wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2023 – 02:46 AM EDT

PDB ID	:	3AB2
Title	:	Crystal structure of aspartate kinase from Corynebacterium glutamicum in complex with threonine
Authors	:	Yoshida, A.; Tomita, T.; Kuzuyama, T.; Nishiyama, M.
Deposited on	:	2009-11-30
Resolution	:	2.59 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 (i)) were used in the production of this report:

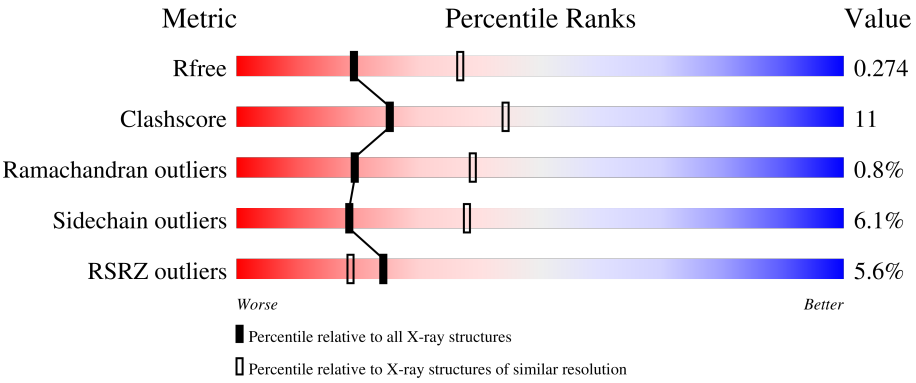
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.59 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))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	421	6% 69% 20% • 8%
1	C	421	4% 73% 15% • 10%
1	E	421	4% 70% 19% • 9%
1	G	421	6% 76% 14% • 9%
1	I	421	4% 70% 18% • 10%

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Mol	Chain	Length	Quality of chain
1	K	421	5% 71% 19% 9%
1	M	421	8% 71% 19% 10%
1	O	421	3% 69% 20% 8%
2	B	178	4% 71% 15% 10%
2	D	178	17% 61% 22% 15%
2	F	178	2% 75% 12% 13%
2	H	178	74% 12% 13%
2	J	178	11% 66% 18% 15%
2	L	178	3% 72% 12% 15%
2	N	178	2% 72% 14% 13%
2	P	178	% 69% 18% 11%

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	THR	A	501	-	-	X	-
3	THR	C	501	-	-	X	-
3	THR	D	501	-	-	X	-
3	THR	F	501	-	-	X	-
3	THR	G	501	-	-	X	-
3	THR	J	501	-	-	X	-
3	THR	K	501	-	-	X	-
3	THR	L	501	-	-	X	-
3	THR	P	501	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 31975 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 Aspartokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			2841	1761	492	574	14			
1	C	380	Total	C	N	O	S	0	0	0
			2793	1737	478	564	14			
1	E	383	Total	C	N	O	S	0	0	0
			2814	1749	484	567	14			
1	G	383	Total	C	N	O	S	0	0	0
			2803	1742	483	564	14			
1	I	377	Total	C	N	O	S	0	0	0
			2748	1711	469	554	14			
1	K	382	Total	C	N	O	S	0	0	0
			2793	1733	480	566	14			
1	M	380	Total	C	N	O	S	0	0	0
			2796	1738	482	562	14			
1	O	386	Total	C	N	O	S	0	0	0
			2851	1767	493	577	14			

- Molecule 2 is a protein called Aspartokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	160	Total	C	N	O	S	0	0	0
			1183	734	202	242	5			
2	D	152	Total	C	N	O	S	0	0	0
			1116	694	191	226	5			
2	F	155	Total	C	N	O	S	0	0	0
			1166	725	202	234	5			
2	H	155	Total	C	N	O	S	0	0	0
			1161	721	202	233	5			
2	J	152	Total	C	N	O	S	0	0	0
			1082	665	193	219	5			
2	L	152	Total	C	N	O	S	0	0	0
			1131	703	193	230	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	155	Total	C	N	O	S	0	0	0
			1135	707	196	227	5			
2	P	159	Total	C	N	O	S	0	0	0
			1196	741	207	243	5			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P26512
B	173	HIS	-	expression tag	UNP P26512
B	174	HIS	-	expression tag	UNP P26512
B	175	HIS	-	expression tag	UNP P26512
B	176	HIS	-	expression tag	UNP P26512
B	177	HIS	-	expression tag	UNP P26512
B	178	HIS	-	expression tag	UNP P26512
D	1	MET	-	initiating methionine	UNP P26512
D	173	HIS	-	expression tag	UNP P26512
D	174	HIS	-	expression tag	UNP P26512
D	175	HIS	-	expression tag	UNP P26512
D	176	HIS	-	expression tag	UNP P26512
D	177	HIS	-	expression tag	UNP P26512
D	178	HIS	-	expression tag	UNP P26512
F	1	MET	-	initiating methionine	UNP P26512
F	173	HIS	-	expression tag	UNP P26512
F	174	HIS	-	expression tag	UNP P26512
F	175	HIS	-	expression tag	UNP P26512
F	176	HIS	-	expression tag	UNP P26512
F	177	HIS	-	expression tag	UNP P26512
F	178	HIS	-	expression tag	UNP P26512
H	1	MET	-	initiating methionine	UNP P26512
H	173	HIS	-	expression tag	UNP P26512
H	174	HIS	-	expression tag	UNP P26512
H	175	HIS	-	expression tag	UNP P26512
H	176	HIS	-	expression tag	UNP P26512
H	177	HIS	-	expression tag	UNP P26512
H	178	HIS	-	expression tag	UNP P26512
J	1	MET	-	initiating methionine	UNP P26512
J	173	HIS	-	expression tag	UNP P26512
J	174	HIS	-	expression tag	UNP P26512
J	175	HIS	-	expression tag	UNP P26512
J	176	HIS	-	expression tag	UNP P26512
J	177	HIS	-	expression tag	UNP P26512

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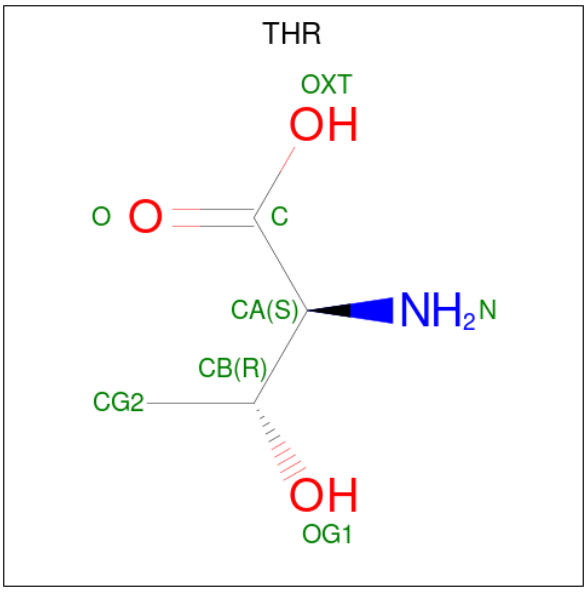
Chain	Residue	Modelled	Actual	Comment	Reference
J	178	HIS	-	expression tag	UNP P26512
L	1	MET	-	initiating methionine	UNP P26512
L	173	HIS	-	expression tag	UNP P26512
L	174	HIS	-	expression tag	UNP P26512
L	175	HIS	-	expression tag	UNP P26512
L	176	HIS	-	expression tag	UNP P26512
L	177	HIS	-	expression tag	UNP P26512
L	178	HIS	-	expression tag	UNP P26512
N	1	MET	-	initiating methionine	UNP P26512
N	173	HIS	-	expression tag	UNP P26512
N	174	HIS	-	expression tag	UNP P26512
N	175	HIS	-	expression tag	UNP P26512
N	176	HIS	-	expression tag	UNP P26512
N	177	HIS	-	expression tag	UNP P26512
N	178	HIS	-	expression tag	UNP P26512
P	1	MET	-	initiating methionine	UNP P26512
P	173	HIS	-	expression tag	UNP P26512
P	174	HIS	-	expression tag	UNP P26512
P	175	HIS	-	expression tag	UNP P26512
P	176	HIS	-	expression tag	UNP P26512
P	177	HIS	-	expression tag	UNP P26512
P	178	HIS	-	expression tag	UNP P26512

- Molecule 3 is THREONINE (three-letter code: THR) (formula: $C_4H_9NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	B	1	Total	C	N	O	0	0
			8	4	1	3		
3	C	1	Total	C	N	O	0	0
			8	4	1	3		
3	D	1	Total	C	N	O	0	0
			8	4	1	3		
3	E	1	Total	C	N	O	0	0
			8	4	1	3		
3	F	1	Total	C	N	O	0	0
			8	4	1	3		
3	G	1	Total	C	N	O	0	0
			8	4	1	3		
3	H	1	Total	C	N	O	0	0
			8	4	1	3		
3	J	1	Total	C	N	O	0	0
			8	4	1	3		
3	K	1	Total	C	N	O	0	0
			8	4	1	3		
3	L	1	Total	C	N	O	0	0
			8	4	1	3		
3	M	1	Total	C	N	O	0	0
			8	4	1	3		
3	N	1	Total	C	N	O	0	0
			8	4	1	3		
3	O	1	Total	C	N	O	0	0
			8	4	1	3		
3	P	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	36	Total	O	0	0
			36	36		
4	B	11	Total	O	0	0
			11	11		
4	C	18	Total	O	0	0
			18	18		
4	D	3	Total	O	0	0
			3	3		
4	E	23	Total	O	0	0
			23	23		

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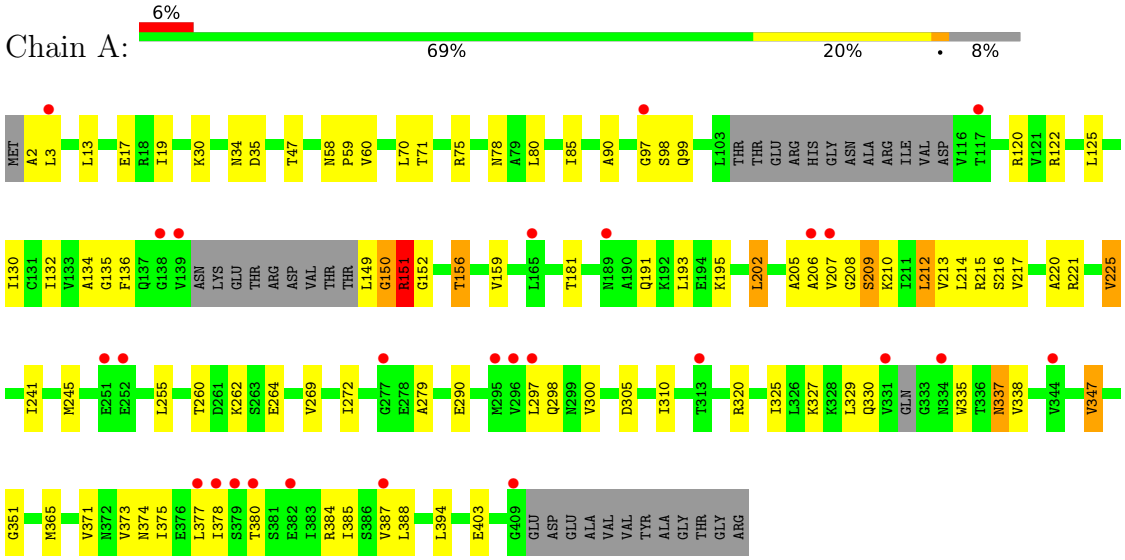
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	8	Total O 8 8	0	0
4	G	18	Total O 18 18	0	0
4	H	9	Total O 9 9	0	0
4	I	16	Total O 16 16	0	0
4	J	6	Total O 6 6	0	0
4	K	25	Total O 25 25	0	0
4	L	5	Total O 5 5	0	0
4	M	21	Total O 21 21	0	0
4	N	4	Total O 4 4	0	0
4	O	31	Total O 31 31	0	0
4	P	12	Total O 12 12	0	0

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 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.

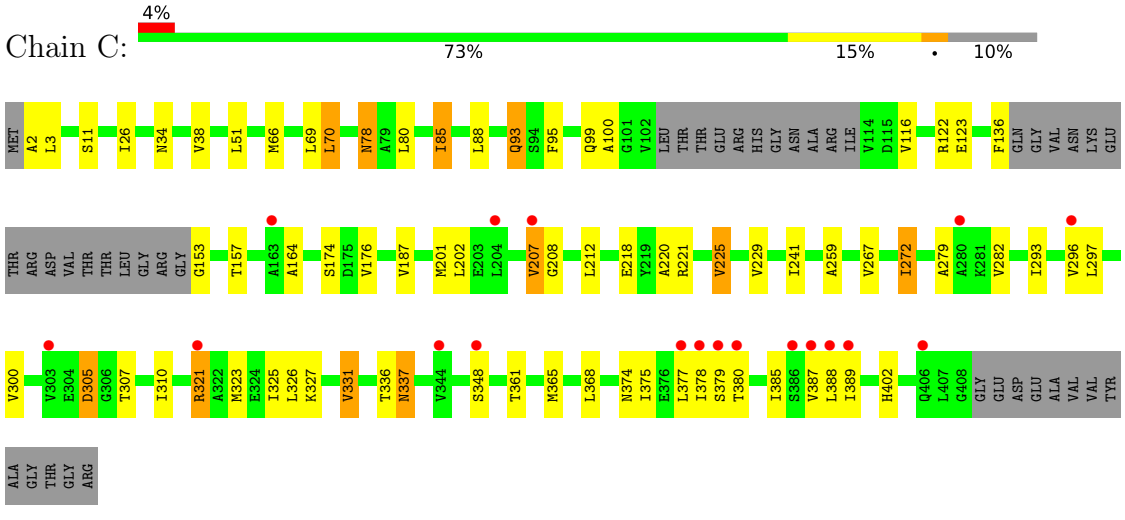
• Molecule 1: Aspartokinase

Chain A:



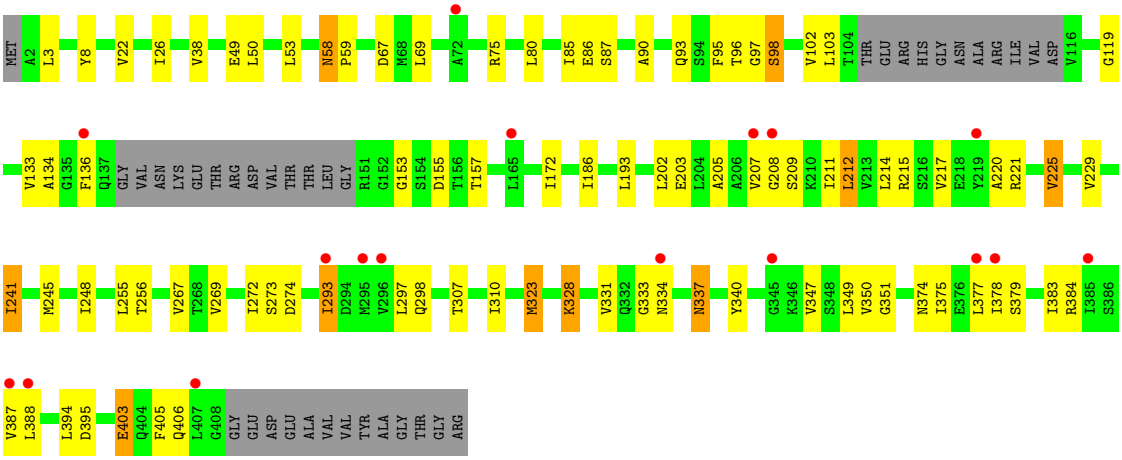
• Molecule 1: Aspartokinase

Chain C:



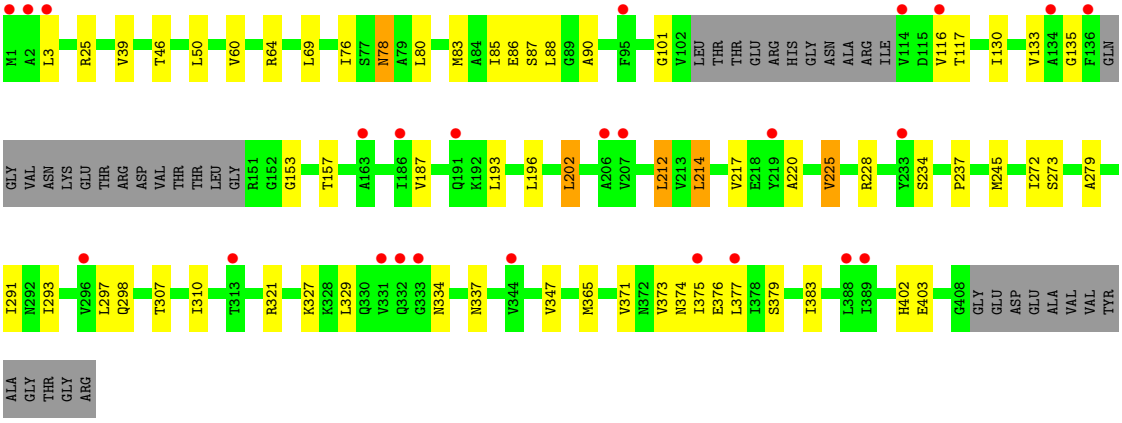
• Molecule 1: Aspartokinase

Chain E:



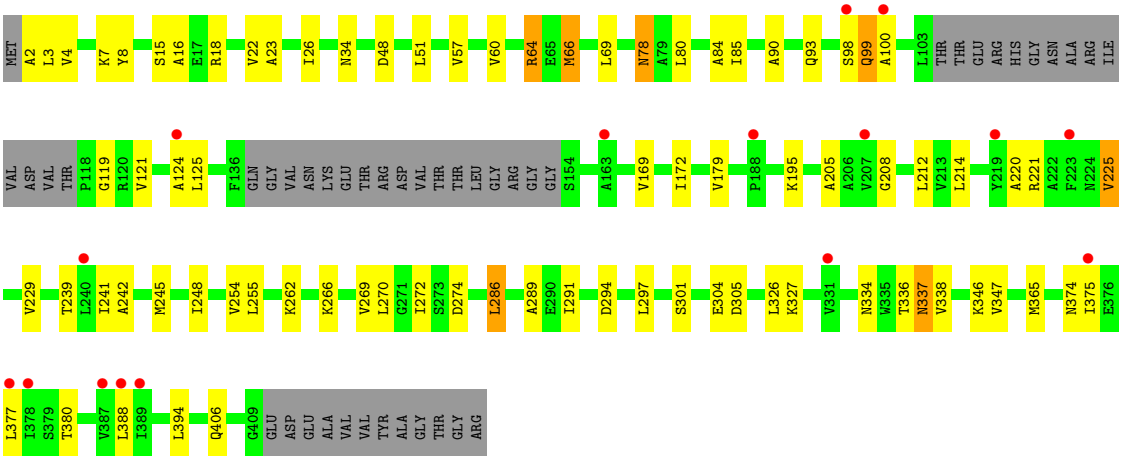
• Molecule 1: Aspartokinase

Chain G:



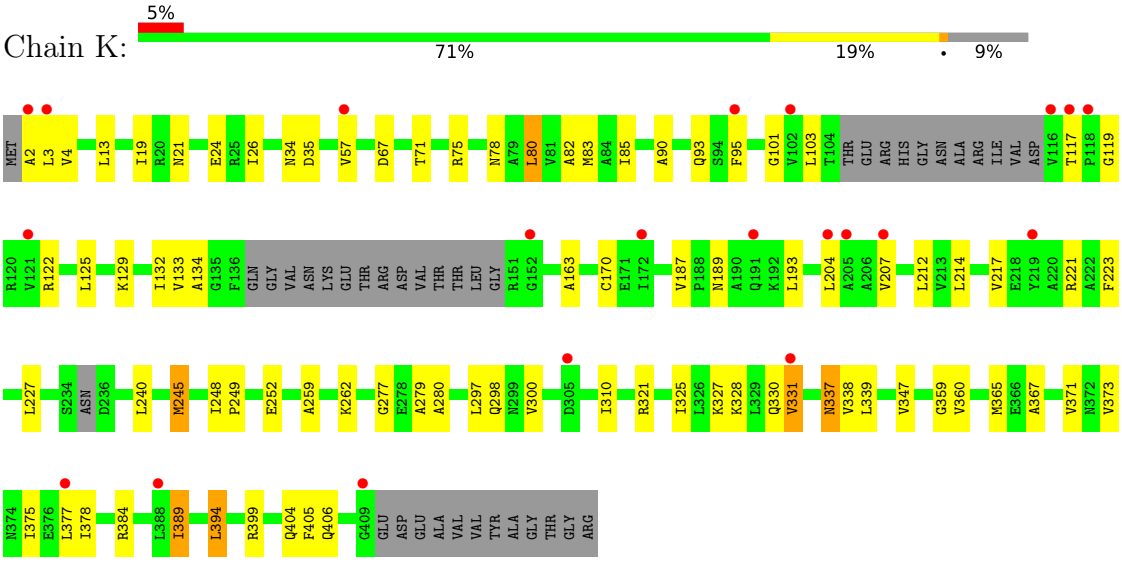
• Molecule 1: Aspartokinase

Chain I:



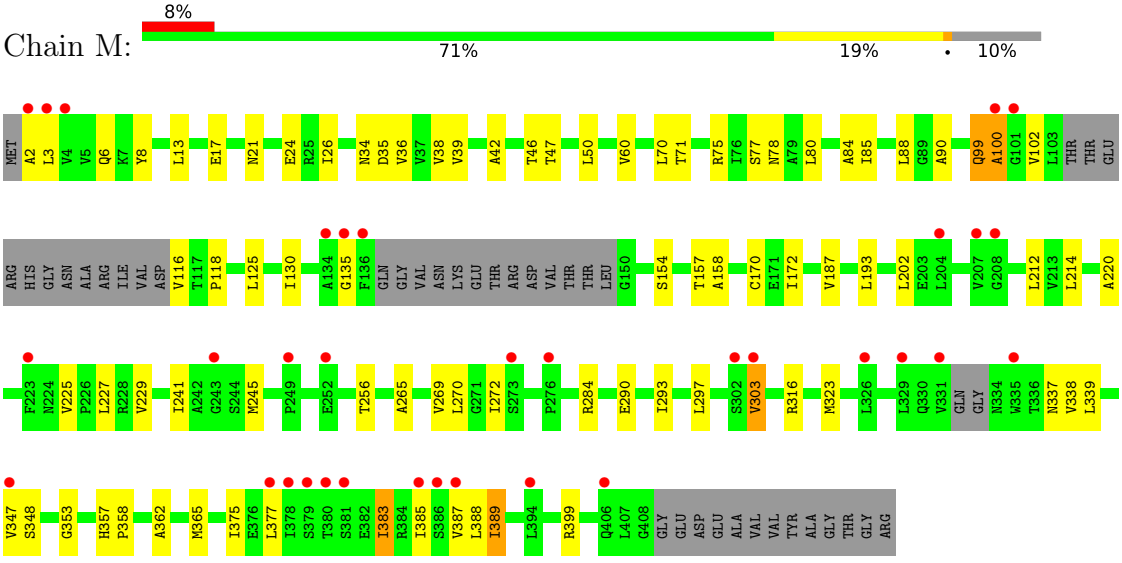
• Molecule 1: Aspartokinase

Chain K:



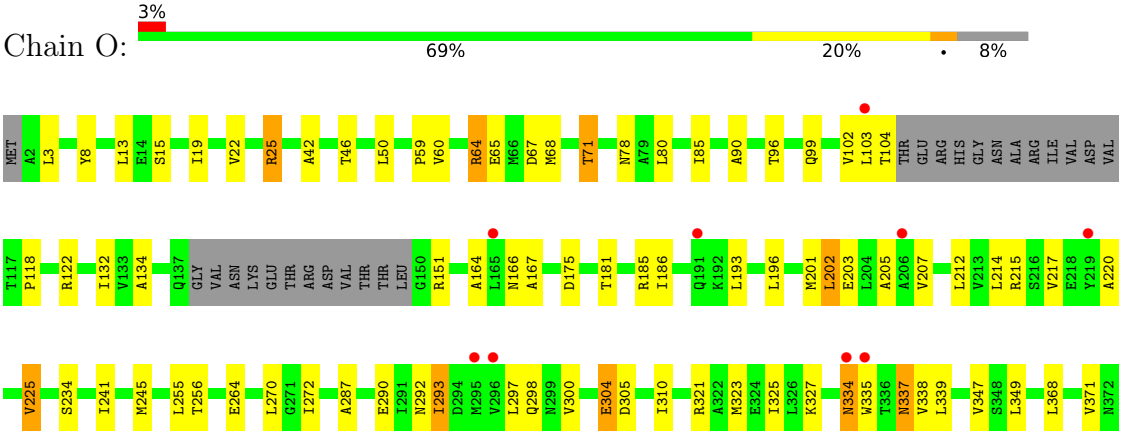
• Molecule 1: Aspartokinase

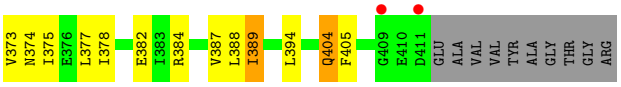
Chain M:



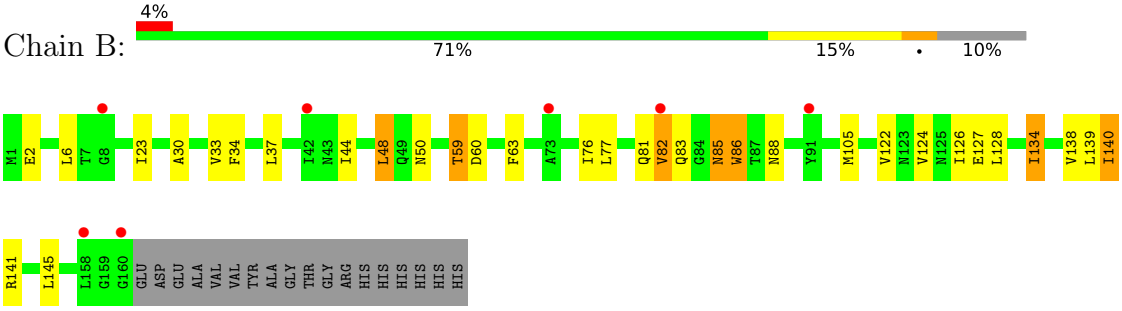
• Molecule 1: Aspartokinase

Chain O:

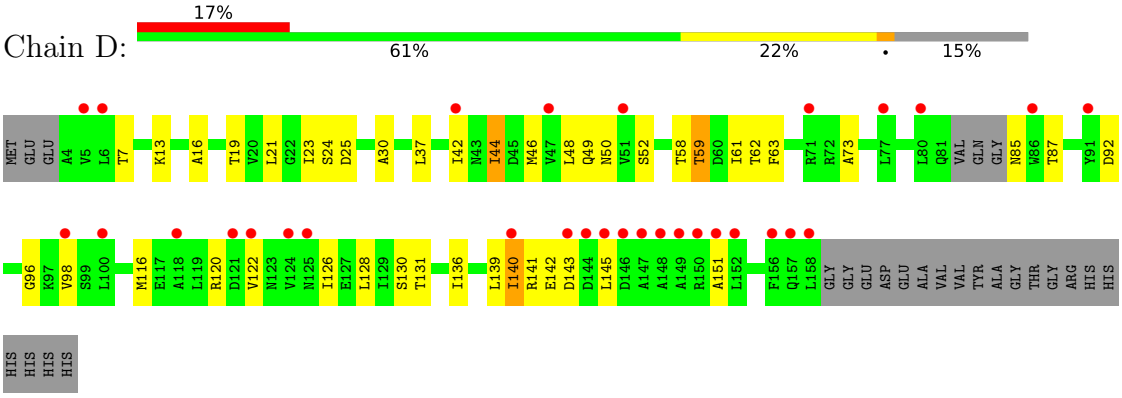




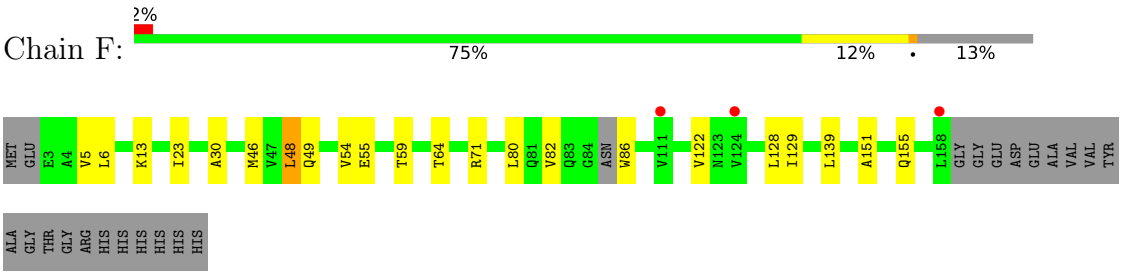
• Molecule 2: Aspartokinase



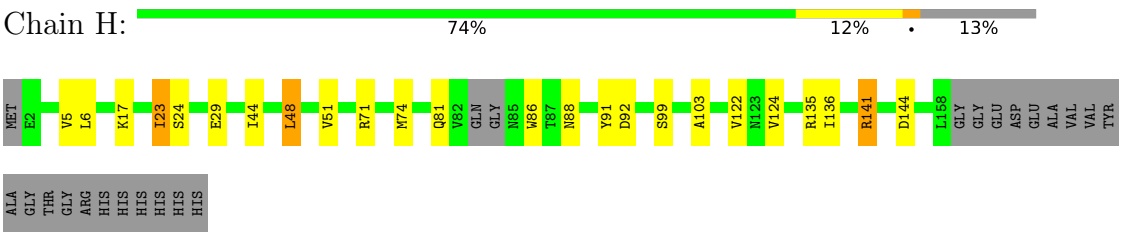
• Molecule 2: Aspartokinase



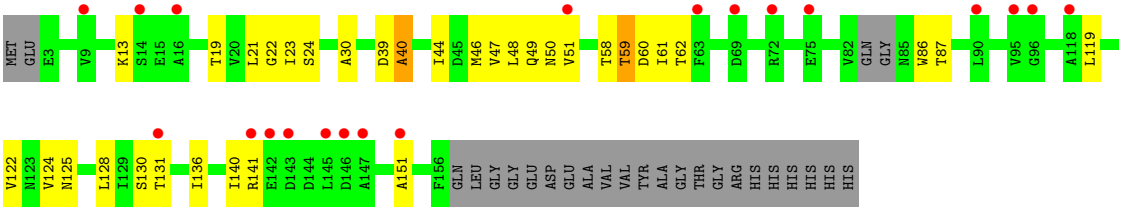
• Molecule 2: Aspartokinase



• Molecule 2: Aspartokinase

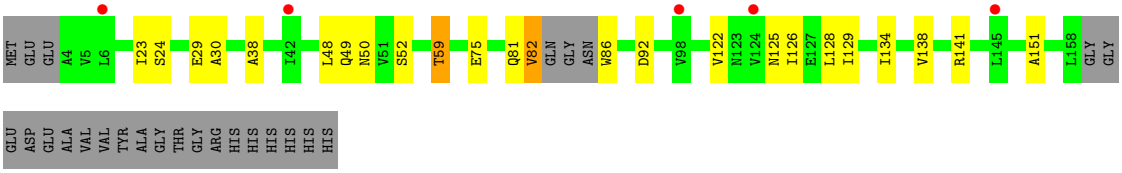


• Molecule 2: Aspartokinase



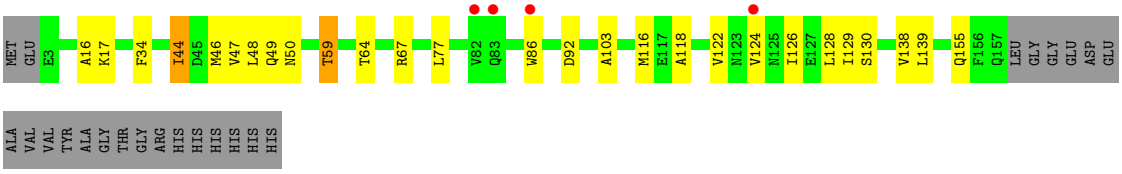
• Molecule 2: Aspartokinase

Chain L:



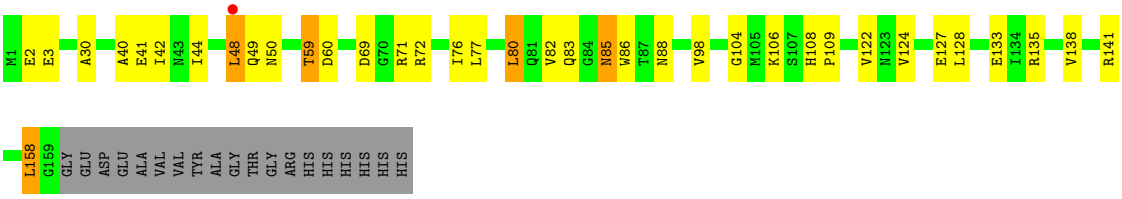
• Molecule 2: Aspartokinase

Chain N:



• Molecule 2: Aspartokinase

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	101.83Å 119.09Å 124.38Å 71.85° 69.48° 72.72°	Depositor
Resolution (Å)	42.04 – 2.59 42.04 – 2.59	Depositor EDS
% Data completeness (in resolution range)	97.1 (42.04-2.59) 97.1 (42.04-2.59)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.232 , 0.280 0.227 , 0.274	Depositor DCC
R_{free} test set	7701 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	66.5	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 56.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	31975	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.32	0/2867	0.53	0/3883
1	C	0.31	0/2820	0.50	0/3825
1	E	0.31	0/2841	0.50	0/3853
1	G	0.32	0/2830	0.52	0/3839
1	I	0.31	0/2774	0.50	0/3765
1	K	0.31	0/2818	0.49	0/3823
1	M	0.30	0/2822	0.49	0/3824
1	O	0.33	0/2878	0.52	0/3899
2	B	0.32	0/1194	0.52	0/1618
2	D	0.29	0/1125	0.49	0/1528
2	F	0.31	0/1176	0.51	0/1590
2	H	0.32	0/1171	0.53	0/1586
2	J	0.28	0/1090	0.46	0/1481
2	L	0.30	0/1141	0.47	0/1547
2	N	0.28	0/1146	0.45	0/1557
2	P	0.33	0/1207	0.56	0/1633
All	All	0.31	0/31900	0.50	0/43251

There are no bond length outliers.

There are no bond angle outliers.

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	2841	0	2834	72	0
1	C	2793	0	2791	60	0
1	E	2814	0	2809	62	0
1	G	2803	0	2793	48	0
1	I	2748	0	2735	66	0
1	K	2793	0	2773	67	0
1	M	2796	0	2799	66	0
1	O	2851	0	2852	82	0
2	B	1183	0	1169	27	0
2	D	1116	0	1094	39	0
2	F	1166	0	1169	18	0
2	H	1161	0	1155	22	0
2	J	1082	0	1027	33	0
2	L	1131	0	1114	22	0
2	N	1135	0	1117	22	0
2	P	1196	0	1194	29	0
3	A	8	0	6	7	0
3	B	8	0	6	1	0
3	C	8	0	6	4	0
3	D	8	0	6	7	0
3	E	8	0	6	1	0
3	F	8	0	6	6	0
3	G	8	0	6	5	0
3	H	8	0	6	3	0
3	J	8	0	6	6	0
3	K	8	0	6	6	0
3	L	8	0	6	4	0
3	M	8	0	6	0	0
3	N	8	0	6	0	0
3	O	8	0	6	0	0
3	P	8	0	6	5	0
4	A	36	0	0	1	0
4	B	11	0	0	0	0
4	C	18	0	0	1	0
4	D	3	0	0	0	0
4	E	23	0	0	0	0
4	F	8	0	0	0	0
4	G	18	0	0	0	0
4	H	9	0	0	0	0
4	I	16	0	0	1	0
4	J	6	0	0	0	0
4	K	25	0	0	0	0
4	L	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	21	0	0	0	0
4	N	4	0	0	0	0
4	O	31	0	0	0	0
4	P	12	0	0	0	0
All	All	31975	0	31515	678	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 11.

The worst 5 of 678 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:L:30:ALA:HB2	3:L:501:THR:HG23	1.26	1.14
2:B:48:LEU:HD11	2:B:128:LEU:HD23	1.30	1.12
1:C:297:LEU:HD13	1:C:377:LEU:HD21	1.31	1.10
2:H:23:ILE:HD11	3:H:501:THR:HG22	1.30	1.10
1:K:279:ALA:HB2	3:K:501:THR:HG22	1.32	1.08

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	378/421 (90%)	356 (94%)	16 (4%)	6 (2%)	9 19
1	C	374/421 (89%)	357 (96%)	15 (4%)	2 (0%)	29 52
1	E	377/421 (90%)	355 (94%)	16 (4%)	6 (2%)	9 19
1	G	377/421 (90%)	356 (94%)	20 (5%)	1 (0%)	41 64
1	I	371/421 (88%)	353 (95%)	14 (4%)	4 (1%)	14 30
1	K	374/421 (89%)	361 (96%)	10 (3%)	3 (1%)	19 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	M	372/421 (88%)	353 (95%)	15 (4%)	4 (1%)	14 30
1	O	380/421 (90%)	369 (97%)	9 (2%)	2 (0%)	29 52
2	B	158/178 (89%)	151 (96%)	6 (4%)	1 (1%)	25 47
2	D	148/178 (83%)	141 (95%)	7 (5%)	0	100 100
2	F	151/178 (85%)	143 (95%)	7 (5%)	1 (1%)	22 43
2	H	151/178 (85%)	149 (99%)	2 (1%)	0	100 100
2	J	148/178 (83%)	136 (92%)	11 (7%)	1 (1%)	22 43
2	L	148/178 (83%)	143 (97%)	5 (3%)	0	100 100
2	N	153/178 (86%)	145 (95%)	8 (5%)	0	100 100
2	P	157/178 (88%)	151 (96%)	3 (2%)	3 (2%)	8 15
All	All	4217/4792 (88%)	4019 (95%)	164 (4%)	34 (1%)	19 39

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	SER
1	A	151	ARG
1	A	209	SER
2	B	82	VAL
1	E	98	SER

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	300/336 (89%)	277 (92%)	23 (8%)	13 25
1	C	296/336 (88%)	276 (93%)	20 (7%)	16 32
1	E	297/336 (88%)	278 (94%)	19 (6%)	17 35
1	G	294/336 (88%)	278 (95%)	16 (5%)	22 44
1	I	288/336 (86%)	274 (95%)	14 (5%)	25 48
1	K	293/336 (87%)	278 (95%)	15 (5%)	24 46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	M	296/336 (88%)	283 (96%)	13 (4%)	28 53
1	O	303/336 (90%)	280 (92%)	23 (8%)	13 26
2	B	126/146 (86%)	113 (90%)	13 (10%)	7 13
2	D	117/146 (80%)	109 (93%)	8 (7%)	16 32
2	F	126/146 (86%)	119 (94%)	7 (6%)	21 42
2	H	125/146 (86%)	118 (94%)	7 (6%)	21 42
2	J	108/146 (74%)	104 (96%)	4 (4%)	34 60
2	L	121/146 (83%)	117 (97%)	4 (3%)	38 64
2	N	119/146 (82%)	115 (97%)	4 (3%)	37 63
2	P	129/146 (88%)	117 (91%)	12 (9%)	9 17
All	All	3338/3856 (87%)	3136 (94%)	202 (6%)	18 38

5 of 202 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	64	ARG
1	K	389	ILE
2	P	135	ARG
1	I	221	ARG
2	J	86	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	21	ASN
1	M	343	GLN
1	K	292	ASN
1	K	406	GLN
1	O	34	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

15 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
3	THR	F	501	-	6,7,7	1.04	1 (16%)	7,9,9	1.42	1 (14%)
3	THR	J	501	-	6,7,7	0.91	1 (16%)	7,9,9	1.27	1 (14%)
3	THR	O	501	-	6,7,7	0.95	1 (16%)	7,9,9	1.28	2 (28%)
3	THR	C	501	-	6,7,7	0.99	1 (16%)	7,9,9	1.34	1 (14%)
3	THR	K	501	-	6,7,7	0.97	1 (16%)	7,9,9	1.23	1 (14%)
3	THR	D	501	-	6,7,7	0.96	1 (16%)	7,9,9	1.23	1 (14%)
3	THR	A	501	-	6,7,7	0.96	1 (16%)	7,9,9	1.31	1 (14%)
3	THR	N	501	-	6,7,7	0.96	1 (16%)	7,9,9	1.27	1 (14%)
3	THR	P	501	-	6,7,7	0.98	1 (16%)	7,9,9	1.37	2 (28%)
3	THR	G	501	-	6,7,7	1.02	1 (16%)	7,9,9	1.33	1 (14%)
3	THR	M	501	-	6,7,7	0.94	1 (16%)	7,9,9	1.41	1 (14%)
3	THR	L	501	-	6,7,7	0.95	1 (16%)	7,9,9	1.15	1 (14%)
3	THR	B	501	-	6,7,7	0.98	1 (16%)	7,9,9	1.41	2 (28%)
3	THR	H	501	-	6,7,7	0.91	1 (16%)	7,9,9	1.26	1 (14%)
3	THR	E	501	-	6,7,7	0.89	1 (16%)	7,9,9	1.44	2 (28%)

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	THR	F	501	-	-	4/8/8/8	-
3	THR	J	501	-	-	1/8/8/8	-
3	THR	O	501	-	-	0/8/8/8	-
3	THR	C	501	-	-	1/8/8/8	-
3	THR	K	501	-	-	0/8/8/8	-
3	THR	D	501	-	-	4/8/8/8	-
3	THR	A	501	-	-	3/8/8/8	-
3	THR	N	501	-	-	0/8/8/8	-
3	THR	P	501	-	-	4/8/8/8	-
3	THR	G	501	-	-	6/8/8/8	-
3	THR	M	501	-	-	0/8/8/8	-
3	THR	L	501	-	-	4/8/8/8	-
3	THR	B	501	-	-	0/8/8/8	-
3	THR	H	501	-	-	0/8/8/8	-
3	THR	E	501	-	-	0/8/8/8	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	501	THR	OXT-C	-2.31	1.23	1.30
3	C	501	THR	OXT-C	-2.24	1.23	1.30
3	G	501	THR	OXT-C	-2.23	1.23	1.30
3	K	501	THR	OXT-C	-2.18	1.23	1.30
3	P	501	THR	OXT-C	-2.17	1.23	1.30

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	501	THR	OXT-C-O	-3.13	116.98	124.09
3	M	501	THR	OXT-C-O	-3.04	117.19	124.09
3	C	501	THR	OXT-C-O	-2.92	117.47	124.09
3	B	501	THR	OXT-C-O	-2.91	117.49	124.09
3	G	501	THR	OXT-C-O	-2.90	117.50	124.09

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	THR	C-CA-CB-OG1

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Mol	Chain	Res	Type	Atoms
3	D	501	THR	N-CA-CB-OG1
3	D	501	THR	C-CA-CB-OG1
3	D	501	THR	C-CA-CB-CG2
3	F	501	THR	N-CA-CB-OG1

There are no ring outliers.

12 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	501	THR	6	0
3	J	501	THR	6	0
3	C	501	THR	4	0
3	K	501	THR	6	0
3	D	501	THR	7	0
3	A	501	THR	7	0
3	P	501	THR	5	0
3	G	501	THR	5	0
3	L	501	THR	4	0
3	B	501	THR	1	0
3	H	501	THR	3	0
3	E	501	THR	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	386/421 (91%)	0.36	26 (6%) 17 13	43, 56, 73, 82	1 (0%)
1	C	380/421 (90%)	0.29	18 (4%) 31 25	43, 61, 86, 96	0
1	E	383/421 (90%)	0.35	17 (4%) 34 27	42, 58, 76, 94	0
1	G	383/421 (90%)	0.35	25 (6%) 18 14	38, 56, 73, 83	0
1	I	377/421 (89%)	0.32	16 (4%) 36 29	50, 69, 90, 98	0
1	K	382/421 (90%)	0.35	21 (5%) 25 19	42, 62, 79, 93	0
1	M	380/421 (90%)	0.45	34 (8%) 9 6	48, 65, 79, 88	0
1	O	386/421 (91%)	0.17	11 (2%) 53 46	37, 50, 69, 82	0
2	B	160/178 (89%)	0.29	7 (4%) 34 27	46, 61, 79, 89	0
2	D	152/178 (85%)	0.98	31 (20%) 1 0	60, 79, 103, 111	0
2	F	155/178 (87%)	0.16	3 (1%) 66 62	43, 59, 79, 87	0
2	H	155/178 (87%)	0.02	0 100 100	34, 50, 73, 83	0
2	J	152/178 (85%)	0.80	20 (13%) 3 2	60, 85, 103, 108	0
2	L	152/178 (85%)	0.27	5 (3%) 46 39	48, 68, 90, 96	0
2	N	155/178 (87%)	0.33	4 (2%) 56 50	59, 75, 93, 104	0
2	P	159/178 (89%)	-0.00	1 (0%) 89 88	36, 47, 66, 72	0
All	All	4297/4792 (89%)	0.34	239 (5%) 24 19	34, 61, 87, 111	1 (0%)

The worst 5 of 239 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	116	VAL	7.1
2	N	82	VAL	6.4
1	A	409	GLY	6.1
1	M	303	VAL	5.9
1	G	114	VAL	5.9

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	THR	M	501	8/8	0.89	0.18	39,39,39,39	0
3	THR	E	501	8/8	0.94	0.12	40,40,41,41	0
3	THR	J	501	8/8	0.94	0.21	51,51,51,51	0
3	THR	L	501	8/8	0.94	0.16	51,52,52,52	0
3	THR	D	501	8/8	0.94	0.12	35,35,35,35	0
3	THR	C	501	8/8	0.95	0.12	71,71,71,71	0
3	THR	K	501	8/8	0.95	0.17	50,50,50,50	0
3	THR	N	501	8/8	0.95	0.14	38,38,38,38	0
3	THR	P	501	8/8	0.95	0.12	35,36,36,36	0
3	THR	F	501	8/8	0.96	0.15	28,28,28,28	0
3	THR	H	501	8/8	0.96	0.14	37,37,37,38	0
3	THR	B	501	8/8	0.97	0.12	38,39,39,39	0
3	THR	G	501	8/8	0.97	0.10	29,30,30,30	0
3	THR	A	501	8/8	0.97	0.09	40,40,40,40	0
3	THR	O	501	8/8	0.99	0.08	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.