825	880	18			
1	D	579	Total	C	H	N	O	S	0	39	0
			9750	3065	4924	841	903	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	598	ALA	ASP	engineered mutation	UNP Q5KWC1
A	823	HIS	ARG	SEE REMARK 999	UNP Q5KWC1
D	598	ALA	ASP	engineered mutation	UNP Q5KWC1
D	823	HIS	ARG	SEE REMARK 999	UNP Q5KWC1

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	9	Total	C	H	N	O	P	0	0	0
			274	85	100	29	52	8			
2	E	9	Total	C	H	N	O	P	0	0	0
			274	85	100	29	52	8			

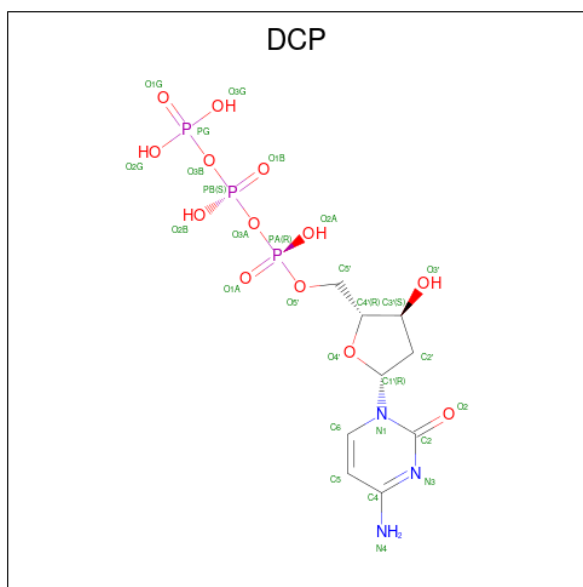
- Molecule 3 is a DNA chain called DNA (5'-D(*C*AP*TP*GP*GP*GP*AP*GP*TP*CP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	12	Total	C	H	N	O	P	0	0	0
			385	119	134	52	69	11			
3	F	12	Total	C	H	N	O	P	0	0	0
			385	119	134	52	69	11			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

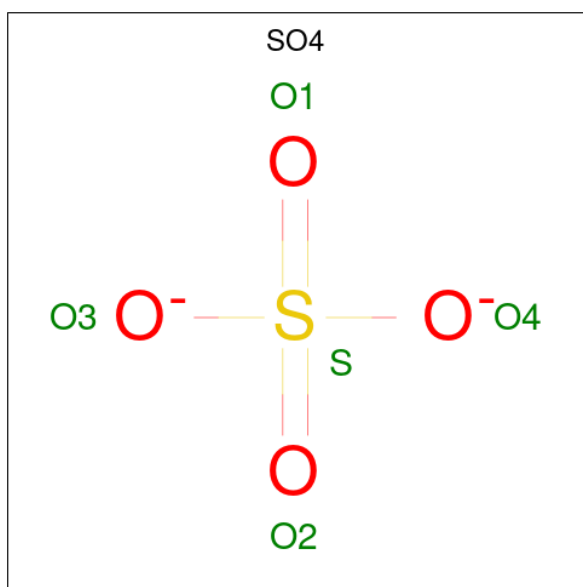
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

- Molecule 5 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (CCD ID: DCP) (formula: $C_9H_{16}N_3O_{13}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	0	0
			40	9	12	3	13	3		
5	A	1	Total	C	H	N	O	P	0	0
			40	9	12	3	13	3		
5	D	1	Total	C	H	N	O	P	0	0
			40	9	12	3	13	3		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

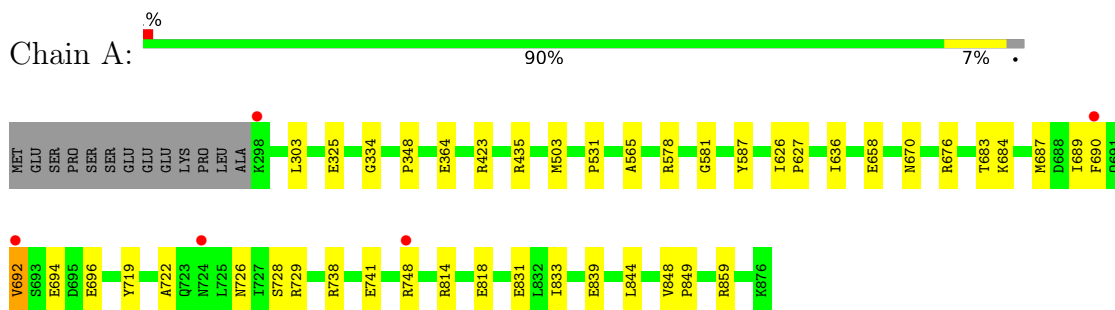
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	583	Total	O	0	0
			583	583		
7	D	820	Total	O	0	0
			820	820		
7	B	38	Total	O	0	0
			38	38		
7	C	77	Total	O	0	0
			77	77		
7	E	40	Total	O	0	0
			40	40		
7	F	78	Total	O	0	0
			78	78		

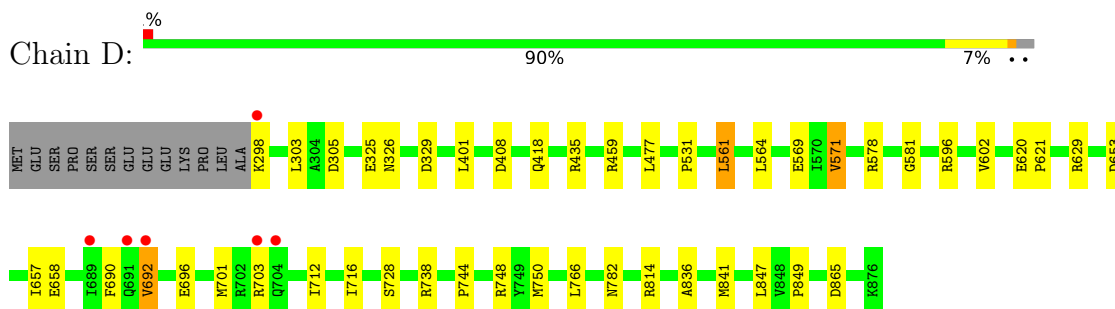
3 Residue-property plots

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.

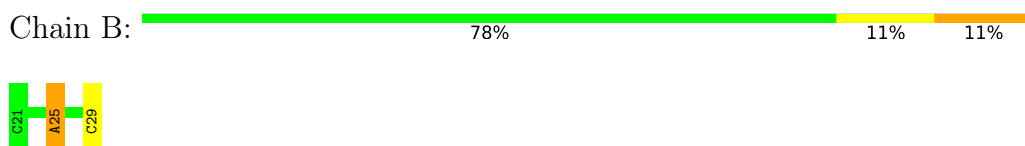
- Molecule 1: DNA polymerase I



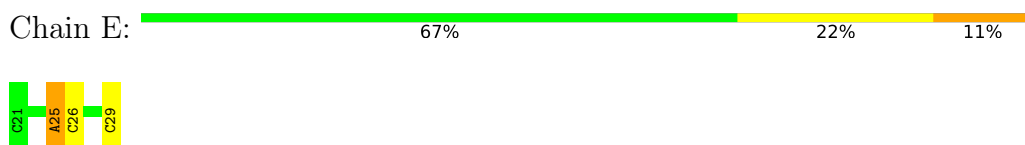
- Molecule 1: DNA polymerase I



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



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



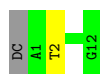
- Molecule 3: DNA (5'-D(*C*AP*TP*GP*GP*GP*AP*GP*TP*CP*AP*GP*G)-3')

Chain C:  92% 8%



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

Chain F:  85% 8% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.68Å 109.36Å 150.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.77 – 1.69 28.77 – 1.69	Depositor EDS
% Data completeness (in resolution range)	86.0 (28.77-1.69) 86.0 (28.77-1.69)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 1.69Å)	Xtriage
Refinement program	PHENIX dev_1026	Depositor
R, R_{free}	0.158 , 0.185 0.159 , 0.186	Depositor DCC
R_{free} test set	6645 reflections (4.48%)	wwPDB-VP
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22370	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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: SO4, DCP, MG, DOC

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	0.57	0/4882	0.74	3/6594 (0.0%)
1	D	0.68	0/5058	0.80	0/6838
2	B	0.48	0/173	1.32	1/264 (0.4%)
2	E	0.59	0/173	1.54	4/264 (1.5%)
3	C	0.50	0/283	1.01	0/437
3	F	0.55	0/283	1.13	0/437
All	All	0.62	0/10852	0.82	8/14834 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	25	DA	C5'-C4'-C3'	8.36	127.45	114.90
2	E	25	DA	P-O5'-C5'	8.09	132.14	120.00
2	E	26	DC	N1-C1'-C2'	-6.73	103.41	113.50
2	B	25	DA	C5'-C4'-C3'	6.54	124.72	114.90
1	A	565	ALA	CA-C-N	-5.58	114.07	119.87
1	A	565	ALA	C-N-CA	-5.58	114.07	119.87
1	A	859	ARG	N-CA-C	-5.57	106.25	113.16
2	E	25	DA	C2'-C3'-O3'	-5.08	103.88	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	4724	4810	4737	34	0
1	D	4826	4924	4751	43	0
2	B	174	100	103	2	0
2	E	174	100	103	2	0
3	C	251	134	136	0	0
3	F	251	134	136	3	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	A	56	24	24	1	0
5	D	28	12	12	0	0
6	A	5	0	0	0	0
6	D	5	0	0	0	0
7	A	583	0	0	13	4
7	B	38	0	0	0	0
7	C	77	0	0	0	0
7	D	820	0	0	25	4
7	E	40	0	0	0	0
7	F	78	0	0	3	0
All	All	12132	10238	10002	80	4

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 4.

All (80) 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:D:298:LYS:NZ	7:D:1768:HOH:O	1.96	0.97
3:F:2:DT:O4	7:F:169:HOH:O	1.83	0.97
1:A:839:GLU:OE1	7:A:1424:HOH:O	1.94	0.86
3:F:2:DT:C4	7:F:169:HOH:O	2.30	0.83
1:D:750:MET:HG3	7:D:1764:HOH:O	1.80	0.79
1:D:782:ASN:HB2	7:D:1781:HOH:O	1.82	0.78
1:A:626:ILE:HG23	1:A:636[B]:ILE:HD11	1.68	0.76
1:D:865:ASP:OD2	7:D:1275:HOH:O	2.03	0.76
1:A:325:GLU:OE2	7:A:1463:HOH:O	2.05	0.74
1:D:782:ASN:CB	7:D:1781:HOH:O	2.34	0.74
1:D:408:ASP:OD1	7:D:1249:HOH:O	2.07	0.72
1:D:602[B]:VAL:HG11	1:D:621:PRO:HG3	1.74	0.70
1:D:561:LEU:O	1:D:571[A]:VAL:HG11	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:TYR:HB3	1:A:636[B]:ILE:HD13	1.75	0.69
1:A:696:GLU:OE2	7:A:1510:HOH:O	2.11	0.69
1:D:581:GLY:HA3	7:D:1743:HOH:O	1.92	0.69
1:D:325:GLU:OE1	7:D:1751:HOH:O	2.10	0.69
1:D:435:ARG:NH1	7:D:1816:HOH:O	2.17	0.68
1:D:766:LEU:HD23	7:D:1707:HOH:O	1.93	0.68
1:A:738:ARG:NE	7:A:1376:HOH:O	2.22	0.66
1:A:627:PRO:HD2	1:A:636[B]:ILE:HD11	1.78	0.64
3:F:2:DT:N3	7:F:169:HOH:O	2.24	0.64
1:A:676:ARG:NH1	7:A:1186:HOH:O	2.32	0.63
1:A:814:ARG:NH1	1:A:818:GLU:OE2	2.32	0.62
1:D:459[A]:ARG:NH2	7:D:1300:HOH:O	2.33	0.61
1:A:581:GLY:HA3	7:A:1563:HOH:O	2.00	0.61
1:A:503[B]:MET:HE1	1:A:636[B]:ILE:HG22	1.84	0.59
1:D:692:VAL:HG11	1:D:701:MET:HE1	1.85	0.59
1:A:692:VAL:HG13	1:A:696:GLU:HB2	1.85	0.58
1:D:703:ARG:NE	7:D:1742:HOH:O	2.21	0.57
1:D:782:ASN:OD1	7:D:1781:HOH:O	2.17	0.56
1:A:364:GLU:HG2	7:A:1522:HOH:O	2.06	0.56
1:D:561:LEU:HB3	1:D:571[A]:VAL:HG13	1.87	0.56
1:D:782:ASN:CG	7:D:1781:HOH:O	2.48	0.55
1:A:578:ARG:NH1	2:B:25:DA:H5"	2.23	0.54
1:D:703:ARG:NH2	7:D:1742:HOH:O	2.37	0.54
1:A:848:VAL:HB	1:A:849:PRO:HD3	1.90	0.53
1:D:814:ARG:NH2	1:D:847[A]:LEU:HD13	2.23	0.53
1:D:435:ARG:NH2	7:D:1280:HOH:O	2.42	0.53
1:D:305:ASP:CG	7:D:1795:HOH:O	2.52	0.52
1:D:418:GLN:NE2	7:D:1337:HOH:O	2.26	0.52
1:A:423:ARG:NE	7:A:1479:HOH:O	2.43	0.51
1:A:738:ARG:O	1:A:741:GLU:HG2	2.10	0.51
1:D:578:ARG:NH1	2:E:25:DA:H5"	2.26	0.51
1:A:435:ARG:NH1	7:A:1417:HOH:O	2.44	0.50
1:D:738:ARG:HD3	7:D:1808:HOH:O	2.11	0.50
1:D:653:ASP:HB2	7:D:1741:HOH:O	2.13	0.48
1:D:744:PRO:O	1:D:748[A]:ARG:HG3	2.12	0.48
1:A:831:GLU:HB3	7:A:1534:HOH:O	2.13	0.48
1:A:719:TYR:OH	7:A:1287:HOH:O	2.19	0.47
1:D:305:ASP:OD1	7:D:1795:HOH:O	2.20	0.47
1:D:329:ASP:OD2	1:D:596:ARG:NH2	2.48	0.47
1:A:587:TYR:HB3	1:A:636[B]:ILE:CD1	2.44	0.46
1:D:712:ILE:HA	1:D:716:ILE:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:629:ARG:NH1	7:D:1685:HOH:O	2.38	0.45
1:A:627:PRO:HD2	1:A:636[B]:ILE:CD1	2.44	0.45
1:D:326:ASN:HD22	1:D:620[A]:GLU:CD	2.25	0.45
1:D:690:PHE:CB	1:D:701:MET:HE3	2.47	0.45
1:D:459[C]:ARG:HG2	7:D:1300:HOH:O	2.16	0.45
1:A:683:THR:HG22	1:A:687:MET:HE2	1.99	0.45
1:D:418:GLN:HA	7:D:1239:HOH:O	2.17	0.44
1:A:325:GLU:H	1:A:325:GLU:CD	2.25	0.44
1:A:658:GLU:CD	5:A:902:DCP:H2'2	2.42	0.43
1:D:657:ILE:HG23	1:D:658:GLU:N	2.34	0.43
1:A:687:MET:HE2	1:A:694:GLU:HG3	2.01	0.43
1:D:569:GLU:CD	7:D:1404:HOH:O	2.62	0.43
1:A:748[A]:ARG:HG2	7:A:1402:HOH:O	2.19	0.43
1:D:531:PRO:HG3	2:E:25:DA:H5'	2.01	0.43
1:A:334:GLY:HA2	1:A:348:PRO:HD3	2.00	0.42
1:D:564:LEU:HB2	1:D:571[A]:VAL:HG21	2.00	0.42
1:A:689:ILE:HG13	1:A:690:PHE:CD1	2.54	0.42
1:D:401:LEU:HD23	1:D:401:LEU:HA	1.91	0.42
1:A:684:LYS:HA	1:A:687:MET:HE3	2.01	0.42
1:A:833:ILE:N	1:A:833:ILE:HD12	2.34	0.42
1:A:531:PRO:HG3	2:B:25:DA:H5'	2.01	0.41
1:D:692:VAL:HG22	1:D:696:GLU:HB2	2.02	0.41
1:A:722:ALA:HB2	1:A:729:ARG:HA	2.03	0.40
1:A:670:ASN:HB3	7:A:1413:HOH:O	2.20	0.40
1:D:836:ALA:HB3	1:D:841:MET:CE	2.52	0.40

All (4) 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)
7:A:1155:HOH:O	7:D:1340:HOH:O[2_745]	1.76	0.44
7:A:1571:HOH:O	7:D:1794:HOH:O[2_745]	1.92	0.28
7:A:1155:HOH:O	7:D:1189:HOH:O[2_745]	2.05	0.15
7:A:1481:HOH:O	7:D:1696:HOH:O[2_745]	2.06	0.14

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	595/592 (100%)	582 (98%)	13 (2%)	0	100	100
1	D	617/592 (104%)	604 (98%)	13 (2%)	0	100	100
All	All	1212/1184 (102%)	1186 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	510/507 (101%)	505 (99%)	5 (1%)	68	58
1	D	534/507 (105%)	527 (99%)	7 (1%)	61	48
All	All	1044/1014 (103%)	1032 (99%)	12 (1%)	65	54

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	LEU
1	A	692	VAL
1	A	726	ASN
1	A	728	SER
1	A	844	LEU
1	D	303	LEU
1	D	477	LEU
1	D	561	LEU

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Mol	Chain	Res	Type
1	D	571[A]	VAL
1	D	571[B]	VAL
1	D	692	VAL
1	D	728	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	543	GLN
1	A	723	GLN
1	A	726	ASN
1	A	867	HIS
1	D	502	GLN
1	D	723	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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
2	DOC	E	29	3,2	16,19,20	0.53	0	20,26,29	1.25	2 (10%)
2	DOC	B	29	3,2	16,19,20	0.58	0	20,26,29	0.70	1 (5%)

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
2	DOC	E	29	3,2	-	0/7/18/19	0/2/2/2
2	DOC	B	29	3,2	-	0/7/18/19	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	29	DOC	O4'-C1'-C2'	3.26	110.28	106.41
2	B	29	DOC	C2'-C1'-N1	2.33	116.81	112.40
2	E	29	DOC	C3'-C2'-C1'	-2.25	100.28	102.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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
5	DCP	A	903	-	28,29,29	2.23	8 (28%)	41,45,45	0.90	2 (4%)
5	DCP	D	902	4	28,29,29	2.22	9 (32%)	41,45,45	1.45	7 (17%)
6	SO4	A	904	-	4,4,4	0.28	0	6,6,6	0.14	0
6	SO4	D	903	-	4,4,4	0.32	0	6,6,6	0.49	0
5	DCP	A	902	4	28,29,29	2.07	7 (25%)	41,45,45	1.52	8 (19%)

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
5	DCP	A	903	-	-	0/22/34/34	0/2/2/2
5	DCP	D	902	4	-	6/22/34/34	0/2/2/2
5	DCP	A	902	4	-	7/22/34/34	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	902	DCP	PB-O3B	-7.70	1.51	1.59
5	A	902	DCP	PB-O3B	-6.15	1.52	1.59
5	A	903	DCP	PB-O3A	-5.66	1.53	1.59
5	A	903	DCP	PB-O3B	-5.57	1.53	1.59
5	A	903	DCP	C2'-C3'	-4.31	1.41	1.52
5	A	902	DCP	O2-C2	4.13	1.31	1.23
5	A	902	DCP	C2'-C3'	-3.76	1.43	1.52
5	D	902	DCP	C2'-C3'	-3.29	1.44	1.52
5	D	902	DCP	PB-O3A	-3.24	1.56	1.59
5	A	903	DCP	C2-N1	-3.18	1.33	1.40
5	A	902	DCP	PA-O3A	3.09	1.62	1.59
5	A	902	DCP	PB-O2B	-3.08	1.41	1.55
5	D	902	DCP	PA-O3A	2.89	1.62	1.59
5	A	903	DCP	O2-C2	2.87	1.29	1.23
5	D	902	DCP	C2-N1	-2.73	1.34	1.40
5	D	902	DCP	C4-N4	2.69	1.40	1.33
5	A	902	DCP	C2-N1	-2.53	1.34	1.40
5	A	903	DCP	C3'-C4'	-2.50	1.46	1.53
5	A	903	DCP	C4-N4	2.47	1.39	1.33
5	A	903	DCP	PB-O2B	-2.45	1.44	1.55
5	D	902	DCP	O2-C2	2.35	1.28	1.23
5	D	902	DCP	C3'-C4'	-2.30	1.47	1.53
5	A	902	DCP	C4-N4	2.19	1.39	1.33
5	D	902	DCP	PB-O2B	-2.10	1.45	1.55

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	902	DCP	O4'-C1'-N1	3.95	114.88	107.86
5	D	902	DCP	O4'-C1'-N1	3.63	114.31	107.86
5	A	902	DCP	O3A-PB-O1B	-3.52	100.13	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	902	DCP	O2B-PB-O3B	2.96	115.28	107.27
5	A	903	DCP	O4'-C1'-N1	2.76	112.76	107.86
5	D	902	DCP	O2-C2-N3	-2.69	118.09	122.33
5	A	902	DCP	O5'-C5'-C4'	2.59	117.81	108.99
5	A	902	DCP	O2B-PB-O3A	2.51	114.06	107.27
5	A	902	DCP	O2-C2-N3	-2.46	118.45	122.33
5	D	902	DCP	O3A-PB-O1B	-2.45	103.33	110.70
5	D	902	DCP	C2'-C1'-N1	-2.39	107.83	113.81
5	A	902	DCP	O2A-PA-O3A	2.13	113.04	107.27
5	D	902	DCP	O2A-PA-O3A	2.10	112.96	107.27
5	D	902	DCP	O3B-PG-O1G	-2.08	100.11	111.04
5	A	903	DCP	O2-C2-N3	-2.08	119.06	122.33
5	D	902	DCP	O3A-PA-O1A	-2.07	104.46	110.70
5	A	902	DCP	C1'-N1-C2	2.03	121.31	117.83

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	902	DCP	PB-O3B-PG-O2G
5	D	902	DCP	PB-O3B-PG-O2G
5	D	902	DCP	PB-O3B-PG-O3G
5	A	902	DCP	PB-O3A-PA-O1A
5	A	902	DCP	PA-O3A-PB-O1B
5	D	902	DCP	PB-O3A-PA-O1A
5	D	902	DCP	PA-O3A-PB-O1B
5	A	902	DCP	PA-O3A-PB-O2B
5	D	902	DCP	PB-O3A-PA-O2A
5	A	902	DCP	PB-O3B-PG-O3G
5	A	902	DCP	PB-O3B-PG-O1G
5	D	902	DCP	PB-O3B-PG-O1G
5	A	902	DCP	PB-O3A-PA-O2A

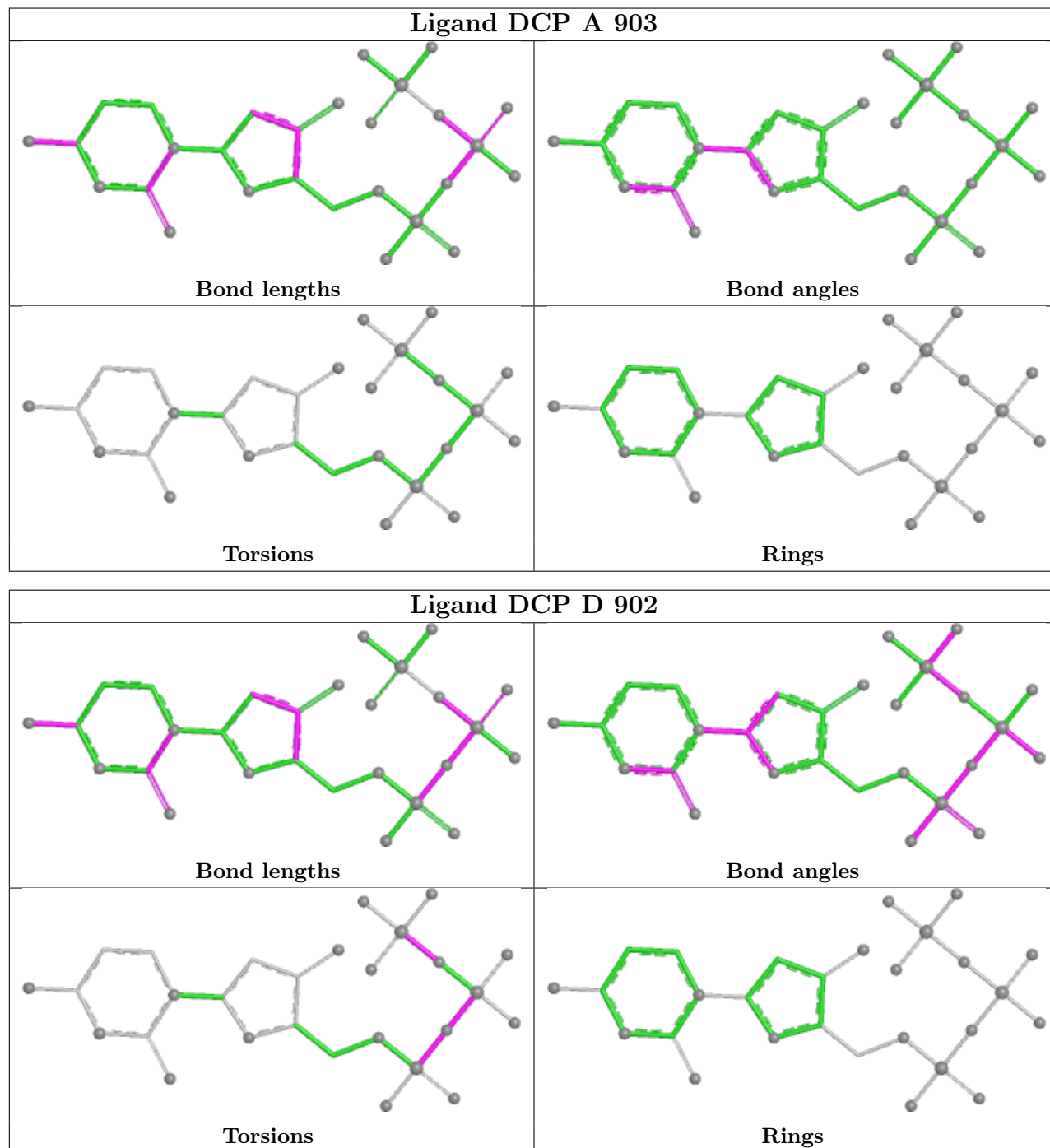
There are no ring outliers.

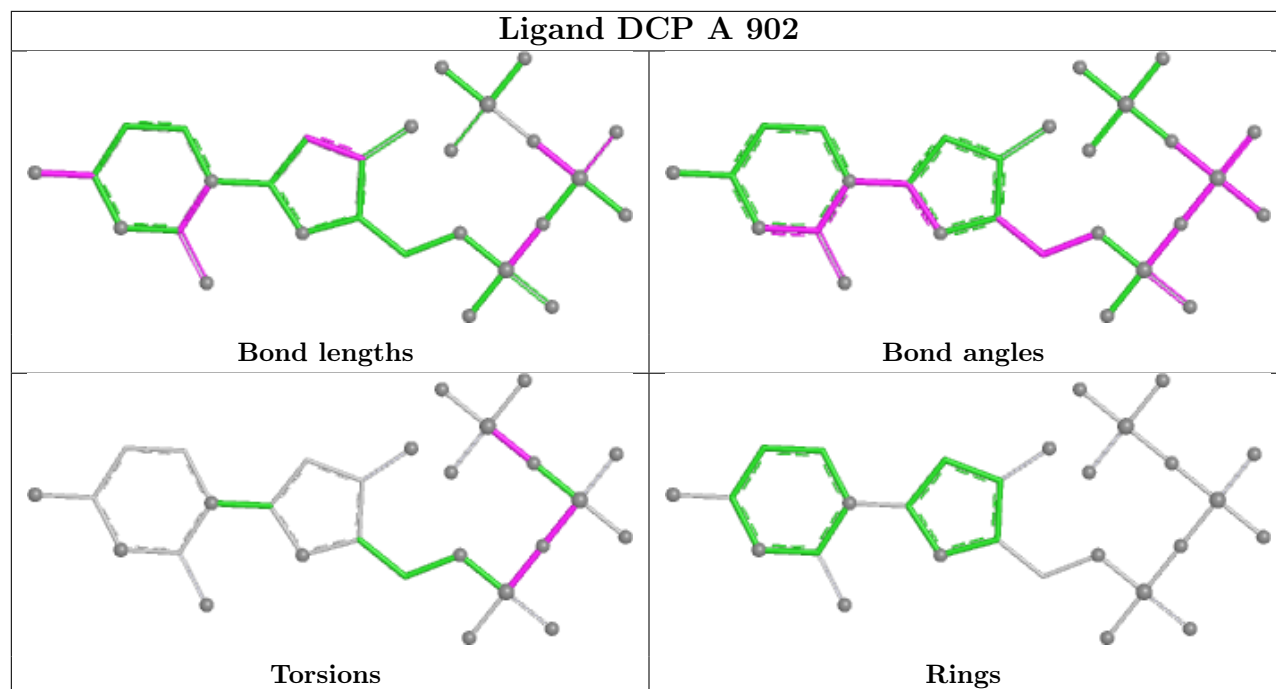
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	902	DCP	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	579/592 (97%)	-0.18	5 (0%) 81 83	8, 30, 57, 89	8 (1%)
1	D	579/592 (97%)	-0.55	6 (1%) 79 82	5, 17, 39, 56	21 (3%)
2	B	8/9 (88%)	-0.60	0 100 100	17, 23, 33, 41	0
2	E	8/9 (88%)	-0.83	0 100 100	11, 17, 27, 37	0
3	C	12/13 (92%)	-0.51	0 100 100	15, 20, 51, 68	0
3	F	12/13 (92%)	-0.70	0 100 100	10, 17, 45, 60	0
All	All	1198/1228 (97%)	-0.37	11 (0%) 81 83	5, 24, 50, 89	29 (2%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748[A]	ARG	6.9
1	D	704	GLN	3.2
1	D	689	ILE	2.7
1	A	724	ASN	2.7
1	D	703	ARG	2.4
1	D	691	GLN	2.3
1	D	298	LYS	2.2
1	D	692	VAL	2.1
1	A	298	LYS	2.1
1	A	692	VAL	2.0
1	A	690	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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($\text{\AA}^2$)	Q<0.9
2	DOC	B	29	18/19	0.98	0.04	16,17,20,22	0
2	DOC	E	29	18/19	0.98	0.04	8,10,15,18	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

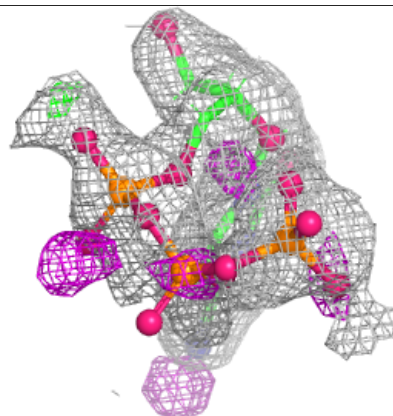
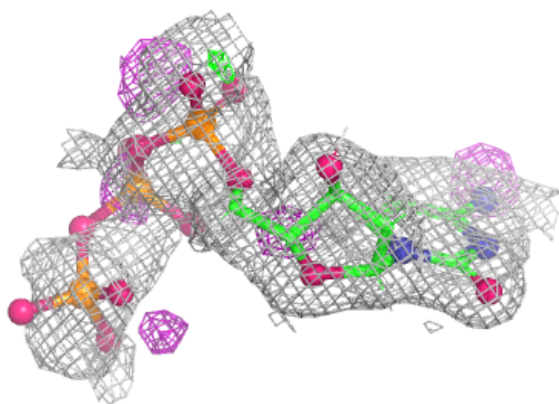
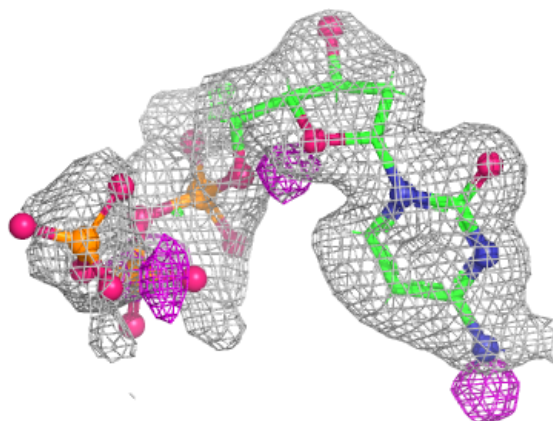
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DCP	A	903	28/28	0.83	0.12	24,50,119,120	0
6	SO4	A	904	5/5	0.89	0.09	40,57,58,65	0
6	SO4	D	903	5/5	0.96	0.08	26,29,44,47	0
5	DCP	A	902	28/28	0.97	0.05	14,18,25,35	0
4	MG	A	901	1/1	0.98	0.04	23,23,23,23	0
5	DCP	D	902	28/28	0.98	0.04	7,13,24,27	0
4	MG	D	901	1/1	0.99	0.02	17,17,17,17	0

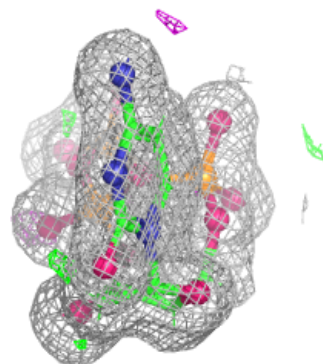
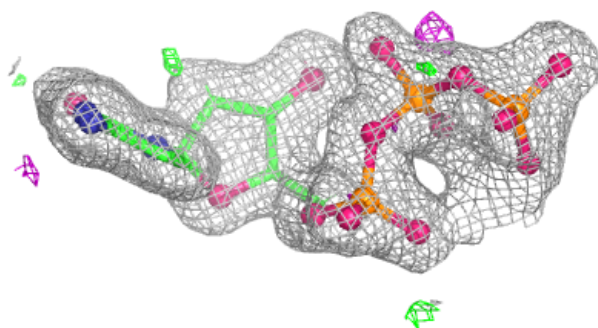
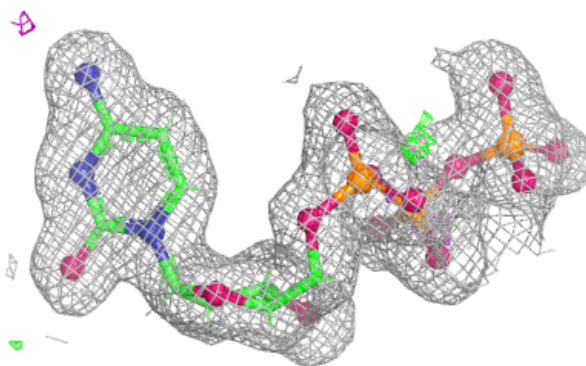
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DCP A 903:

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

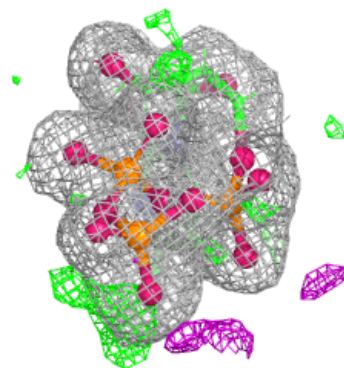
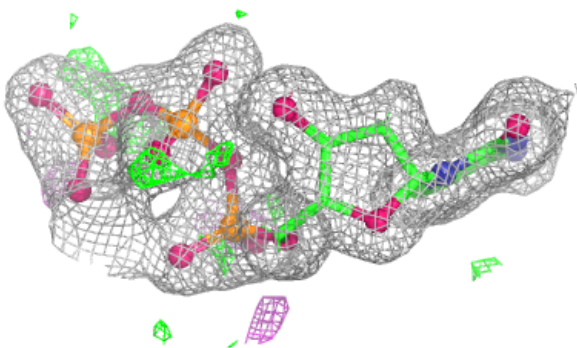
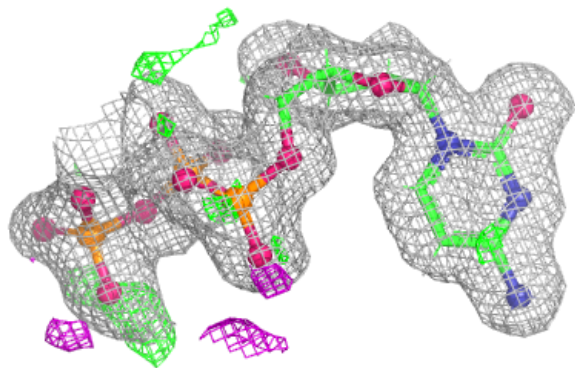
**Electron density around DCP A 902:**

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



Electron density around DCP D 902:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.