



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 12:56 am BST

PDB ID : 1R0B
Title : Aspartate Transcarbamylase (ATCase) of Escherichia coli: A New Crystalline R State Bound to PALA, or to Product Analogues Phosphate and Citrate
Authors : Huang, J.; Lipscomb, W.N.
Deposited on : 2003-09-19
Resolution : 2.90 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 ⓘ symbol.

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	:	2.11
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)	:	2.11

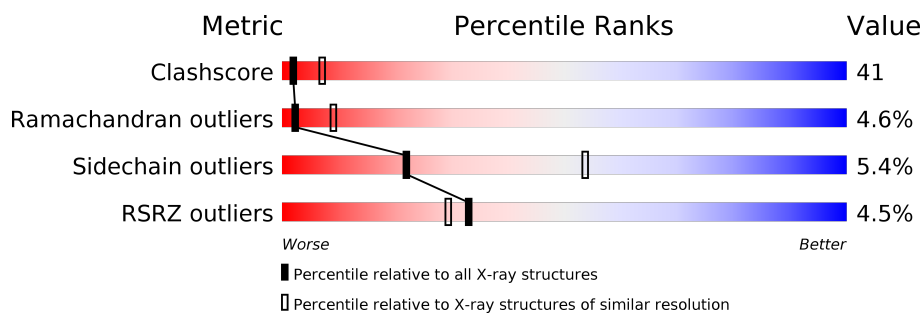
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 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 $\leq 5\%$. 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	<div> <div style="width: 52%;"></div> <div style="width: 43%;"></div> <div style="width: 5%;"></div> </div>
1	B	310	<div> <div style="width: 50%;"></div> <div style="width: 45%;"></div> <div style="width: 5%;"></div> </div>
1	C	310	<div> <div style="width: 50%;"></div> <div style="width: 43%;"></div> <div style="width: 7%;"></div> </div>
1	D	310	<div> <div style="width: 50%;"></div> <div style="width: 45%;"></div> <div style="width: 5%;"></div> </div>
1	E	310	<div> <div style="width: 53%;"></div> <div style="width: 43%;"></div> <div style="width: 4%;"></div> </div>
1	F	310	<div> <div style="width: 49%;"></div> <div style="width: 46%;"></div> <div style="width: 5%;"></div> </div>
2	G	153	<div> <div style="width: 14%;"></div> <div style="width: 21%;"></div> <div style="width: 69%;"></div> <div style="width: 8%;"></div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	153	
2	I	153	
2	J	153	
2	K	153	
2	L	153	

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	FLC	A	2001	-	-	X	-
3	FLC	B	2002	-	-	X	-
3	FLC	C	2003	-	-	X	-
3	FLC	D	2004	-	-	X	-
3	FLC	E	2005	-	-	X	-
4	PO4	A	3001	-	X	X	-
4	PO4	B	3002	-	X	-	-
4	PO4	C	3003	-	X	-	-
4	PO4	E	3005	-	X	-	-
4	PO4	F	3006	-	X	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22698 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.

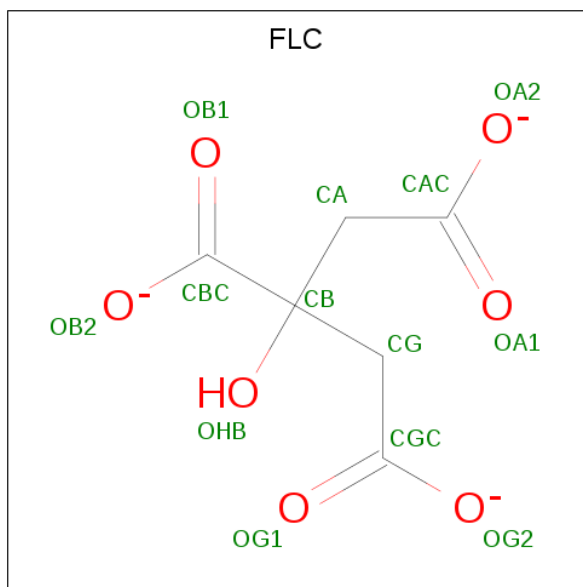
- Molecule 1 is a protein called Aspartate carbamoyltransferase catalytic chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	B	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	C	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	D	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	E	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	F	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			

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

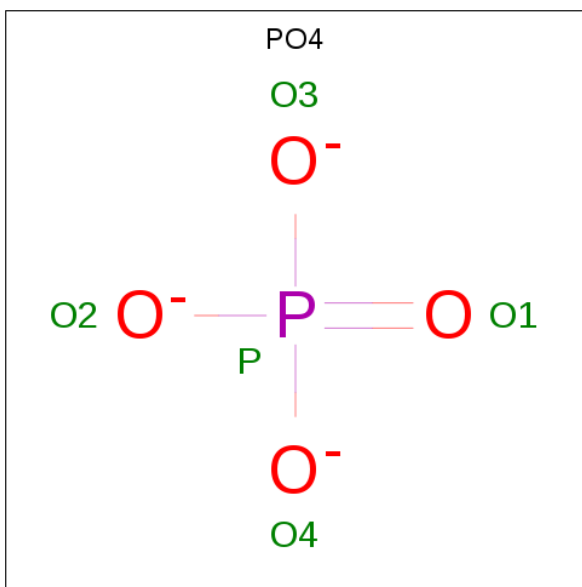
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			
2	H	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			
2	I	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			
2	J	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			
2	K	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			
2	L	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: C₆H₅O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	D	1	Total	C	O	0	0
			13	6	7		
3	E	1	Total	C	O	0	0
			13	6	7		
3	F	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Zn	0	0
			1	1		
5	J	1	Total	Zn	0	0
			1	1		
5	K	1	Total	Zn	0	0
			1	1		
5	H	1	Total	Zn	0	0
			1	1		
5	I	1	Total	Zn	0	0
			1	1		
5	L	1	Total	Zn	0	0
			1	1		

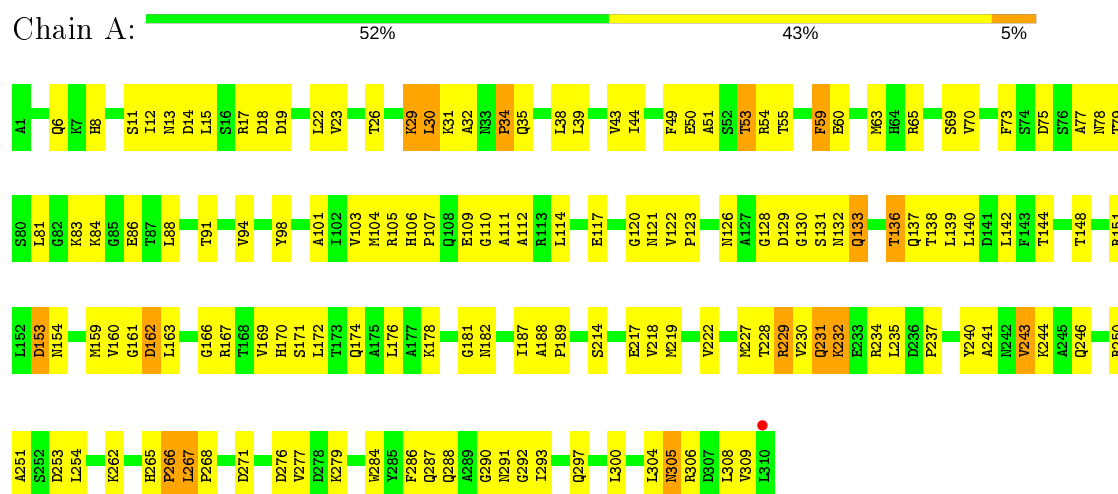
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	84	Total 84	O 84	0	0
6	B	95	Total 95	O 95	0	0
6	C	113	Total 113	O 113	0	0
6	G	65	Total 65	O 65	0	0
6	H	59	Total 59	O 59	0	0
6	I	45	Total 45	O 45	0	0
6	D	102	Total 102	O 102	0	0
6	E	86	Total 86	O 86	0	0
6	F	82	Total 82	O 82	0	0
6	J	51	Total 51	O 51	0	0
6	K	51	Total 51	O 51	0	0
6	L	55	Total 55	O 55	0	0

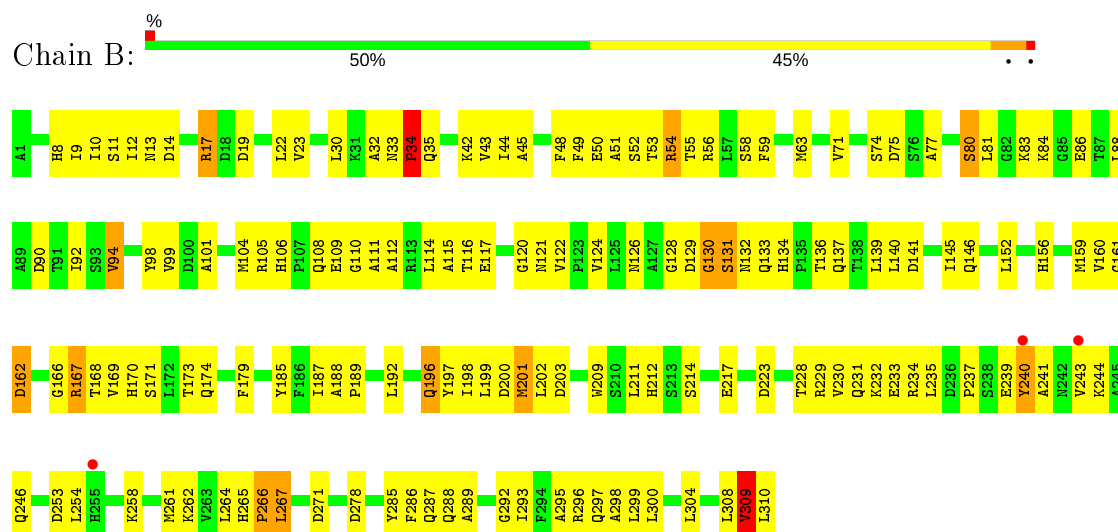
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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

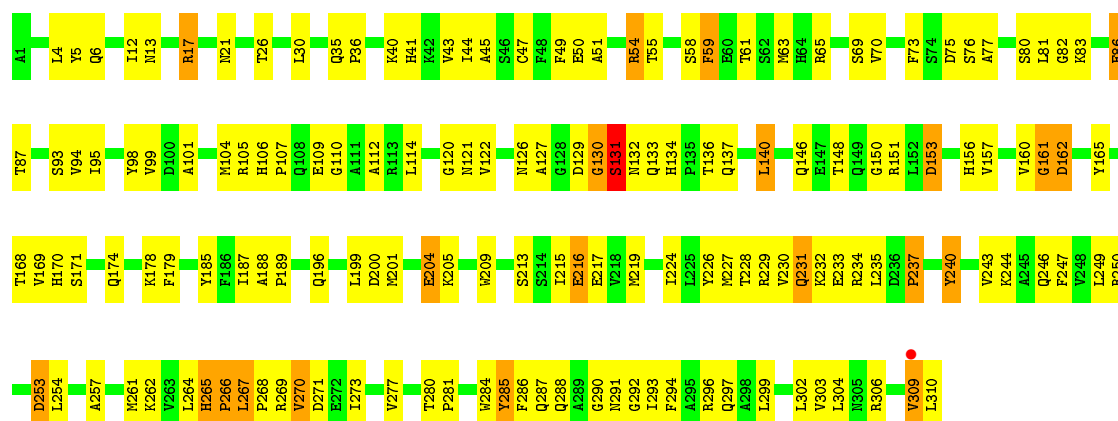


- Molecule 1: Aspartate carbamoyltransferase catalytic chain

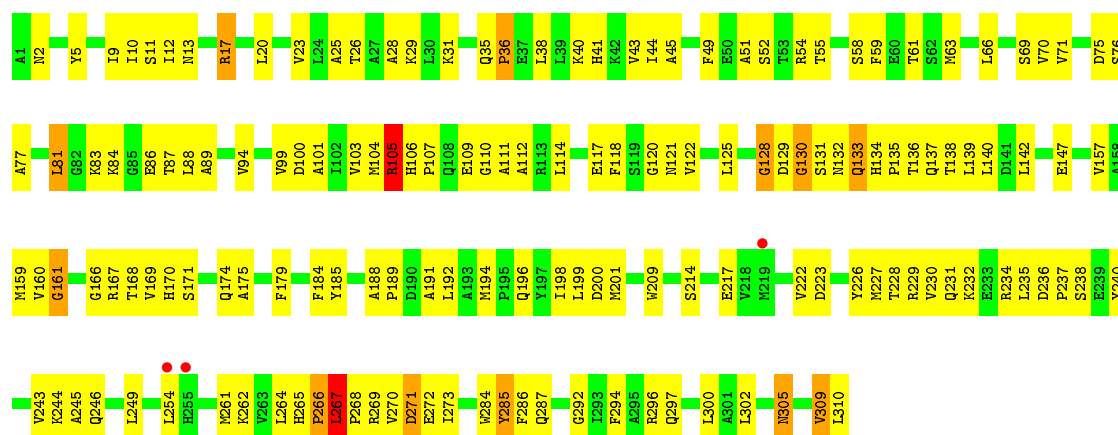


- Molecule 1: Aspartate carbamoyltransferase catalytic chain

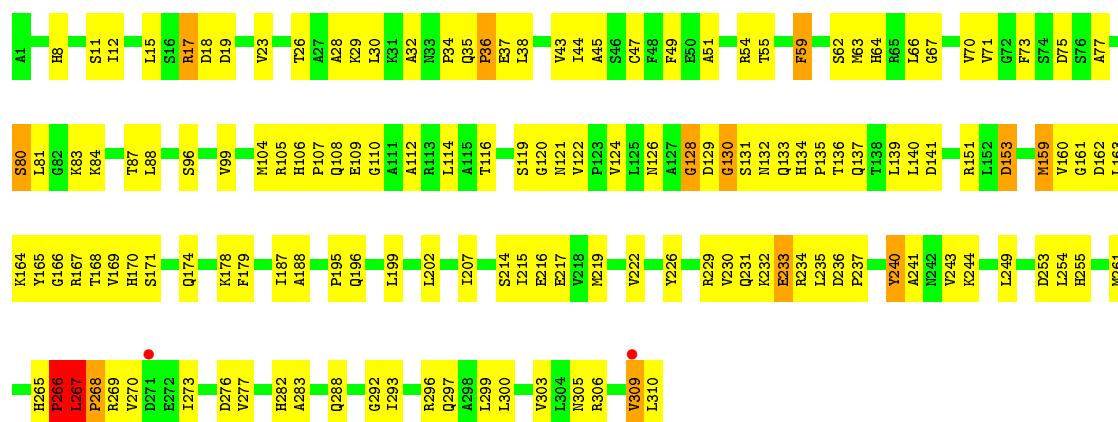




• Molecule 1: Aspartate carbamoyltransferase catalytic chain

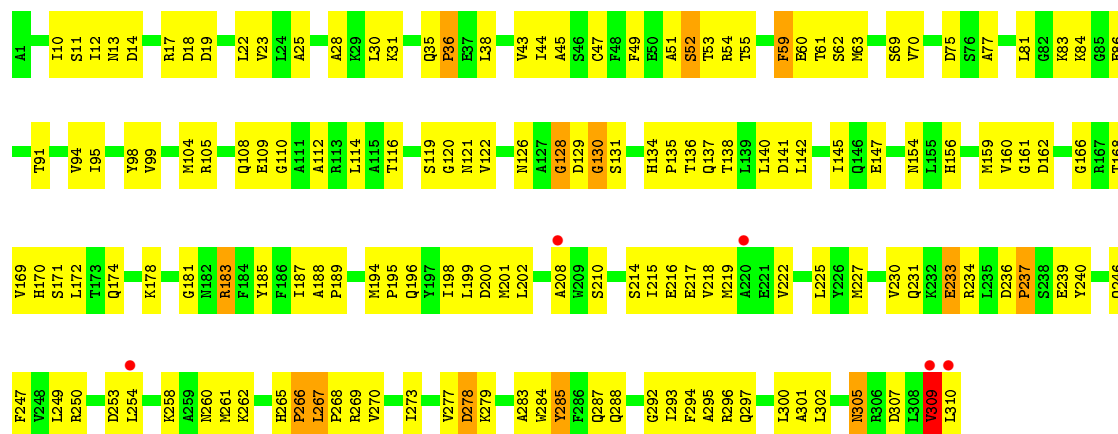


• Molecule 1: Aspartate carbamoyltransferase catalytic chain

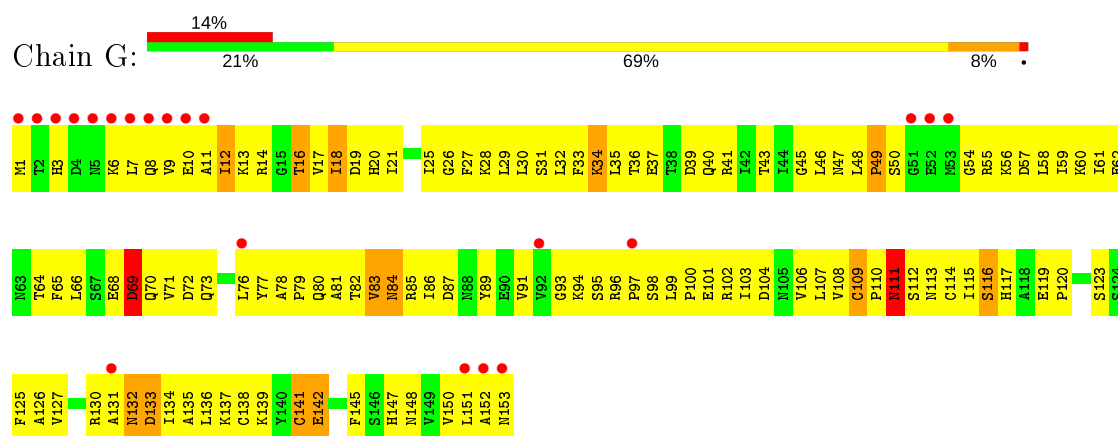


• Molecule 1: Aspartate carbamoyltransferase catalytic chain

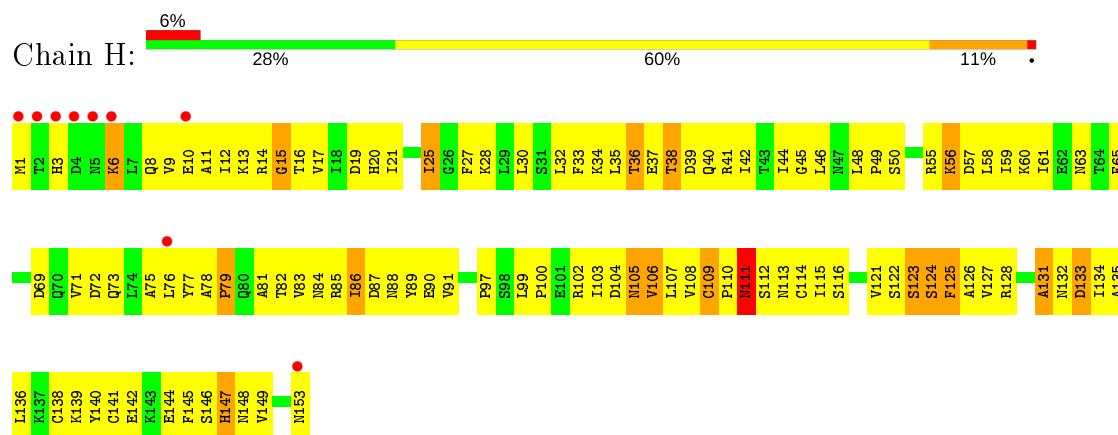




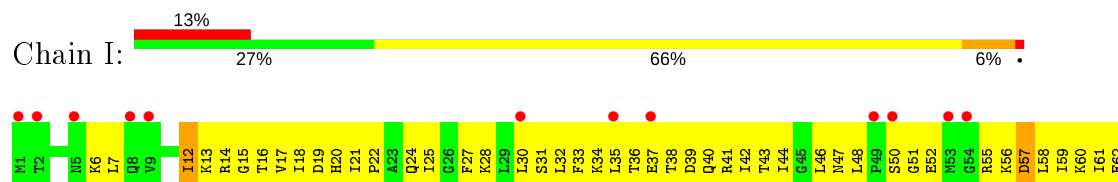
• Molecule 2: Aspartate carbamoyltransferase regulatory chain

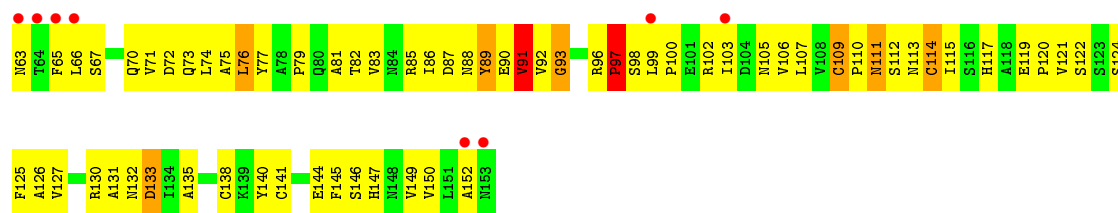


• Molecule 2: Aspartate carbamoyltransferase regulatory chain

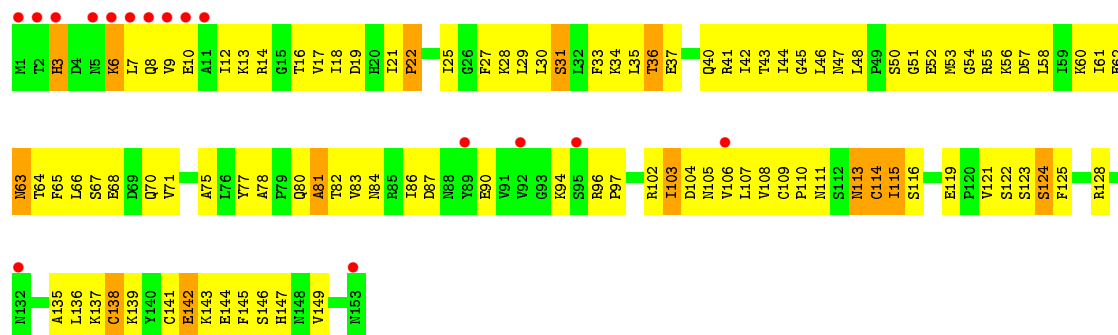


• Molecule 2: Aspartate carbamoyltransferase regulatory chain

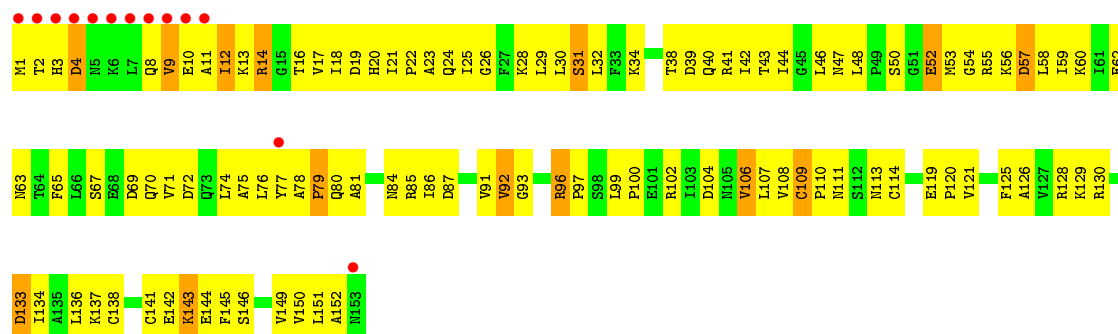




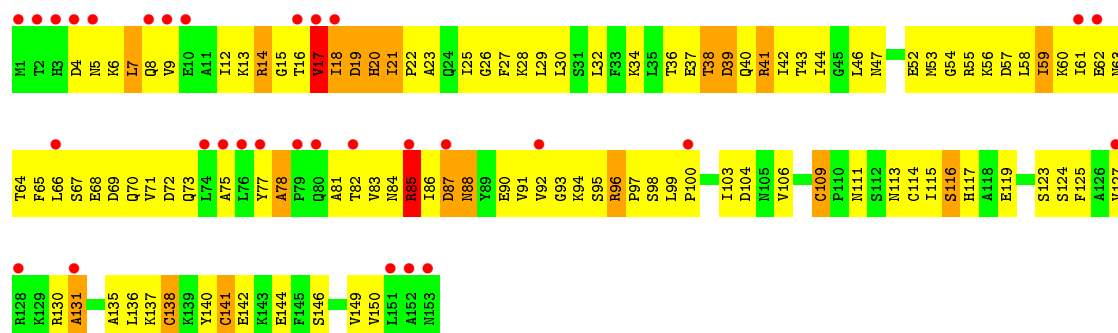
• Molecule 2: Aspartate carbamoyltransferase regulatory chain



• Molecule 2: Aspartate carbamoyltransferase regulatory chain



• Molecule 2: Aspartate carbamoyltransferase regulatory chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	120.69 Å 155.40 Å 194.96 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 42.82 – 2.86	Depositor EDS
% Data completeness (in resolution range)	72.5 (50.00-2.90) 70.5 (42.82-2.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.86 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.240 , 0.300 0.234 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	57.4	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22698	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: PO4, FLC, ZN

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	0.41	0/2461	0.75	3/3339 (0.1%)
1	B	0.38	0/2461	0.75	4/3339 (0.1%)
1	C	0.39	0/2461	0.72	4/3339 (0.1%)
1	D	0.37	0/2461	0.69	3/3339 (0.1%)
1	E	0.37	0/2461	0.69	3/3339 (0.1%)
1	F	0.34	0/2461	0.67	4/3339 (0.1%)
2	G	0.37	0/1219	0.66	0/1647
2	H	0.43	0/1219	0.79	0/1647
2	I	0.39	0/1219	0.70	0/1647
2	J	0.37	0/1219	0.73	1/1647 (0.1%)
2	K	0.39	0/1219	0.70	0/1647
2	L	0.39	0/1219	0.83	2/1647 (0.1%)
All	All	0.38	0/22080	0.72	24/29916 (0.1%)

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	267	LEU	N-CA-C	9.60	136.91	111.00
1	F	267	LEU	N-CA-C	9.08	135.52	111.00
1	A	267	LEU	N-CA-C	9.05	135.44	111.00
1	B	267	LEU	N-CA-C	8.47	133.88	111.00
1	C	266	PRO	N-CA-C	-8.28	90.57	112.10

There are no chirality outliers.

There are no planarity outliers.

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	2415	0	2422	155	0
1	B	2415	0	2422	162	0
1	C	2415	0	2422	166	0
1	D	2415	0	2422	175	0
1	E	2415	0	2422	150	0
1	F	2415	0	2422	167	0
2	G	1201	0	1219	159	0
2	H	1201	0	1219	143	0
2	I	1201	0	1219	161	0
2	J	1201	0	1219	141	0
2	K	1201	0	1219	135	0
2	L	1201	0	1219	216	0
3	A	13	0	5	7	0
3	B	13	0	5	4	0
3	C	13	0	5	4	0
3	D	13	0	5	7	0
3	E	13	0	5	4	0
3	F	13	0	5	1	0
4	A	5	0	0	5	0
4	B	5	0	0	1	0
4	C	5	0	0	0	0
4	D	5	0	0	1	0
4	E	5	0	0	1	0
4	F	5	0	0	2	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
6	A	84	0	0	1	0
6	B	95	0	0	3	0
6	C	113	0	0	4	0
6	D	102	0	0	2	0
6	E	86	0	0	3	0
6	F	82	0	0	8	0
6	G	65	0	0	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	59	0	0	4	0
6	I	45	0	0	5	0
6	J	51	0	0	0	0
6	K	51	0	0	4	0
6	L	55	0	0	2	0
All	All	22698	0	21876	1795	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 41.

The worst 5 of 1795 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:J:109:CYS:HB3	2:J:138:CYS:SG	1.64	1.36
1:F:114:LEU:HD22	2:L:115:ILE:CD1	1.62	1.28
2:L:21:ILE:O	2:L:21:ILE:HD12	1.35	1.25
2:J:114:CYS:SG	2:J:116:SER:HB3	1.81	1.20
2:L:21:ILE:HG22	2:L:56:LYS:HD3	1.25	1.19

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%)	260 (84%)	38 (12%)	10 (3%)	4	16
1	B	308/310 (99%)	257 (83%)	39 (13%)	12 (4%)	3	12
1	C	308/310 (99%)	260 (84%)	37 (12%)	11 (4%)	3	14
1	D	308/310 (99%)	265 (86%)	32 (10%)	11 (4%)	3	14
1	E	308/310 (99%)	262 (85%)	36 (12%)	10 (3%)	4	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	308/310 (99%)	263 (85%)	36 (12%)	9 (3%)	4	18
2	G	151/153 (99%)	105 (70%)	33 (22%)	13 (9%)	1	2
2	H	151/153 (99%)	104 (69%)	34 (22%)	13 (9%)	1	2
2	I	151/153 (99%)	112 (74%)	33 (22%)	6 (4%)	3	11
2	J	151/153 (99%)	104 (69%)	38 (25%)	9 (6%)	1	4
2	K	151/153 (99%)	125 (83%)	20 (13%)	6 (4%)	3	11
2	L	151/153 (99%)	94 (62%)	40 (26%)	17 (11%)	0	1
All	All	2754/2778 (99%)	2211 (80%)	416 (15%)	127 (5%)	2	9

5 of 127 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	30	LEU
1	A	133	GLN
1	A	243	VAL
1	B	131	SER

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%)	249 (95%)	12 (5%)	27	60
1	B	261/261 (100%)	249 (95%)	12 (5%)	27	60
1	C	261/261 (100%)	247 (95%)	14 (5%)	22	54
1	D	261/261 (100%)	253 (97%)	8 (3%)	40	74
1	E	261/261 (100%)	251 (96%)	10 (4%)	33	67
1	F	261/261 (100%)	248 (95%)	13 (5%)	24	57
2	G	137/137 (100%)	129 (94%)	8 (6%)	20	50
2	H	137/137 (100%)	126 (92%)	11 (8%)	12	33
2	I	137/137 (100%)	127 (93%)	10 (7%)	14	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	137/137 (100%)	126 (92%)	11 (8%)	12	33
2	K	137/137 (100%)	125 (91%)	12 (9%)	10	30
2	L	137/137 (100%)	128 (93%)	9 (7%)	16	44
All	All	2388/2388 (100%)	2258 (95%)	130 (5%)	22	54

5 of 130 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	52	GLU
1	D	285	TYR
2	K	149	VAL
2	I	76	LEU
2	I	147	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 88 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	147	HIS
1	D	305	ASN
2	K	20	HIS
1	D	13	ASN
1	D	64	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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	PO4	D	3004	-	4,4,4	1.92	1 (25%)	6,6,6	1.86	2 (33%)
3	FLC	B	2002	-	3,12,12	2.88	2 (66%)	3,17,17	1.21	0
3	FLC	F	2006	-	3,12,12	4.39	2 (66%)	3,17,17	2.69	1 (33%)
4	PO4	C	3003	-	4,4,4	2.20	1 (25%)	6,6,6	1.79	3 (50%)
3	FLC	E	2005	-	3,12,12	4.97	2 (66%)	3,17,17	2.02	1 (33%)
4	PO4	E	3005	-	4,4,4	2.10	1 (25%)	6,6,6	2.00	3 (50%)
4	PO4	B	3002	-	4,4,4	2.20	2 (50%)	6,6,6	2.06	2 (33%)
3	FLC	A	2001	-	3,12,12	5.10	2 (66%)	3,17,17	1.93	1 (33%)
3	FLC	D	2004	-	3,12,12	4.64	3 (100%)	3,17,17	2.00	1 (33%)
4	PO4	F	3006	-	4,4,4	2.06	1 (25%)	6,6,6	1.93	3 (50%)
4	PO4	A	3001	-	4,4,4	1.70	1 (25%)	6,6,6	2.22	4 (66%)
3	FLC	C	2003	-	3,12,12	4.50	2 (66%)	3,17,17	1.43	0

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
3	FLC	B	2002	-	-	4/6/16/16	-
3	FLC	F	2006	-	-	0/6/16/16	-
3	FLC	E	2005	-	-	4/6/16/16	-
3	FLC	A	2001	-	-	5/6/16/16	-
3	FLC	D	2004	-	-	3/6/16/16	-
3	FLC	C	2003	-	-	2/6/16/16	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2003	FLC	CG-CB	6.64	1.64	1.54
3	A	2001	FLC	CA-CB	6.41	1.63	1.54
3	E	2005	FLC	CA-CB	6.35	1.63	1.54
3	A	2001	FLC	CG-CB	5.86	1.63	1.54
3	E	2005	FLC	CG-CB	5.79	1.63	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2006	FLC	CB-CA-CAC	4.52	122.23	114.98
4	A	3001	PO4	O4-P-O1	-3.25	99.00	110.89
3	D	2004	FLC	CB-CA-CAC	3.22	120.14	114.98
3	E	2005	FLC	CB-CA-CAC	3.20	120.10	114.98
3	A	2001	FLC	CB-CA-CAC	3.09	119.93	114.98

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2002	FLC	CAC-CA-CB-CBC
3	B	2002	FLC	CAC-CA-CB-CG
3	B	2002	FLC	CAC-CA-CB-OHB
3	E	2005	FLC	CAC-CA-CB-CBC
3	E	2005	FLC	CAC-CA-CB-CG

There are no ring outliers.

11 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3004	PO4	1	0
3	B	2002	FLC	4	0
3	F	2006	FLC	1	0
3	E	2005	FLC	4	0
4	E	3005	PO4	1	0
4	B	3002	PO4	1	0
3	A	2001	FLC	7	0
3	D	2004	FLC	7	0
4	F	3006	PO4	2	0
4	A	3001	PO4	5	0
3	C	2003	FLC	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.36	1 (0%) 94 94	15, 42, 66, 78	0
1	B	310/310 (100%)	-0.13	3 (0%) 82 82	20, 60, 91, 113	0
1	C	310/310 (100%)	-0.30	1 (0%) 94 94	19, 46, 69, 97	0
1	D	310/310 (100%)	-0.19	3 (0%) 82 82	31, 59, 83, 109	0
1	E	310/310 (100%)	-0.19	2 (0%) 89 89	34, 54, 85, 103	0
1	F	310/310 (100%)	-0.12	5 (1%) 72 71	36, 66, 91, 118	0
2	G	153/153 (100%)	0.57	21 (13%) 3 2	45, 92, 161, 182	0
2	H	153/153 (100%)	0.05	9 (5%) 22 18	40, 63, 133, 171	0
2	I	153/153 (100%)	0.61	20 (13%) 3 2	57, 99, 144, 161	0
2	J	153/153 (100%)	0.60	16 (10%) 6 5	49, 89, 164, 192	0
2	K	153/153 (100%)	0.31	13 (8%) 10 8	34, 63, 149, 181	0
2	L	153/153 (100%)	1.08	31 (20%) 1 0	62, 126, 163, 170	0
All	All	2778/2778 (100%)	0.03	125 (4%) 33 29	15, 61, 130, 192	0

The worst 5 of 125 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	3	HIS	11.6
2	J	1	MET	10.7
2	G	1	MET	10.0
2	J	7	LEU	9.7
2	K	4	ASP	9.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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(\AA^2)	Q<0.9
5	ZN	J	1004	1/1	0.81	0.09	52,52,52,52	0
5	ZN	I	1003	1/1	0.87	0.17	67,67,67,67	0
3	FLC	D	2004	13/13	0.88	0.23	63,65,68,70	0
3	FLC	A	2001	13/13	0.91	0.23	34,48,52,55	0
3	FLC	C	2003	13/13	0.91	0.23	46,50,55,55	0
3	FLC	B	2002	13/13	0.92	0.26	65,68,69,71	0
3	FLC	E	2005	13/13	0.93	0.23	68,70,72,72	0
3	FLC	F	2006	13/13	0.93	0.24	61,64,67,68	0
5	ZN	K	1005	1/1	0.93	0.15	64,64,64,64	0
4	PO4	F	3006	5/5	0.96	0.22	49,49,51,51	0
4	PO4	E	3005	5/5	0.97	0.23	41,41,42,43	0
5	ZN	L	1006	1/1	0.97	0.14	63,63,63,63	0
4	PO4	A	3001	5/5	0.98	0.20	26,26,30,32	0
4	PO4	B	3002	5/5	0.98	0.28	37,37,40,41	0
4	PO4	C	3003	5/5	0.98	0.23	38,39,41,41	0
5	ZN	H	1002	1/1	0.99	0.14	56,56,56,56	0
5	ZN	G	1001	1/1	0.99	0.11	57,57,57,57	0
4	PO4	D	3004	5/5	0.99	0.19	29,30,33,34	0

6.5 Other polymers ⓘ

There are no such residues in this entry.