Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:56 PM GMT

PDB ID	:	1RAI
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

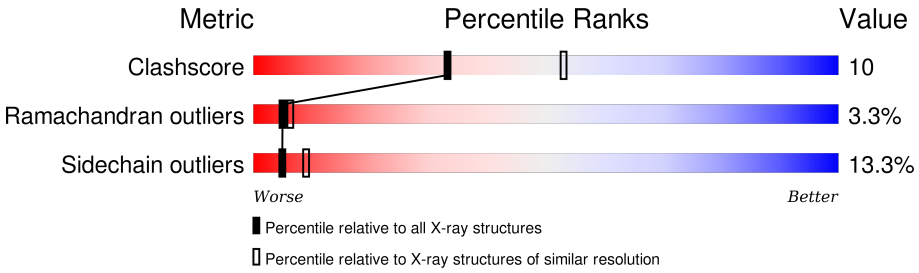
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	310	64% 29% 5% •
1	C	310	70% 21% 6% •
2	B	153	54% 34% 7% 5%
2	D	153	54% 29% 11% • 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7310 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
			2415	1527	423	456	9			
1	C	310	Total	C	N	O	S	0	1	0
			2420	1529	426	456	9			

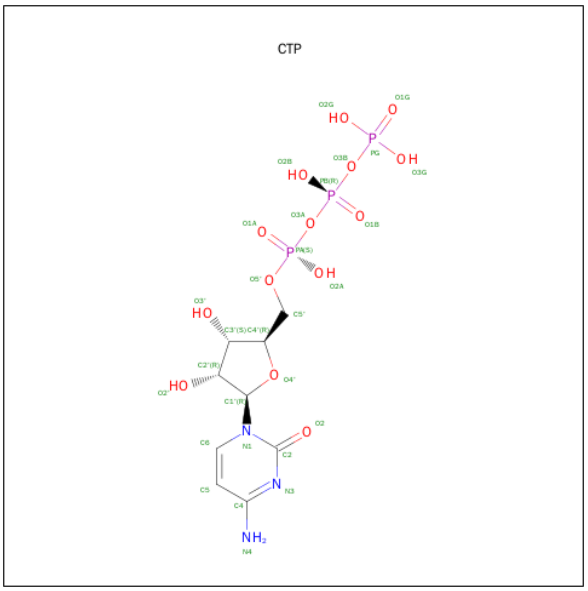
- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	153	Total	C	N	O	S	0	0	0
			1196	749	212	229	6			
2	D	146	Total	C	N	O	S	0	0	0
			1138	714	201	218	5			

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

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

- 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
4	B	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
4	D	1	Total	C	N	O	P	0	0
			29	9	3	14	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total	O	0	0
			26	26		
5	B	9	Total	O	0	0
			9	9		
5	C	37	Total	O	0	0
			37	37		
5	D	9	Total	O	0	0
			9	9		

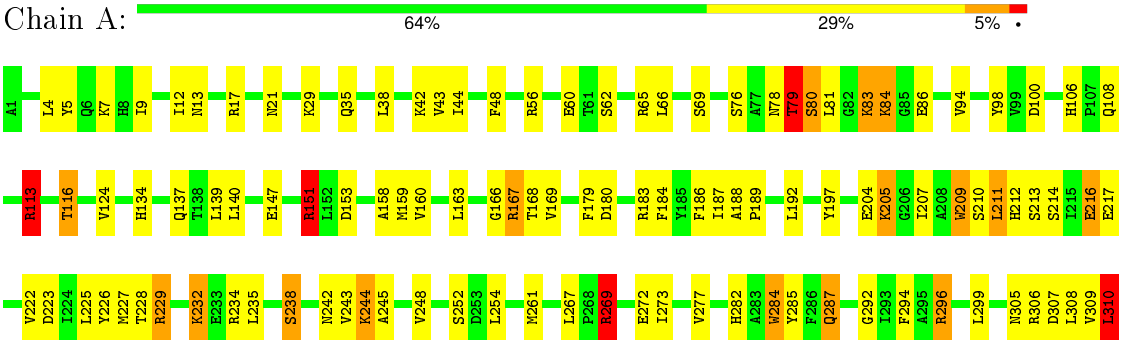
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

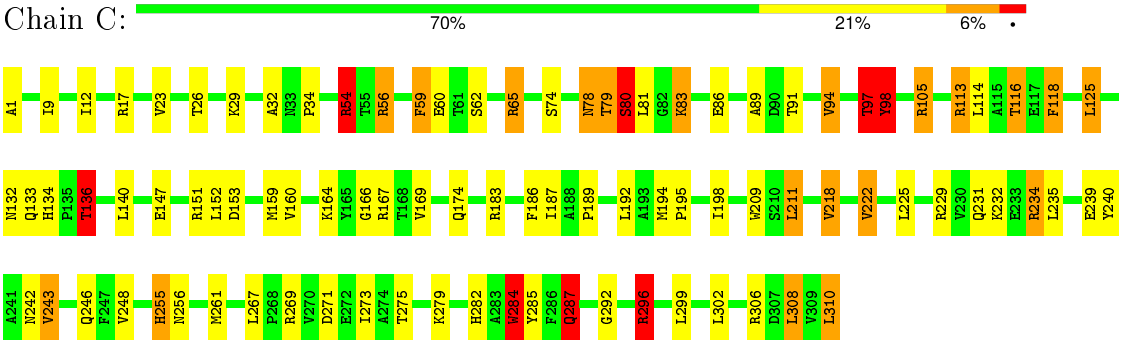
- Molecule 1: Aspartate carbamoyltransferase catalytic chain

Chain A:



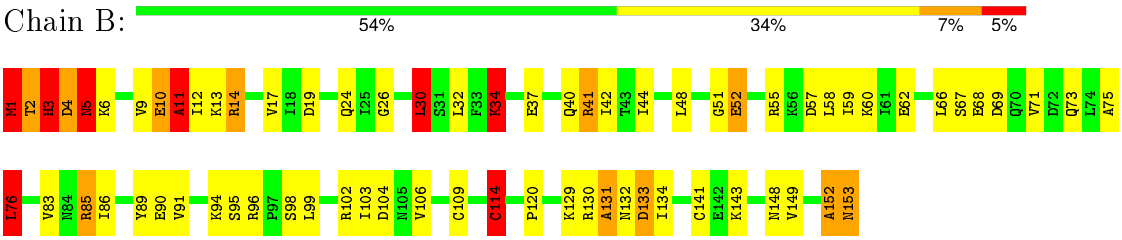
- Molecule 1: Aspartate carbamoyltransferase catalytic chain

Chain C:



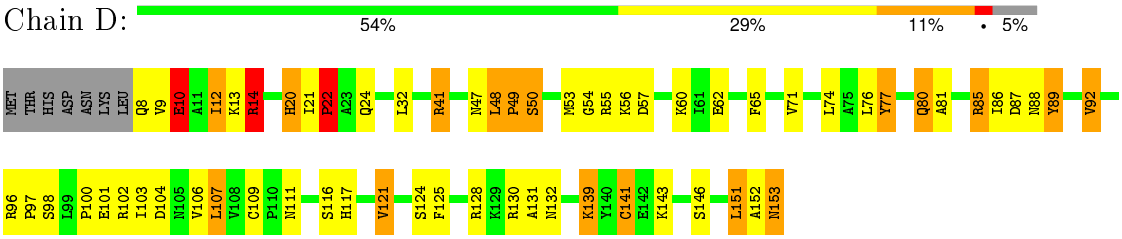
- Molecule 2: Aspartate carbamoyltransferase regulatory chain

Chain B:



- Molecule 2: Aspartate carbamoyltransferase regulatory chain

Chain D:


54%
29%
11%
5%
MET THR HIS ASP ASN LYS LEU Q8 V9 E10 A11 I12 K13 R14 H20 I21 F22 A23 Q24 L32 R41 N47 L48 P49 S50 M53 G54 R55 K56 D57 K60 I61 E62 F65 V71 L74 A75 L76 Y77 Q80 A81 R85 I86 D87 N88 Y89 V92
R96 P97 S98 L99 P100 E101 R102 I103 D104 N105 V106 L107 V108 C109 P110 N111 S116 H117 V121 S124 F125 R128 K129 R130 A131 N132 K139 Y140 C141 E142 K143 S146 L151 A152 N153

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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}	0.182 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7310	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.98	4/2461 (0.2%)	1.78	45/3339 (1.3%)
1	C	0.99	2/2472 (0.1%)	1.80	51/3353 (1.5%)
2	B	0.90	0/1214	1.77	28/1640 (1.7%)
2	D	0.97	4/1155 (0.3%)	1.72	19/1561 (1.2%)
All	All	0.97	10/7302 (0.1%)	1.77	143/9893 (1.4%)

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	4
1	C	0	2
2	B	0	1
2	D	0	1
All	All	0	8

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	147	GLU	CD-OE2	8.25	1.34	1.25
1	A	147	GLU	CD-OE1	7.67	1.34	1.25
2	D	141	CYS	CB-SG	-6.33	1.71	1.82
1	A	60	GLU	CD-OE2	6.26	1.32	1.25
2	D	9	VAL	CA-CB	5.89	1.67	1.54
1	A	69	SER	CA-CB	-5.86	1.44	1.52
2	D	141	CYS	CA-CB	-5.60	1.41	1.53
1	C	60	GLU	CD-OE2	5.27	1.31	1.25
2	D	121	VAL	CB-CG2	-5.27	1.41	1.52
1	A	56	ARG	CA-CB	-5.23	1.42	1.53

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	56	ARG	NE-CZ-NH2	-14.01	113.30	120.30
1	A	269	ARG	NE-CZ-NH1	13.51	127.06	120.30
1	C	296	ARG	NE-CZ-NH1	11.28	125.94	120.30
1	C	56	ARG	NE-CZ-NH2	-11.27	114.67	120.30
1	A	229	ARG	NE-CZ-NH1	11.20	125.90	120.30
1	A	296	ARG	NE-CZ-NH1	11.16	125.88	120.30
1	A	56	ARG	NE-CZ-NH1	10.28	125.44	120.30
1	A	209	TRP	CD1-CG-CD2	9.92	114.24	106.30
1	C	209	TRP	CD1-CG-CD2	9.67	114.04	106.30
2	D	141	CYS	CA-CB-SG	9.65	131.37	114.00
1	A	269	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	C	284	TRP	CD1-CG-CD2	8.54	113.14	106.30
1	C	54[A]	ARG	CA-CB-CG	8.28	131.62	113.40
1	C	54[B]	ARG	CA-CB-CG	8.28	131.62	113.40
1	A	234	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	C	209	TRP	CE2-CD2-CG	-8.10	100.82	107.30
1	C	97	THR	N-CA-CB	-8.04	95.03	110.30
2	B	96	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	C	159	MET	CG-SD-CE	-7.95	87.48	100.20
2	B	133	ASP	N-CA-C	7.89	132.31	111.00
2	D	141	CYS	CB-CA-C	-7.83	94.73	110.40
1	C	140	LEU	CA-CB-CG	7.82	133.28	115.30
1	C	284	TRP	CE2-CD2-CG	-7.75	101.10	107.30
2	B	96	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	A	209	TRP	CE2-CD2-CG	-7.71	101.13	107.30
1	C	113	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	C	98	TYR	CB-CG-CD2	-7.39	116.57	121.00
2	D	9	VAL	CA-C-N	-7.32	101.11	117.20
1	A	17	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	C	284	TRP	CB-CG-CD1	-7.25	117.58	127.00
2	D	96	ARG	NE-CZ-NH2	-7.19	116.70	120.30
2	B	75	ALA	CA-C-N	7.15	132.92	117.20
2	B	11	ALA	N-CA-C	7.12	130.24	111.00
1	A	79	THR	N-CA-C	7.08	130.11	111.00
1	C	248	VAL	CG1-CB-CG2	-7.05	99.63	110.90
1	C	125	LEU	CA-CB-CG	7.03	131.46	115.30
1	A	167	ARG	NE-CZ-NH2	-7.00	116.80	120.30
2	B	130	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	A	167	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	284	TRP	CD1-CG-CD2	6.90	111.82	106.30
1	A	80	SER	N-CA-C	6.85	129.49	111.00
1	C	234	ARG	NE-CZ-NH1	6.82	123.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	26	THR	CA-CB-CG2	6.81	121.94	112.40
1	A	44	ILE	CG1-CB-CG2	-6.79	96.47	111.40
1	A	296	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	A	113	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	A	284	TRP	CE2-CD2-CG	-6.66	101.97	107.30
1	A	209	TRP	CG-CD1-NE1	-6.65	103.45	110.10
2	B	52	GLU	N-CA-C	6.54	128.66	111.00
1	C	209	TRP	CG-CD1-NE1	-6.52	103.58	110.10
1	A	84	LYS	N-CA-C	-6.50	93.46	111.00
1	C	284	TRP	CG-CD2-CE3	6.47	139.72	133.90
2	B	114	CYS	CA-CB-SG	6.45	125.62	114.00
1	C	56	ARG	CG-CD-NE	-6.42	98.31	111.80
1	A	269	ARG	CA-CB-CG	6.40	127.48	113.40
1	C	222	VAL	CA-CB-CG1	6.38	120.46	110.90
1	C	65	ARG	NE-CZ-NH2	-6.35	117.12	120.30
2	D	128	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	C	56	ARG	NE-CZ-NH1	6.25	123.43	120.30
2	B	85	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	C	80	SER	N-CA-C	6.20	127.73	111.00
2	D	89	TYR	N-CA-C	6.17	127.67	111.00
1	A	234	ARG	CA-CB-CG	6.17	126.97	113.40
1	A	310	LEU	CA-CB-CG	6.17	129.48	115.30
1	C	222	VAL	CA-CB-CG2	-6.15	101.67	110.90
1	A	42	LYS	CA-CB-CG	-6.15	99.87	113.40
1	A	197	TYR	CA-CB-CG	6.15	125.08	113.40
2	B	76	LEU	CA-CB-CG	6.10	129.32	115.30
1	C	26	THR	CA-CB-OG1	-6.09	96.22	109.00
2	B	149	VAL	CA-C-N	6.05	130.52	117.20
2	B	57	ASP	CB-CG-OD1	6.05	123.75	118.30
2	D	55	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	C	94	VAL	CA-C-N	6.03	130.47	117.20
2	B	66	LEU	CA-CB-CG	5.94	128.95	115.30
1	A	269	ARG	CG-CD-NE	-5.92	99.36	111.80
1	A	62	SER	CA-CB-OG	-5.86	95.38	111.20
2	B	131	ALA	N-CA-C	5.81	126.70	111.00
1	A	5	TYR	CB-CG-CD1	-5.77	117.54	121.00
1	C	284	TRP	CG-CD1-NE1	-5.76	104.34	110.10
1	A	116	THR	N-CA-CB	-5.73	99.41	110.30
1	C	255	HIS	CB-CA-C	-5.73	98.94	110.40
2	D	128	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	C	94	VAL	O-C-N	-5.66	113.64	122.70
1	C	174	GLN	CA-CB-CG	-5.66	100.95	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	133	ASP	CA-C-N	-5.65	104.78	117.20
2	D	88	ASN	N-CA-C	-5.65	95.75	111.00
1	C	275	THR	CA-CB-OG1	-5.62	97.20	109.00
2	D	96	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	C	105	ARG	CG-CD-NE	-5.62	100.00	111.80
1	C	275	THR	CA-CB-CG2	5.60	120.24	112.40
2	D	128	ARG	CB-CG-CD	-5.59	97.07	111.60
1	C	242	ASN	CA-C-N	-5.59	104.91	117.20
1	C	113	ARG	NE-CZ-NH2	-5.58	117.51	120.30
2	B	106	VAL	N-CA-CB	-5.56	99.27	111.50
1	C	116	THR	N-CA-CB	-5.56	99.74	110.30
2	B	130	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	A	306	ARG	NE-CZ-NH2	-5.51	117.54	120.30
2	B	1	MET	CA-CB-CG	5.51	122.67	113.30
2	D	77	TYR	CB-CG-CD1	-5.50	117.70	121.00
1	A	211	LEU	CB-CG-CD1	-5.50	101.65	111.00
2	B	109	CYS	CA-CB-SG	-5.47	104.16	114.00
1	C	229	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	94	VAL	CG1-CB-CG2	-5.45	102.19	110.90
1	A	113	ARG	NE-CZ-NH1	5.44	123.02	120.30
2	D	14	ARG	NE-CZ-NH1	5.43	123.02	120.30
2	B	13	LYS	CA-CB-CG	5.41	125.30	113.40
1	C	183	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	216	GLU	CA-CB-CG	5.38	125.25	113.40
1	A	42	LYS	CG-CD-CE	-5.38	95.77	111.90
1	C	23	VAL	CG1-CB-CG2	-5.36	102.32	110.90
1	C	136	THR	N-CA-CB	-5.34	100.15	110.30
1	C	62	SER	CA-CB-OG	5.33	125.60	111.20
1	C	218	VAL	CA-CB-CG2	-5.32	102.92	110.90
2	B	34	LYS	CA-CB-CG	5.31	125.09	113.40
2	B	91	VAL	CA-CB-CG2	-5.30	102.94	110.90
1	C	273	ILE	N-CA-C	-5.30	96.69	111.00
1	C	83	LYS	CA-C-N	-5.29	105.55	117.20
1	A	151	ARG	CG-CD-NE	-5.29	100.69	111.80
1	A	69	SER	CA-CB-OG	-5.28	96.94	111.20
2	D	89	TYR	CB-CG-CD1	-5.28	117.83	121.00
1	C	105	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	C	78	ASN	N-CA-C	5.27	125.23	111.00
2	B	30	LEU	CA-CB-CG	5.27	127.41	115.30
1	C	32	ALA	CA-C-N	5.25	128.75	117.20
1	C	114	LEU	CA-CB-CG	5.25	127.36	115.30
2	D	92	VAL	CA-CB-CG2	-5.23	103.05	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	41	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	43	VAL	CG1-CB-CG2	-5.22	102.56	110.90
2	B	132	ASN	C-N-CA	5.21	134.72	121.70
2	B	37	GLU	CA-CB-CG	-5.19	101.98	113.40
2	D	102	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	C	287	GLN	CG-CD-NE2	5.18	129.13	116.70
1	A	284	TRP	CB-CG-CD1	-5.18	120.27	127.00
2	D	22	PRO	N-CA-C	5.16	125.51	112.10
2	B	5	ASN	O-C-N	-5.13	114.48	122.70
1	A	65	ARG	NE-CZ-NH1	5.12	122.86	120.30
2	B	52	GLU	CA-C-N	-5.09	106.00	117.20
1	A	100	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	116	THR	CA-CB-CG2	5.07	119.50	112.40
1	A	56	ARG	CG-CD-NE	-5.05	101.20	111.80
1	A	159	MET	CA-CB-CG	-5.02	104.76	113.30
2	B	10	GLU	CA-C-N	-5.02	106.15	117.20
2	D	102	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	226	TYR	Sidechain
1	A	294	PHE	Sidechain
1	A	48	PHE	Sidechain
1	A	98	TYR	Sidechain
2	B	152	ALA	Peptide
1	C	118	PHE	Sidechain
1	C	98	TYR	Sidechain
2	D	20	HIS	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	45	0
1	C	2420	0	2427	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1196	0	1212	33	0
2	D	1138	0	1152	34	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	B	29	0	12	2	0
4	D	29	0	12	0	0
5	A	26	0	0	1	0
5	B	9	0	0	1	0
5	C	37	0	0	4	0
5	D	9	0	0	1	0
All	All	7310	0	7237	149	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.

All (149) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:THR:HG23	1:C:296:ARG:HH11	1.19	1.01
1:C:54[B]:ARG:NH2	1:C:267:LEU:HB3	1.74	1.00
2:B:6:LYS:HB3	2:D:10:GLU:HG3	1.47	0.97
1:C:54[B]:ARG:NH1	1:C:54[B]:ARG:HG2	1.92	0.83
2:B:76:LEU:HD11	2:B:103:ILE:HD11	1.61	0.83
1:C:54[B]:ARG:HH21	1:C:267:LEU:HB3	1.43	0.81
1:A:308:LEU:HG	1:A:310:LEU:HD22	1.63	0.81
1:C:54[B]:ARG:NH2	1:C:267:LEU:CB	2.43	0.80
2:B:4:ASP:HA	2:B:10:GLU:HB2	1.65	0.77
2:B:114:CYS:HB2	2:B:141:CYS:HB3	1.67	0.76
1:A:106:HIS:HD2	1:A:108:GLN:H	1.33	0.74
2:D:76:LEU:HD22	2:D:103:ILE:HD13	1.70	0.74
2:B:58:LEU:HD21	2:B:60:LYS:HE3	1.69	0.73
1:A:83:LYS:HB3	1:A:86:GLU:HB3	1.70	0.72
2:B:17:VAL:HG22	2:B:60:LYS:HG2	1.71	0.71
2:B:2:THR:HG22	2:B:10:GLU:HB3	1.74	0.70
2:B:6:LYS:HZ2	2:D:12:ILE:HG12	1.58	0.67
2:D:20:HIS:HB2	5:D:1008:HOH:O	1.94	0.67
1:C:54[B]:ARG:HH22	1:C:267:LEU:HB3	1.59	0.66
2:D:116:SER:HA	2:D:121:VAL:HG11	1.75	0.66
1:C:292:GLY:O	1:C:296:ARG:HB2	1.96	0.65
1:C:29:LYS:HD3	1:C:310:LEU:HD22	1.77	0.65
1:A:151:ARG:HD2	1:A:153:ASP:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:ARG:O	1:C:116:THR:HB	1.98	0.64
2:D:65:PHE:HB3	2:D:85:ARG:HH22	1.61	0.64
1:C:94:VAL:O	1:C:97:THR:HB	1.98	0.64
2:B:12:ILE:HB	2:B:62:GLU:HG2	1.80	0.63
1:A:261:MET:O	1:A:282:HIS:HD2	1.81	0.63
2:B:6:LYS:HE2	2:D:41:ARG:HD2	1.81	0.63
2:D:14:ARG:HB3	2:D:87:ASP:HA	1.80	0.62
1:A:284:TRP:HA	1:A:287:GLN:NE2	2.14	0.62
1:A:187:ILE:HG13	1:A:212:HIS:HB2	1.81	0.61
2:D:32:LEU:HD22	2:D:106:VAL:HG13	1.80	0.61
1:C:136:THR:HG23	1:C:296:ARG:NH1	2.03	0.61
2:B:41:ARG:HD3	2:D:48:LEU:HA	1.83	0.60
1:C:136:THR:CG2	1:C:296:ARG:HH11	2.03	0.60
2:D:65:PHE:HB3	2:D:85:ARG:NH2	2.17	0.60
2:D:22:PRO:HG3	2:D:80:GLN:OE1	2.03	0.59
1:A:153:ASP:HB3	1:A:180:ASP:O	2.03	0.59
1:C:97:THR:HG22	1:C:98:TYR:CD2	2.37	0.59
2:D:20:HIS:HA	2:D:56:LYS:HD2	1.85	0.58
1:C:54[B]:ARG:HH21	1:C:267:LEU:CB	2.12	0.58
2:B:48:LEU:O	2:B:55:ARG:HA	2.03	0.58
2:D:81:ALA:O	2:D:97:PRO:HD2	2.03	0.57
1:C:235:LEU:HB3	1:C:239:GLU:HB3	1.86	0.57
2:D:21:ILE:HB	2:D:57:ASP:HB2	1.87	0.57
1:C:255:HIS:HB2	5:C:318:HOH:O	2.04	0.57
2:B:11:ALA:HA	4:B:999:CTP:N3	2.20	0.56
2:B:41:ARG:NE	2:D:49:PRO:HD3	2.20	0.55
1:A:214:SER:O	1:A:217:GLU:HG2	2.06	0.55
1:A:269:ARG:HA	1:A:272:GLU:OE2	2.06	0.55
1:C:302:LEU:HD23	1:C:308:LEU:HD13	1.89	0.55
1:A:292:GLY:O	1:A:296:ARG:HG3	2.07	0.54
2:D:12:ILE:HG21	2:D:62:GLU:HB3	1.89	0.54
1:C:284:TRP:HA	1:C:287:GLN:NE2	2.22	0.54
1:C:9:ILE:HG21	1:C:299:LEU:HD21	1.91	0.53
1:A:227:MET:HG3	1:A:273:ILE:HD11	1.91	0.53
1:A:29:LYS:HE2	1:A:310:LEU:HD23	1.91	0.52
1:A:38:LEU:HD23	1:A:66:LEU:HD22	1.91	0.52
1:C:97:THR:HG22	1:C:98:TYR:HD2	1.72	0.52
1:A:184:PHE:O	1:A:209:TRP:HA	2.11	0.51
1:C:231:GLN:HB2	1:C:234:ARG:HG2	1.91	0.51
1:A:189:PRO:HG2	1:A:192:LEU:HB2	1.92	0.51
1:A:287:GLN:H	1:A:287:GLN:NE2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:VAL:HG22	1:A:187:ILE:HB	1.93	0.50
1:A:106:HIS:CD2	1:A:108:GLN:H	2.20	0.50
2:D:141:CYS:HB2	2:D:143:LYS:H	1.74	0.50
2:B:14:ARG:HA	2:B:86:ILE:O	2.12	0.50
1:C:261:MET:O	1:C:282:HIS:HD2	1.95	0.49
2:B:42:ILE:HA	2:B:60:LYS:O	2.13	0.49
1:C:86:GLU:HA	5:C:324:HOH:O	2.13	0.48
2:B:94:LYS:HE2	4:B:999:CTP:O2G	2.13	0.48
1:A:287:GLN:H	1:A:287:GLN:HE21	1.61	0.47
2:B:5:ASN:O	2:B:9:VAL:HA	2.13	0.47
1:C:83:LYS:NZ	1:C:83:LYS:HA	2.29	0.47
2:D:151:LEU:HD13	2:D:151:LEU:HA	1.71	0.47
1:C:189:PRO:HG2	1:C:192:LEU:HD12	1.96	0.47
2:D:124:SER:HB3	2:D:139:LYS:HG2	1.97	0.47
1:A:232:LYS:HA	1:A:235:LEU:HD12	1.97	0.47
1:A:29:LYS:HE2	1:A:310:LEU:CD2	2.45	0.47
2:B:152:ALA:O	2:B:153:ASN:C	2.52	0.47
1:C:80:SER:O	1:C:83:LYS:HB2	2.15	0.47
1:C:59:PHE:CE2	1:C:136:THR:HG21	2.50	0.46
2:B:4:ASP:HA	2:B:10:GLU:CB	2.41	0.46
1:A:223:ASP:O	1:A:261:MET:HA	2.15	0.46
2:B:4:ASP:HA	2:B:10:GLU:H	1.80	0.46
1:C:186:PHE:HB2	1:C:211:LEU:HD12	1.97	0.46
2:D:10:GLU:O	2:D:60:LYS:HE2	2.16	0.46
1:C:1:ALA:HB2	1:C:306:ARG:NH2	2.31	0.46
1:C:287:GLN:HE21	1:C:287:GLN:H	1.64	0.45
2:B:44:ILE:HG23	2:B:59:ILE:HG12	1.98	0.45
1:A:248:VAL:HG12	1:A:272:GLU:HA	1.99	0.45
2:D:109:CYS:HA	2:D:125:PHE:HZ	1.80	0.45
1:C:287:GLN:NE2	1:C:287:GLN:H	2.14	0.45
1:A:261:MET:O	1:A:282:HIS:CD2	2.67	0.45
2:D:111:ASN:O	2:D:117:HIS:CE1	2.69	0.45
2:B:4:ASP:HA	2:B:10:GLU:N	2.32	0.45
1:C:160:VAL:HG22	1:C:187:ILE:HB	1.98	0.45
2:B:26:GLY:O	2:B:30:LEU:HD22	2.17	0.45
1:C:59:PHE:CE1	1:C:296:ARG:HG3	2.52	0.44
1:A:113:ARG:O	1:A:116:THR:HB	2.17	0.44
2:D:12:ILE:HD11	2:D:60:LYS:HB3	1.98	0.44
1:A:205:LYS:HB3	1:A:207:ILE:HG13	1.99	0.44
1:A:21:ASN:HD21	1:A:179:PHE:HE1	1.65	0.44
1:A:163:LEU:HG	1:A:188:ALA:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:LYS:HA	1:C:195:PRO:HD3	2.00	0.44
1:C:132:ASN:OD1	1:C:133:GLN:HG2	2.17	0.44
2:B:4:ASP:HB2	2:D:8:GLN:C	2.38	0.44
2:B:152:ALA:O	2:B:153:ASN:O	2.36	0.44
1:A:137:GLN:HG2	1:A:168:THR:HG22	2.00	0.43
2:D:50:SER:O	2:D:54:GLY:N	2.51	0.43
1:C:232:LYS:HA	1:C:240:TYR:CD2	2.53	0.43
1:C:198:ILE:HD13	1:C:198:ILE:HA	1.81	0.43
2:B:41:ARG:HG2	2:D:47:ASN:O	2.19	0.43
1:C:194:MET:SD	1:C:198:ILE:HG21	2.58	0.43
1:A:4:LEU:O	1:A:7:LYS:HB2	2.19	0.43
2:B:24:GLN:HA	5:B:1003:HOH:O	2.16	0.43
1:A:254:LEU:HD11	1:A:277:VAL:HG13	2.00	0.43
1:C:1:ALA:HA	1:C:306:ARG:O	2.18	0.43
1:A:238:SER:O	1:A:242:ASN:HB2	2.19	0.43
1:C:166:GLY:O	1:C:169:VAL:HG22	2.18	0.43
2:D:13:LYS:O	2:D:86:ILE:HG22	2.18	0.43
2:B:71:VAL:HG13	2:B:83:VAL:HG21	2.01	0.42
1:C:136:THR:HG22	5:C:315:HOH:O	2.19	0.42
1:A:232:LYS:H	1:A:232:LYS:HE3	1.84	0.42
2:D:20:HIS:O	2:D:20:HIS:CG	2.73	0.42
1:C:17:ARG:NH1	5:C:335:HOH:O	2.52	0.42
2:D:106:VAL:O	2:D:107:LEU:HG	2.20	0.42
2:B:41:ARG:CZ	2:D:49:PRO:HD3	2.49	0.42
1:A:158:ALA:HB2	1:A:222:VAL:HG21	2.02	0.42
2:D:77:TYR:CE1	2:D:151:LEU:HD11	2.55	0.42
1:A:166:GLY:O	1:A:169:VAL:HG22	2.19	0.42
2:D:152:ALA:O	2:D:153:ASN:HB2	2.20	0.42
2:B:1:MET:N	2:B:89:TYR:OH	2.52	0.41
1:A:189:PRO:HG2	1:A:192:LEU:HD12	2.01	0.41
2:B:3:HIS:N	2:B:3:HIS:ND1	2.69	0.41
1:A:163:LEU:CD1	1:A:186:PHE:HB3	2.50	0.41
1:A:244:LYS:HB3	1:A:245:ALA:H	1.75	0.41
1:C:81:LEU:HD21	1:C:91:THR:HG21	2.01	0.41
2:D:71:VAL:HA	2:D:74:LEU:HD12	2.02	0.41
1:A:139:LEU:HD23	1:A:139:LEU:HA	1.81	0.41
1:C:79:THR:O	1:C:81:LEU:N	2.53	0.41
1:A:204:GLU:HG3	5:A:314:HOH:O	2.20	0.41
2:B:19:ASP:OD1	2:B:58:LEU:HD12	2.19	0.41
1:A:12:ILE:HD12	1:A:12:ILE:HA	1.99	0.41
1:A:140:LEU:HD22	1:A:292:GLY:HA2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:ALA:HB1	1:C:118:PHE:CE1	2.56	0.40
1:A:267:LEU:HD23	1:A:269:ARG:HB3	2.04	0.40
1:A:9:ILE:HG21	1:A:299:LEU:HD21	2.04	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%)	280 (91%)	22 (7%)	6 (2%)	10	16
1	C	309/310 (100%)	284 (92%)	22 (7%)	3 (1%)	19	34
2	B	151/153 (99%)	123 (82%)	15 (10%)	13 (9%)	1	1
2	D	144/153 (94%)	122 (85%)	14 (10%)	8 (6%)	2	2
All	All	912/926 (98%)	809 (89%)	73 (8%)	30 (3%)	5	6

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	SER
1	A	83	LYS
1	A	84	LYS
2	B	3	HIS
2	B	11	ALA
2	B	68	GLU
2	B	131	ALA
2	B	133	ASP
2	B	134	ILE
1	C	80	SER
1	C	243	VAL
2	D	24	GLN

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Mol	Chain	Res	Type
2	D	89	TYR
2	B	4	ASP
1	C	78	ASN
2	D	10	GLU
2	D	107	LEU
2	D	132	ASN
2	B	52	GLU
2	B	129	LYS
2	D	22	PRO
2	D	131	ALA
1	A	79	THR
1	A	243	VAL
1	A	244	LYS
2	B	14	ARG
2	B	51	GLY
2	B	120	PRO
2	D	53	MET
2	B	34	LYS

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	261/261 (100%)	231 (88%)	30 (12%)	7 13
1	C	262/261 (100%)	228 (87%)	34 (13%)	5 9
2	B	136/137 (99%)	112 (82%)	24 (18%)	2 4
2	D	129/137 (94%)	111 (86%)	18 (14%)	4 8
All	All	788/796 (99%)	682 (86%)	106 (14%)	5 9

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	35	GLN
1	A	76	SER

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Mol	Chain	Res	Type
1	A	78	ASN
1	A	79	THR
1	A	81	LEU
1	A	113	ARG
1	A	124	VAL
1	A	134	HIS
1	A	151	ARG
1	A	167	ARG
1	A	183	ARG
1	A	205	LYS
1	A	210	SER
1	A	211	LEU
1	A	213	SER
1	A	216	GLU
1	A	225	LEU
1	A	228	THR
1	A	229	ARG
1	A	232	LYS
1	A	238	SER
1	A	252	SER
1	A	269	ARG
1	A	285	TYR
1	A	287	GLN
1	A	305	ASN
1	A	307	ASP
1	A	309	VAL
1	A	310	LEU
2	B	1	MET
2	B	2	THR
2	B	3	HIS
2	B	5	ASN
2	B	30	LEU
2	B	32	LEU
2	B	34	LYS
2	B	40	GLN
2	B	41	ARG
2	B	67	SER
2	B	69	ASP
2	B	73	GLN
2	B	76	LEU
2	B	85	ARG
2	B	90	GLU

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Mol	Chain	Res	Type
2	B	95	SER
2	B	98	SER
2	B	99	LEU
2	B	102	ARG
2	B	104	ASP
2	B	114	CYS
2	B	143	LYS
2	B	148	ASN
2	B	153	ASN
1	C	12	ILE
1	C	34	PRO
1	C	54[A]	ARG
1	C	54[B]	ARG
1	C	56	ARG
1	C	59	PHE
1	C	65	ARG
1	C	74	SER
1	C	79	THR
1	C	97	THR
1	C	105	ARG
1	C	125	LEU
1	C	134	HIS
1	C	136	THR
1	C	151	ARG
1	C	152	LEU
1	C	153	ASP
1	C	167	ARG
1	C	211	LEU
1	C	218	VAL
1	C	222	VAL
1	C	225	LEU
1	C	243	VAL
1	C	246	GLN
1	C	256	ASN
1	C	269	ARG
1	C	271	ASP
1	C	279	LYS
1	C	284	TRP
1	C	285	TYR
1	C	287	GLN
1	C	296	ARG
1	C	308	LEU

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Mol	Chain	Res	Type
1	C	310	LEU
2	D	10	GLU
2	D	12	ILE
2	D	14	ARG
2	D	48	LEU
2	D	49	PRO
2	D	50	SER
2	D	80	GLN
2	D	85	ARG
2	D	92	VAL
2	D	98	SER
2	D	100	PRO
2	D	101	GLU
2	D	104	ASP
2	D	130	ARG
2	D	139	LYS
2	D	146	SER
2	D	151	LEU
2	D	153	ASN

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

Mol	Chain	Res	Type
1	A	106	HIS
1	A	146	GLN
1	A	282	HIS
1	A	287	GLN
2	B	147	HIS
2	B	148	ASN
1	C	21	ASN
1	C	255	HIS
1	C	282	HIS
1	C	287	GLN
2	D	117	HIS

5.3.3 RNA

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 carbohydrates 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	B	999	-	21,30,30	1.32	4 (19%)	31,47,47	2.34	8 (25%)
4	CTP	D	999	-	21,30,30	1.21	2 (9%)	31,47,47	2.19	7 (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
4	CTP	B	999	-	-	0/18/38/38	0/2/2/2
4	CTP	D	999	-	-	0/18/38/38	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	999	CTP	C6-N1	-2.82	1.31	1.35
4	B	999	CTP	C4-N3	-2.12	1.31	1.35
4	D	999	CTP	C6-N1	-2.01	1.33	1.35
4	B	999	CTP	PB-O1B	2.08	1.58	1.51
4	B	999	CTP	PG-O1G	2.14	1.58	1.51
4	D	999	CTP	PG-O1G	2.45	1.59	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	999	CTP	PB-O3A-PA	-7.19	112.53	132.73
4	B	999	CTP	PB-O3A-PA	-7.13	112.69	132.73
4	D	999	CTP	PB-O3B-PG	-6.47	110.96	132.67
4	B	999	CTP	PB-O3B-PG	-5.26	115.03	132.67
4	B	999	CTP	C4'-O4'-C1'	-4.82	104.42	109.72
4	D	999	CTP	C6-N1-C2	-3.16	116.17	121.28
4	B	999	CTP	C6-N1-C2	-3.04	116.35	121.28
4	D	999	CTP	C5-C4-N3	-2.06	119.20	121.80
4	B	999	CTP	C5'-C4'-C3'	-2.05	107.07	115.21
4	D	999	CTP	O4'-C1'-N1	2.37	113.07	108.08
4	B	999	CTP	O4'-C1'-N1	2.43	113.21	108.08
4	D	999	CTP	O3A-PA-O5'	2.95	110.75	102.94
4	B	999	CTP	C2-N3-C4	3.32	120.30	115.61
4	B	999	CTP	O3A-PA-O5'	4.00	113.55	102.94
4	D	999	CTP	C2-N3-C4	4.09	121.38	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	999	CTP	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.