

wwPDB X-ray Structure Validation Summary Report (i)

Feb 5, 2024 – 07:44 AM EST

PDB ID : 8AT1

Title: CRYSTAL STRUCTURES OF ASPARTATE CARBAMOYLTRANS-

FERASE LIGATED WITH PHOSPHONOACETAMIDE, MALONATE, AND CTP OR ATP AT 2.8-ANGSTROMS RESOLUTION AND NEUTRAL

P*H

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Deposited on : 1989-09-22

Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : NOT EXECUTED

EDS : NOT EXECUTED

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

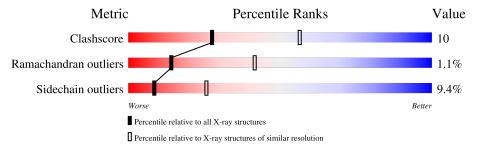
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain						
1	A	310	69%	25% • •					
1	С	310	76%	18% 5%					
2	В	153	51%	37% 7% • 5%					
2	D	153	54%	35% 7% • 5%					
3	Е	2	50%	50%					
3	F	2	50%	50%					

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 crite-



ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density	
3	GLC	Е	2	X	X	=	-	
3	GLC	F	2	X	X	=	-	



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7196 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 (R STATE), CATALYTIC CHAIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	310	Total 2415	C 1527	11	O 456	S 9	0	0	0
1	С	310		C 1527		O 456	S 9	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	GLN	GLU	conflict	UNP P0A786
A	147	GLN	GLU	conflict	UNP P0A786
A	149	GLU	GLN	conflict	UNP P0A786
A	196	GLU	GLN	conflict	UNP P0A786
С	60	GLN	GLU	conflict	UNP P0A786
С	147	GLN	GLU	conflict	UNP P0A786
С	149	GLU	GLN	conflict	UNP P0A786
С	196	GLU	GLN	conflict	UNP P0A786

• Molecule 2 is a protein called ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
2	В	146	Total 1138			S 5	0	0	0
2	D	146	Total 1138			S 5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue Modelled Actua		Actual	Comment	Reference
В	8	GLY	GLN	conflict	UNP P0A7F3
D	8	GLY	GLN	conflict	UNP P0A7F3

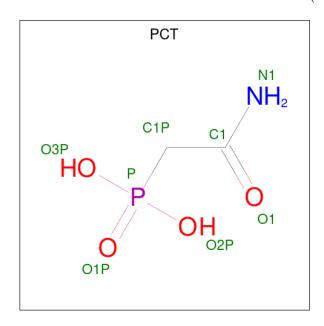


• Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	E	2	Total C O 7 4 3	0	0	1
3	F	2	Total C O 7 4 3	0	0	1

 \bullet Molecule 4 is PHOSPHONOACETAMIDE (three-letter code: PCT) (formula: $\mathrm{C_2H_6NO_4P}).$



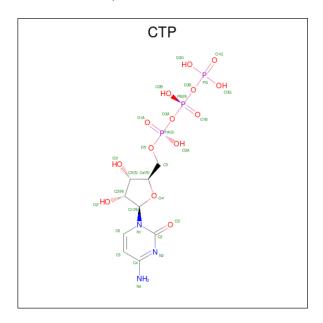
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
1	Λ	1	Total	С	N	О	Р	0	0
4	A	1	8	2	1	4	1	0	
4	С	1	Total	С	N	О	Р	0	0
4		1	8	2	1	4	1	0	U

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

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



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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	В	1	Total 29					0	0
6	D	1	Total 29		N 3		P 3	0	0

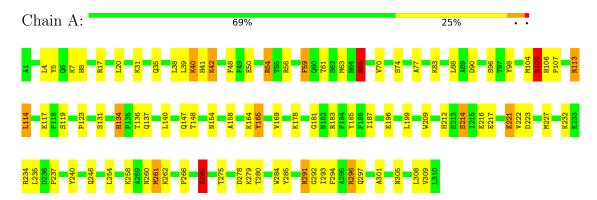


3 Residue-property plots (i)

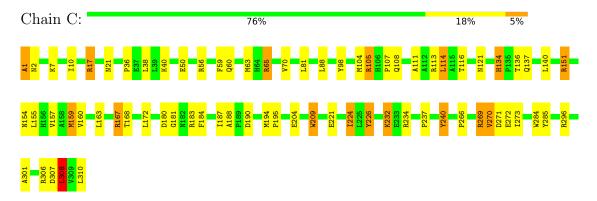
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

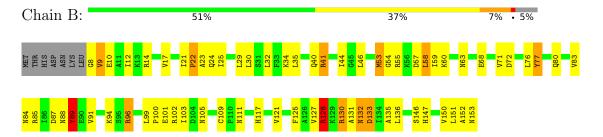
• Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE (R STATE), CATALYTIC CHAIN



• Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE (R STATE), CATALYTIC CHAIN

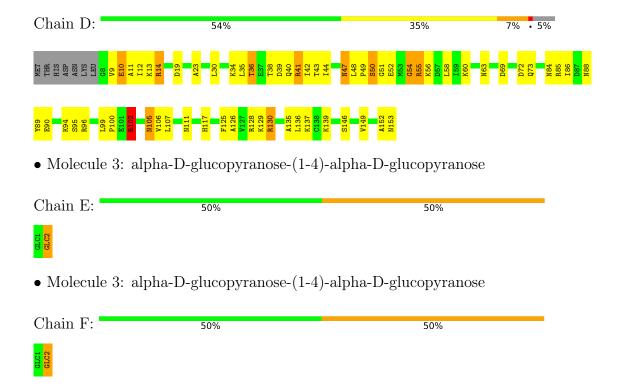


• Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN



• Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN







4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	P 3 2 1	Depositor	
Cell constants	122.20Å 122.20Å 155.20Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	6.00 - 2.80	Depositor	
% Data completeness	(Not available) (6.00-2.80)	Depositor	
(in resolution range)	(1100 available) (0.00 2.00)	Берозног	
R_{merge}	(Not available)	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	X-PLOR	Depositor	
R, R_{free}	0.167 , (Not available)	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	7196	wwPDB-VP	
Average B, all atoms (Å ²)	33.0	wwPDB-VP	



5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, PCT, ZN, CTP

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	
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.81	0/2461	1.58	$34/3339 \ (1.0\%)$
1	С	0.83	0/2461	1.58	29/3339~(0.9%)
2	В	0.77	0/1155	1.51	$10/1561 \ (0.6\%)$
2	D	0.74	0/1155	1.49	$12/1561 \ (0.8\%)$
All	All	0.80	0/7232	1.55	85/9800 (0.9%)

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	С	0	1
2	В	0	2
2	D	0	1
All	All	0	7

There are no bond length outliers.

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	С	105	ARG	NE-CZ-NH2	15.21	127.91	120.30
1	С	105	ARG	NE-CZ-NH1	-14.38	113.11	120.30
1	A	105	ARG	NE-CZ-NH2	13.44	127.02	120.30
1	A	269	ARG	NE-CZ-NH2	13.42	127.01	120.30
1	A	269	ARG	NE-CZ-NH1	-11.28	114.66	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	165	TYR	Sidechain
1	A	185	TYR	Sidechain
1	A	5	TYR	Sidechain
2	В	77	TYR	Sidechain
2	В	89	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2415	0	2422	42	0
1	С	2415	0	2422	29	0
2	В	1138	0	1154	37	0
2	D	1138	0	1154	40	0
3	Ε	7	0	0	0	0
3	F	7	0	0	0	0
4	A	8	0	4	1	0
4	С	8	0	4	0	0
5	В	1	0	0	0	0
5	D	1	0	0	0	0
6	В	29	0	12	3	0
6	D	29	0	12	2	0
All	All	7196	0	7184	144	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 10.

The worst 5 of 144 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:C:10:ILE:HD11	1:C:116:THR:HG21	1.43	0.98
1:C:137:GLN:HG2	1:C:168:THR:HG22	1.71	0.72
2:B:14:ARG:HG3	2:B:87:ASP:HA	1.70	0.72
2:D:30:LEU:HD12	2:D:36:THR:HG23	1.70	0.71
1:C:301:ALA:HB1	1:C:308:LEU:HD11	1.73	0.71

There are no symmetry-related clashes.



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	Perce	entiles
1	A	308/310 (99%)	295 (96%)	13 (4%)	0	100	100
1	C	308/310~(99%)	296 (96%)	11 (4%)	1 (0%)	41	72
2	В	144/153 (94%)	125 (87%)	15 (10%)	4 (3%)	5	17
2	D	144/153 (94%)	126 (88%)	13 (9%)	5 (4%)	3	12
All	All	904/926~(98%)	842 (93%)	52 (6%)	10 (1%)	14	41

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	34	LYS
2	В	132	ASN
2	D	51	GLY
2	D	54	GLY
2	D	105	ASN

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	Perc	entiles
1	A	261/261 (100%)	241 (92%)	20 (8%)	13	35
1	С	$261/261 \; (100\%)$	239 (92%)	22 (8%)	11	31
2	В	129/136 (95%)	112 (87%)	17 (13%)	4	12
2	D	129/136~(95%)	115 (89%)	14 (11%)	6	19
All	All	780/794 (98%)	707 (91%)	73 (9%)	8	26



\sim	c	70	• 1	• , 1			• 1	1 .		1 1	1 1
Э	Οİ	73	residues	with.	a	non-rotameric	Side	echain	are	listed	below:

Mol	Chain	Res	Type
1	С	308	LEU
2	D	137	LYS
2	D	34	LYS
2	D	52	GLU
2	В	53	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	С	154	ASN
1	С	13	ASN
2	В	63	ASN
2	В	153	ASN
2	В	47	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

Of 4 monosaccharides modelled in this entry, 2 were used 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	Ad True Chain Dea Link		B	Bond lengths			Bond angles			
MIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLC	Е	2	3	5,5,12	3.92	3 (60%)	5,5,17	1.92	2 (40%)
3	GLC	F	2	3	5,5,12	3.73	3 (60%)	5,5,17	2.04	2 (40%)



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.

Mo	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	Е	2	3	2/2/1/5	1/3/3/22	-
3	GLC	F	2	3	2/2/1/5	1/3/3/22	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$Ideal(\AA)$
3	Ε	2	GLC	C4-C3	-6.30	1.23	1.51
3	F	2	GLC	C4-C3	-6.11	1.24	1.51
3	E	2	GLC	O3-C3	-4.75	1.22	1.43
3	F	2	GLC	O3-C3	-4.43	1.24	1.43
3	Е	2	GLC	O5-C1	-3.73	1.22	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	F	2	GLC	O3-C3-C4	3.40	124.13	109.38
3	Е	2	GLC	O3-C3-C4	2.63	120.77	109.38
3	F	2	GLC	O5-C1-C2	2.33	119.47	111.31
3	Е	2	GLC	O5-C1-C2	2.32	119.44	111.31

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	Ε	2	GLC	C1
3	Ε	2	GLC	С3
3	F	2	GLC	C1
3	F	2	GLC	СЗ

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Е	2	GLC	C1-C2-C3-C4
3	F	2	GLC	C1-C2-C3-C4

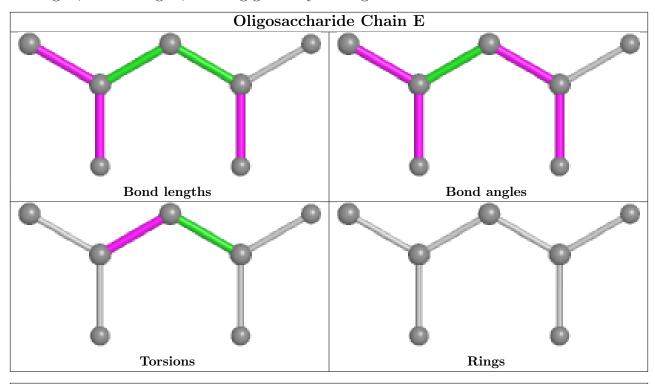
There are no ring outliers.

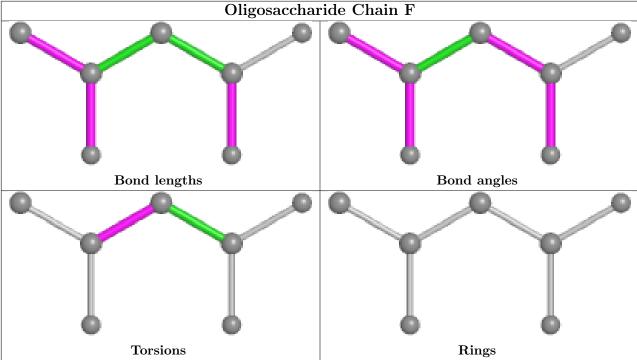
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,



bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are 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	Trus	Chain	n Res Link		Вс	Bond lengths			Bond angles		
MIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
6	CTP	В	155	-	26,30,30	1.40	5 (19%)	39,47,47	2.45	8 (20%)	
6	CTP	D	155	-	26,30,30	1.39	6 (23%)	39,47,47	2.38	8 (20%)	
4	PCT	A	311	-	7,7,7	1.77	2 (28%)	9,10,10	3.14	2 (22%)	
4	PCT	С	311	-	7,7,7	1.61	2 (28%)	9,10,10	1.95	2 (22%)	

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
6	CTP	В	155	-	-	7/22/38/38	0/2/2/2
6	CTP	D	155	-	-	4/22/38/38	0/2/2/2
4	PCT	A	311	-	-	3/4/5/5	-
4	PCT	С	311	-	-	3/4/5/5	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	Ideal(A)
4	A	311	PCT	P-O1P	3.42	1.57	1.50
4	С	311	PCT	P-O1P	3.09	1.56	1.50
6	В	155	CTP	C2-N1	-2.94	1.33	1.40
6	D	155	CTP	PG-O1G	2.87	1.59	1.50
6	D	155	CTP	C2-N1	-2.79	1.33	1.40

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
4	A	311	PCT	O1-C1-C1P	7.51	127.41	119.72
6	D	155	CTP	O2-C2-N3	-7.32	110.42	122.33
6	В	155	CTP	O2-C2-N3	-6.96	111.00	122.33
6	D	155	CTP	PB-O3A-PA	-6.79	109.54	132.83
6	В	155	CTP	PB-O3A-PA	-6.75	109.66	132.83

There are no chirality outliers.



5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	311	PCT	C1-C1P-P-O1P
4	A	311	PCT	C1-C1P-P-O3P
4	С	311	PCT	C1-C1P-P-O1P
4	С	311	PCT	C1-C1P-P-O2P
4	С	311	PCT	C1-C1P-P-O3P

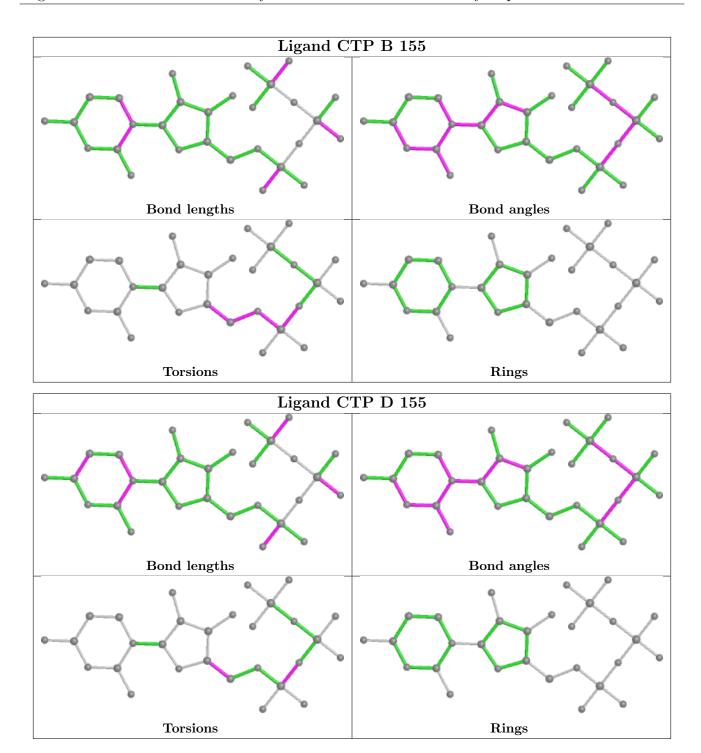
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	В	155	CTP	3	0
6	D	155	CTP	2	0
4	A	311	PCT	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 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.





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

