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 16, 2021 – 06:45 PM EDT

PDB ID	:	1TUG
Title	:	Aspartate Transcarbamoylase Catalytic Chain Mutant E50A Complex with Phosphonoacetamide, Malonate, and Cytidine-5-Prime-Triphosphate (CTP)
Authors	:	Stieglitz, K.; Stec, B.; Baker, D.P.; Kantrowitz, E.R.
Deposited on	:	2004-06-24
Resolution	:	2.10 Å(reported)

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

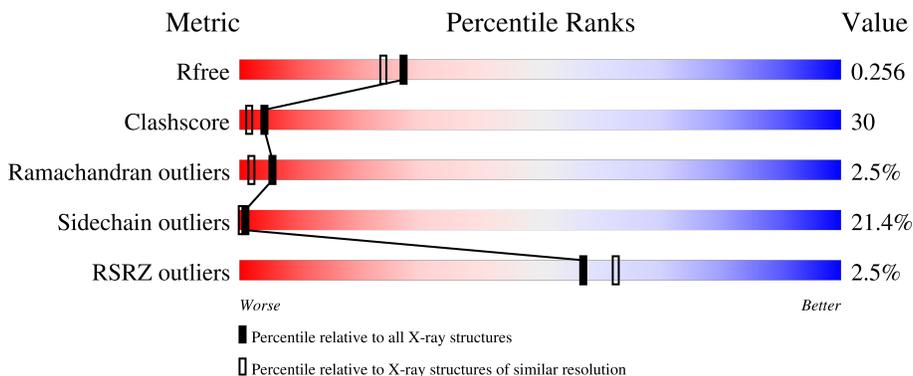|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.256
Clashscore		30
Ramachandran outliers		2.5%
Sidechain outliers		21.4%
RSRZ outliers		2.5%

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))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	310	4% / 43% 43% 14%
1	C	310	.% / 56% 32% 9% •
2	B	153	2% / 27% 50% 20% •
2	D	153	4% / 27% 50% 20% •

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
3	MLI	A	1312	-	-	-	X
3	MLI	C	1311	-	-	X	X
4	PCT	C	1313	-	X	X	-

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 8012 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 protein called Aspartate carbamoyltransferase catalytic chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2411	1525	423	454	9			
1	C	310	Total	C	N	O	S	0	0	0
			2411	1525	423	454	9			

There are 2 discrepancies between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
A	50	ALA	GLU	engineered mutation	UNP P0A786
C	50	ALA	GLU	engineered mutation	UNP P0A786

- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			
2	D	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P0A7F3
D	1	MET	-	initiating methionine	UNP P0A7F3

- Molecule 3 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).

MLI

C1 C2

O7 O⁻

C3

O9 O⁻

O6 O

O8 O
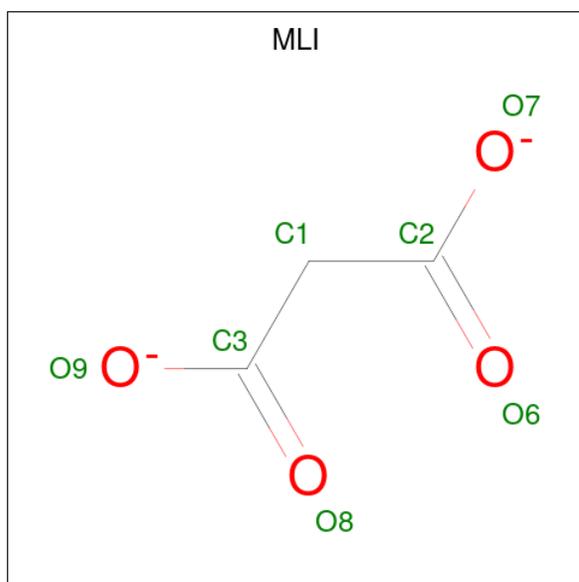
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 7	C 3	O 4	0	0
3	C	1	Total 7	C 3	O 4	0	0

- Molecule 4 is PHOSPHONOACETAMIDE (three-letter code: PCT) (formula: $C_2H_6NO_4P$).

PCT

N1 NH₂

C1P C1

O3P HO P

O1 O

O2P OH

O1P O
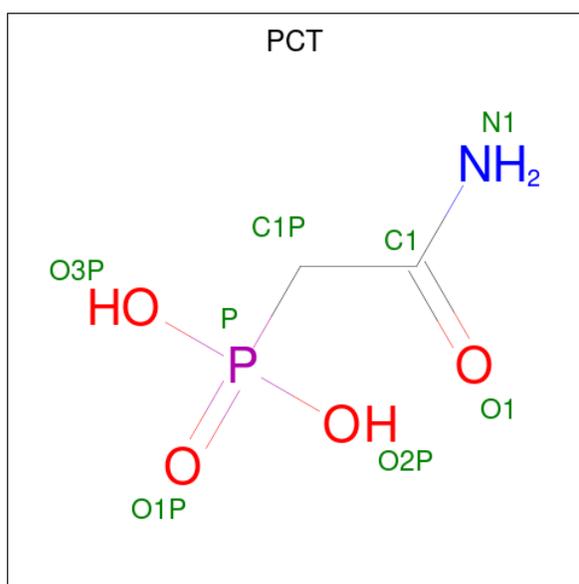
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 8	C 2	N 1	O 4	P 1	0	0
4	C	1	Total 8	C 2	N 1	O 4	P 1	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Zn 1	0	0
5	D	1	Total 1	Zn 1	0	0

- Molecule 6 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula: $C_9H_{16}N_3O_{14}P_3$).

CTP
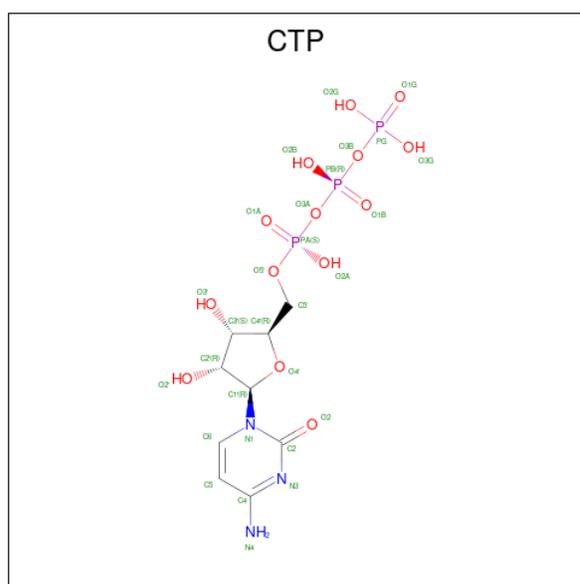
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total 29	C 9	N 3	O 14	P 3	0	0
6	D	1	Total 29	C 9	N 3	O 14	P 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	211	Total 211	O 211	0	0
7	B	101	Total 101	O 101	0	0
7	C	265	Total 265	O 265	0	0
7	D	121	Total 121	O 121	0	0

3 Residue-property plots ⓘ

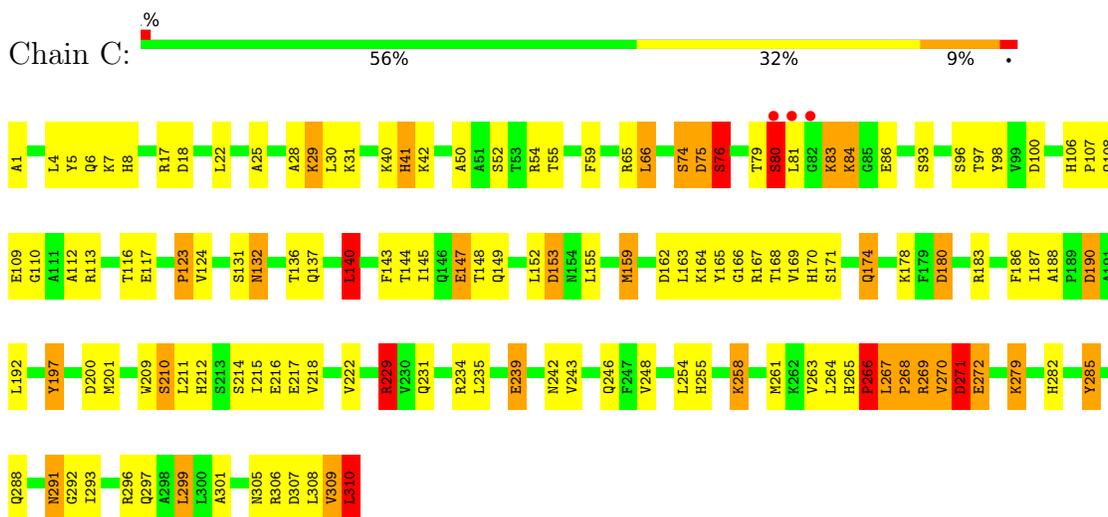These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Aspartate carbamoyltransferase catalytic chain
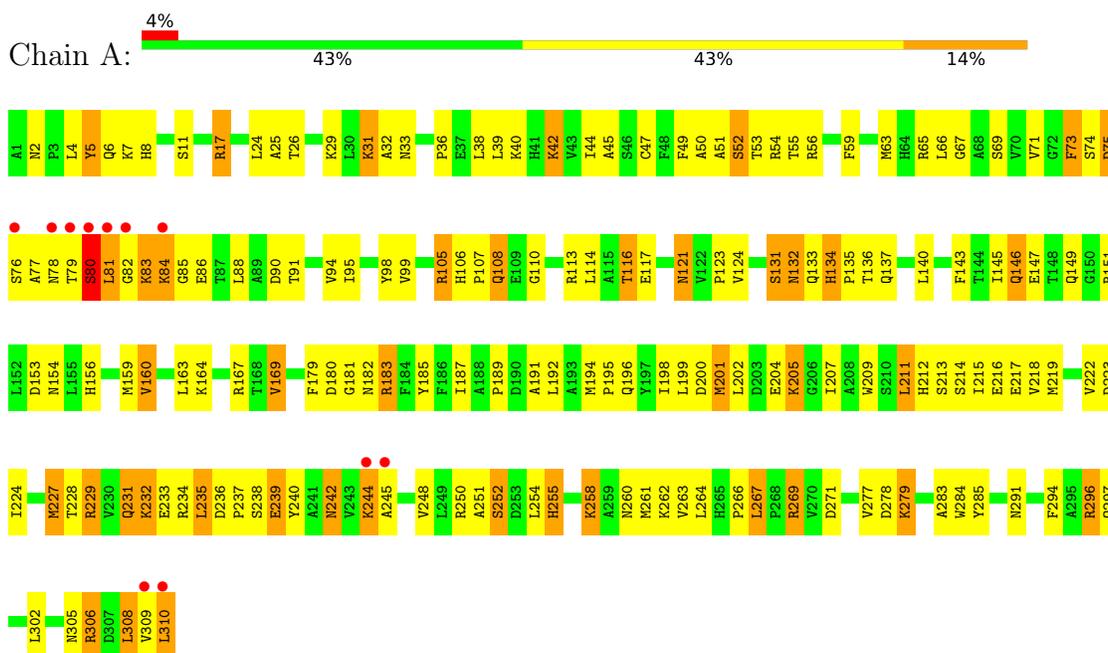
- Molecule 1: Aspartate carbamoyltransferase catalytic chain

- Molecule 2: Aspartate carbamoyltransferase regulatory chain

Chain B:

2%

27%　　　　　　　　　　　50%　　　　　　　　　20%

M1 T2 H3 D4 N5 K6 L7 Q8 V9 E10 A11 I12 K13 R14 V17 I18 D19 H20 I21 P22 A23 Q24 I25 G26 F27 K28 L29 L30 S31 L32 F33 K34 L35 T36 E37 T38 D39 Q40 R41 L46 N47 L48 P49 S50 G51 E52 M53 G54 R55 K56 D57 L58 I59 K60 I61 E62 N63 T64

F65 L66 S67 E68 D69 Q70 V71 D72 Q73 L74 A75 L76 Y77 A78 P79 Q80 A81 T82 V83 N84 R85 I86 D87 N88 Y89 E90 V91 V92 S95 R96 P97 S98 L99 P100 E101 R102 I103 D104 N105 V106 L107 N113 C114 I115 E119 P120 V121 S122 S123 S124 F125 A126 V127 R128 K129 R130 A131

N132 D133 I134 A135 L136 K137 C138 K139 Y140 C141 E142 K143 N148 V149 V150 L151 A152 N153

• Molecule 2: Aspartate carbamoyltransferase regulatory chain

Chain D:

4%

27%　　　　　　　　　　　50%　　　　　　　　　20%

M1 T2 H3 D4 N5 K6 L7 Q8 V9 E10 A11 I12 K13 R14 G15 T16 V17 I18 D19 H20 I21 P22 A23 Q24 I25 G26 F27 K28 L29 L30 K34 L35 T36 E37 T38 D39 Q40 R41 I42 G45 L46 N47 L48 G51 E52 M53 G54 R55 K56 D57 L58 I59 K60 I61 E62 N63 T64

F65 L66 S67 E68 D69 Q70 V71 D72 Q73 L74 A75 L76 Y77 A78 P79 Q80 A81 T82 V83 N84 R85 I86 D87 N88 Y89 E90 V91 V92 S95 R96 P97 S98 L99 P100 E101 R102 I103 D104 N105 V106 L107 V108 C109 I115 S116 H117 A118 E119 P120 V121 S122 S123 S124 F125 A126 V127 R128 K129

R130 A131 N132 D133 I134 A135 L136 K137 C138 K139 Y140 C141 E142 K143 E144 F145 S146 H147 N148 V149 V150 L151 A152 N153

4   Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	122.29Å 122.29Å 142.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.10 59.09 – 2.08	Depositor EDS
% Data completeness (in resolution range)	88.1 (30.00-2.10) 90.8 (59.09-2.08)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.86 (at 2.08Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.230 , 0.272 0.234 , 0.256	Depositor DCC
R_{free} test set	3367 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	13.6	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 435.5	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8012	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[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: PCT, ZN, CTP, MLI

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	0.71	9/2457 (0.4%)	1.27	19/3334 (0.6%)
1	C	0.70	7/2457 (0.3%)	1.24	24/3334 (0.7%)
2	B	0.93	7/1219 (0.6%)	1.13	8/1647 (0.5%)
2	D	0.90	10/1219 (0.8%)	1.57	28/1647 (1.7%)
All	All	0.78	33/7352 (0.4%)	1.29	79/9962 (0.8%)

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
1	A	0	3
1	C	0	4
2	B	0	1
2	D	0	6
All	All	0	14

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	133	ASP	C-N	-20.57	0.86	1.34
1	C	310	LEU	C-OXT	-15.38	0.94	1.23
2	D	153	ASN	C-OXT	15.01	1.51	1.23
1	C	271	ASP	C-N	13.87	1.66	1.34
2	B	134	ILE	C-N	-13.59	1.02	1.34

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	6	LYS	CB-CA-C	15.81	142.02	110.40
1	A	79	THR	O-C-N	15.43	147.38	122.70
2	D	105	ASN	O-C-N	-14.76	99.08	122.70
1	A	80	SER	O-C-N	-13.77	100.68	122.70
2	D	6	LYS	CA-C-N	11.68	142.89	117.20

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	242	ASN	Mainchain
1	A	73	PHE	Mainchain
1	A	82	GLY	Mainchain
2	B	133	ASP	Peptide
1	C	76	SER	Mainchain

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	2411	0	2420	149	0
1	C	2411	0	2421	91	0
2	B	1201	0	1216	116	0
2	D	1201	0	1218	92	0
3	A	7	0	2	0	0
3	C	7	0	2	4	0
4	A	8	0	4	3	0
4	C	8	0	4	5	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	B	29	0	12	7	0
6	D	29	0	12	7	0
7	A	211	0	0	26	0
7	B	101	0	0	13	0
7	C	265	0	0	20	0
7	D	121	0	0	14	0
All	All	8012	0	7311	436	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 30.

The worst 5 of 436 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1313:PCT:H1P2	7:C:1461:HOH:O	1.31	1.25
1:A:67:GLY:HA2	7:A:1510:HOH:O	1.39	1.20
2:B:133:ASP:O	2:B:134:ILE:N	1.78	1.15
1:C:200:ASP:HB3	7:C:1516:HOH:O	1.49	1.11
1:C:234:ARG:NH1	3:C:1311:MLI:H11	1.65	1.11

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	308/310 (99%)	284 (92%)	22 (7%)	2 (1%)	25	21
1	C	308/310 (99%)	286 (93%)	17 (6%)	5 (2%)	9	5
2	B	151/153 (99%)	123 (82%)	21 (14%)	7 (5%)	2	0
2	D	151/153 (99%)	124 (82%)	18 (12%)	9 (6%)	1	0
All	All	918/926 (99%)	817 (89%)	78 (8%)	23 (2%)	5	2

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	3	HIS
2	B	12	ILE
2	B	106	VAL
2	D	6	LYS
2	D	9	VAL

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	260/260 (100%)	208 (80%)	52 (20%)	1	0
1	C	260/260 (100%)	217 (84%)	43 (16%)	2	1
2	B	137/137 (100%)	98 (72%)	39 (28%)	0	0
2	D	137/137 (100%)	101 (74%)	36 (26%)	0	0
All	All	794/794 (100%)	624 (79%)	170 (21%)	1	0

5 of 170 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	183	ARG
2	D	48	LEU
1	C	216	GLU
1	C	299	LEU
2	D	76	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	8	HIS
2	D	84	ASN
1	C	137	GLN
2	D	63	ASN
1	C	108	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	PCT	A	1314	-	7,7,7	3.04	4 (57%)	9,10,10	1.41	2 (22%)
3	MLI	C	1311	-	0,6,6	-	-	0,7,7	-	-
6	CTP	B	1156	-	23,30,30	2.50	6 (26%)	30,47,47	3.45	13 (43%)
4	PCT	C	1313	-	7,7,7	3.09	4 (57%)	9,10,10	1.51	2 (22%)
6	CTP	D	1157	-	23,30,30	2.53	7 (30%)	30,47,47	3.12	12 (40%)
3	MLI	A	1312	-	0,6,6	-	-	0,7,7	-	-

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
4	PCT	A	1314	-	-	1/4/5/5	-
3	MLI	C	1311	-	-	0/0/4/4	-
6	CTP	B	1156	-	-	6/20/38/38	0/2/2/2
4	PCT	C	1313	-	-	3/4/5/5	-
6	CTP	D	1157	-	-	1/20/38/38	0/2/2/2
3	MLI	A	1312	-	-	0/0/4/4	-

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1157	CTP	C4-N3	8.40	1.49	1.35
6	B	1156	CTP	C4-N3	8.36	1.49	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1157	CTP	C2-N3	5.86	1.49	1.38
6	B	1156	CTP	C2-N3	5.77	1.49	1.38
4	A	1314	PCT	P-O1P	5.08	1.60	1.50

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1156	CTP	O2G-PG-O3B	8.75	133.99	104.64
6	B	1156	CTP	PB-O3A-PA	-8.59	103.35	132.83
6	D	1157	CTP	O3G-PG-O3B	-7.59	79.19	104.64
6	B	1156	CTP	C6-N1-C2	-7.33	109.56	121.20
6	D	1157	CTP	PB-O3A-PA	-7.15	108.30	132.83

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1314	PCT	O1-C1-C1P-P
4	C	1313	PCT	O1-C1-C1P-P
6	B	1156	CTP	C5'-O5'-PA-O2A
6	B	1156	CTP	PB-O3B-PG-O3G
4	C	1313	PCT	C1-C1P-P-O2P

There are no ring outliers.

5 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1314	PCT	3	0
3	C	1311	MLI	4	0
6	B	1156	CTP	7	0
4	C	1313	PCT	5	0
6	D	1157	CTP	7	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 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 CTP B 1156

Bond lengths   Bond angles

Torsions   Rings

Ligand CTP D 1157

Bond lengths   Bond angles

Torsions   Rings
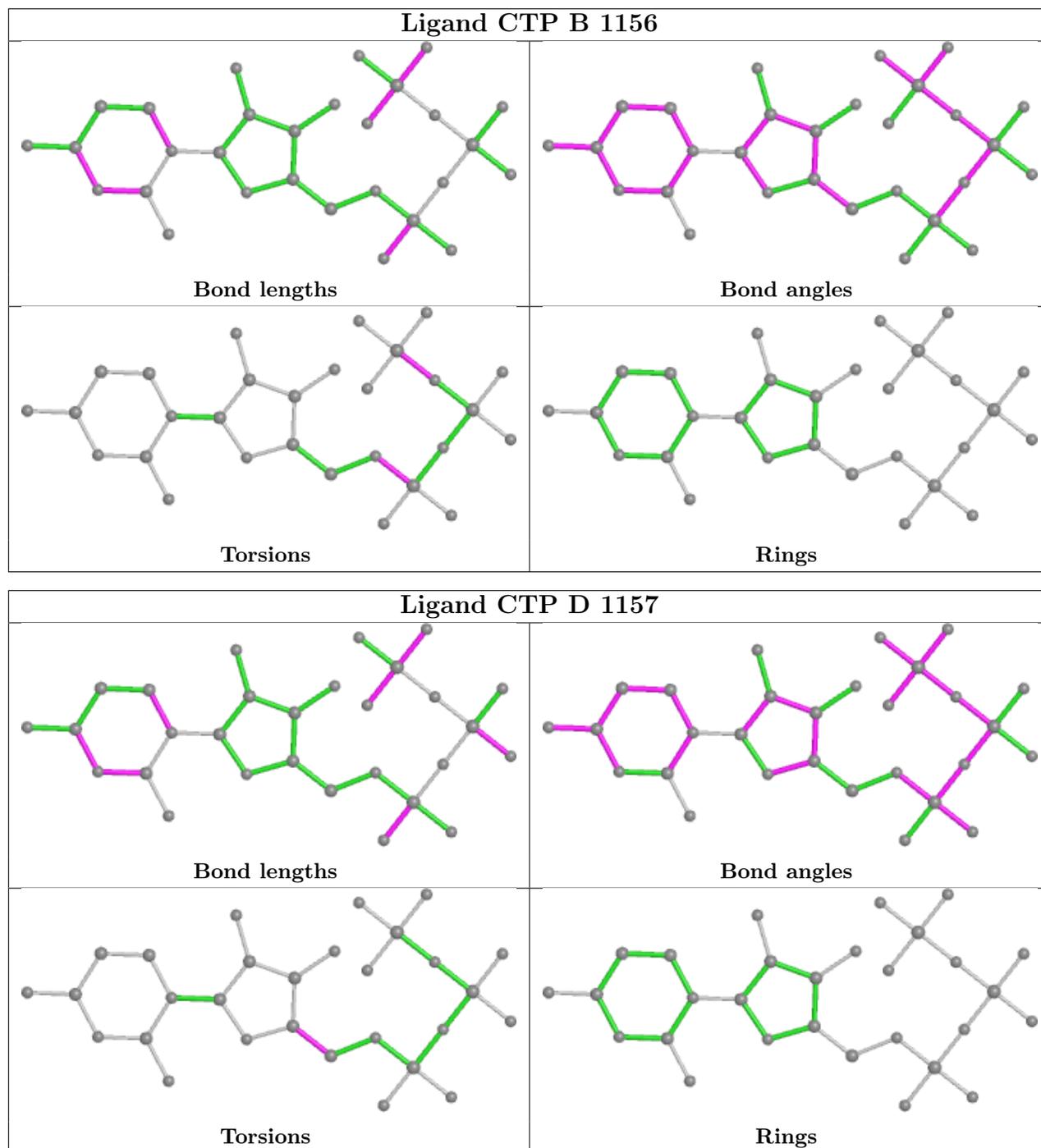
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

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

The worst 5 of 9 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	271:ASP	C	272:GLU	N	1.65
1	A	79:THR	C	80:SER	N	1.64
1	A	80:SER	C	81:LEU	N	1.63
1	D	8:GLN	C	9:VAL	N	1.63
1	D	104:ASP	C	105:ASN	N	1.19

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	310/310 (100%)	-0.69	11 (3%)	44	50	7, 25, 95, 158	0
1	C	310/310 (100%)	-0.86	3 (0%)	82	85	6, 18, 86, 158	0
2	B	153/153 (100%)	-0.38	3 (1%)	65	69	14, 45, 157, 158	0
2	D	153/153 (100%)	-0.24	6 (3%)	39	45	13, 47, 156, 158	0
All	All	926/926 (100%)	-0.62	23 (2%)	57	62	6, 30, 133, 158	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	81	LEU	10.3
1	A	80	SER	7.4
2	D	5	ASN	6.1
1	A	82	GLY	6.1
2	D	7	LEU	5.9

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

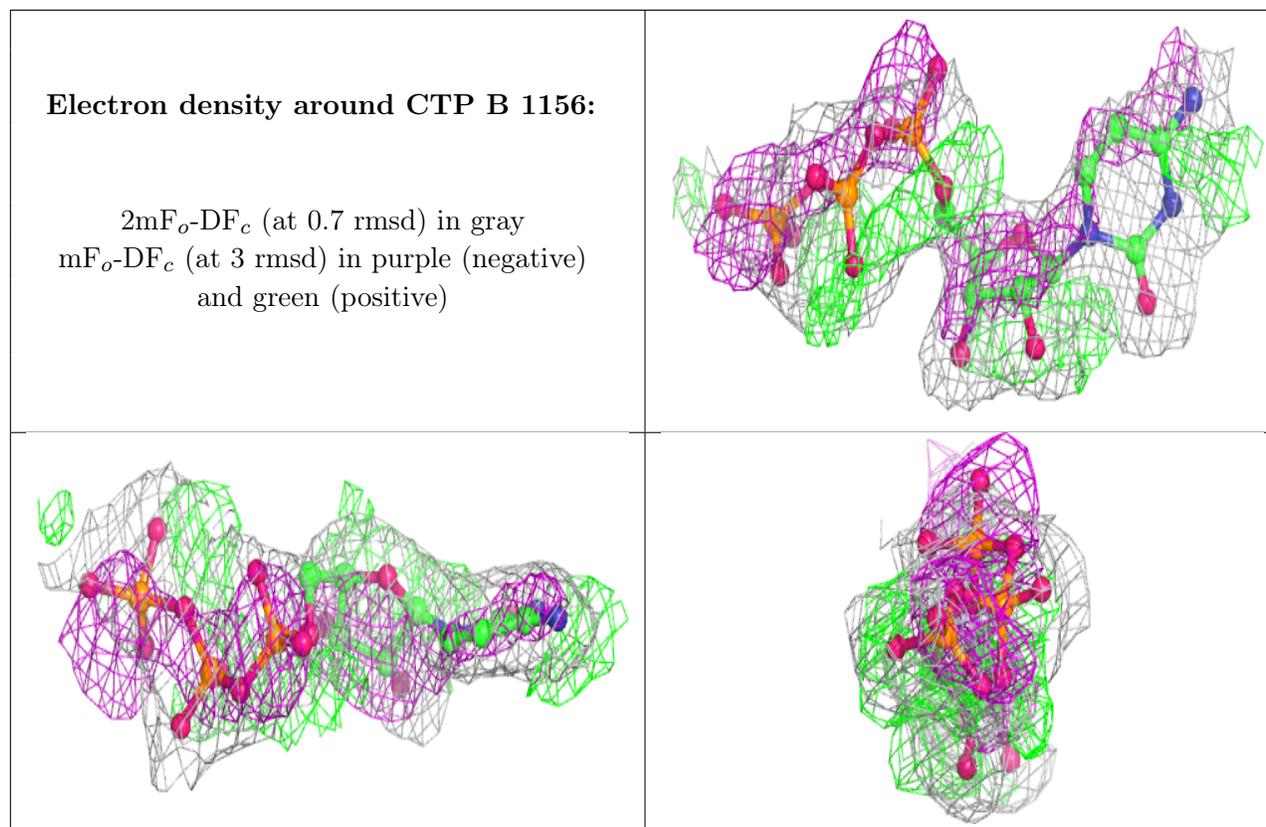There are no non-standard protein/DNA/RNA residues in this entry.

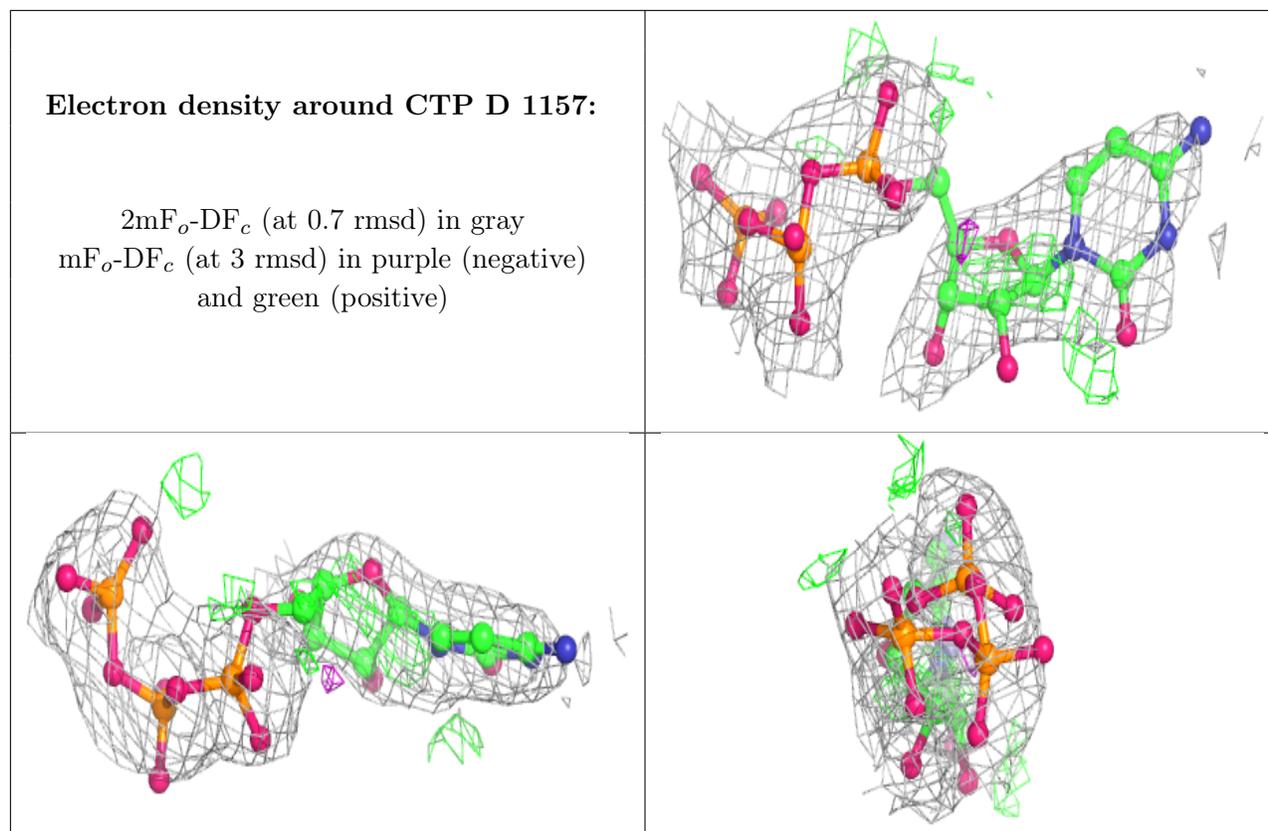## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MLI	C	1311	7/7	0.35	0.65	80,81,87,87	7
3	MLI	A	1312	7/7	0.47	0.82	36,56,74,76	7
4	PCT	A	1314	8/8	0.73	0.36	52,72,78,92	8
6	CTP	B	1156	29/29	0.82	0.15	25,40,73,80	0
4	PCT	C	1313	8/8	0.84	0.21	39,53,79,86	8
6	CTP	D	1157	29/29	0.89	0.16	56,79,88,90	29
5	ZN	D	155	1/1	0.98	0.06	121,121,121,121	1
5	ZN	B	154	1/1	1.00	0.05	19,19,19,19	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 CTP B 1156:

$2\text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray
$\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

Electron density around CTP D 1157:

$2mF_o$-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.