



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:24 PM UTC

PDB ID : 4DQR / pdb_00004dqr
Title : Ternary complex of Bacillus DNA Polymerase I Large Fragment E658A, DNA duplex, and rCTP (paired with dG of template) in presence of Mn²⁺
Authors : Wang, W.; Beese, L.S.
Deposited on : 2012-02-16
Resolution : 1.95 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

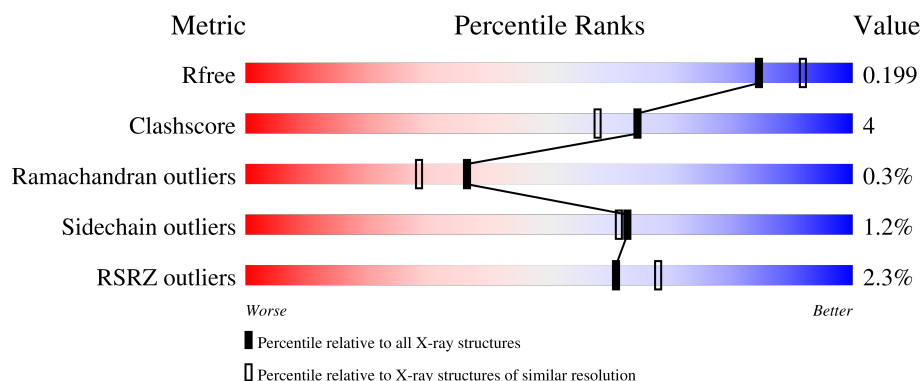
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	4% 89% 9% .
1	D	592	90% 8% .
2	B	9	67% 33%
2	E	9	78% 22%
3	C	13	62% 23% 15%

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Mol	Chain	Length	Quality of chain
3	F	13	77%15%8%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 21345 atoms, of which 10147 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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	580	Total	C	H	N	O	S	0	16	0
			9514	2995	4801	822	878	18			
1	D	579	Total	C	H	N	O	S	0	23	0
			9561	3012	4823	823	885	18			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	598	ALA	ASP	engineered mutation	UNP Q5KWC1
A	658	ALA	GLU	engineered mutation	UNP Q5KWC1
A	823	HIS	ARG	engineered mutation	UNP Q5KWC1
D	598	ALA	ASP	engineered mutation	UNP Q5KWC1
D	658	ALA	GLU	engineered mutation	UNP Q5KWC1
D	823	HIS	ARG	engineered mutation	UNP Q5KWC1

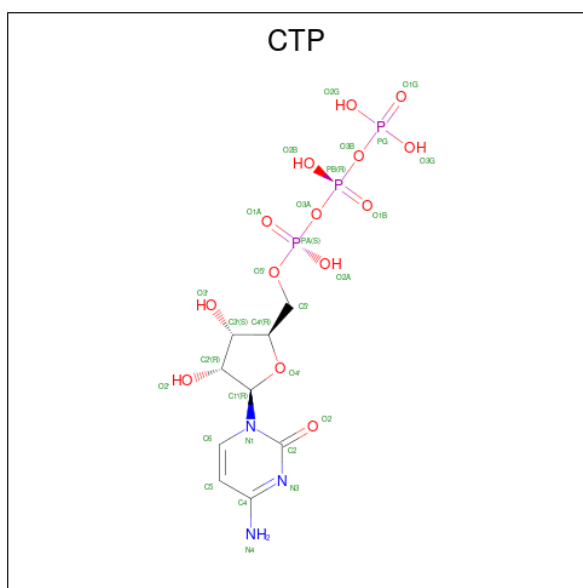
- Molecule 2 is a DNA chain called DNA (5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*(DOC))-3').

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(*CP*AP*TP*GP*GP*GP*AP*GP*TP*CP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	11	Total	C	H	N	O	P	0	0	0
			356	109	123	47	66	11			
3	F	12	Total	C	H	N	O	P	0	0	0
			385	119	134	52	69	11			

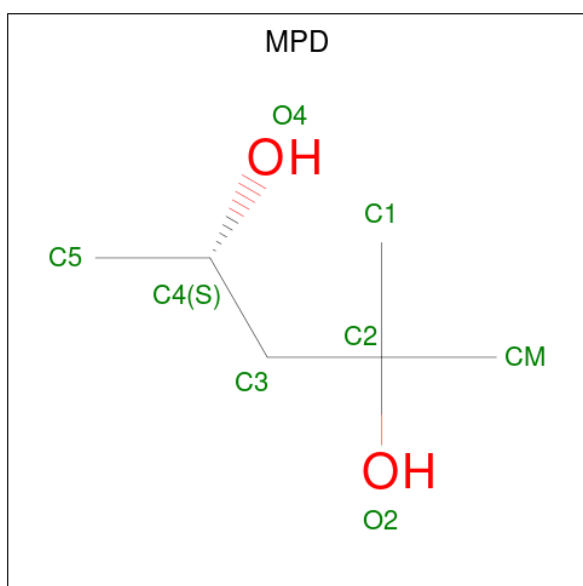
- Molecule 4 is CYTIDINE-5'-TRIPHOSPHATE (CCD ID: CTP) (formula: $C_9H_{16}N_3O_{14}P_3$).





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 (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			22	6	14	2		
7	D	1	Total	C	H	O	0	0
			22	6	14	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	H	O	0	0
			22	6	14	2		

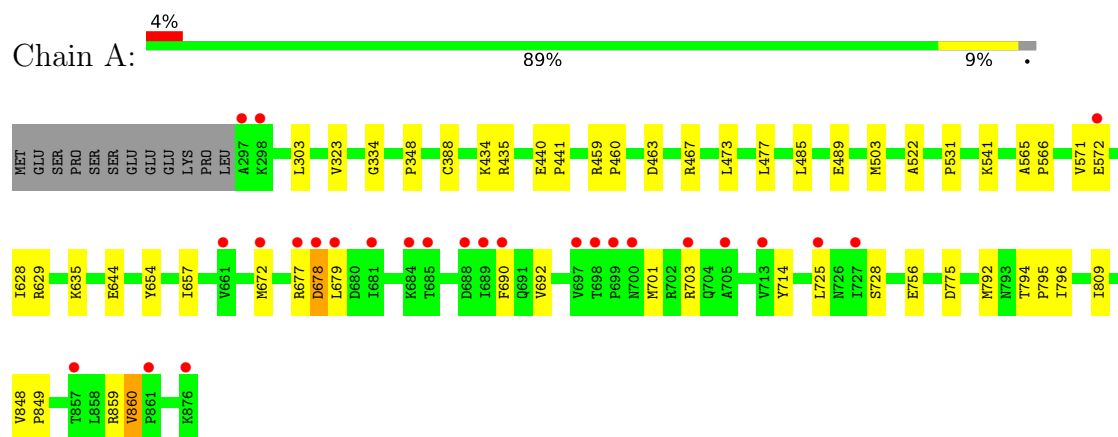
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	239	Total	O	0	0
			239	239		
8	D	447	Total	O	0	0
			447	447		
8	B	22	Total	O	0	0
			22	22		
8	C	39	Total	O	0	0
			39	39		
8	E	29	Total	O	0	0
			29	29		
8	F	45	Total	O	0	0
			45	45		

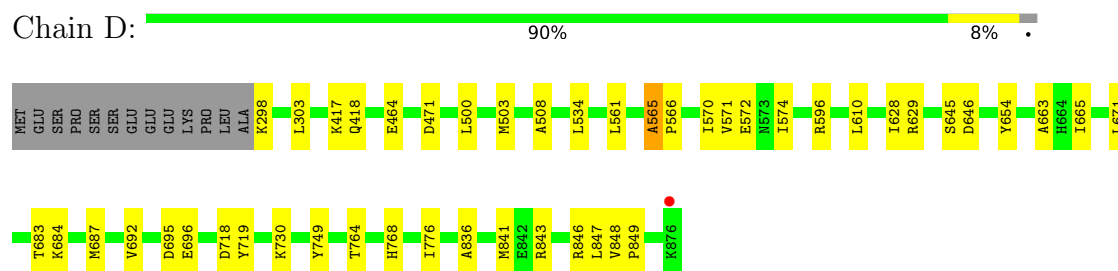
3 Residue-property plots [i](#)

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.

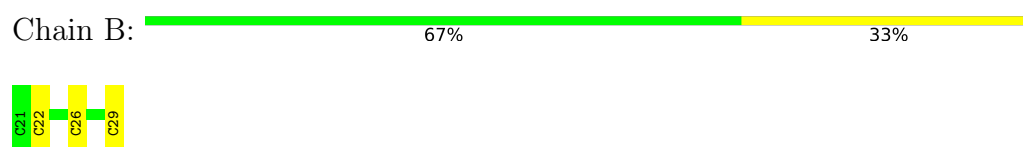
• Molecule 1: DNA polymerase



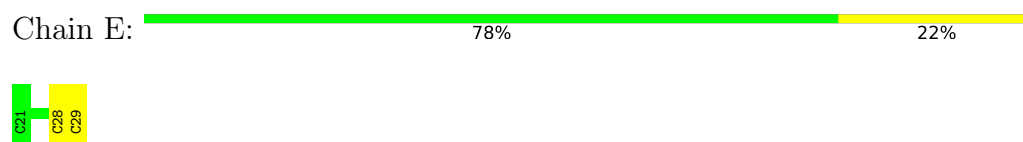
• Molecule 1: DNA polymerase



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

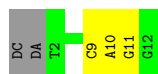


• Molecule 2: DNA (5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*(DOC))-3')



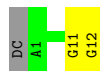
- Molecule 3: DNA (5'-D(*CP*AP*TP*GP*GP*GP*AP*GP*TP*CP*AP*GP*G)-3')

Chain C:  62% 23% 15%



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

Chain F:  77% 15% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.90Å 108.85Å 149.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.79 – 1.95 36.79 – 1.95	Depositor EDS
% Data completeness (in resolution range)	94.1 (36.79-1.95) 94.1 (36.79-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.97 (at 1.95Å)	Xtriage
Refinement program	PHENIX dev_1026	Depositor
R, R_{free}	0.166 , 0.198 0.168 , 0.199	Depositor DCC
R_{free} test set	4479 reflections (4.24%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21345	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: MPD, SO4, DOC, CTP, 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	A	0.60	0/4854	0.77	1/6558 (0.0%)
1	D	0.75	0/4911	0.82	2/6637 (0.0%)
2	B	0.44	0/173	1.27	2/264 (0.8%)
2	E	0.53	0/173	1.24	0/264
3	C	0.46	0/262	0.98	0/404
3	F	0.51	0/283	1.10	0/437
All	All	0.66	0/10656	0.83	5/14564 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	26	DC	N1-C1'-C2'	-6.04	104.44	113.50
2	B	22	DC	C4'-C3'-O3'	-5.83	101.25	110.00
1	A	859	ARG	N-CA-C	-5.29	105.68	111.82
1	D	565	ALA	CA-C-N	-5.15	114.47	120.04
1	D	565	ALA	C-N-CA	-5.15	114.47	120.04

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	A	4713	4801	4726	36	0
1	D	4738	4823	4711	34	0
2	B	174	100	103	1	0
2	E	174	100	103	1	0
3	C	233	123	124	2	0
3	F	251	134	136	5	0
4	A	29	12	12	0	0
4	D	29	12	12	1	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	5	0	0	0	0
6	D	5	0	0	0	0
7	A	8	14	14	0	0
7	D	16	28	28	2	0
8	A	239	0	0	12	0
8	B	22	0	0	0	0
8	C	39	0	0	1	0
8	D	447	0	0	13	0
8	E	29	0	0	0	0
8	F	45	0	0	5	0
All	All	11198	10147	9969	80	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 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:A:388:CYS:SG	8:A:1194:HOH:O	2.13	1.06
3:C:11:DG:OP1	8:C:123:HOH:O	1.91	0.88
1:D:764[B]:THR:HG21	8:D:1304:HOH:O	1.77	0.84
1:A:792:MET:SD	8:A:1215:HOH:O	2.38	0.82
3:F:12:DG:N3	8:F:143:HOH:O	2.11	0.82
1:D:654:TYR:O	8:D:1090:HOH:O	1.99	0.81
3:F:11:DG:OP2	8:F:122:HOH:O	2.03	0.76
1:A:434:LYS:NZ	8:A:1223:HOH:O	2.21	0.73
1:A:323:VAL:O	1:A:435:ARG:NH2	2.24	0.71
7:D:904:MPD:HM2	8:D:1059:HOH:O	1.89	0.71
1:D:418:GLN:OE1	8:D:1329:HOH:O	2.10	0.69
1:D:843:ARG:HD2	8:D:1101:HOH:O	1.92	0.69
1:D:684:LYS:NZ	8:D:1303:HOH:O	2.27	0.68
4:D:901:CTP:O2G	8:D:1158:HOH:O	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:MET:HG3	1:A:860:VAL:HG12	1.76	0.66
1:A:434:LYS:CE	8:A:1223:HOH:O	2.44	0.65
1:D:846:ARG:NH1	8:D:1306:HOH:O	2.08	0.65
1:D:683:THR:HG22	1:D:687:MET:CE	2.27	0.64
1:A:672:MET:HG3	1:A:860:VAL:CG1	2.29	0.62
1:A:565:ALA:HA	1:A:571:VAL:CG2	2.30	0.62
1:D:683:THR:HG22	1:D:687:MET:HE2	1.83	0.61
1:A:756:GLU:OE1	8:A:1147:HOH:O	2.17	0.58
1:D:508:ALA:O	8:D:1316:HOH:O	2.17	0.58
1:A:477:LEU:HD12	1:A:809:ILE:HD12	1.86	0.57
1:A:565:ALA:HA	1:A:571:VAL:HG21	1.87	0.56
1:A:629:ARG:HH22	2:B:29:DOC:H5	1.69	0.56
1:A:714:TYR:HE1	1:A:796:ILE:HD12	1.70	0.56
1:A:692:VAL:HG21	1:A:701:MET:HE1	1.89	0.55
1:A:629:ARG:HD3	1:A:703:ARG:CZ	2.38	0.53
1:A:531:PRO:HD2	8:A:1219:HOH:O	2.09	0.53
3:F:12:DG:C4'	8:F:121:HOH:O	2.57	0.52
3:F:12:DG:H1'	8:F:143:HOH:O	2.09	0.52
1:D:596:ARG:HD2	8:D:1438:HOH:O	2.10	0.52
1:D:610[B]:LEU:HD12	8:D:1188:HOH:O	2.10	0.51
1:D:417:LYS:NZ	1:D:464:GLU:OE2	2.39	0.51
1:D:683:THR:HG22	1:D:687:MET:HE3	1.93	0.50
1:D:692:VAL:HB	1:D:696:GLU:HB2	1.94	0.49
1:A:848:VAL:HB	1:A:849:PRO:HD3	1.94	0.48
1:A:434:LYS:HD2	8:A:1223:HOH:O	2.13	0.48
1:D:561:LEU:O	1:D:571:VAL:HG11	2.14	0.48
1:D:570:ILE:O	1:D:574[B]:ILE:HG12	2.13	0.48
1:A:459:ARG:HB3	1:A:460:PRO:HD3	1.96	0.48
1:D:629:ARG:HD3	2:E:28:DC:P	2.54	0.47
1:A:463:ASP:O	1:A:467[B]:ARG:HG3	2.14	0.47
1:D:565:ALA:N	1:D:566:PRO:CD	2.78	0.47
1:D:561:LEU:HB3	1:D:571:VAL:HG13	1.97	0.46
1:D:565:ALA:N	1:D:566:PRO:HD2	2.30	0.46
1:D:665:ILE:HG22	1:D:749[A]:TYR:CE1	2.51	0.45
1:D:663:ALA:HB2	1:D:671:LEU:HG	1.98	0.45
1:D:534:LEU:HD11	1:D:574[A]:ILE:HD13	1.98	0.45
1:A:565:ALA:N	1:A:566:PRO:HD2	2.33	0.44
1:A:654:TYR:HB3	1:A:657:ILE:HB	1.99	0.44
1:A:334:GLY:HA2	1:A:348:PRO:HD3	1.99	0.44
1:D:836:ALA:HB3	1:D:841:MET:CE	2.47	0.44
3:C:9:DC:H2'	3:C:10:DA:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:764[B]:THR:CG2	1:D:768:HIS:HA	2.48	0.44
1:A:531:PRO:N	8:A:1219:HOH:O	2.49	0.44
3:F:12:DG:H4'	8:F:121:HOH:O	2.18	0.44
7:D:905:MPD:O2	8:D:1193:HOH:O	2.20	0.44
1:A:677:ARG:HD2	1:A:679:LEU:HD21	1.99	0.43
1:D:848:VAL:HB	1:D:849:PRO:HD3	2.00	0.43
1:D:596:ARG:CG	8:D:1438:HOH:O	2.66	0.43
1:D:764[B]:THR:HG22	1:D:768:HIS:HA	1.99	0.43
1:D:610[A]:LEU:C	1:D:610[A]:LEU:HD23	2.43	0.43
1:A:690:PHE:O	1:A:692:VAL:HG13	2.19	0.43
1:A:522:ALA:O	1:A:541:LYS:HE2	2.19	0.43
1:A:775:ASP:HB2	8:A:1055:HOH:O	2.19	0.43
1:D:847:LEU:C	1:D:847:LEU:HD23	2.44	0.43
1:A:531:PRO:CD	8:A:1219:HOH:O	2.67	0.42
1:D:645:SER:O	1:D:646:ASP:HB2	2.20	0.42
1:A:440:GLU:HB3	1:A:441:PRO:HD3	2.01	0.42
1:D:718:ASP:OD2	1:D:719:TYR:N	2.52	0.42
1:A:485:LEU:O	1:A:489:GLU:HG3	2.19	0.41
1:A:572:GLU:HB2	8:A:1158:HOH:O	2.20	0.41
1:A:794:THR:N	1:A:795:PRO:CD	2.83	0.41
1:D:471:ASP:OD1	1:D:471:ASP:N	2.52	0.41
1:A:467[B]:ARG:HD2	8:A:1101:HOH:O	2.21	0.41
1:D:500:LEU:HA	1:D:503:MET:HE3	2.03	0.41
1:A:503[B]:MET:HE1	1:A:635:LYS:O	2.20	0.41
1:A:473:LEU:HD12	1:A:477:LEU:HD23	2.03	0.40

There are no symmetry-related clashes.

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	594/592 (100%)	583 (98%)	9 (2%)	2 (0%)	36 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	600/592 (101%)	585 (98%)	14 (2%)	1 (0%)	43	36
All	All	1194/1184 (101%)	1168 (98%)	23 (2%)	3 (0%)	36	28

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	678	ASP
1	D	628	ILE
1	A	628	ILE

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	
1	A	508/506 (100%)	502 (99%)	6 (1%)	63	61
1	D	517/506 (102%)	511 (99%)	6 (1%)	63	61
All	All	1025/1012 (101%)	1013 (99%)	12 (1%)	63	61

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

Mol	Chain	Res	Type
1	A	303	LEU
1	A	644	GLU
1	A	678	ASP
1	A	725	LEU
1	A	728	SER
1	A	860	VAL
1	D	298	LYS
1	D	303	LEU
1	D	572	GLU
1	D	695	ASP
1	D	730	LYS
1	D	776	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	670	ASN
1	A	709	ASN
1	A	755	GLN
1	A	812	ASN
1	D	573	ASN
1	D	579	GLN
1	D	704	GLN
1	D	782	ASN

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	B	29	3,2	16,19,20	0.72	0	20,26,29	0.63	0
2	DOC	E	29	3,2	16,19,20	0.56	0	20,26,29	0.81	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	B	29	3,2	-	0/7/18/19	0/2/2/2
2	DOC	E	29	3,2	-	0/7/18/19	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	29	DOC	O4'-C1'-C2'	2.02	108.81	106.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	29	DOC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	$\# Z > 2$
6	SO4	D	903	-	4,4,4	0.38	0	6,6,6	0.51	0
7	MPD	D	904	-	7,7,7	0.32	0	9,10,10	0.96	0
7	MPD	D	905	-	7,7,7	0.53	0	9,10,10	0.57	0
6	SO4	A	903	-	4,4,4	0.27	0	6,6,6	0.14	0
7	MPD	A	904	-	7,7,7	0.36	0	9,10,10	1.33	1 (11%)
4	CTP	D	901	5	29,30,30	1.93	6 (20%)	43,47,47	1.22	4 (9%)
4	CTP	A	901	5	29,30,30	1.89	4 (13%)	43,47,47	1.38	6 (13%)

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
7	MPD	D	904	-	-	2/5/5/5	-
7	MPD	D	905	-	-	0/5/5/5	-
7	MPD	A	904	-	-	1/5/5/5	-
4	CTP	D	901	5	-	2/22/38/38	0/2/2/2
4	CTP	A	901	5	-	2/22/38/38	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	CTP	O2-C2	6.86	1.36	1.23
4	D	901	CTP	O2-C2	4.99	1.33	1.23
4	D	901	CTP	PB-O3B	-4.06	1.55	1.59
4	A	901	CTP	C4-N4	3.64	1.42	1.33
4	D	901	CTP	C4-N4	3.57	1.42	1.33
4	A	901	CTP	C2-N3	2.89	1.42	1.36
4	D	901	CTP	PA-O3A	-2.66	1.56	1.59
4	D	901	CTP	PB-O3A	-2.07	1.57	1.59
4	A	901	CTP	C4-N3	2.03	1.38	1.34
4	D	901	CTP	C6-C5	2.02	1.39	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	CTP	O2B-PB-O3B	4.10	118.37	107.27
4	D	901	CTP	O2A-PA-O3A	3.72	117.33	107.27
4	A	901	CTP	O2G-PG-O3B	3.23	115.47	104.64
4	D	901	CTP	O2G-PG-O3B	3.02	114.75	104.64
4	A	901	CTP	O4'-C1'-N1	2.93	115.00	108.36
4	A	901	CTP	O3G-PG-O3B	2.84	114.15	104.64
7	A	904	MPD	O2-C2-C3	-2.83	98.67	109.27
4	A	901	CTP	O2B-PB-O1B	-2.25	101.97	112.44
4	A	901	CTP	O2A-PA-O3A	2.24	113.34	107.27
4	D	901	CTP	O3A-PB-O1B	-2.13	104.28	110.70
4	D	901	CTP	O2A-PA-O1A	-2.01	103.09	112.44

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	CTP	PG-O3B-PB-O2B

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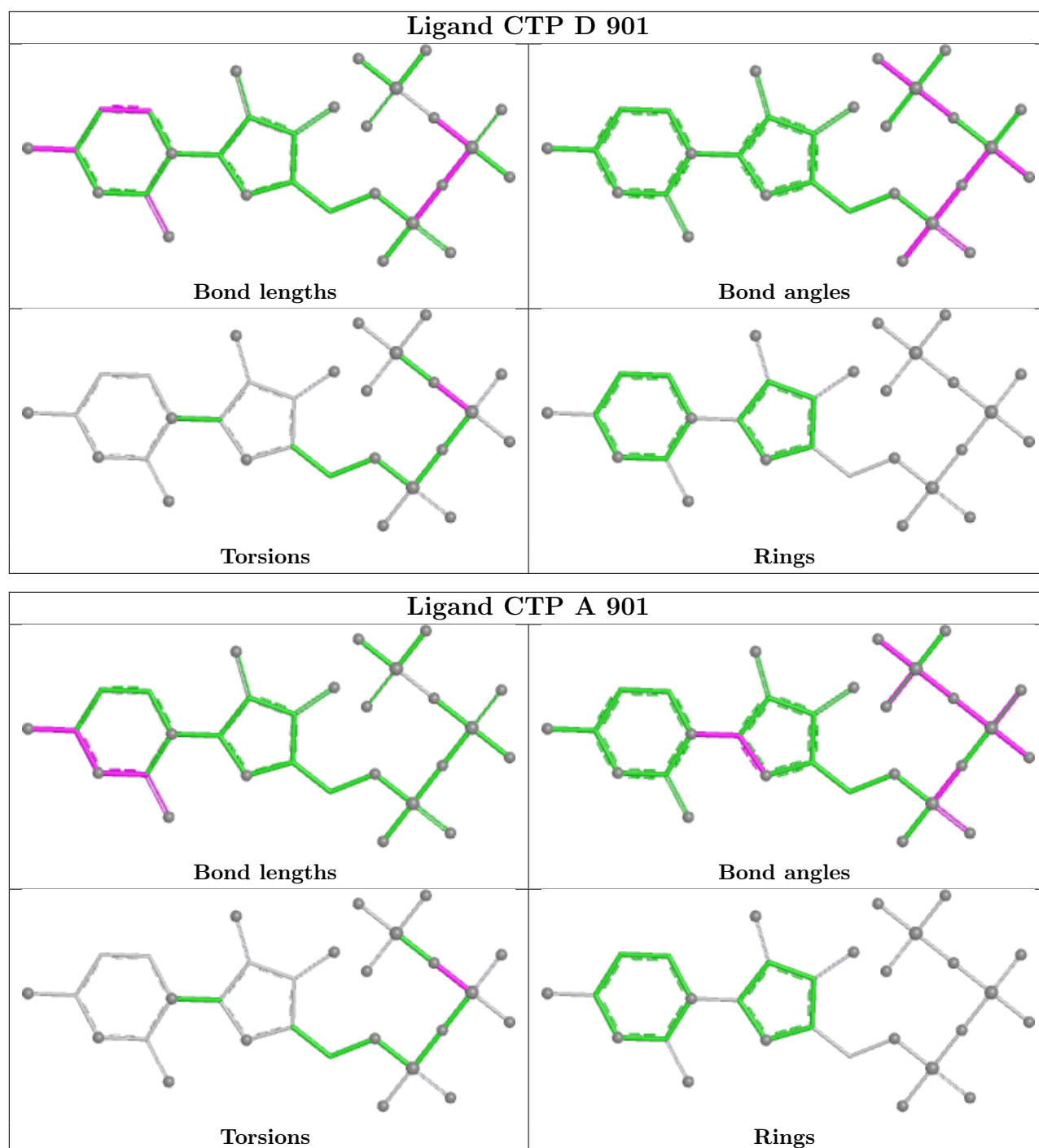
Mol	Chain	Res	Type	Atoms
4	A	901	CTP	PG-O3B-PB-O1B
4	D	901	CTP	PG-O3B-PB-O2B
7	A	904	MPD	O2-C2-C3-C4
7	D	904	MPD	O2-C2-C3-C4
7	D	904	MPD	C1-C2-C3-C4
4	D	901	CTP	PG-O3B-PB-O1B

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	904	MPD	1	0
7	D	905	MPD	1	0
4	D	901	CTP	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	580/592 (97%)	0.20	26 (4%) 38 44	13, 46, 84, 119	8 (1%)
1	D	579/592 (97%)	-0.43	1 (0%) 91 92	8, 27, 58, 84	12 (2%)
2	B	8/9 (88%)	-0.51	0 100 100	27, 30, 53, 75	0
2	E	8/9 (88%)	-0.62	0 100 100	21, 28, 49, 66	0
3	C	11/13 (84%)	-0.45	0 100 100	23, 31, 61, 83	0
3	F	12/13 (92%)	-0.53	0 100 100	19, 27, 72, 86	0
All	All	1198/1228 (97%)	-0.13	27 (2%) 61 68	8, 37, 75, 119	20 (1%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	679	LEU	5.4
1	A	297	ALA	4.0
1	D	876	LYS	3.9
1	A	681	ILE	3.6
1	A	689	ILE	3.0
1	A	876	LYS	3.0
1	A	685	THR	2.9
1	A	677	ARG	2.9
1	A	857	THR	2.8
1	A	298	LYS	2.8
1	A	699	PRO	2.6
1	A	713	VAL	2.5
1	A	690	PHE	2.4
1	A	727	ILE	2.3
1	A	572	GLU	2.3
1	A	684	LYS	2.3
1	A	697	VAL	2.3
1	A	678	ASP	2.2
1	A	688	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	661	VAL	2.1
1	A	698	THR	2.1
1	A	725	LEU	2.1
1	A	861	PRO	2.1
1	A	705	ALA	2.1
1	A	672	MET	2.0
1	A	700	ASN	2.0
1	A	703	ARG	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(Å ²)	Q<0.9
2	DOC	B	29	18/19	0.96	0.07	23,29,35,37	0
2	DOC	E	29	18/19	0.97	0.05	16,20,26,26	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.

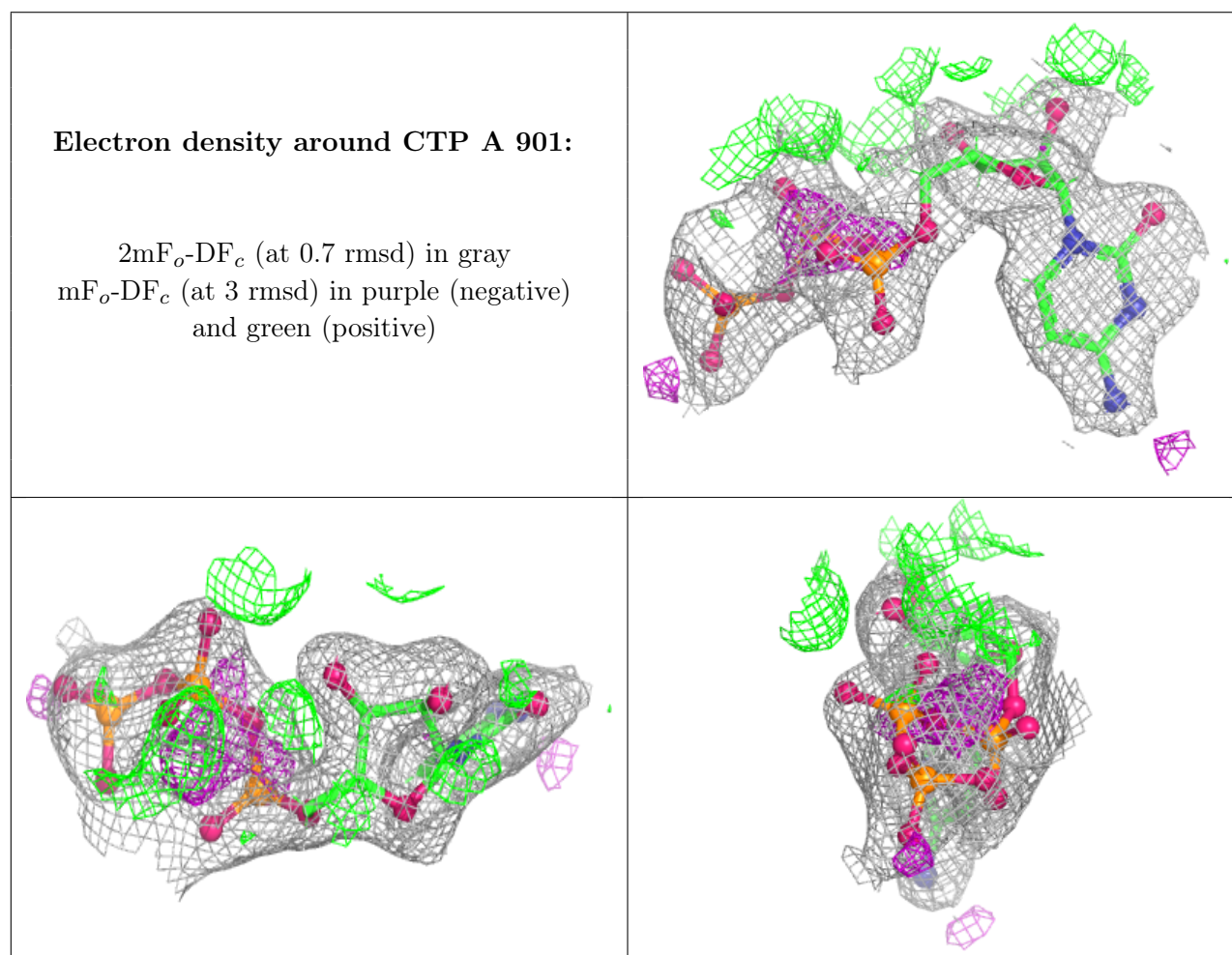
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SO4	A	903	5/5	0.90	0.09	52,52,58,61	0
5	MN	A	902	1/1	0.91	0.08	59,59,59,59	0
4	CTP	A	901	29/29	0.92	0.09	25,35,59,66	0
7	MPD	A	904	8/8	0.92	0.10	26,37,46,50	0
7	MPD	D	904	8/8	0.92	0.11	24,40,53,57	0
7	MPD	D	905	8/8	0.95	0.09	31,48,58,58	0
6	SO4	D	903	5/5	0.97	0.06	31,35,37,44	0
4	CTP	D	901	29/29	0.98	0.04	17,22,27,31	0

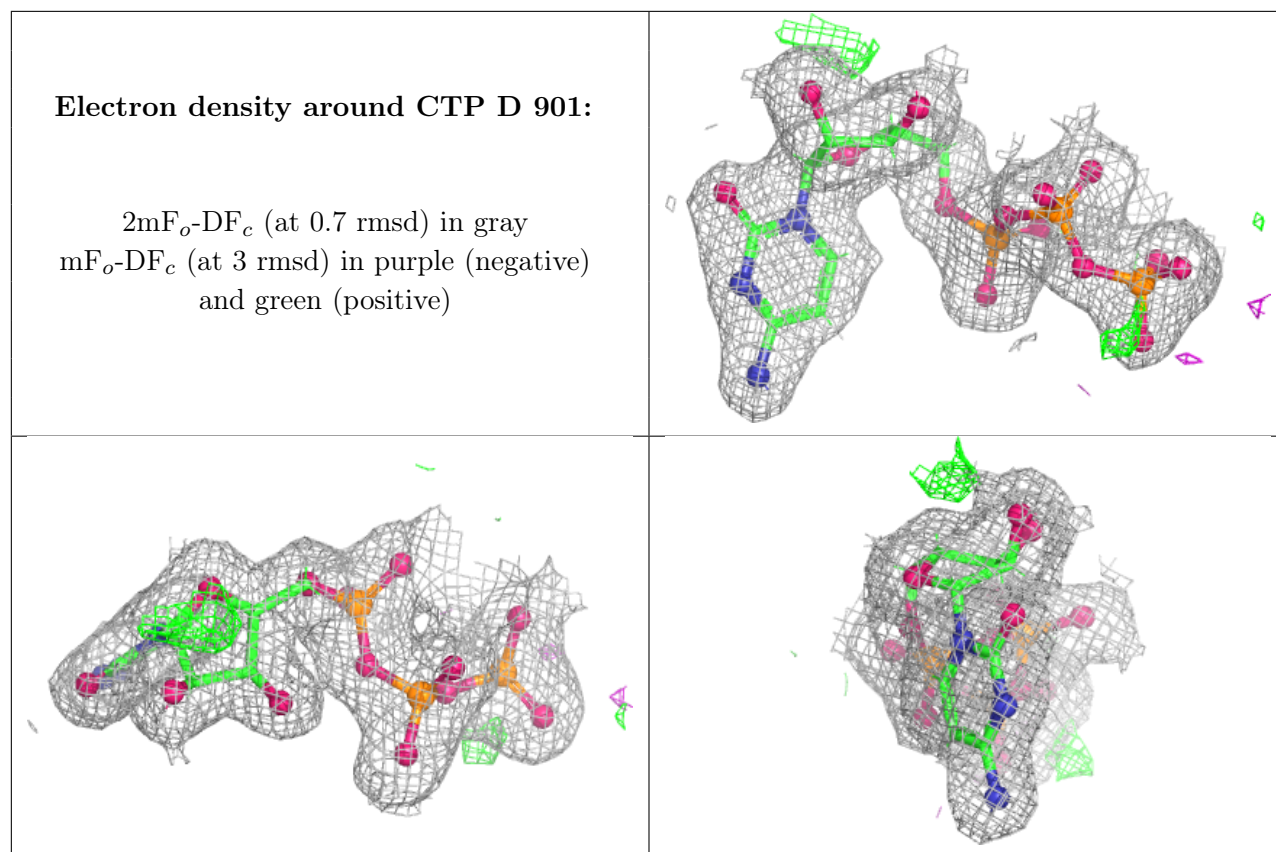
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MN	D	902	1/1	0.99	0.03	30,30,30,30	0

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.