Full wwPDB X-ray Structure Validation Report (i)

Feb 4, 2024 – 03:12 PM EST

PDB ID	:	1RAE
Title	:	CRYSTAL STRUCTURE OF CTP-LIGATED T STATE ASPARTATE TRANSCARBAMOYLASE AT 2.5 ANGSTROMS RESOLUTION: IMPLICATIONS FOR ATCASE MUTANTS AND THE MECHANISM OF NEGATIVE COOPERATIVITY
Authors	:	Kosman, R.P.; Gouaux, J.E.; Lipscomb, W.N.
Deposited on	:	1992-08-14
Resolution	:	2.50 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 (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:

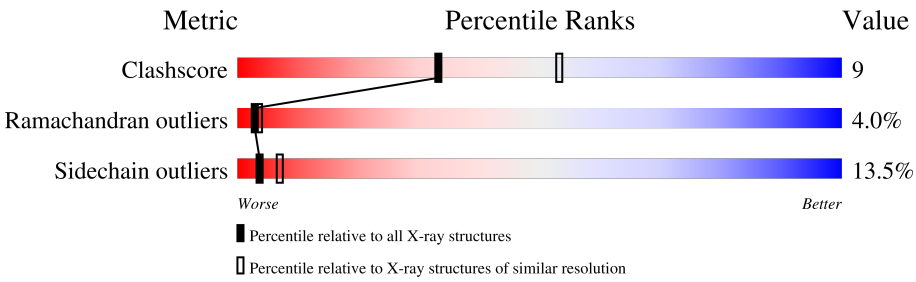
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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	65% 28% 6% •
1	C	310	70% 21% 8% •
2	B	153	60% 27% 8% •
2	D	153	58% 29% 10% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7375 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
			Total	C	N	O	S			
1	A	310	2415	1527	423	456	9	0	0	0
1	C	310	2415	1527	423	456	9	0	0	0

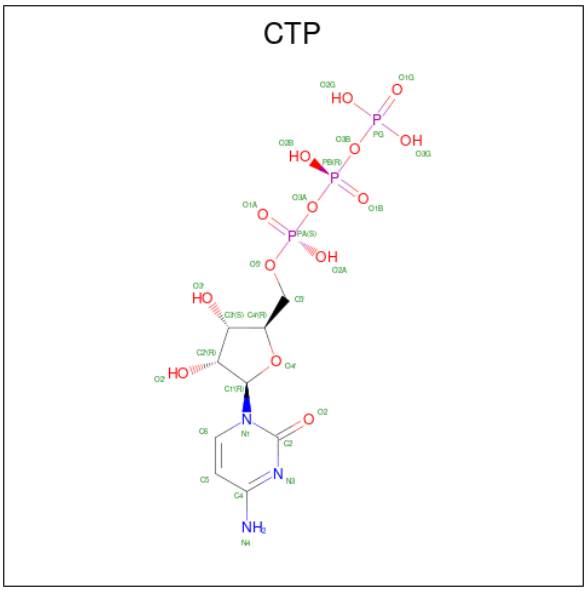
- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	153	1196	749	212	229	6	0	0	0
2	D	153	1196	749	212	229	6	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	30	30	30	0	0
5	B	10	10	10	0	0
5	C	44	44	44	0	0
5	D	9	9	9	0	0

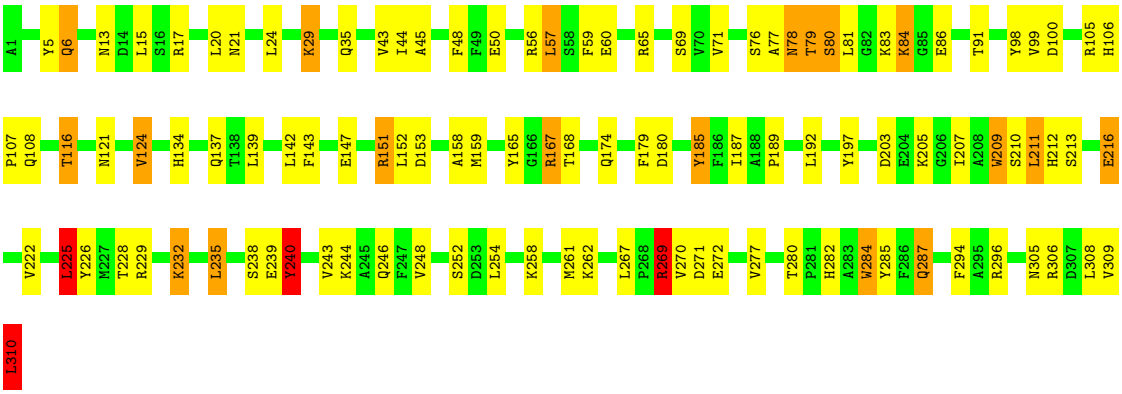
3 Residue-property plots (i)

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.

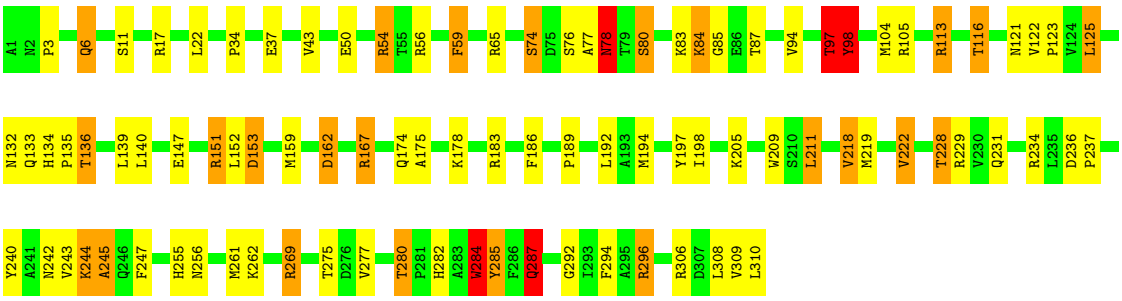
• Molecule 1: Aspartate carbamoyltransferase catalytic chain

Chain A: 65% 28% 6%



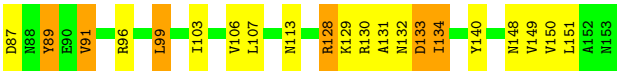
• Molecule 1: Aspartate carbamoyltransferase catalytic chain

Chain C: 70% 21% 8%



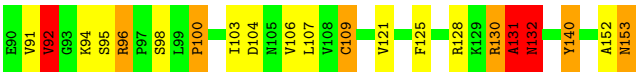
• Molecule 2: Aspartate carbamoyltransferase regulatory chain

Chain B: 60% 27% 8%



• Molecule 2: Aspartate carbamoyltransferase regulatory chain

Chain D:



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 a, b, c, α, β, γ	122.13Å 122.13Å 142.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.189 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7375	wwPDB-VP
Average B, all atoms ($Å^2$)	25.0	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: 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	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.96	3/2461 (0.1%)	1.80	47/3339 (1.4%)
1	C	1.02	2/2461 (0.1%)	1.86	63/3339 (1.9%)
2	B	0.90	0/1214	1.76	20/1640 (1.2%)
2	D	0.91	0/1214	1.78	24/1640 (1.5%)
All	All	0.97	5/7350 (0.1%)	1.81	154/9958 (1.5%)

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	6
1	C	0	2
2	B	0	2
2	D	0	2
All	All	0	12

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	147	GLU	CD-OE1	8.24	1.34	1.25
1	A	147	GLU	CD-OE2	7.77	1.34	1.25
1	A	60	GLU	CD-OE2	6.67	1.32	1.25
1	A	69	SER	CA-CB	-5.44	1.44	1.52
1	C	11	SER	CA-CB	-5.04	1.45	1.52

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ARG	NE-CZ-NH2	-17.72	111.44	120.30
1	A	269	ARG	NE-CZ-NH1	17.36	128.98	120.30
1	C	269	ARG	NE-CZ-NH1	16.00	128.30	120.30
1	A	65	ARG	NE-CZ-NH1	13.00	126.80	120.30
1	C	104	MET	CG-SD-CE	-11.65	81.56	100.20
1	C	296	ARG	NE-CZ-NH1	11.10	125.85	120.30
1	C	269	ARG	NE-CZ-NH2	-10.86	114.87	120.30
1	C	65	ARG	NE-CZ-NH2	-10.06	115.27	120.30
1	C	209	TRP	CD1-CG-CD2	9.31	113.75	106.30
1	A	209	TRP	CD1-CG-CD2	9.27	113.72	106.30
2	B	52	GLU	CA-C-N	-9.17	97.02	117.20
1	C	309	VAL	CA-C-N	-9.01	97.39	117.20
2	D	2	THR	CA-C-N	-8.98	97.45	117.20
1	A	56	ARG	NE-CZ-NH1	8.95	124.77	120.30
1	C	56	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	A	6	GLN	CA-CB-CG	8.55	132.22	113.40
1	C	183	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	A	269	ARG	NE-CZ-NH2	-8.33	116.14	120.30
1	A	209	TRP	CE2-CD2-CG	-7.86	101.01	107.30
1	C	209	TRP	CE2-CD2-CG	-7.81	101.05	107.30
2	B	133	ASP	N-CA-C	7.79	132.02	111.00
1	C	54	ARG	CA-CB-CG	7.76	130.48	113.40
2	D	121	VAL	CA-CB-CG2	-7.73	99.30	110.90
1	C	97	THR	N-CA-CB	-7.71	95.65	110.30
1	C	284	TRP	CD1-CG-CD2	7.68	112.44	106.30
1	C	284	TRP	CG-CD2-CE3	7.56	140.71	133.90
1	C	284	TRP	CE2-CD2-CG	-7.55	101.26	107.30
2	B	1	MET	CA-CB-CG	7.54	126.11	113.30
1	C	174	GLN	CA-CB-CG	-7.54	96.82	113.40
2	B	133	ASP	CA-C-N	-7.51	100.69	117.20
2	D	3	HIS	N-CA-C	-7.45	90.89	111.00
1	C	105	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	C	284	TRP	CB-CG-CD1	-7.34	117.45	127.00
1	C	125	LEU	CA-CB-CG	7.34	132.17	115.30
1	A	284	TRP	CE2-CD2-CG	-7.28	101.48	107.30
1	C	244	LYS	CA-C-N	7.27	133.18	117.20
1	C	218	VAL	CA-CB-CG2	-7.25	100.03	110.90
1	C	80	SER	N-CA-C	7.24	130.56	111.00
1	A	43	VAL	CG1-CB-CG2	-7.20	99.38	110.90
2	B	11	ALA	N-CA-C	7.18	130.38	111.00
1	A	296	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	C	309	VAL	O-C-N	7.12	134.09	122.70
1	A	222	VAL	CG1-CB-CG2	-7.05	99.62	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	167	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	A	284	TRP	CD1-CG-CD2	6.96	111.87	106.30
2	D	55	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	A	44	ILE	CG1-CB-CG2	-6.89	96.25	111.40
1	A	269	ARG	CA-CB-CG	6.85	128.47	113.40
1	A	79	THR	N-CA-CB	-6.82	97.33	110.30
1	C	287	GLN	CG-CD-NE2	6.82	133.08	116.70
1	C	280	THR	N-CA-CB	-6.72	97.53	110.30
1	C	56	ARG	CG-CD-NE	-6.68	97.76	111.80
1	A	167	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	C	285	TYR	CB-CG-CD1	-6.62	117.03	121.00
1	C	222	VAL	CA-CB-CG2	-6.58	101.03	110.90
1	A	211	LEU	CB-CG-CD1	-6.58	99.82	111.00
1	A	56	ARG	CG-CD-NE	-6.56	98.02	111.80
2	B	66	LEU	CA-CB-CG	6.51	130.28	115.30
1	C	98	TYR	CB-CG-CD2	-6.44	117.14	121.00
1	A	310	LEU	CA-CB-CG	6.42	130.07	115.30
1	C	104	MET	N-CA-CB	-6.41	99.06	110.60
1	A	100	ASP	CB-CG-OD1	6.39	124.05	118.30
1	C	296	ARG	NE-CZ-NH2	-6.31	117.15	120.30
1	A	258	LYS	CB-CG-CD	-6.26	95.31	111.60
1	A	197	TYR	CA-CB-CG	6.24	125.25	113.40
1	C	113	ARG	NE-CZ-NH1	6.21	123.40	120.30
2	D	131	ALA	CA-C-N	-6.21	103.54	117.20
2	B	106	VAL	N-CA-CB	-6.18	97.89	111.50
1	A	185	TYR	CB-CG-CD2	-6.18	117.29	121.00
2	D	132	ASN	N-CA-C	-6.15	94.39	111.00
1	A	80	SER	N-CA-C	6.15	127.61	111.00
1	A	203	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	C	54	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	284	TRP	CG-CD2-CE3	6.10	139.39	133.90
1	A	209	TRP	CG-CD1-NE1	-6.09	104.01	110.10
1	C	151	ARG	CG-CD-NE	-6.05	99.09	111.80
1	A	84	LYS	N-CA-C	-6.05	94.67	111.00
1	A	57	LEU	CB-CG-CD1	-6.00	100.80	111.00
2	D	49	PRO	CA-C-N	-5.97	104.06	117.20
1	C	113	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	C	209	TRP	CG-CD1-NE1	-5.95	104.15	110.10
1	C	37	GLU	CA-CB-CG	-5.93	100.36	113.40
2	D	130	ARG	NE-CZ-NH2	-5.89	117.35	120.30
2	B	23	ALA	N-CA-CB	5.88	118.33	110.10
2	B	30	LEU	CA-CB-CG	5.87	128.81	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	140	TYR	CB-CG-CD1	-5.87	117.48	121.00
1	C	222	VAL	CA-CB-CG1	5.86	119.69	110.90
2	D	106	VAL	N-CA-C	-5.76	95.45	111.00
1	C	87	THR	O-C-N	-5.74	113.52	122.70
2	B	14	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	C	104	MET	CA-CB-CG	5.72	123.02	113.30
1	C	122	VAL	N-CA-C	-5.68	95.65	111.00
2	D	32	LEU	CA-CB-CG	5.63	128.25	115.30
1	A	211	LEU	CA-CB-CG	5.61	128.21	115.30
2	D	96	ARG	NE-CZ-NH1	5.61	123.11	120.30
2	D	109	CYS	CA-CB-SG	-5.59	103.93	114.00
1	C	275	THR	CA-CB-CG2	5.58	120.22	112.40
1	A	6	GLN	N-CA-C	5.57	126.03	111.00
1	A	116	THR	N-CA-CB	-5.57	99.72	110.30
2	D	130	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	124	VAL	CG1-CB-CG2	-5.55	102.02	110.90
1	C	116	THR	N-CA-CB	-5.55	99.75	110.30
1	C	84	LYS	CA-CB-CG	-5.54	101.21	113.40
1	C	140	LEU	CA-CB-CG	5.53	128.02	115.30
1	C	219	MET	CG-SD-CE	5.53	109.05	100.20
2	B	128	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	284	TRP	CB-CG-CD1	-5.51	119.84	127.00
1	A	17	ARG	NE-CZ-NH1	5.49	123.04	120.30
2	D	77	TYR	CB-CG-CD1	-5.48	117.71	121.00
1	C	78	ASN	N-CA-C	5.48	125.80	111.00
1	A	216	GLU	CA-CB-CG	5.48	125.45	113.40
2	B	10	GLU	CA-C-N	-5.47	105.16	117.20
2	D	94	LYS	N-CA-C	-5.46	96.26	111.00
1	C	197	TYR	CA-CB-CG	5.45	123.75	113.40
2	B	58	LEU	CA-CB-CG	5.42	127.77	115.30
1	A	165	TYR	CA-C-N	5.39	126.97	116.20
1	C	84	LYS	CA-C-N	5.37	126.93	116.20
1	C	43	VAL	CG1-CB-CG2	-5.36	102.33	110.90
1	C	306	ARG	CA-CB-CG	5.35	125.17	113.40
1	A	29	LYS	CB-CG-CD	-5.32	97.76	111.60
2	B	52	GLU	O-C-N	5.32	131.21	122.70
1	A	229	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	C	247	PHE	N-CA-C	-5.31	96.66	111.00
2	B	53	MET	N-CA-C	-5.29	96.72	111.00
1	C	275	THR	CA-CB-OG1	-5.27	97.93	109.00
1	A	15	LEU	CB-CG-CD1	-5.26	102.06	111.00
2	B	149	VAL	CA-C-N	5.25	128.76	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	71	VAL	CA-C-N	5.25	126.70	116.20
1	A	167	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	A	222	VAL	CA-CB-CG1	5.23	118.74	110.90
2	D	11	ALA	N-CA-C	-5.20	96.95	111.00
1	A	79	THR	N-CA-C	5.20	125.04	111.00
2	D	55	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	C	228	THR	CA-CB-CG2	5.17	119.64	112.40
2	B	22	PRO	CA-N-CD	-5.14	104.30	111.50
1	C	287	GLN	OE1-CD-NE2	-5.14	110.09	121.90
1	C	87	THR	CA-C-N	5.13	128.48	117.20
2	D	30	LEU	CB-CG-CD1	-5.13	102.28	111.00
2	D	92	VAL	CA-CB-CG2	-5.13	103.21	110.90
2	D	3	HIS	CA-C-N	-5.12	105.93	117.20
1	C	147	GLU	CA-C-N	5.12	128.46	117.20
2	B	134	ILE	CB-CA-C	-5.11	101.39	111.60
2	D	128	ARG	NE-CZ-NH1	5.10	122.85	120.30
2	B	23	ALA	N-CA-C	-5.10	97.23	111.00
2	D	25	ILE	CG1-CB-CG2	-5.09	100.20	111.40
1	C	74	SER	N-CA-C	-5.09	97.27	111.00
1	C	284	TRP	CG-CD1-NE1	-5.08	105.02	110.10
2	B	133	ASP	O-C-N	5.08	130.83	122.70
1	C	228	THR	CA-CB-OG1	-5.07	98.35	109.00
1	A	225	LEU	O-C-N	-5.07	114.59	122.70
1	C	162	ASP	N-CA-C	-5.04	97.39	111.00
1	C	222	VAL	N-CA-CB	-5.01	100.47	111.50
2	D	89	TYR	N-CA-C	5.01	124.54	111.00
1	A	211	LEU	CB-CG-CD2	5.00	119.51	111.00

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	PHE	Sidechain
1	A	226	TYR	Sidechain
1	A	240	TYR	Sidechain
1	A	294	PHE	Sidechain
1	A	48	PHE	Sidechain
1	A	98	TYR	Sidechain
2	B	140	TYR	Sidechain
2	B	89	TYR	Sidechain
1	C	294	PHE	Sidechain
1	C	98	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	D	140	TYR	Sidechain
2	D	48	LEU	Peptide

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	43	0
1	C	2415	0	2422	33	0
2	B	1196	0	1212	31	0
2	D	1196	0	1212	25	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	B	29	0	12	1	0
4	D	29	0	12	0	0
5	A	30	0	0	0	0
5	B	10	0	0	0	0
5	C	44	0	0	1	0
5	D	9	0	0	0	0
All	All	7375	0	7292	125	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 9.

All (125) 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)
2:B:4:ASP:HA	2:B:10:GLU:HB2	1.49	0.93
1:A:106:HIS:HD2	1:A:108:GLN:H	1.27	0.82
1:A:308:LEU:HG	1:A:310:LEU:HD22	1.67	0.75
2:D:76:LEU:HD22	2:D:103:ILE:HD13	1.69	0.73
2:B:6:LYS:HB3	2:D:10:GLU:HG3	1.70	0.72
1:C:113:ARG:O	1:C:116:THR:HB	1.91	0.70
1:A:209:TRP:HZ3	1:A:211:LEU:HG	1.57	0.69
1:C:277:VAL:O	1:C:280:THR:HB	1.93	0.68
2:B:41:ARG:HH21	2:D:49:PRO:HB2	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:THR:CG2	1:C:296:ARG:HH11	2.06	0.67
1:C:97:THR:HG22	1:C:98:TYR:CD2	2.30	0.66
1:C:136:THR:HB	5:C:317:HOH:O	1.97	0.65
2:D:5:ASN:ND2	2:D:6:LYS:HD2	2.12	0.64
1:A:287:GLN:NE2	1:A:287:GLN:H	1.97	0.63
1:A:189:PRO:HG2	1:A:192:LEU:HB2	1.81	0.63
2:D:152:ALA:O	2:D:153:ASN:HB2	1.99	0.62
2:B:1:MET:HA	2:D:7:LEU:HD21	1.81	0.62
1:A:151:ARG:HD2	1:A:153:ASP:O	2.00	0.62
2:B:2:THR:HG22	2:B:11:ALA:HB3	1.81	0.61
2:B:76:LEU:HD12	2:B:103:ILE:HD11	1.81	0.61
2:D:17:VAL:HG22	2:D:60:LYS:HG2	1.82	0.60
2:B:14:ARG:NH1	2:B:63:ASN:HA	2.16	0.60
1:A:153:ASP:HB3	1:A:180:ASP:O	2.01	0.60
2:B:65:PHE:CE1	2:B:85:ARG:HG3	2.36	0.60
1:A:284:TRP:HA	1:A:287:GLN:NE2	2.17	0.59
1:A:45:ALA:HB2	1:A:99:VAL:HG11	1.86	0.58
1:C:136:THR:CG2	1:C:296:ARG:HD3	2.33	0.58
1:C:97:THR:HG22	1:C:98:TYR:HD2	1.66	0.57
2:B:5:ASN:OD1	2:B:7:LEU:HG	2.05	0.57
1:C:136:THR:HG23	1:C:296:ARG:HD3	1.85	0.57
2:B:76:LEU:HD12	2:B:103:ILE:CD1	2.35	0.56
2:B:6:LYS:HA	2:B:9:VAL:HG22	1.88	0.56
1:C:50:GLU:HA	1:C:76:SER:OG	2.05	0.56
1:C:242:ASN:O	1:C:244:LYS:N	2.39	0.56
2:B:48:LEU:O	2:B:55:ARG:HA	2.05	0.55
1:C:231:GLN:HB2	1:C:234:ARG:HG2	1.86	0.55
2:D:72:ASP:HB3	2:D:100:PRO:HB3	1.87	0.55
1:C:94:VAL:O	1:C:97:THR:HB	2.07	0.55
2:B:86:ILE:HG13	2:B:91:VAL:HA	1.89	0.55
2:D:65:PHE:HB3	2:D:85:ARG:NH2	2.22	0.55
1:A:50:GLU:HB2	1:A:107:PRO:HD3	1.89	0.55
2:B:6:LYS:CB	2:D:10:GLU:HG3	2.37	0.55
1:C:284:TRP:HA	1:C:287:GLN:NE2	2.22	0.54
1:C:6:GLN:HG3	1:C:123:PRO:HG3	1.90	0.54
1:A:76:SER:O	1:A:78:ASN:HB2	2.08	0.54
2:D:65:PHE:HB3	2:D:85:ARG:HH22	1.73	0.53
2:B:107:LEU:HD22	2:B:150:VAL:HG12	1.90	0.53
1:A:235:LEU:HG	1:A:239:GLU:HG3	1.91	0.53
1:A:232:LYS:HD3	1:A:240:TYR:HE2	1.74	0.52
2:B:14:ARG:HH11	2:B:14:ARG:HG2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:LYS:HG2	2:B:132:ASN:OD1	2.09	0.52
2:D:20:HIS:O	2:D:20:HIS:ND1	2.44	0.52
1:A:269:ARG:HA	1:A:272:GLU:OE2	2.11	0.51
2:D:29:LEU:HD13	2:D:74:LEU:HD22	1.91	0.51
1:A:5:TYR:CD1	1:A:306:ARG:HA	2.46	0.51
2:B:1:MET:N	2:B:89:TYR:OH	2.45	0.50
1:A:21:ASN:HD21	1:A:179:PHE:HE2	1.58	0.50
2:B:17:VAL:HG22	2:B:60:LYS:HG2	1.92	0.50
1:A:5:TYR:CZ	1:A:306:ARG:HG2	2.47	0.49
1:A:81:LEU:HD12	1:A:91:THR:HG23	1.93	0.49
1:C:240:TYR:O	1:C:245:ALA:HB2	2.12	0.49
2:D:50:SER:HB3	2:D:56:LYS:HE3	1.94	0.49
1:A:142:LEU:HD22	1:A:152:LEU:HD13	1.94	0.49
1:A:261:MET:SD	1:A:262:LYS:N	2.86	0.48
1:A:243:VAL:O	1:A:246:GLN:HA	2.14	0.48
1:A:187:ILE:HG12	1:A:212:HIS:HB2	1.96	0.48
1:C:280:THR:HG22	1:C:282:HIS:H	1.78	0.48
2:D:131:ALA:O	2:D:132:ASN:HB2	2.14	0.47
1:A:137:GLN:HG2	1:A:168:THR:HG22	1.96	0.47
2:D:21:ILE:HB	2:D:57:ASP:HB2	1.95	0.47
1:A:106:HIS:CD2	1:A:108:GLN:H	2.18	0.47
2:B:6:LYS:HE3	2:B:6:LYS:HB2	1.63	0.47
2:B:27:PHE:HA	2:B:30:LEU:HD23	1.97	0.47
2:D:109:CYS:HA	2:D:125:PHE:HZ	1.81	0.46
1:A:232:LYS:HD3	1:A:240:TYR:CE2	2.49	0.46
1:A:248:VAL:HG12	1:A:272:GLU:HA	1.98	0.45
2:B:41:ARG:HE	2:D:49:PRO:HD2	1.82	0.45
1:A:205:LYS:HB2	1:A:207:ILE:HD12	1.98	0.45
2:B:11:ALA:HA	4:B:999:CTP:N3	2.30	0.45
1:C:292:GLY:O	1:C:296:ARG:HG3	2.16	0.45
1:C:59:PHE:CE2	1:C:136:THR:HG21	2.52	0.45
1:C:186:PHE:HB2	1:C:211:LEU:HD12	1.97	0.45
1:C:132:ASN:OD1	1:C:133:GLN:HG2	2.17	0.45
1:C:162:ASP:HA	1:C:192:LEU:HB3	1.99	0.45
2:D:130:ARG:HD2	2:D:130:ARG:HA	1.55	0.45
1:A:81:LEU:HD12	1:A:91:THR:OG1	2.16	0.44
2:B:14:ARG:HA	2:B:86:ILE:O	2.17	0.44
1:C:261:MET:C	1:C:261:MET:SD	2.96	0.44
1:A:270:VAL:HG23	1:A:271:ASP:H	1.82	0.44
2:B:41:ARG:NE	2:D:49:PRO:HD2	2.33	0.44
1:A:209:TRP:CZ3	1:A:211:LEU:HG	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:ASN:O	2:B:9:VAL:HA	2.17	0.44
2:B:22:PRO:HB2	2:B:25:ILE:HD13	1.99	0.44
1:C:310:LEU:H	1:C:310:LEU:HG	1.68	0.44
1:A:108:GLN:HG2	2:B:113:ASN:OD1	2.18	0.43
1:A:29:LYS:HD2	1:A:310:LEU:HG	2.00	0.43
1:A:235:LEU:HG	1:A:239:GLU:CG	2.47	0.43
1:C:189:PRO:CG	1:C:192:LEU:HD12	2.47	0.43
1:C:3:PRO:HD2	1:C:22:LEU:CD2	2.49	0.43
1:C:175:ALA:O	1:C:178:LYS:HB2	2.17	0.43
2:D:14:ARG:HA	2:D:86:ILE:O	2.18	0.43
1:A:262:LYS:HG3	1:A:284:TRP:HB2	2.00	0.43
1:C:151:ARG:HD2	1:C:153:ASP:O	2.18	0.42
1:A:185:TYR:HD1	1:A:212:HIS:NE2	2.17	0.42
1:A:158:ALA:HB3	1:A:225:LEU:HD23	2.00	0.42
2:B:12:ILE:HB	2:B:62:GLU:HG2	2.02	0.42
1:A:267:LEU:HD23	1:A:269:ARG:HB3	2.01	0.42
1:C:194:MET:SD	1:C:198:ILE:HG21	2.59	0.42
1:C:135:PRO:O	1:C:139:LEU:HG	2.20	0.42
2:D:6:LYS:HB2	2:D:9:VAL:HG22	2.01	0.42
1:A:235:LEU:HD12	1:A:235:LEU:HA	1.84	0.41
1:A:254:LEU:HD12	1:A:280:THR:HG21	2.02	0.41
2:B:99:LEU:HB2	2:B:130:ARG:HD3	2.02	0.41
1:A:261:MET:O	1:A:282:HIS:HD2	2.04	0.41
1:A:139:LEU:HD23	1:A:139:LEU:HA	1.86	0.41
2:B:7:LEU:H	2:B:7:LEU:HD23	1.85	0.41
1:C:17:ARG:HH11	1:C:17:ARG:HD3	1.69	0.41
2:D:13:LYS:O	2:D:86:ILE:HG22	2.20	0.41
1:C:198:ILE:HD13	1:C:198:ILE:HA	1.98	0.40
1:C:261:MET:O	1:C:282:HIS:HD2	2.03	0.40
1:A:20:LEU:O	1:A:24:LEU:HD13	2.21	0.40
1:A:254:LEU:HD11	1:A:277:VAL:HG13	2.02	0.40
1:C:229:ARG:CZ	1:C:229:ARG:HB2	2.51	0.40
2:D:67:SER:HA	2:D:71:VAL:HG23	2.03	0.40
2:D:92:VAL:HG13	2:D:92:VAL:O	2.22	0.40

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	Percentiles
1	A	308/310 (99%)	281 (91%)	19 (6%)	8 (3%)	5 8
1	C	308/310 (99%)	284 (92%)	17 (6%)	7 (2%)	6 10
2	B	151/153 (99%)	121 (80%)	19 (13%)	11 (7%)	1 1
2	D	151/153 (99%)	125 (83%)	15 (10%)	11 (7%)	1 1
All	All	918/926 (99%)	811 (88%)	70 (8%)	37 (4%)	3 3

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	THR
1	A	80	SER
2	B	3	HIS
2	B	11	ALA
2	B	14	ARG
2	B	23	ALA
2	B	131	ALA
2	B	133	ASP
2	B	134	ILE
1	C	78	ASN
1	C	80	SER
1	C	243	VAL
2	D	4	ASP
2	D	5	ASN
2	D	7	LEU
2	D	24	GLN
2	D	89	TYR
2	D	107	LEU
2	D	132	ASN
1	A	84	LYS
2	B	4	ASP
1	C	245	ALA

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Mol	Chain	Res	Type
1	A	83	LYS
1	A	116	THR
1	A	244	LYS
2	B	22	PRO
2	B	68	GLU
2	B	91	VAL
1	C	77	ALA
2	D	68	GLU
1	A	77	ALA
1	C	84	LYS
2	D	131	ALA
1	A	6	GLN
2	D	23	ALA
1	C	85	GLY
2	D	91	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	261/261 (100%)	231 (88%)	30 (12%)	5 11
1	C	261/261 (100%)	230 (88%)	31 (12%)	5 10
2	B	136/137 (99%)	114 (84%)	22 (16%)	2 4
2	D	136/137 (99%)	112 (82%)	24 (18%)	2 3
All	All	794/796 (100%)	687 (86%)	107 (14%)	4 7

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	35	GLN
1	A	57	LEU
1	A	59	PHE
1	A	78	ASN
1	A	86	GLU

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Mol	Chain	Res	Type
1	A	105	ARG
1	A	121	ASN
1	A	124	VAL
1	A	134	HIS
1	A	151	ARG
1	A	159	MET
1	A	167	ARG
1	A	174	GLN
1	A	210	SER
1	A	213	SER
1	A	216	GLU
1	A	225	LEU
1	A	228	THR
1	A	232	LYS
1	A	235	LEU
1	A	238	SER
1	A	240	TYR
1	A	252	SER
1	A	269	ARG
1	A	285	TYR
1	A	287	GLN
1	A	305	ASN
1	A	309	VAL
1	A	310	LEU
2	B	1	MET
2	B	2	THR
2	B	3	HIS
2	B	4	ASP
2	B	7	LEU
2	B	14	ARG
2	B	30	LEU
2	B	32	LEU
2	B	34	LYS
2	B	36	THR
2	B	37	GLU
2	B	49	PRO
2	B	56	LYS
2	B	67	SER
2	B	68	GLU
2	B	76	LEU
2	B	87	ASP
2	B	96	ARG

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Mol	Chain	Res	Type
2	B	99	LEU
2	B	128	ARG
2	B	148	ASN
2	B	151	LEU
1	C	6	GLN
1	C	34	PRO
1	C	54	ARG
1	C	59	PHE
1	C	74	SER
1	C	78	ASN
1	C	83	LYS
1	C	97	THR
1	C	121	ASN
1	C	125	LEU
1	C	134	HIS
1	C	136	THR
1	C	152	LEU
1	C	153	ASP
1	C	159	MET
1	C	167	ARG
1	C	205	LYS
1	C	211	LEU
1	C	218	VAL
1	C	222	VAL
1	C	228	THR
1	C	236	ASP
1	C	237	PRO
1	C	255	HIS
1	C	256	ASN
1	C	262	LYS
1	C	269	ARG
1	C	284	TRP
1	C	285	TYR
1	C	287	GLN
1	C	308	LEU
2	D	3	HIS
2	D	4	ASP
2	D	5	ASN
2	D	6	LYS
2	D	9	VAL
2	D	10	GLU
2	D	14	ARG

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Mol	Chain	Res	Type
2	D	16	THR
2	D	31	SER
2	D	43	THR
2	D	49	PRO
2	D	66	LEU
2	D	67	SER
2	D	73	GLN
2	D	85	ARG
2	D	88	ASN
2	D	92	VAL
2	D	95	SER
2	D	96	ARG
2	D	98	SER
2	D	100	PRO
2	D	104	ASP
2	D	132	ASN
2	D	153	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	106	HIS
1	A	282	HIS
1	A	287	GLN
1	A	297	GLN
1	C	33	ASN
1	C	78	ASN
1	C	282	HIS
1	C	287	GLN
2	D	5	ASN
2	D	117	HIS

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
4	CTP	D	999	-	26,30,30	1.30	5 (19%)	39,47,47	1.79	8 (20%)
4	CTP	B	999	-	26,30,30	1.39	6 (23%)	39,47,47	1.77	5 (12%)

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	CTP	D	999	-	-	4/22/38/38	0/2/2/2
4	CTP	B	999	-	-	6/22/38/38	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	999	CTP	PG-O1G	2.54	1.58	1.50
4	D	999	CTP	C5-C4	-2.46	1.37	1.42
4	D	999	CTP	C6-N1	-2.44	1.32	1.38
4	B	999	CTP	C2-N3	-2.44	1.31	1.36
4	B	999	CTP	PG-O1G	2.39	1.58	1.50
4	B	999	CTP	C6-N1	-2.29	1.32	1.38
4	B	999	CTP	C2-N1	-2.28	1.35	1.40
4	B	999	CTP	C5-C4	-2.21	1.37	1.42
4	D	999	CTP	PB-O1B	2.16	1.58	1.50
4	B	999	CTP	PB-O1B	2.12	1.58	1.50
4	D	999	CTP	PA-O1A	2.10	1.58	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	999	CTP	PB-O3A-PA	-6.60	110.18	132.83
4	B	999	CTP	PB-O3A-PA	-5.94	112.45	132.83
4	B	999	CTP	O2-C2-N3	-4.64	114.78	122.33
4	D	999	CTP	PB-O3B-PG	-4.56	117.18	132.83
4	B	999	CTP	PB-O3B-PG	-4.16	118.54	132.83
4	D	999	CTP	O2-C2-N3	-3.90	115.99	122.33
4	B	999	CTP	N1-C2-N3	2.46	123.28	118.81
4	B	999	CTP	C6-N1-C2	-2.42	116.30	120.49
4	D	999	CTP	C6-N1-C2	-2.39	116.35	120.49
4	D	999	CTP	N1-C2-N3	2.14	122.70	118.81
4	D	999	CTP	C3'-C2'-C1'	2.12	105.45	101.43
4	D	999	CTP	O4'-C1'-N1	2.11	113.18	108.36
4	D	999	CTP	O2'-C2'-C1'	-2.01	103.31	110.02

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	999	CTP	O4'-C4'-C5'-O5'
4	B	999	CTP	C5'-O5'-PA-O1A
4	B	999	CTP	C5'-O5'-PA-O2A
4	B	999	CTP	C5'-O5'-PA-O3A
4	D	999	CTP	O4'-C4'-C5'-O5'
4	B	999	CTP	C3'-C4'-C5'-O5'
4	D	999	CTP	PB-O3A-PA-O5'
4	B	999	CTP	PB-O3A-PA-O1A
4	D	999	CTP	PB-O3A-PA-O1A
4	D	999	CTP	C3'-C4'-C5'-O5'

There are no ring outliers.

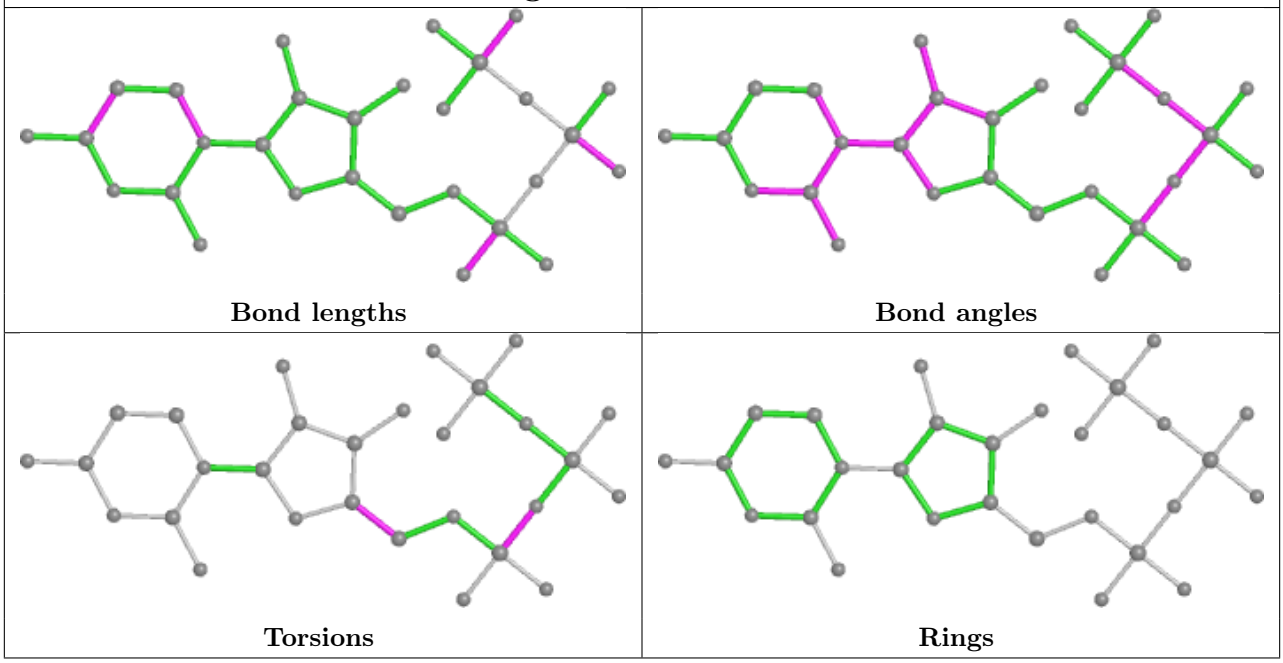
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	999	CTP	1	0

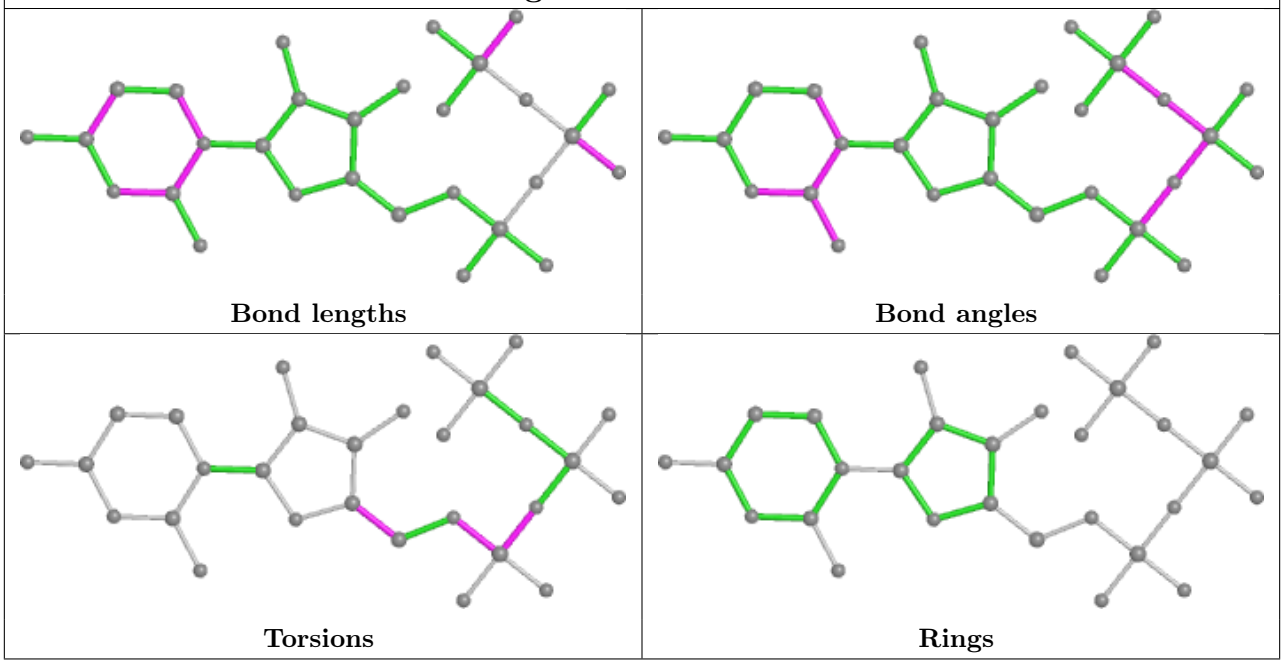
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 D 999



Ligand CTP B 999



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.