



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:50 AM UTC

PDB ID : 3PX4 / pdb_00003px4
Title : Crystal Structure of Bacillus DNA Polymerase I Large Fragment Bound to DNA and ddCTP-dA Mismatch (wobble) in Ajar Conformation
Authors : Wang, W.; Beese, L.S.
Deposited on : 2010-12-09
Resolution : 1.58 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

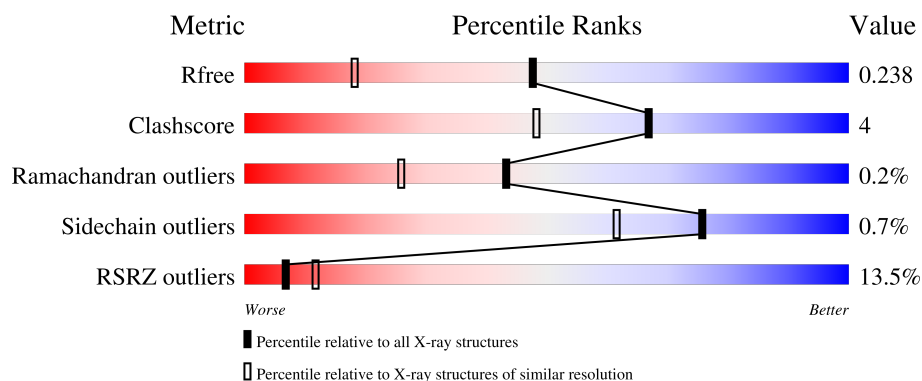
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

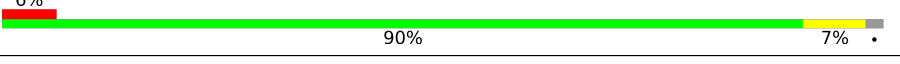
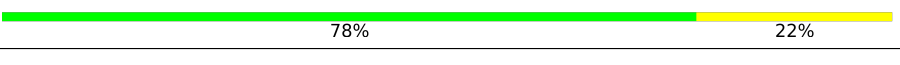
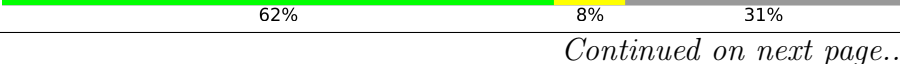
The reported resolution of this entry is 1.58 Å.

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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	 20% 84% 8% 7%
1	D	592	 6% 90% 7%
2	B	9	 78% 22%
2	E	9	 78% 22%
3	C	13	 62% 8% 31%

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Mol	Chain	Length	Quality of chain
3	F	13	23% 92% 8%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 21056 atoms, of which 9648 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	549	Total	C	H	N	O	S	0	2	0
			8887	2811	4476	764	821	15			
1	D	579	Total	C	H	N	O	S	0	7	0
			9405	2969	4730	810	879	17			

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	710	TYR	PHE	engineered mutation	UNP Q5KWC1
A	823	HIS	ARG	SEE REMARK 999	UNP Q5KWC1
D	598	ALA	ASP	engineered mutation	UNP Q5KWC1
D	710	TYR	PHE	engineered mutation	UNP Q5KWC1
D	823	HIS	ARG	SEE REMARK 999	UNP Q5KWC1

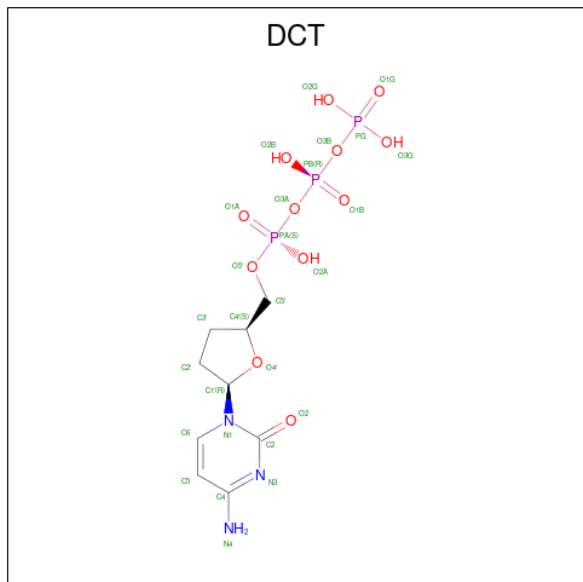
- Molecule 2 is a DNA chain called DNA (5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*(DOC))-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	9	Total	C	H	N	O	P	0	0	0
			275	85	101	29	52	8			
2	E	9	Total	C	H	N	O	P	0	0	0
			275	85	101	29	52	8			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	9	Total	C	H	N	O	P	0	0	0
			292	89	101	40	53	9			
3	F	12	Total	C	H	N	O	P	0	0	0
			383	119	133	52	68	11			

- Molecule 4 is 2',3'-DIDEOXYCYTIDINE 5'-TRIPHOSPHATE (CCD ID: DCT) (formula: $C_9H_{16}N_3O_{12}P_3$).

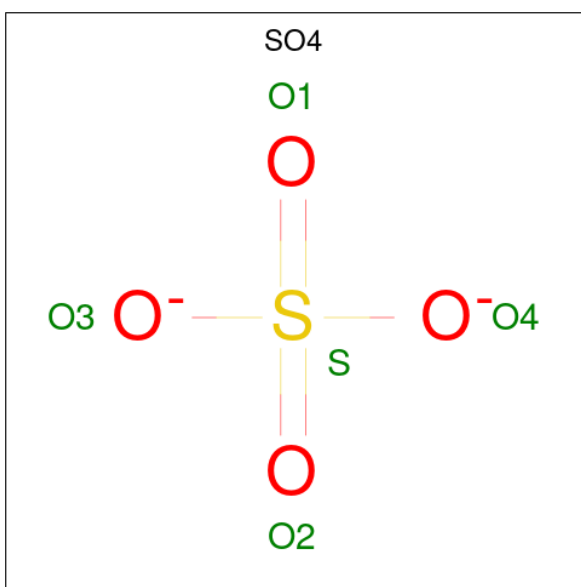


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P	0	0
			31	9	4	3	12	3		
4	D	1	Total	C	H	N	O	P	0	0
			29	9	2	3	12	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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



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

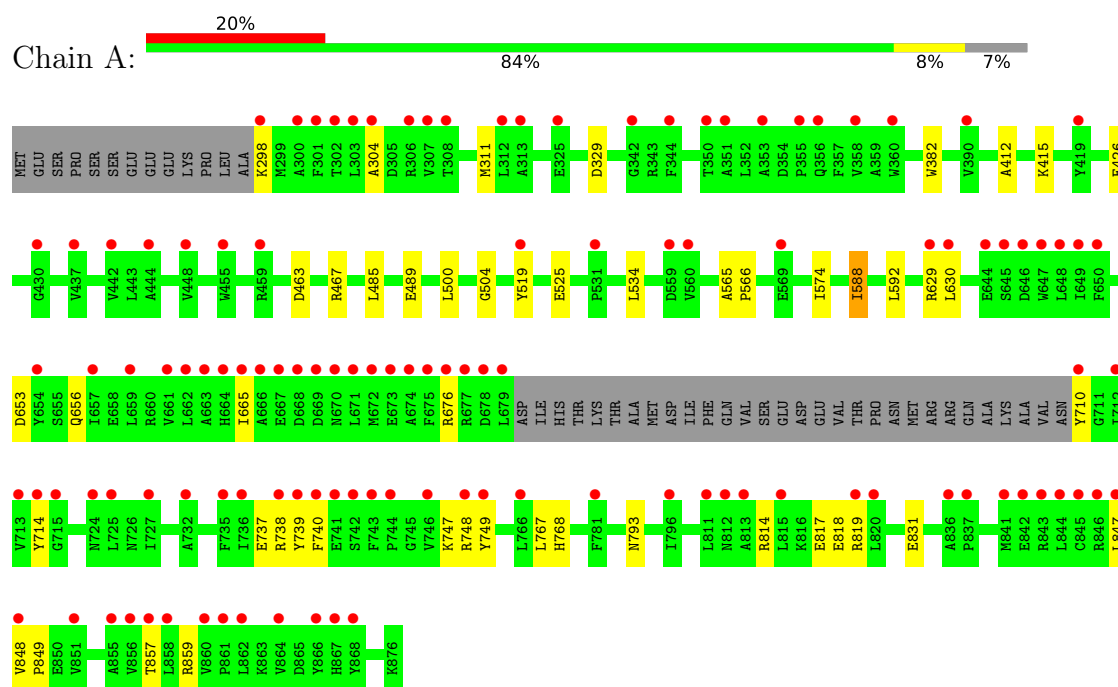
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	503	Total	O	0	0
			503	503		
7	D	775	Total	O	0	0
			775	775		
7	B	31	Total	O	0	0
			31	31		
7	C	50	Total	O	0	0
			50	50		
7	E	41	Total	O	0	0
			41	41		
7	F	68	Total	O	0	0
			68	68		

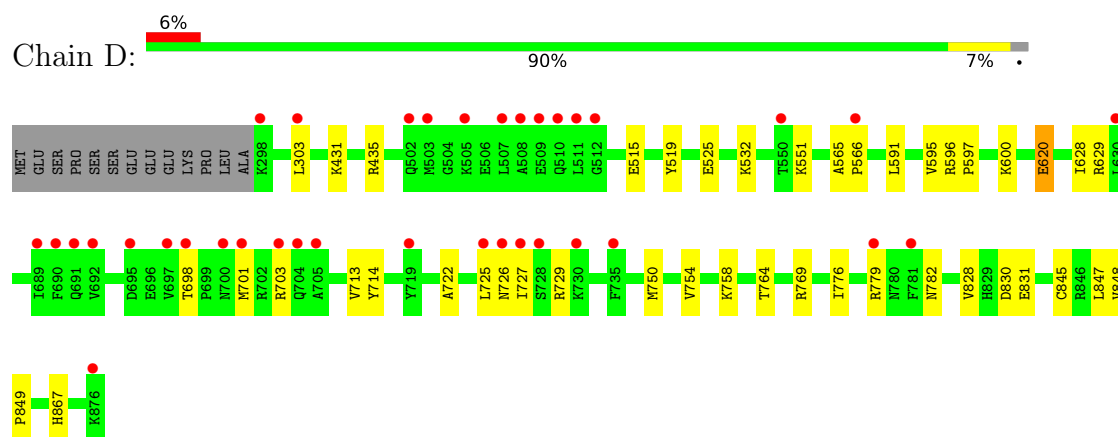
3 Residue-property plots

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')

Chain B:  78% 22%



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

Chain E:  78% 22%



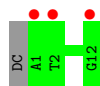
- Molecule 3: DNA (5'-D(*CP*AP*TP*AP*GP*GP*AP*GP*TP*CP*AP*GP*G)-3')

Chain C:  62% 8% 31%



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

Chain F:  23% 92% 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 109.19Å 150.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.10 – 1.58 71.10 – 1.58	Depositor EDS
% Data completeness (in resolution range)	89.6 (71.10-1.58) 89.7 (71.10-1.58)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 1.58Å)	Xtriage
Refinement program	PHENIX 1.7.1_743, REFMAC 5.5.0109	Depositor
R, R_{free}	0.211 , 0.239 0.210 , 0.238	Depositor DCC
R_{free} test set	8586 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 41.9	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	0.95	EDS
Total number of atoms	21056	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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: DCT, MG, DOC, SO4

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	0.44	0/4500	0.71	0/6082
1	D	0.59	0/4782	0.77	1/6464 (0.0%)
2	B	0.35	0/173	1.01	0/264
2	E	0.39	0/173	1.01	0/264
3	C	0.35	0/215	0.96	0/331
3	F	0.46	0/282	0.99	0/435
All	All	0.51	0/10125	0.77	1/13840 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	620	GLU	CB-CA-C	-5.31	106.38	111.00

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	4411	4476	4456	34	0
1	D	4675	4730	4686	33	1
2	B	174	101	103	3	0
2	E	174	101	103	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	191	101	101	1	0
3	F	250	133	136	0	0
4	A	27	4	12	0	0
4	D	27	2	12	2	0
5	D	1	0	0	0	0
6	D	10	0	0	0	0
7	A	503	0	0	10	2
7	B	31	0	0	0	0
7	C	50	0	0	1	0
7	D	775	0	0	13	6
7	E	41	0	0	0	0
7	F	68	0	0	0	0
All	All	11408	9648	9609	72	6

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 (72) 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:710:TYR:HB2	7:A:1447:HOH:O	1.89	0.72
1:A:665:ILE:HG22	1:A:749:TYR:CE1	2.28	0.69
1:D:830[B]:ASP:HB3	7:D:969:HOH:O	1.91	0.69
1:D:600:LYS:NZ	7:D:1403:HOH:O	2.30	0.64
1:D:830[A]:ASP:OD1	1:D:831[A]:GLU:HG2	1.99	0.60
1:A:629:ARG:HG3	1:A:630:LEU:HG	1.84	0.59
1:A:738:ARG:NH1	7:A:1108:HOH:O	2.35	0.59
1:D:830[B]:ASP:OD2	4:D:202:DCT:O1A	2.20	0.59
1:A:534:LEU:HD11	1:A:574:ILE:HD13	1.85	0.58
1:A:740:PHE:HB3	1:A:747:LYS:HD2	1.85	0.58
1:D:725:LEU:O	1:D:727:ILE:HG23	2.04	0.58
1:A:748:ARG:HD2	7:A:1245:HOH:O	2.04	0.57
1:A:519:TYR:CD2	1:A:525:GLU:HG2	2.41	0.56
1:D:828:VAL:HB	1:D:831[B]:GLU:CG	2.35	0.56
1:A:848:VAL:HB	1:A:849:PRO:HD3	1.87	0.56
1:D:776:ILE:HG22	7:D:1129:HOH:O	2.05	0.55
1:D:629:ARG:NH1	7:D:1271:HOH:O	2.39	0.55
1:D:726:ASN:CG	7:D:1433:HOH:O	2.50	0.55
1:D:565:ALA:N	1:D:566:PRO:CD	2.70	0.54
1:A:714:TYR:HB2	7:A:1018:HOH:O	2.08	0.53
1:D:515:GLU:HG2	1:D:519:TYR:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:629:ARG:NH2	7:D:1216:HOH:O	2.34	0.53
1:A:504:GLY:HA2	1:A:588:ILE:HD12	1.89	0.52
1:D:551:LYS:NZ	7:D:1046:HOH:O	2.42	0.52
2:B:22:DC:C6	2:B:22:DC:H5'	2.45	0.51
1:D:435:ARG:NH2	7:D:1463:HOH:O	2.35	0.51
1:A:629:ARG:HD2	7:A:1131:HOH:O	2.10	0.50
1:A:304:ALA:CB	1:A:311:MET:HE1	2.42	0.50
1:D:828:VAL:HB	1:D:831[A]:GLU:HG3	1.94	0.50
1:D:776:ILE:CG2	7:D:1129:HOH:O	2.57	0.49
1:A:412:ALA:HA	1:A:415:LYS:HD3	1.95	0.49
1:D:714:TYR:HB3	7:D:908:HOH:O	2.13	0.49
1:D:845:CYS:SG	7:D:883:HOH:O	2.48	0.48
1:A:767:LEU:O	1:A:768:HIS:HB2	2.13	0.48
1:D:620:GLU:HB2	7:D:1209:HOH:O	2.13	0.48
2:B:22:DC:H5'	2:B:22:DC:H6	1.78	0.48
1:A:298:LYS:N	7:A:1036:HOH:O	2.47	0.47
1:D:725:LEU:HB2	1:D:727:ILE:HG12	1.96	0.47
1:A:676:ARG:NH2	1:A:859:ARG:O	2.47	0.47
1:D:848:VAL:HB	1:D:849:PRO:HD3	1.97	0.47
1:A:485:LEU:O	1:A:489:GLU:HG3	2.14	0.46
1:A:426:GLU:HG3	7:A:1258:HOH:O	2.14	0.46
1:A:565:ALA:N	1:A:566:PRO:CD	2.78	0.46
1:A:817:GLU:HG3	1:A:818:GLU:N	2.30	0.45
1:D:519:TYR:CD2	1:D:525:GLU:HG2	2.50	0.45
1:A:814:ARG:HB3	1:A:847:LEU:HD11	1.97	0.45
1:A:739:TYR:CD2	1:A:739:TYR:C	2.94	0.45
1:D:867:HIS:HD2	7:D:1205:HOH:O	2.00	0.45
1:A:463:ASP:O	1:A:467:ARG:HG3	2.17	0.45
1:D:725:LEU:O	1:D:726:ASN:C	2.60	0.44
1:D:698:THR:OG1	1:D:701:MET:HG3	2.18	0.44
1:A:737:GLU:CD	7:A:1458:HOH:O	2.60	0.44
1:A:500:LEU:HD23	1:A:592:LEU:HG	1.99	0.44
1:D:847:LEU:C	1:D:847:LEU:HD23	2.43	0.44
1:A:665:ILE:CG2	1:A:749:TYR:CE1	2.98	0.43
1:A:814:ARG:O	1:A:818:GLU:HG2	2.18	0.43
1:A:793:ASN:HB2	7:A:1046:HOH:O	2.16	0.43
4:D:202:DCT:H6	4:D:202:DCT:O5'	2.18	0.43
1:D:722:ALA:HB2	1:D:729:ARG:HA	2.00	0.43
1:A:817:GLU:HG3	1:A:818:GLU:H	1.83	0.43
1:D:754:VAL:CG1	1:D:758:LYS:HE2	2.49	0.43
3:C:4:DG:H5''	7:C:215:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:GLN:NE2	7:A:1417:HOH:O	2.36	0.42
1:D:764:THR:HA	1:D:769:ARG:O	2.19	0.42
1:A:329:ASP:H	1:A:382:TRP:CD1	2.36	0.42
1:D:591:LEU:O	1:D:595:VAL:HG23	2.20	0.41
1:D:596:ARG:HA	1:D:597:PRO:HD3	1.96	0.41
1:D:754:VAL:HG12	1:D:758:LYS:HE2	2.02	0.41
2:E:28:DC:H2'	2:E:29:DOC:H6	2.02	0.41
1:A:653:ASP:CB	1:A:831:GLU:HG2	2.51	0.41
1:A:629:ARG:HH12	2:B:27:DT:P	2.45	0.40
1:D:713:VAL:O	1:D:750:MET:HE3	2.21	0.40

All (6) 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:D:1210:HOH:O	7:D:1238:HOH:O[4_445]	1.69	0.51
7:A:1211:HOH:O	7:D:1208:HOH:O[2_745]	1.82	0.38
1:D:779:ARG:HH22	7:D:1406:HOH:O[4_545]	1.39	0.21
7:D:1027:HOH:O	7:D:1028:HOH:O[4_545]	2.03	0.17
7:A:990:HOH:O	7:D:942:HOH:O[4_545]	2.14	0.06
7:D:1397:HOH:O	7:D:1407:HOH:O[4_445]	2.17	0.03

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
1	A	547/592 (92%)	531 (97%)	15 (3%)	1 (0%)	43 26
1	D	584/592 (99%)	571 (98%)	12 (2%)	1 (0%)	43 26
All	All	1131/1184 (96%)	1102 (97%)	27 (2%)	2 (0%)	43 26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	819	ARG
1	D	628	ILE

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	469/507 (92%)	467 (100%)	2 (0%)	84	75
1	D	501/507 (99%)	496 (99%)	5 (1%)	68	49
All	All	970/1014 (96%)	963 (99%)	7 (1%)	76	61

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	588	ILE
1	A	857	THR
1	D	303	LEU
1	D	431	LYS
1	D	532	LYS
1	D	703	ARG
1	D	782	ASN

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

Mol	Chain	Res	Type
1	A	418	GLN
1	A	726	ASN
1	D	759	GLN
1	D	854	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	B	29	2,3	16,19,20	0.47	0	20,26,29	0.61	0
2	DOC	E	29	2,3	16,19,20	0.49	0	20,26,29	0.65	0

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

There are no bond length outliers.

There are no bond angle outliers.

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	E	29	DOC	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	DCT	D	202	5	27,28,28	1.12	2 (7%)	37,43,43	1.31	4 (10%)
4	DCT	A	203	-	27,28,28	0.97	0	37,43,43	1.35	3 (8%)
6	SO4	D	2	-	4,4,4	0.28	0	6,6,6	0.14	0
6	SO4	D	877	-	4,4,4	0.25	0	6,6,6	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DCT	D	202	5	-	0/22/31/31	0/2/2/2
4	DCT	A	203	-	-	2/22/31/31	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	202	DCT	PA-O3A	3.14	1.62	1.59
4	D	202	DCT	PB-O3B	2.36	1.62	1.59

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	202	DCT	C2'-C1'-N1	-3.66	105.46	112.40
4	A	203	DCT	O4'-C4'-C5'	3.38	115.43	109.34
4	D	202	DCT	O2B-PB-O3A	3.20	115.92	107.27
4	A	203	DCT	C2'-C1'-N1	-3.00	106.71	112.40
4	D	202	DCT	O3A-PB-O1B	-2.82	102.23	110.70
4	A	203	DCT	C3'-C2'-C1'	2.63	105.90	102.87
4	D	202	DCT	O2B-PB-O3B	2.54	114.14	107.27

There are no chirality outliers.

All (2) torsion outliers are listed below:

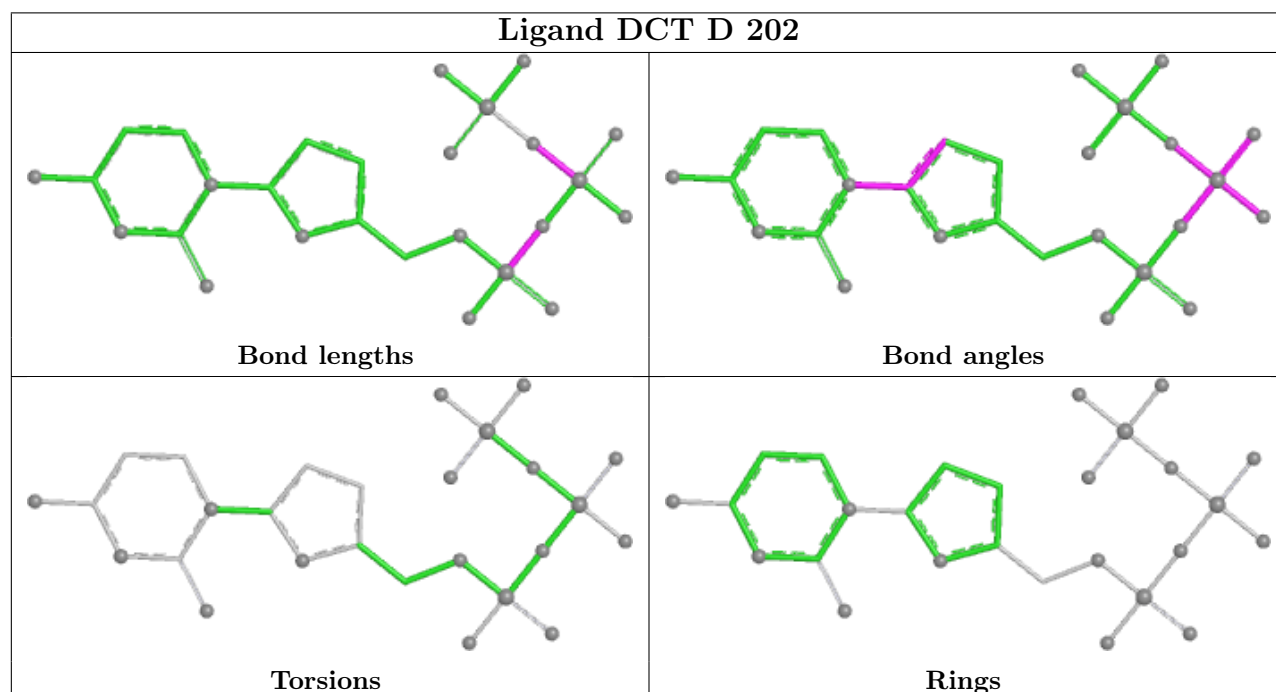
Mol	Chain	Res	Type	Atoms
4	A	203	DCT	C3'-C4'-C5'-O5'
4	A	203	DCT	O4'-C4'-C5'-O5'

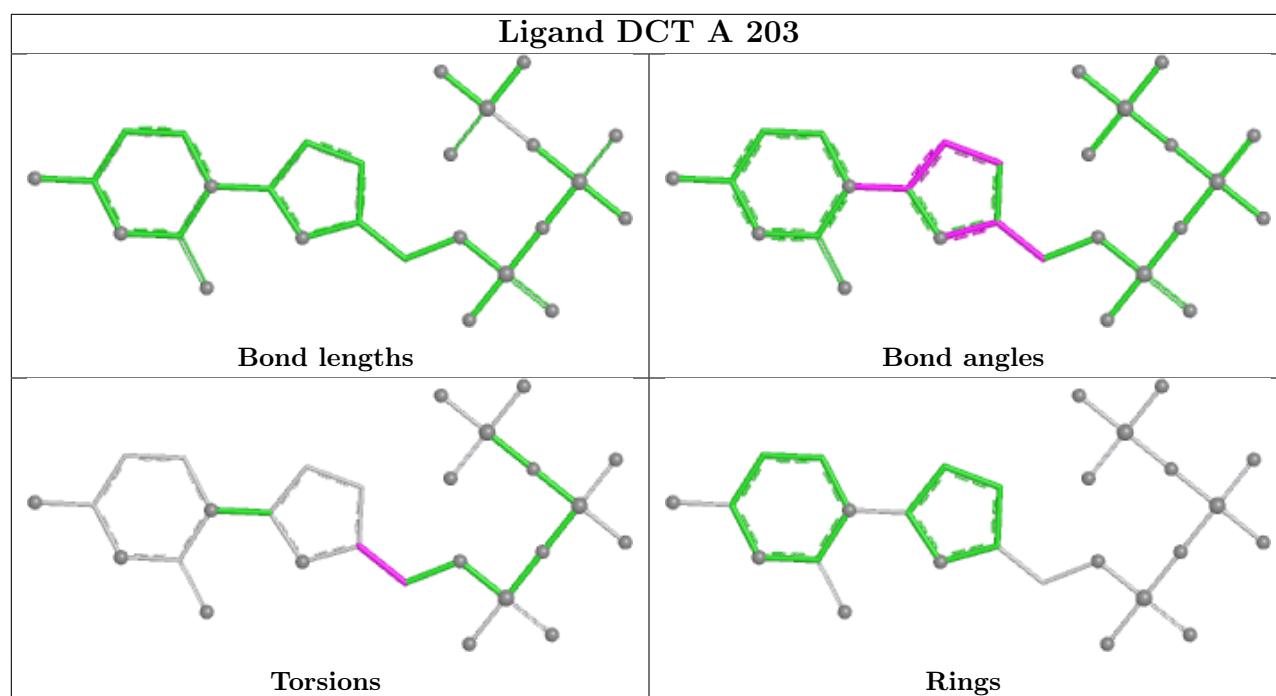
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	202	DCT	2	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	549/592 (92%)	1.13	118 (21%) 2 4	9, 33, 55, 73	1 (0%)
1	D	579/592 (97%)	0.22	36 (6%) 26 36	6, 20, 42, 56	4 (0%)
2	B	8/9 (88%)	0.31	0 100 100	21, 27, 44, 52	0
2	E	8/9 (88%)	0.21	0 100 100	16, 24, 40, 53	0
3	C	9/13 (69%)	0.00	0 100 100	17, 21, 30, 37	0
3	F	12/13 (92%)	0.40	3 (25%) 2 2	13, 21, 46, 62	0
All	All	1165/1228 (94%)	0.65	157 (13%) 7 12	6, 27, 51, 73	5 (0%)

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	671	LEU	6.6
1	A	679	LEU	6.3
1	A	847	LEU	5.2
1	A	743	PHE	5.1
1	A	675	PHE	4.6
1	A	858	LEU	4.4
1	A	670	ASN	4.4
1	A	866	TYR	4.3
1	A	298	LYS	4.2
1	A	300	ALA	4.1
1	A	710	TYR	4.1
1	A	714	TYR	4.0
1	A	860	VAL	4.0
1	A	735	PHE	3.9
1	A	740	PHE	3.9
1	A	851	VAL	3.9
1	A	862	LEU	3.9
1	A	647	TRP	3.8
1	D	507	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	698	THR	3.8
1	A	674	ALA	3.8
1	A	856	VAL	3.7
1	D	690	PHE	3.7
1	A	739	TYR	3.7
1	A	864	VAL	3.6
1	A	303	LEU	3.6
1	D	692	VAL	3.5
1	A	844	LEU	3.5
1	A	845	CYS	3.5
1	D	725	LEU	3.4
1	A	712	ILE	3.4
1	D	509	GLU	3.4
1	A	725	LEU	3.4
1	A	459	ARG	3.3
1	A	672	MET	3.3
3	F	1	DA	3.3
1	D	727	ILE	3.3
1	D	781	PHE	3.3
1	A	843	ARG	3.3
1	A	307	VAL	3.3
1	D	303	LEU	3.2
1	A	677	ARG	3.2
1	D	700	ASN	3.2
1	A	819	ARG	3.2
1	D	730	LYS	3.1
1	A	727	ILE	3.1
1	A	736	ILE	3.1
1	D	735	PHE	3.1
1	A	742	SER	3.1
1	D	695	ASP	3.1
1	A	820	LEU	3.0
1	A	855	ALA	3.0
1	A	749	TYR	3.0
1	D	697	VAL	3.0
1	D	566	PRO	3.0
1	A	857	THR	3.0
1	A	744	PRO	3.0
1	D	689	ILE	2.9
1	A	713	VAL	2.9
1	D	508	ALA	2.9
1	A	673	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	836	ALA	2.9
1	A	301	PHE	2.9
1	A	815	LEU	2.9
1	A	741	GLU	2.9
1	A	304	ALA	2.8
1	A	663	ALA	2.8
1	A	861	PRO	2.8
1	A	746	VAL	2.7
1	A	645	SER	2.7
1	D	505	LYS	2.7
1	A	669	ASP	2.7
1	A	444	ALA	2.7
1	D	298	LYS	2.7
1	A	813	ALA	2.6
1	A	868	TYR	2.6
1	A	659	LEU	2.6
1	A	353	ALA	2.6
1	A	665	ILE	2.6
1	A	738	ARG	2.6
1	D	728	SER	2.6
1	D	550	THR	2.5
1	A	342	GLY	2.5
1	A	430	GLY	2.5
1	A	661	VAL	2.5
1	D	876	LYS	2.5
1	A	766	LEU	2.5
1	A	350	THR	2.5
1	A	629	ARG	2.5
1	A	657	ILE	2.5
1	D	779	ARG	2.4
3	F	2	DT	2.4
1	A	360	TRP	2.4
1	A	390	VAL	2.4
1	A	442	VAL	2.4
1	A	560	VAL	2.4
1	A	848	VAL	2.4
1	A	867	HIS	2.4
1	A	649	ILE	2.4
1	A	306	ARG	2.4
1	D	512	GLY	2.4
1	A	455	TRP	2.3
1	A	312	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	569	GLU	2.3
1	A	419	TYR	2.3
1	D	691	GLN	2.3
1	A	676	ARG	2.3
1	A	308	THR	2.3
1	A	715	GLY	2.3
1	A	841	MET	2.3
1	A	531	PRO	2.3
1	A	448	VAL	2.3
1	A	664	HIS	2.3
1	A	351	ALA	2.2
1	A	732	ALA	2.2
1	A	837	PRO	2.2
1	D	503	MET	2.2
1	D	701	MET	2.2
3	F	12	DG	2.2
1	A	842	GLU	2.2
1	A	811	LEU	2.2
1	A	630	LEU	2.2
1	A	796	ILE	2.2
1	A	654	TYR	2.2
1	A	812	ASN	2.2
1	D	726	ASN	2.2
1	A	646	ASP	2.2
1	A	678	ASP	2.2
1	A	437	VAL	2.2
1	D	704	GLN	2.1
1	A	325	GLU	2.1
1	A	559	ASP	2.1
1	A	344	PHE	2.1
1	A	358	VAL	2.1
1	A	748	ARG	2.1
1	D	703	ARG	2.1
1	A	313	ALA	2.1
1	A	662	LEU	2.1
1	A	666	ALA	2.1
1	D	719	TYR	2.1
1	A	781	PHE	2.1
1	D	511	LEU	2.1
1	D	630	LEU	2.1
1	A	846	ARG	2.1
1	D	502	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	724	ASN	2.1
1	A	355	PRO	2.1
1	A	648	LEU	2.0
1	A	644	GLU	2.0
1	A	667	GLU	2.0
1	A	668	ASP	2.0
1	A	302	THR	2.0
1	A	356	GLN	2.0
1	D	510	GLN	2.0
1	D	705	ALA	2.0
1	A	650	PHE	2.0
1	A	519	TYR	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	0.08	15,24,32,35	0
2	DOC	E	29	18/19	0.97	0.06	10,14,19,22	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.

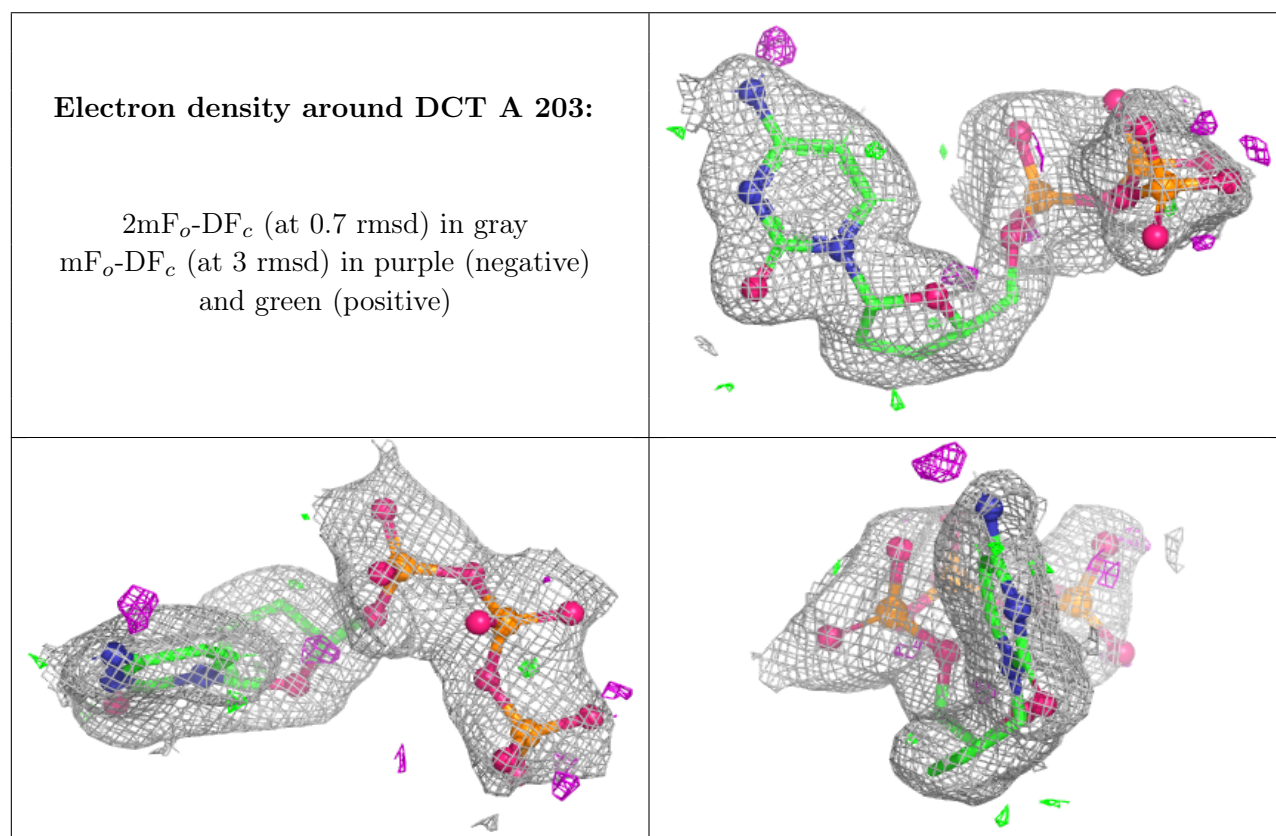
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	DCT	A	203	27/27	0.85	0.13	19,36,62,65	0
6	SO4	D	2	5/5	0.90	0.12	27,29,32,38	0
5	MG	D	1	1/1	0.96	0.10	29,29,29,29	0
4	DCT	D	202	27/27	0.96	0.08	14,20,29,31	0

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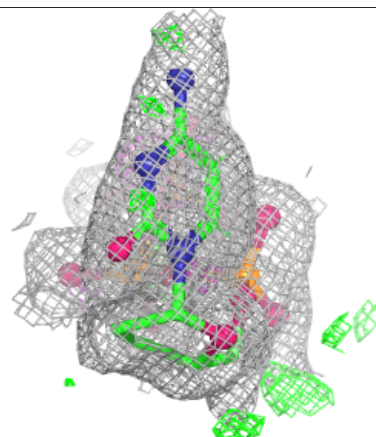
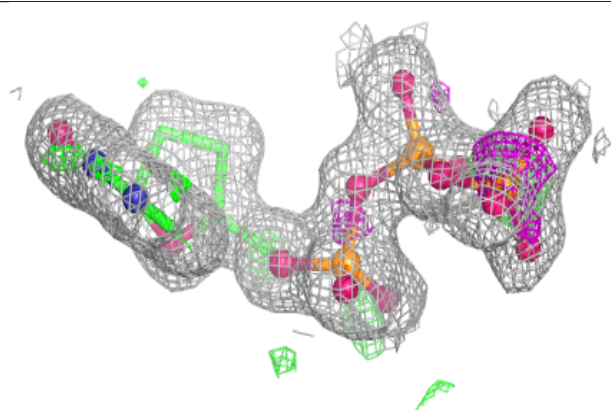
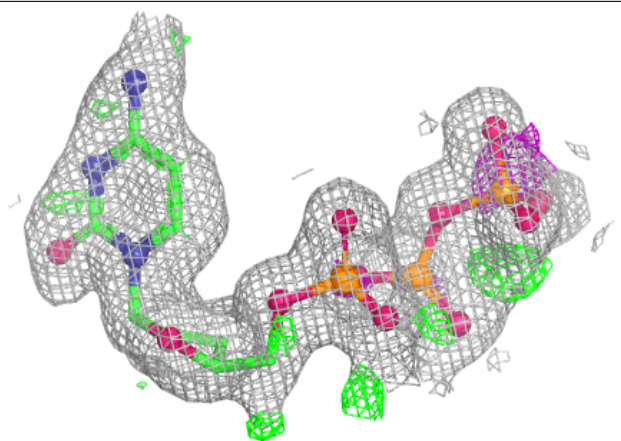
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	D	877	5/5	0.97	0.08	26,26,37,42	0

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 DCT D 202:

$2mF_o-DF_c$ (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.