W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2021 – 04:01 PM EDT

PDB ID	:	3E0D
Title	:	Insights into the Replisome from the Crystal Structure of the Ternary Complex of the Eubacterial DNA Polymerase III alpha-subunit
Authors	:	Wing, R.A.; Bailey, S.; Steitz, T.A.
Deposited on	:	2008-07-31
Resolution	:	4.60 Å(reported)

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

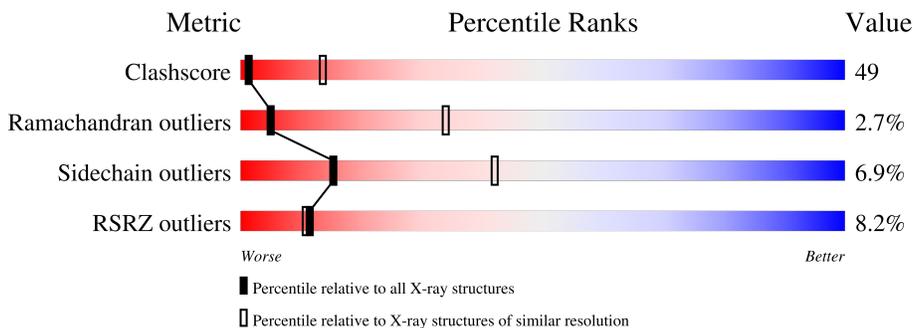|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 4.60 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	Percentile Ranks	Value
Clashscore		49
Ramachandran outliers		2.7%
Sidechain outliers		6.9%
RSRZ outliers		8.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1130 (5.40-3.80)
Ramachandran outliers	138981	1074 (5.40-3.80)
Sidechain outliers	138945	1055 (5.40-3.80)
RSRZ outliers	127900	1113 (5.50-3.70)

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 <=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	C	27	4% 67% 26%
1	E	27	70% 26%
2	D	21	5% 57% 24% 5% 10%
2	F	21	81% 10% 10%
3	A	1220	9% 61% 28% 6%
3	B	1220	7% 61% 28% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DOC	D	21	-	-	X	-
2	DOC	F	21	-	-	X	-
5	DTP	A	1222	-	-	X	-
5	DTP	B	1222	-	-	X	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 19982 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 DNA substrate template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	20	Total	C	N	O	P	0	0	0
			407	195	69	124	19			
1	E	20	Total	C	N	O	P	0	0	0
			407	195	69	124	19			

- Molecule 2 is a DNA chain called DNA substrate primer strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	19	Total	C	N	O	P	0	0	0
			385	183	78	106	18			
2	F	19	Total	C	N	O	P	0	0	0
			385	183	78	106	18			

- Molecule 3 is a protein called DNA polymerase III subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1148	Total	C	N	O	S	0	0	0
			9168	5847	1605	1688	28			
3	B	1148	Total	C	N	O	S	0	0	0
			9168	5847	1605	1688	28			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ASN	ASP	engineered mutation	UNP Q9XDH5
A	212	ASN	ASP	engineered mutation	UNP Q9XDH5
A	539	PHE	ILE	engineered mutation	UNP Q9XDH5
A	540	GLU	GLN	engineered mutation	UNP Q9XDH5
A	541	ALA	VAL	engineered mutation	UNP Q9XDH5
A	542	GLU	VAL	engineered mutation	UNP Q9XDH5
B	20	ASN	ASP	engineered mutation	UNP Q9XDH5
B	212	ASN	ASP	engineered mutation	UNP Q9XDH5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	539	PHE	ILE	engineered mutation	UNP Q9XDH5
B	540	GLU	GLN	engineered mutation	UNP Q9XDH5
B	541	ALA	VAL	engineered mutation	UNP Q9XDH5
B	542	GLU	VAL	engineered mutation	UNP Q9XDH5

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Ca 1	0	0
4	B	1	Total 1	Ca 1	0	0

- Molecule 5 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).
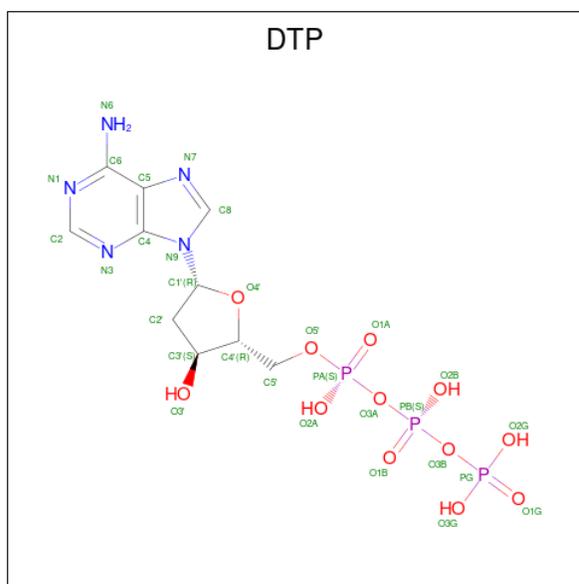
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 30	C 10	N 5	O 12	P 3	0	0
5	B	1	Total 30	C 10	N 5	O 12	P 3	0	0

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 substrate template strand
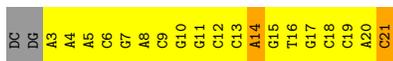
Chain C:

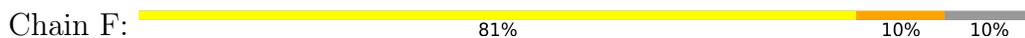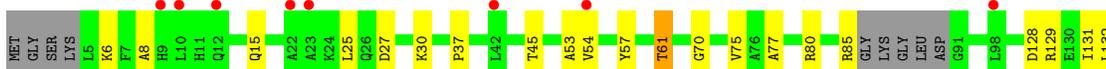• Molecule 1: DNA substrate template strand
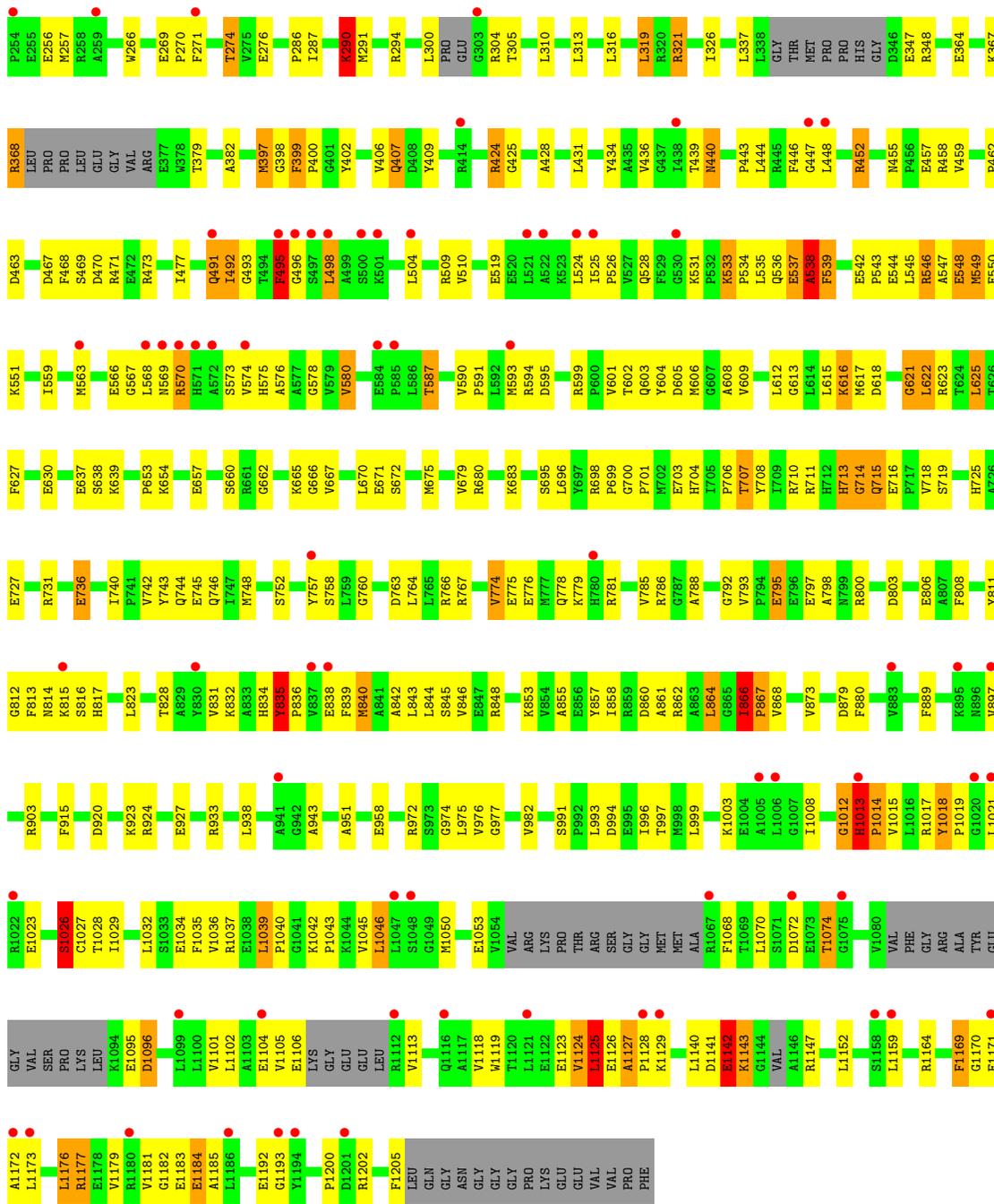
Chain E:
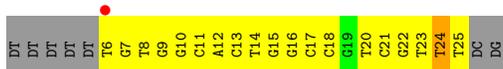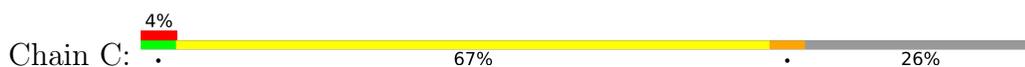
• Molecule 2: DNA substrate primer strand

Chain D:

• Molecule 2: DNA substrate primer strand

Chain F:

• Molecule 3: DNA polymerase III subunit alpha

Chain A:

• Molecule 3: DNA polymerase III subunit alpha

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	149.55Å 149.55Å 163.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.60 49.85 – 4.59	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-4.60) 99.5 (49.85-4.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 4.64Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.287 , 0.271 0.303 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	215.6	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 198.0	EDS
L-test for twinning[2]	$< |L| > = 0.38, < L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.347 for h,-k,-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	19982	wwPDB-VP
Average B, all atoms (Å^2)	233.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: DTP, DOC, CA

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	C	2.18	1/454 (0.2%)	1.01	3/700 (0.4%)
1	E	0.74	1/454 (0.2%)	0.88	0/700
2	D	1.93	1/413 (0.2%)	1.24	6/635 (0.9%)
2	F	0.85	1/413 (0.2%)	0.95	0/635
3	A	0.68	13/9348 (0.1%)	1.00	21/12615 (0.2%)
3	B	0.79	14/9346 (0.1%)	0.84	20/12608 (0.2%)
All	All	0.84	31/20428 (0.2%)	0.94	50/27893 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	3
3	A	3	8
3	B	4	11
All	All	7	22

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	24	DT	O3'-P	43.89	2.13	1.61
3	B	713	HIS	C-N	34.20	1.94	1.33
3	B	397	MET	C-N	29.55	1.86	1.33
2	D	3	DA	O3'-P	29.28	1.96	1.61
3	A	567	GLY	C-N	28.47	1.99	1.34

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	495	PHE	O-C-N	-47.05	43.21	123.20
3	A	699	PRO	CA-C-N	-41.86	32.49	116.20
3	A	699	PRO	C-N-CA	-39.91	38.49	122.30
3	A	1127	ALA	C-N-CD	-29.66	55.35	120.60
3	A	495	PHE	C-N-CA	-28.34	62.79	122.30

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	538	ALA	CA
3	A	1013	HIS	CA
3	A	1120	THR	CB
3	B	538	ALA	CA
3	B	866	ILE	CA

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	285	LEU	Mainchain
3	A	337	LEU	Mainchain
2	D	11	DG	Sidechain
2	D	20	DA	Sidechain
2	D	7	DG	Sidechain

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	C	407	0	230	199	0
1	E	407	0	229	139	0
2	D	385	0	212	143	1
2	F	385	0	212	79	0
3	A	9168	0	9186	856	33
3	B	9168	0	9182	793	35
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	30	0	12	24	0
5	B	30	0	11	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	19982	0	19274	1892	36

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 49.

The worst 5 of 1892 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)
3:A:1013:HIS:CE1	3:A:1073:GLU:HB3	1.26	1.68
3:A:858:ILE:HD11	3:A:889:PHE:CZ	1.24	1.65
3:A:844:LEU:HB3	3:A:880:PHE:CE1	1.24	1.64
3:B:831:VAL:HG12	3:B:839:PHE:CD1	1.14	1.63
3:B:832:LYS:HB2	3:B:839:PHE:CE2	1.26	1.63

The worst 5 of 36 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)
3:A:1177:ARG:NH2	3:B:972:ARG:CA[3_655]	0.82	1.38
3:A:1154:GLU:O	3:B:157:ASP:OD2[1_655]	0.99	1.21
3:A:657:GLU:OE2	3:B:654:LYS:N[2_655]	1.00	1.20
3:A:1177:ARG:NH2	3:B:972:ARG:CB[3_655]	1.14	1.06
3:A:654:LYS:N	3:B:657:GLU:OE2[2_655]	1.22	0.98

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	
3	A	1124/1220 (92%)	1006 (90%)	88 (8%)	30 (3%)	5	34
3	B	1120/1220 (92%)	1007 (90%)	82 (7%)	31 (3%)	5	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2244/2440 (92%)	2013 (90%)	170 (8%)	61 (3%)	5	34

5 of 61 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	286	PRO
3	A	537	GLU
3	A	538	ALA
3	A	774	VAL
3	A	836	PRO

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	
3	A	953/1008 (94%)	889 (93%)	64 (7%)	16	43
3	B	953/1008 (94%)	886 (93%)	67 (7%)	15	41
All	All	1906/2016 (94%)	1775 (93%)	131 (7%)	15	42

5 of 131 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	1013	HIS
3	B	1032	LEU
3	B	1192	GLU
3	A	958	GLU
3	A	927	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	569	ASN
3	B	746	GLN
3	B	725	HIS

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Mol	Chain	Res	Type
3	B	778	GLN
3	A	746	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	D	21	2,1	14,19,20	1.07	2 (14%)	13,26,29	1.38	2 (15%)
2	DOC	F	21	2,1	14,19,20	1.07	1 (7%)	13,26,29	1.37	1 (7%)

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	D	21	2,1	-	2/4/18/19	0/2/2/2
2	DOC	F	21	2,1	-	2/4/18/19	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	21	DOC	O5'-C5'	-2.22	1.39	1.44
2	D	21	DOC	C6-C5	-2.20	1.33	1.38
2	F	21	DOC	C6-C5	-2.13	1.33	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	21	DOC	C2-N3-C4	3.83	120.23	116.34
2	D	21	DOC	C2-N3-C4	3.80	120.19	116.34
2	D	21	DOC	C3'-C2'-C1'	2.32	105.45	102.78

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	21	DOC	C3'-C4'-C5'-O5'
2	D	21	DOC	C4'-C5'-O5'-P
2	F	21	DOC	C4'-C5'-O5'-P
2	F	21	DOC	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	21	DOC	25	0
2	F	21	DOC	16	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 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	#$|Z| > 2$
5	DTP	A	1222	4	26,32,32	1.27	2 (7%)	30,50,50	1.28	4 (13%)
5	DTP	B	1222	4	26,32,32	1.27	2 (7%)	30,50,50	1.28	4 (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
5	DTP	A	1222	4	-	5/18/34/34	0/3/3/3
5	DTP	B	1222	4	-	5/18/34/34	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1222	DTP	O4'-C1'	-3.10	1.35	1.42
5	A	1222	DTP	O4'-C1'	-3.09	1.35	1.42
5	B	1222	DTP	PA-O2A	-2.69	1.42	1.55
5	A	1222	DTP	PA-O2A	-2.66	1.42	1.55

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1222	DTP	C2'-C1'-N9	-3.07	107.20	114.27
5	B	1222	DTP	C2'-C1'-N9	-3.03	107.28	114.27
5	B	1222	DTP	O3'-C3'-C4'	2.91	121.23	110.10
5	A	1222	DTP	O3'-C3'-C4'	2.89	121.17	110.10
5	A	1222	DTP	O3G-PG-O3B	-2.84	95.11	104.64

There are no chirality outliers.
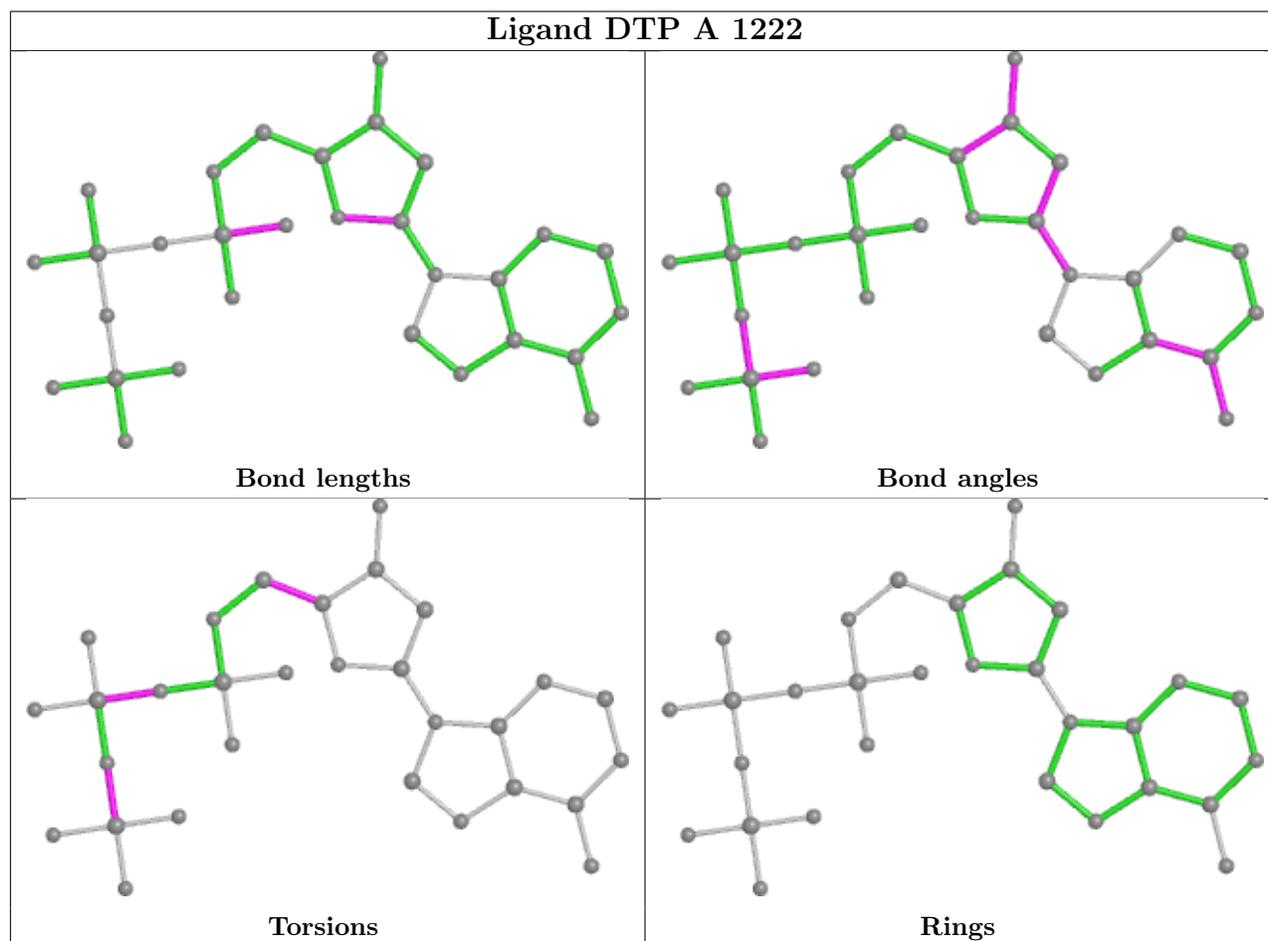
5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1222	DTP	PB-O3B-PG-O3G
5	B	1222	DTP	PB-O3B-PG-O3G
5	A	1222	DTP	O4'-C4'-C5'-O5'
5	B	1222	DTP	O4'-C4'-C5'-O5'
5	A	1222	DTP	PA-O3A-PB-O1B

There are no ring outliers.

2 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1222	DTP	24	0
5	B	1222	DTP	14	0

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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 then 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.

Ligand DTP A 1222

Bond lengths

Bond angles

Torsions

Rings

Ligand DTP B 1222

Bond lengths

Bond angles

Torsions

Rings
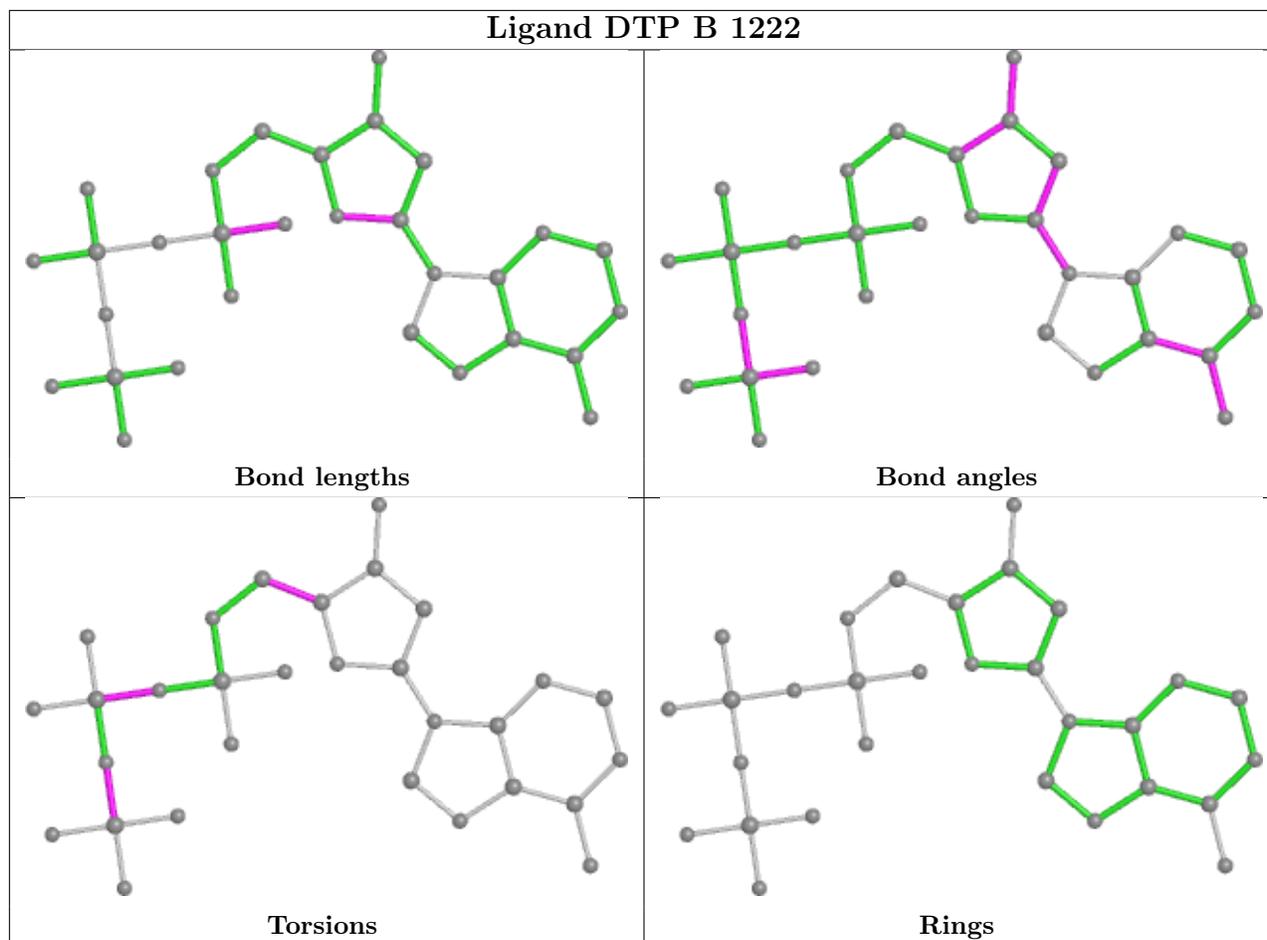
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	B	12
3	A	9
1	C	1
2	D	1

The worst 5 of 23 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	575:HIS	C	576:ALA	N	3.18
1	B	575:HIS	C	576:ALA	N	3.14

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	812:GLY	C	813:PHE	N	2.78
1	B	812:GLY	C	813:PHE	N	2.56
1	B	285:LEU	C	286:PRO	N	2.49

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	C	20/27 (74%)	-0.30	1 (5%)	28	25	228, 228, 228, 228	0
1	E	20/27 (74%)	-0.63	0	100	100	228, 228, 228, 228	0
2	D	18/21 (85%)	-0.50	0	100	100	66, 228, 228, 228	0
2	F	18/21 (85%)	-0.50	0	100	100	228, 228, 228, 228	0
3	A	1148/1220 (94%)	0.34	105 (9%)	9	8	201, 226, 296, 326	0
3	B	1148/1220 (94%)	0.33	88 (7%)	13	12	201, 226, 296, 326	0
All	All	2372/2536 (93%)	0.31	194 (8%)	11	11	66, 226, 296, 326	0

The worst 5 of 194 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	1026	SER	8.0
3	B	496	GLY	7.8
3	B	569	ASN	7.2
3	B	1129	LYS	6.4
3	B	524	LEU	6.3

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

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.

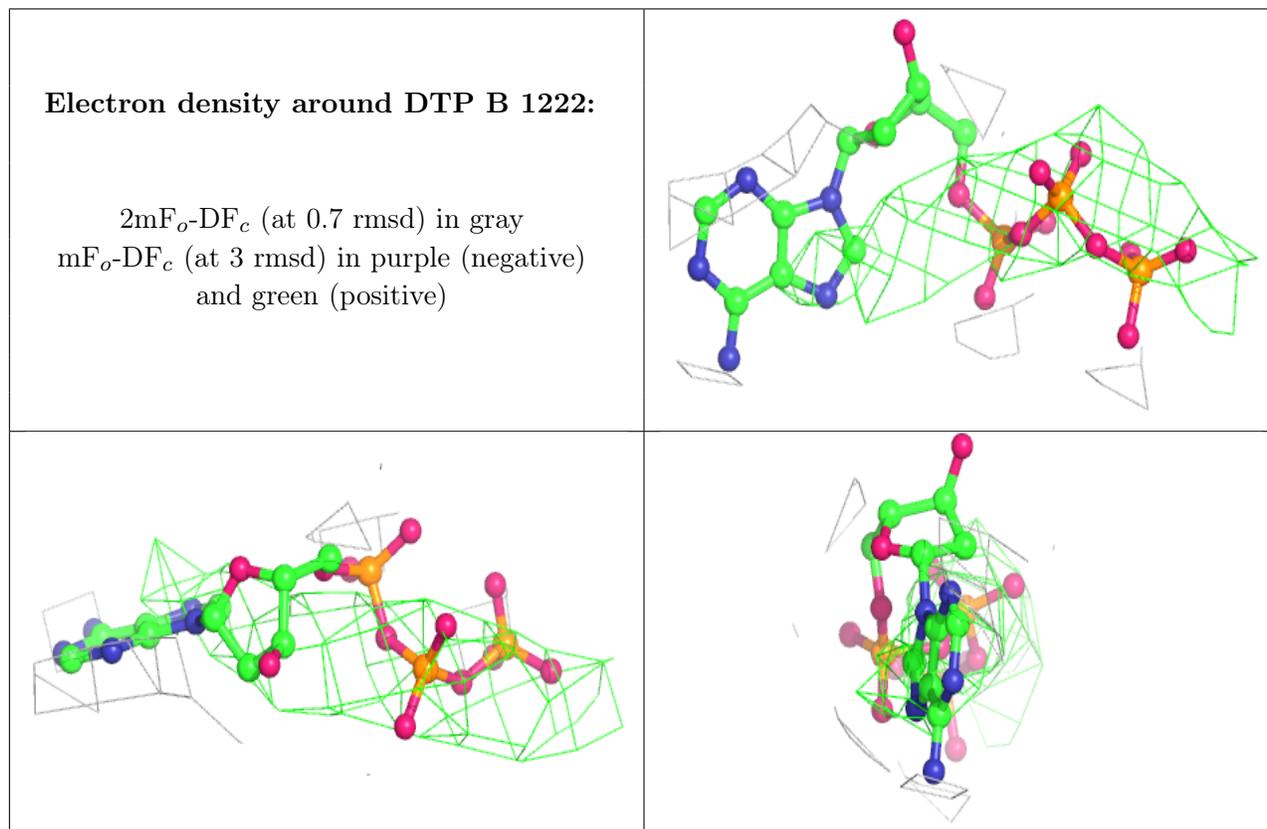| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DOC	F	21	18/19	0.67	0.26	227,227,227,227	0
2	DOC	D	21	18/19	0.78	0.19	227,227,227,227	0

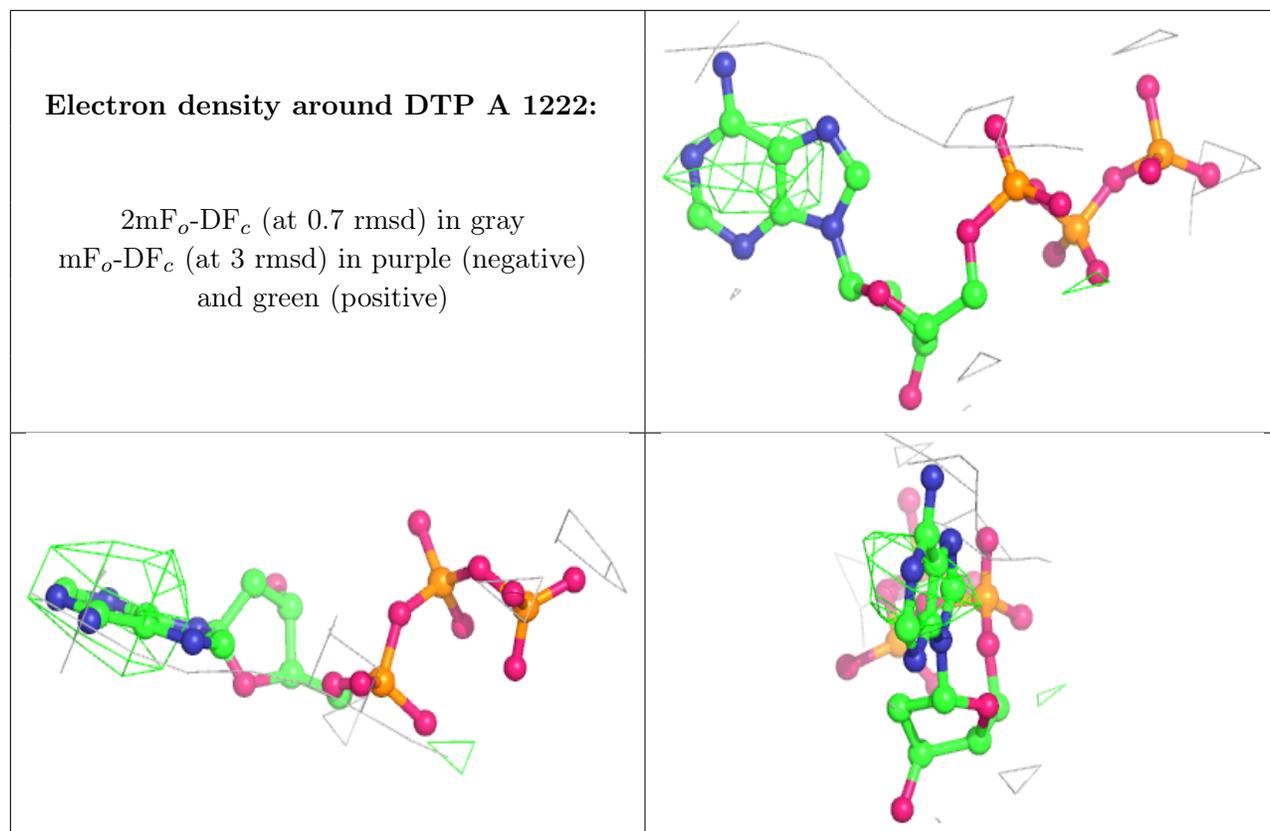## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DTP	B	1222	30/30	0.80	0.28	242,242,242,242	0
5	DTP	A	1222	30/30	0.83	0.25	242,242,242,242	0
4	CA	B	1221	1/1	0.96	0.24	47,47,47,47	0
4	CA	A	1221	1/1	0.97	0.26	47,47,47,47	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 DTP B 1222:

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

Electron density around DTP A 1222:

$2mF_o$-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.