wwPDB X-ray Structure Validation Summary Report (i)

Jan 30, 2021 – 10:35 PM EST

PDB ID	:	3TVI
Title	:	Crystal structure of Clostridium acetobutylicum aspartate kinase (CaAK): An important allosteric enzyme for industrial amino acids production
Authors	:	Manjasetty, B.A.; Chance, M.R.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2011-09-20
Resolution	:	3.00 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 following versions of software and data (see references (1)) were used in the production of this report:

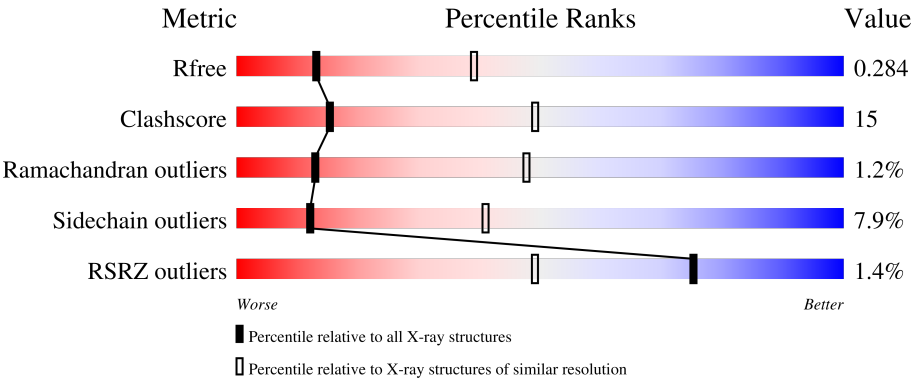
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	446	69% 26%
1	B	446	72% 23%
1	C	446	72% 22%
1	D	446	70% 25%
1	E	446	67% 28%

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Mol	Chain	Length	Quality of chain
1	F	446	70% 24%
1	G	446	66% 28%
1	H	446	67% 26%
1	I	446	2% 68% 26%
1	J	446	% 70% 23%
1	K	446	4% 66% 27%
1	L	446	7% 69% 26%

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
2	ASP	A	451	-	-	-	X
2	ASP	G	457	-	-	-	X
2	ASP	H	458	-	-	-	X
2	ASP	L	462	-	-	-	X
3	LYS	A	501	-	-	-	X
3	LYS	C	503	-	-	-	X
3	LYS	D	504	-	-	-	X
3	LYS	G	507	-	-	X	X
3	LYS	H	508	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 39043 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	429	Total	C	N	O	S	Se	0	0	0
			3228	2045	530	638	7	8			
1	B	438	Total	C	N	O	S	Se	0	0	0
			3304	2104	538	647	7	8			
1	C	433	Total	C	N	O	S	Se	0	0	0
			3271	2078	536	643	7	7			
1	D	437	Total	C	N	O	S	Se	0	0	0
			3296	2093	539	649	7	8			
1	E	439	Total	C	N	O	S	Se	0	0	0
			3293	2091	539	648	7	8			
1	F	434	Total	C	N	O	S	Se	0	0	0
			3267	2073	533	647	7	7			
1	G	436	Total	C	N	O	S	Se	0	1	0
			3288	2089	537	648	7	7			
1	H	435	Total	C	N	O	S	Se	0	0	0
			3217	2041	524	638	6	8			
1	I	428	Total	C	N	O	S	Se	0	0	0
			3191	2024	521	633	6	7			
1	J	433	Total	C	N	O	S	Se	0	0	0
			3204	2032	525	633	6	8			
1	K	429	Total	C	N	O	S	Se	0	0	0
			3170	2005	518	633	6	8			
1	L	428	Total	C	N	O	S	Se	0	0	0
			3192	2021	522	636	6	7			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q97MC0
A	1	LEU	-	expression tag	UNP Q97MC0
A	438	GLU	-	expression tag	UNP Q97MC0
A	439	GLY	-	expression tag	UNP Q97MC0
A	440	HIS	-	expression tag	UNP Q97MC0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	441	HIS	-	expression tag	UNP Q97MC0
A	442	HIS	-	expression tag	UNP Q97MC0
A	443	HIS	-	expression tag	UNP Q97MC0
A	444	HIS	-	expression tag	UNP Q97MC0
A	445	HIS	-	expression tag	UNP Q97MC0
B	0	SER	-	expression tag	UNP Q97MC0
B	1	LEU	-	expression tag	UNP Q97MC0
B	438	GLU	-	expression tag	UNP Q97MC0
B	439	GLY	-	expression tag	UNP Q97MC0
B	440	HIS	-	expression tag	UNP Q97MC0
B	441	HIS	-	expression tag	UNP Q97MC0
B	442	HIS	-	expression tag	UNP Q97MC0
B	443	HIS	-	expression tag	UNP Q97MC0
B	444	HIS	-	expression tag	UNP Q97MC0
B	445	HIS	-	expression tag	UNP Q97MC0
C	0	SER	-	expression tag	UNP Q97MC0
C	1	LEU	-	expression tag	UNP Q97MC0
C	438	GLU	-	expression tag	UNP Q97MC0
C	439	GLY	-	expression tag	UNP Q97MC0
C	440	HIS	-	expression tag	UNP Q97MC0
C	441	HIS	-	expression tag	UNP Q97MC0
C	442	HIS	-	expression tag	UNP Q97MC0
C	443	HIS	-	expression tag	UNP Q97MC0
C	444	HIS	-	expression tag	UNP Q97MC0
C	445	HIS	-	expression tag	UNP Q97MC0
D	0	SER	-	expression tag	UNP Q97MC0
D	1	LEU	-	expression tag	UNP Q97MC0
D	438	GLU	-	expression tag	UNP Q97MC0
D	439	GLY	-	expression tag	UNP Q97MC0
D	440	HIS	-	expression tag	UNP Q97MC0
D	441	HIS	-	expression tag	UNP Q97MC0
D	442	HIS	-	expression tag	UNP Q97MC0
D	443	HIS	-	expression tag	UNP Q97MC0
D	444	HIS	-	expression tag	UNP Q97MC0
D	445	HIS	-	expression tag	UNP Q97MC0
E	0	SER	-	expression tag	UNP Q97MC0
E	1	LEU	-	expression tag	UNP Q97MC0
E	438	GLU	-	expression tag	UNP Q97MC0
E	439	GLY	-	expression tag	UNP Q97MC0
E	440	HIS	-	expression tag	UNP Q97MC0
E	441	HIS	-	expression tag	UNP Q97MC0
E	442	HIS	-	expression tag	UNP Q97MC0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	443	HIS	-	expression tag	UNP Q97MC0
E	444	HIS	-	expression tag	UNP Q97MC0
E	445	HIS	-	expression tag	UNP Q97MC0
F	0	SER	-	expression tag	UNP Q97MC0
F	1	LEU	-	expression tag	UNP Q97MC0
F	438	GLU	-	expression tag	UNP Q97MC0
F	439	GLY	-	expression tag	UNP Q97MC0
F	440	HIS	-	expression tag	UNP Q97MC0
F	441	HIS	-	expression tag	UNP Q97MC0
F	442	HIS	-	expression tag	UNP Q97MC0
F	443	HIS	-	expression tag	UNP Q97MC0
F	444	HIS	-	expression tag	UNP Q97MC0
F	445	HIS	-	expression tag	UNP Q97MC0
G	0	SER	-	expression tag	UNP Q97MC0
G	1	LEU	-	expression tag	UNP Q97MC0
G	438	GLU	-	expression tag	UNP Q97MC0
G	439	GLY	-	expression tag	UNP Q97MC0
G	440	HIS	-	expression tag	UNP Q97MC0
G	441	HIS	-	expression tag	UNP Q97MC0
G	442	HIS	-	expression tag	UNP Q97MC0
G	443	HIS	-	expression tag	UNP Q97MC0
G	444	HIS	-	expression tag	UNP Q97MC0
G	445	HIS	-	expression tag	UNP Q97MC0
H	0	SER	-	expression tag	UNP Q97MC0
H	1	LEU	-	expression tag	UNP Q97MC0
H	438	GLU	-	expression tag	UNP Q97MC0
H	439	GLY	-	expression tag	UNP Q97MC0
H	440	HIS	-	expression tag	UNP Q97MC0
H	441	HIS	-	expression tag	UNP Q97MC0
H	442	HIS	-	expression tag	UNP Q97MC0
H	443	HIS	-	expression tag	UNP Q97MC0
H	444	HIS	-	expression tag	UNP Q97MC0
H	445	HIS	-	expression tag	UNP Q97MC0
I	0	SER	-	expression tag	UNP Q97MC0
I	1	LEU	-	expression tag	UNP Q97MC0
I	438	GLU	-	expression tag	UNP Q97MC0
I	439	GLY	-	expression tag	UNP Q97MC0
I	440	HIS	-	expression tag	UNP Q97MC0
I	441	HIS	-	expression tag	UNP Q97MC0
I	442	HIS	-	expression tag	UNP Q97MC0
I	443	HIS	-	expression tag	UNP Q97MC0
I	444	HIS	-	expression tag	UNP Q97MC0

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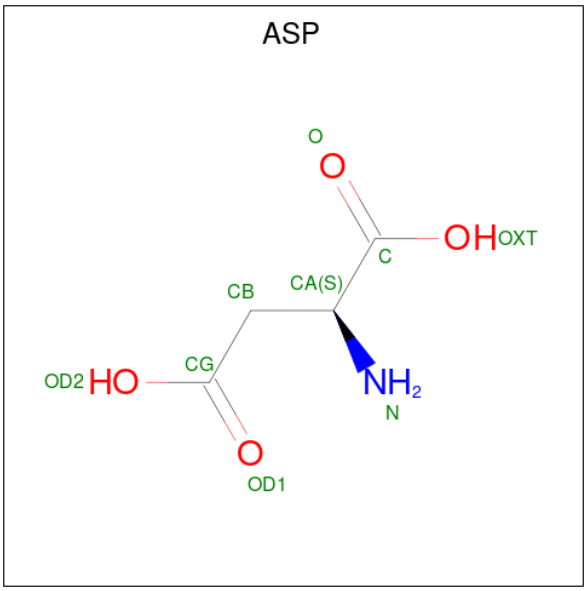
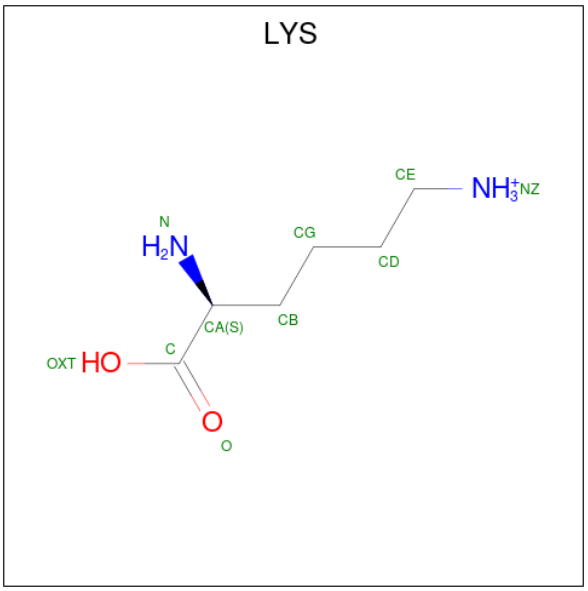
Chain	Residue	Modelled	Actual	Comment	Reference
I	445	HIS	-	expression tag	UNP Q97MC0
J	0	SER	-	expression tag	UNP Q97MC0
J	1	LEU	-	expression tag	UNP Q97MC0
J	438	GLU	-	expression tag	UNP Q97MC0
J	439	GLY	-	expression tag	UNP Q97MC0
J	440	HIS	-	expression tag	UNP Q97MC0
J	441	HIS	-	expression tag	UNP Q97MC0
J	442	HIS	-	expression tag	UNP Q97MC0
J	443	HIS	-	expression tag	UNP Q97MC0
J	444	HIS	-	expression tag	UNP Q97MC0
J	445	HIS	-	expression tag	UNP Q97MC0
K	0	SER	-	expression tag	UNP Q97MC0
K	1	LEU	-	expression tag	UNP Q97MC0
K	438	GLU	-	expression tag	UNP Q97MC0
K	439	GLY	-	expression tag	UNP Q97MC0
K	440	HIS	-	expression tag	UNP Q97MC0
K	441	HIS	-	expression tag	UNP Q97MC0
K	442	HIS	-	expression tag	UNP Q97MC0
K	443	HIS	-	expression tag	UNP Q97MC0
K	444	HIS	-	expression tag	UNP Q97MC0
K	445	HIS	-	expression tag	UNP Q97MC0
L	0	SER	-	expression tag	UNP Q97MC0
L	1	LEU	-	expression tag	UNP Q97MC0
L	438	GLU	-	expression tag	UNP Q97MC0
L	439	GLY	-	expression tag	UNP Q97MC0
L	440	HIS	-	expression tag	UNP Q97MC0
L	441	HIS	-	expression tag	UNP Q97MC0
L	442	HIS	-	expression tag	UNP Q97MC0
L	443	HIS	-	expression tag	UNP Q97MC0
L	444	HIS	-	expression tag	UNP Q97MC0
L	445	HIS	-	expression tag	UNP Q97MC0

- Molecule 2 is ASPARTIC ACID (three-letter code: ASP) (formula: $C_4H_7NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 9 4 1 4	0	0
2	D	1	Total C N O 9 4 1 4	0	0
2	E	1	Total C N O 9 4 1 4	0	0
2	G	1	Total C N O 9 4 1 4	0	0
2	H	1	Total C N O 9 4 1 4	0	0
2	I	1	Total C N O 8 4 1 3	0	0
2	L	1	Total C N O 9 4 1 4	0	0

- Molecule 3 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



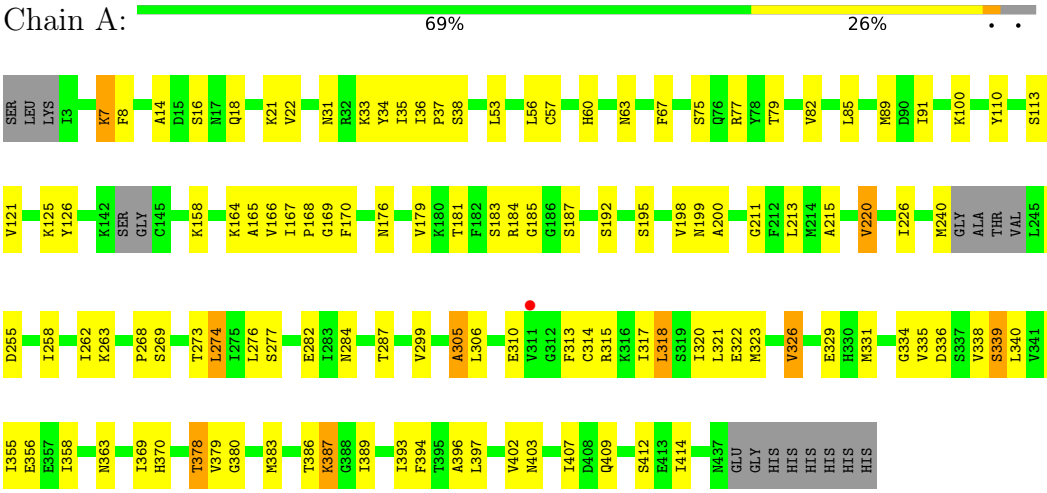
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 10 6 2 2	0	0
3	B	1	Total C N O 10 6 2 2	0	0
3	C	1	Total C N O 10 6 2 2	0	0
3	D	1	Total C N O 10 6 2 2	0	0
3	G	1	Total C N O 10 6 2 2	0	0
3	H	1	Total C N O 10 6 2 2	0	0

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.

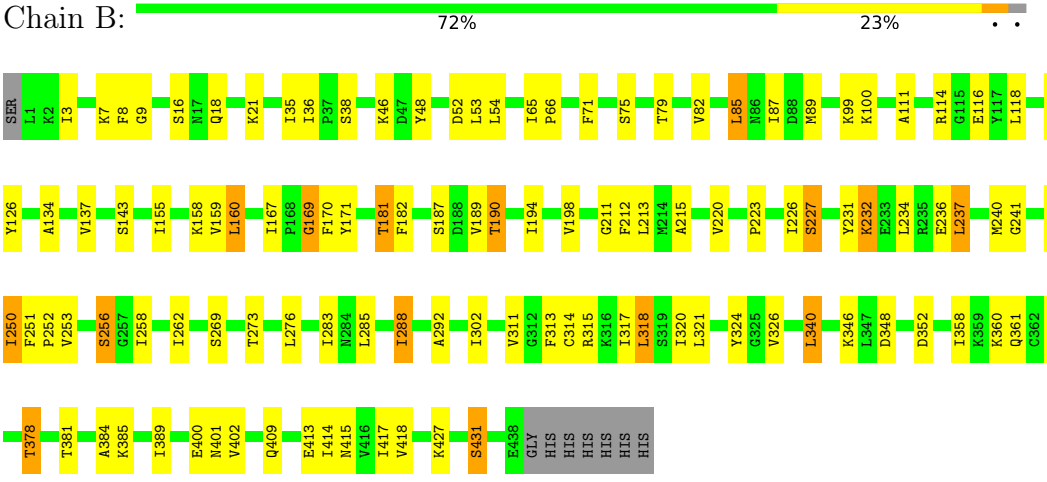
- Molecule 1: Aspartokinase

Chain A:



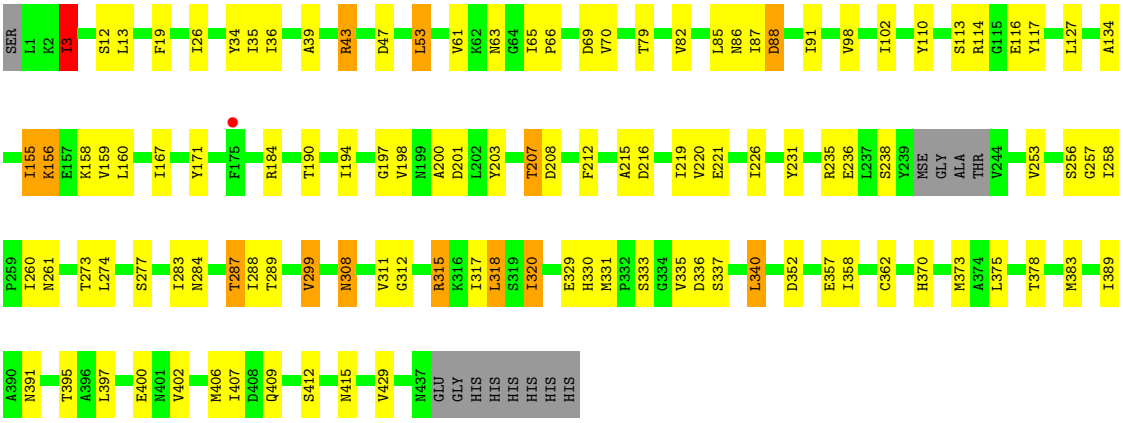
- Molecule 1: Aspartokinase

Chain B:



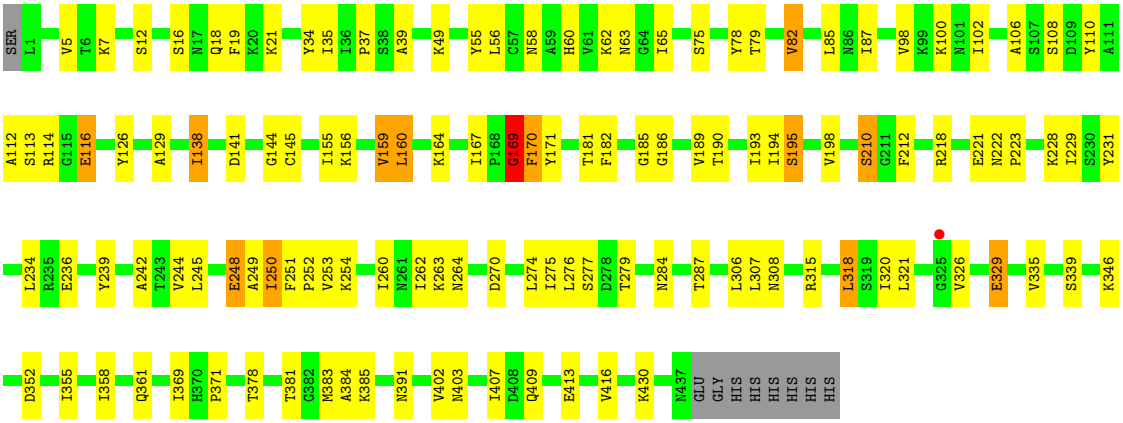
- Molecule 1: Aspartokinase

Chain C:



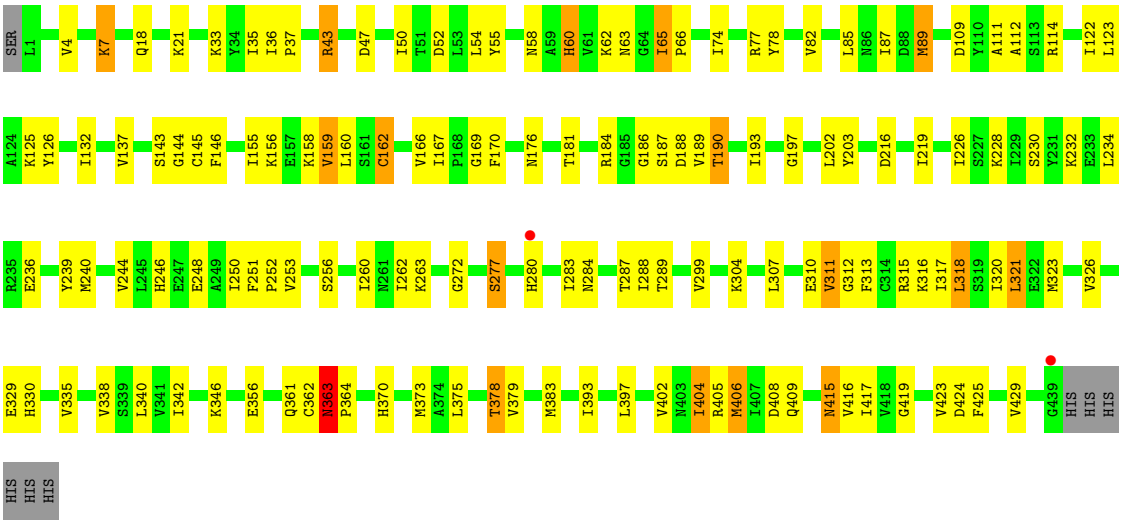
• Molecule 1: Aspartokinase

Chain D:



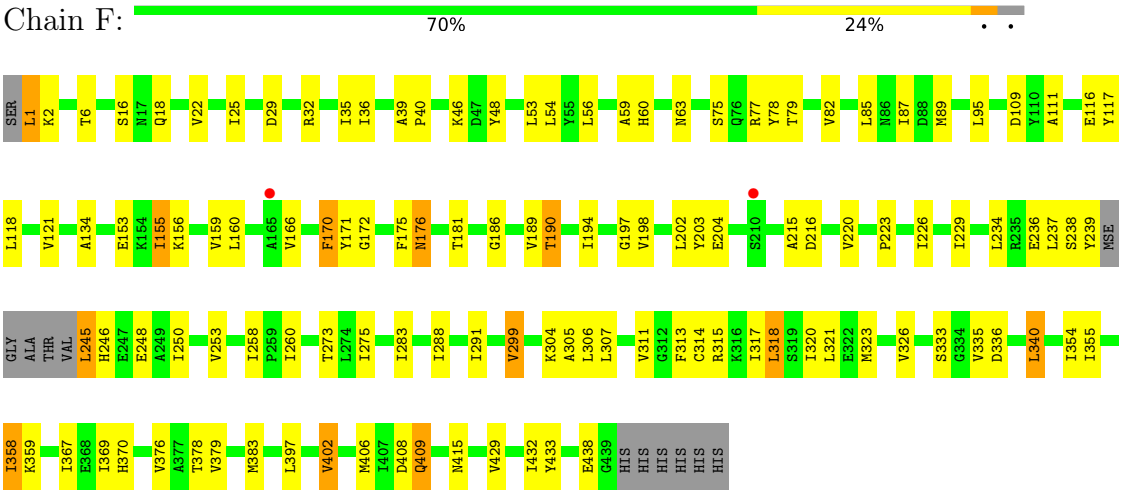
• Molecule 1: Aspartokinase

Chain E:



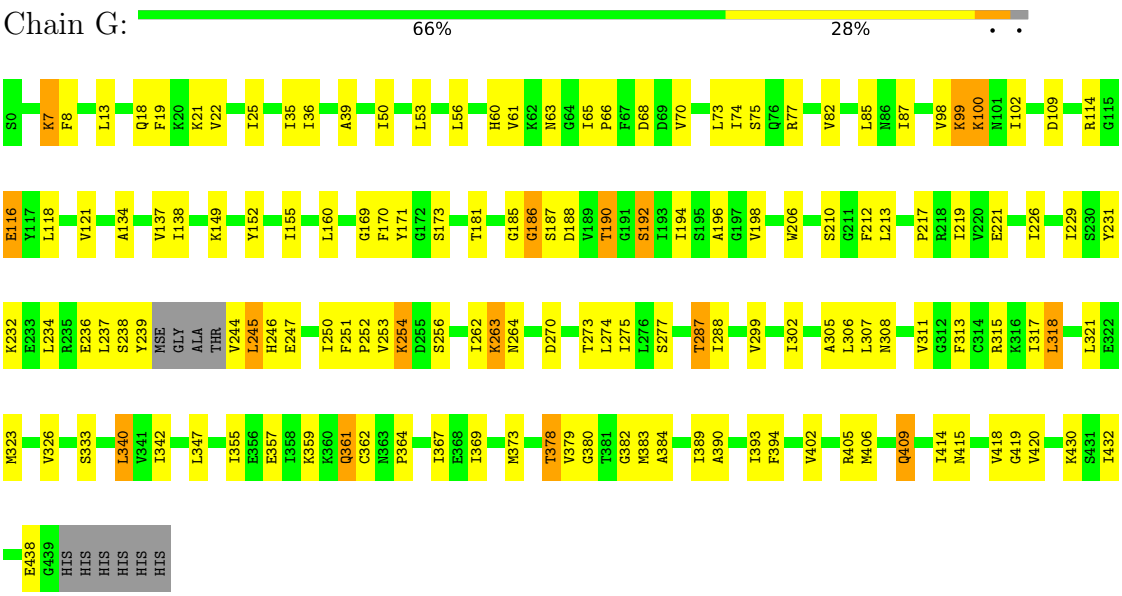
• Molecule 1: Aspartokinase

Chain F:



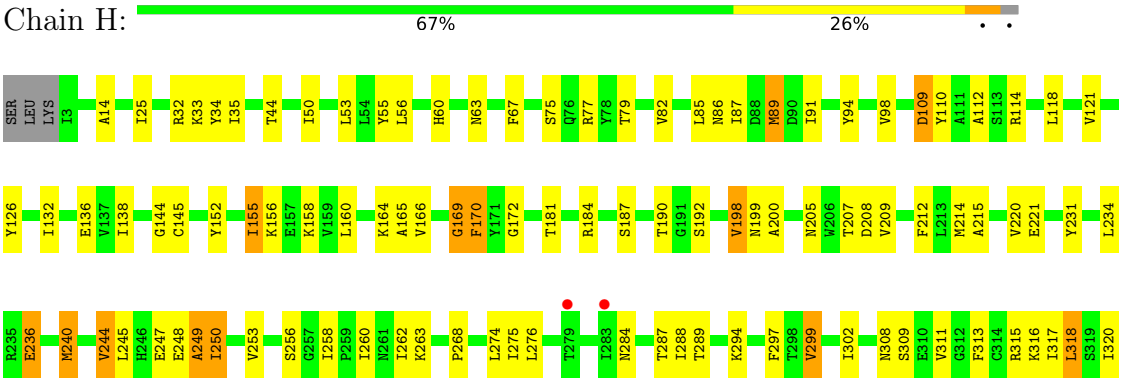
• Molecule 1: Aspartokinase

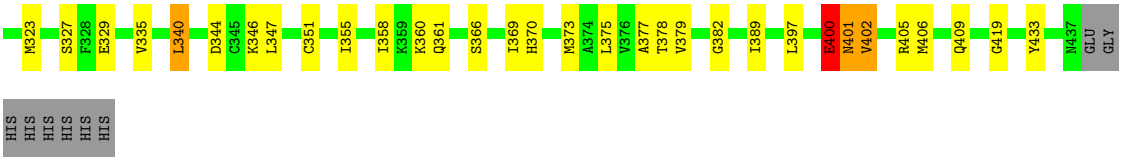
Chain G:



• Molecule 1: Aspartokinase

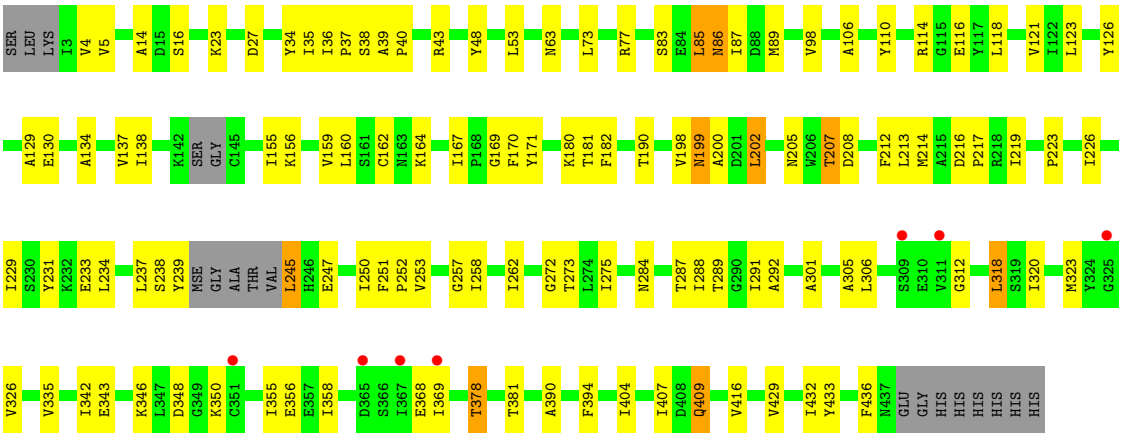
Chain H:





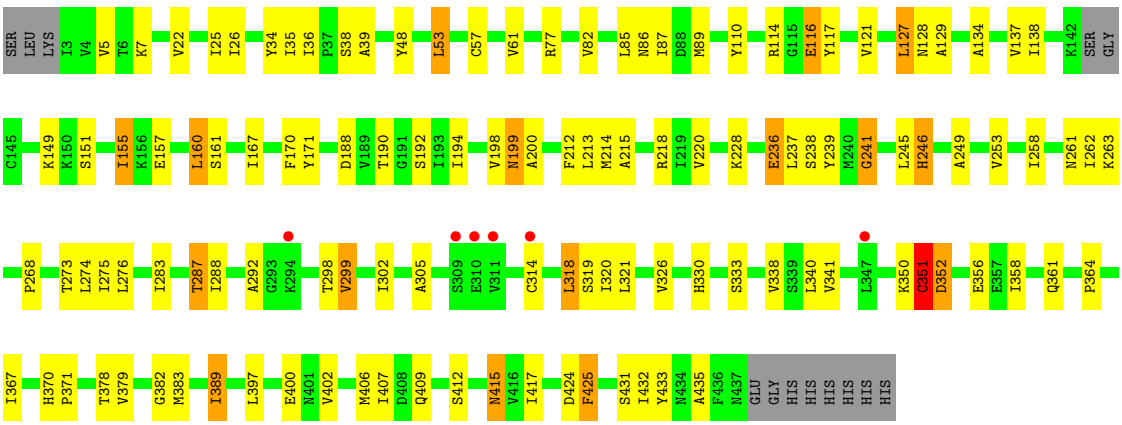
• Molecule 1: Aspartokinase

Chain I:



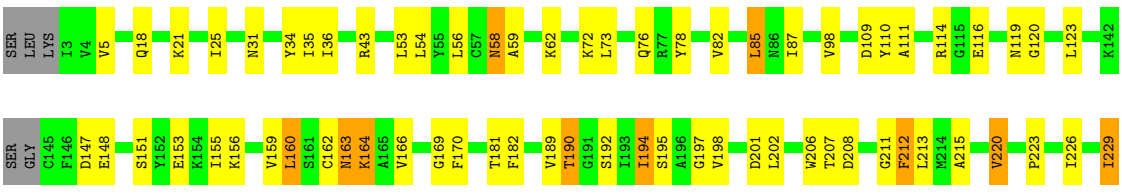
• Molecule 1: Aspartokinase

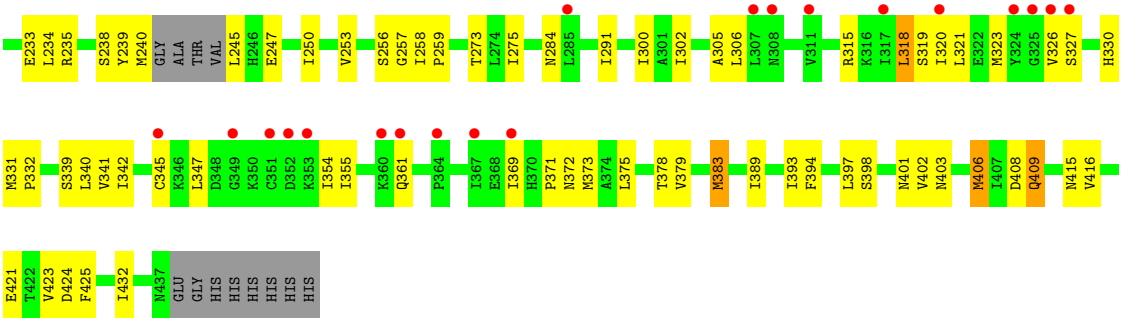
Chain J:



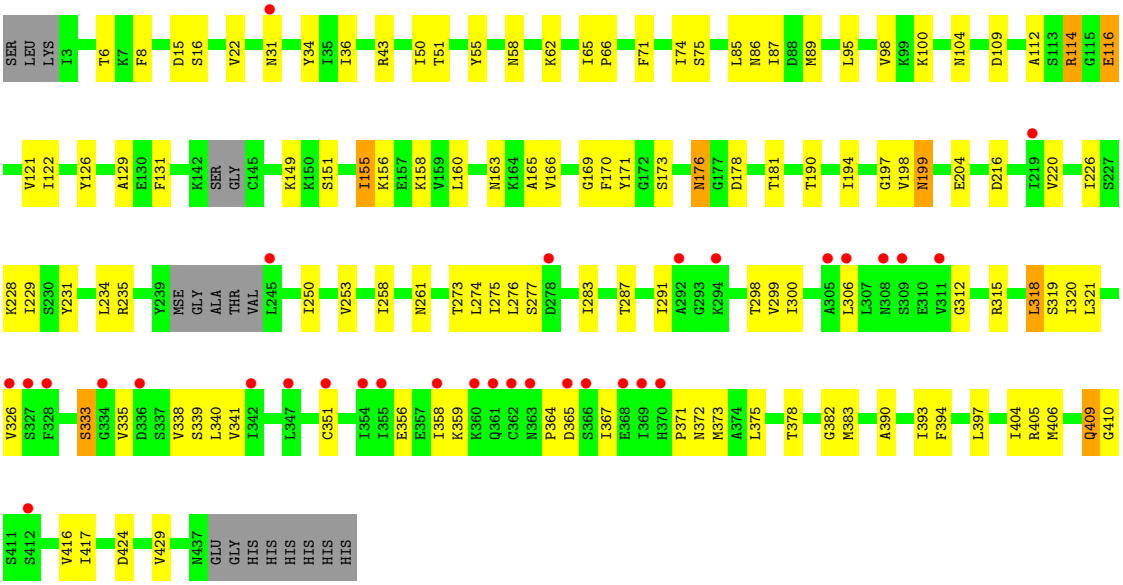
• Molecule 1: Aspartokinase

Chain K:





• Molecule 1: Aspartokinase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	109.04Å 274.22Å 114.04Å 90.00° 113.69° 90.00°	Depositor
Resolution (Å)	44.16 – 3.00 44.16 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.1 (44.16-3.00) 92.2 (44.16-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.92 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.206 , 0.273 0.209 , 0.284	Depositor DCC
R_{free} test set	924 reflections (0.82%)	wwPDB-VP
Wilson B-factor (Å^2)	77.3	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 41.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	39043	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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	0.40	0/3270	0.58	0/4409
1	B	0.38	0/3349	0.57	0/4516
1	C	0.37	0/3317	0.55	0/4479
1	D	0.43	0/3341	0.58	0/4509
1	E	0.38	0/3339	0.56	0/4510
1	F	0.35	0/3311	0.51	0/4471
1	G	0.40	0/3338	0.58	0/4504
1	H	0.37	0/3260	0.57	1/4407 (0.0%)
1	I	0.34	0/3234	0.50	0/4371
1	J	0.35	0/3245	0.53	0/4383
1	K	0.36	0/3210	0.51	0/4336
1	L	0.35	0/3234	0.51	0/4369
All	All	0.37	0/39448	0.55	1/53264 (0.0%)

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	B	0	1
1	D	0	1
1	H	0	2
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	400	GLU	N-CA-C	5.09	124.74	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	169	GLY	Peptide
1	D	169	GLY	Peptide
1	H	169	GLY	Peptide
1	H	400	GLU	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	3228	0	3156	81	0
1	B	3304	0	3281	88	0
1	C	3271	0	3214	107	0
1	D	3296	0	3257	95	0
1	E	3293	0	3224	112	0
1	F	3267	0	3209	93	0
1	G	3288	0	3244	118	0
1	H	3217	0	3103	103	0
1	I	3191	0	3092	105	0
1	J	3204	0	3116	103	0
1	K	3170	0	3042	109	0
1	L	3192	0	3093	110	0
2	A	9	0	3	2	0
2	D	9	0	3	0	0
2	E	9	0	3	1	0
2	G	9	0	3	1	0
2	H	9	0	3	1	0
2	I	8	0	3	0	0
2	L	9	0	3	0	0
3	A	10	0	12	0	0
3	B	10	0	12	0	0
3	C	10	0	12	3	0
3	D	10	0	12	0	0
3	G	10	0	12	7	0
3	H	10	0	12	1	0
All	All	39043	0	38124	1150	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 15.

The worst 5 of 1150 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:K:169:GLY:O	1:K:190:THR:HG21	1.41	1.19
1:D:189:VAL:HA	1:D:249:ALA:CB	1.76	1.14
1:D:189:VAL:HA	1:D:249:ALA:HB3	1.30	1.08
1:G:288:ILE:HD13	1:G:383:MSE:HE2	1.35	1.08
1:L:160:LEU:HD13	1:L:198:VAL:HG13	1.37	1.06

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	423/446 (95%)	385 (91%)	34 (8%)	4 (1%)	17	55
1	B	436/446 (98%)	406 (93%)	28 (6%)	2 (0%)	29	68
1	C	429/446 (96%)	381 (89%)	45 (10%)	3 (1%)	22	60
1	D	435/446 (98%)	397 (91%)	33 (8%)	5 (1%)	14	50
1	E	437/446 (98%)	401 (92%)	28 (6%)	8 (2%)	8	37
1	F	430/446 (96%)	387 (90%)	38 (9%)	5 (1%)	13	48
1	G	433/446 (97%)	400 (92%)	28 (6%)	5 (1%)	13	48
1	H	433/446 (97%)	386 (89%)	40 (9%)	7 (2%)	9	40
1	I	422/446 (95%)	377 (89%)	39 (9%)	6 (1%)	11	43
1	J	429/446 (96%)	386 (90%)	36 (8%)	7 (2%)	9	40
1	K	423/446 (95%)	381 (90%)	37 (9%)	5 (1%)	13	48
1	L	422/446 (95%)	383 (91%)	36 (8%)	3 (1%)	22	60
All	All	5152/5352 (96%)	4670 (91%)	422 (8%)	60 (1%)	13	48

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	307	LEU
1	E	144	GLY
1	G	170	PHE
1	H	199	ASN
1	I	199	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	348/377 (92%)	318 (91%)	30 (9%)	10	37
1	B	359/377 (95%)	328 (91%)	31 (9%)	10	37
1	C	354/377 (94%)	325 (92%)	29 (8%)	11	39
1	D	358/377 (95%)	326 (91%)	32 (9%)	9	35
1	E	354/377 (94%)	320 (90%)	34 (10%)	8	32
1	F	353/377 (94%)	327 (93%)	26 (7%)	13	44
1	G	357/377 (95%)	328 (92%)	29 (8%)	11	40
1	H	338/377 (90%)	312 (92%)	26 (8%)	13	42
1	I	340/377 (90%)	326 (96%)	14 (4%)	30	67
1	J	339/377 (90%)	314 (93%)	25 (7%)	13	44
1	K	334/377 (89%)	304 (91%)	30 (9%)	9	35
1	L	341/377 (90%)	319 (94%)	22 (6%)	17	50
All	All	4175/4524 (92%)	3847 (92%)	328 (8%)	12	41

5 of 328 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	338	VAL
1	G	75	SER
1	K	406	MSE
1	E	404	ILE

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Mol	Chain	Res	Type
1	F	190	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	17	ASN
1	G	58	ASN
1	K	437	ASN
1	F	18	GLN
1	F	222	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

13 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	$\#\|Z\| > 2$
2	ASP	A	451	-	2,8,8	0.31	0	1,10,10	0.80	0
2	ASP	E	455	-	2,8,8	0.41	0	1,10,10	1.41	0
3	LYS	H	508	-	5,9,9	0.63	0	4,10,10	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ASP	H	458	-	2,8,8	0.36	0	1,10,10	1.02	0
3	LYS	B	502	-	5,9,9	0.28	0	4,10,10	0.25	0
2	ASP	I	459	-	4,7,8	2.23	1 (25%)	3,8,10	1.64	1 (33%)
2	ASP	G	457	-	2,8,8	0.30	0	1,10,10	1.53	0
3	LYS	C	503	-	5,9,9	0.25	0	4,10,10	0.41	0
3	LYS	A	501	-	5,9,9	0.47	0	4,10,10	0.43	0
2	ASP	D	454	-	2,8,8	0.26	0	1,10,10	0.54	0
2	ASP	L	462	-	2,8,8	0.25	0	1,10,10	0.36	0
3	LYS	D	504	-	5,9,9	0.51	0	4,10,10	0.45	0
3	LYS	G	507	-	5,9,9	0.57	0	4,10,10	0.33	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
2	ASP	A	451	-	-	0/2/8/8	-
2	ASP	E	455	-	-	1/2/8/8	-
3	LYS	H	508	-	-	0/5/9/9	-
2	ASP	H	458	-	-	1/2/8/8	-
3	LYS	B	502	-	-	0/5/9/9	-
2	ASP	I	459	-	-	2/4/6/8	-
2	ASP	G	457	-	-	0/2/8/8	-
3	LYS	C	503	-	-	0/5/9/9	-
3	LYS	A	501	-	-	0/5/9/9	-
2	ASP	D	454	-	-	1/2/8/8	-
2	ASP	L	462	-	-	0/2/8/8	-
3	LYS	D	504	-	-	0/5/9/9	-
3	LYS	G	507	-	-	2/5/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	459	ASP	OXT-C	-4.43	1.23	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	459	ASP	OXT-C-CA	2.47	121.27	111.52

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	455	ASP	N-CA-CB-CG
2	H	458	ASP	N-CA-CB-CG
2	I	459	ASP	N-CA-CB-CG
2	I	459	ASP	C-CA-CB-CG
3	G	507	LYS	C-CA-CB-CG

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	451	ASP	2	0
2	E	455	ASP	1	0
3	H	508	LYS	1	0
2	H	458	ASP	1	0
2	G	457	ASP	1	0
3	C	503	LYS	3	0
3	G	507	LYS	7	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

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	421/446 (94%)	-0.45	1 (0%) 95 87	42, 62, 111, 135	0
1	B	430/446 (96%)	-0.37	0 100 100	43, 66, 108, 135	1 (0%)
1	C	426/446 (95%)	-0.38	1 (0%) 95 87	53, 82, 112, 133	0
1	D	429/446 (96%)	-0.41	1 (0%) 95 87	36, 58, 123, 175	1 (0%)
1	E	431/446 (96%)	-0.38	2 (0%) 91 75	48, 74, 111, 142	1 (0%)
1	F	427/446 (95%)	-0.26	2 (0%) 91 75	58, 101, 135, 154	0
1	G	429/446 (96%)	-0.51	0 100 100	39, 61, 87, 101	0
1	H	427/446 (95%)	-0.38	2 (0%) 91 75	51, 80, 110, 140	0
1	I	421/446 (94%)	-0.10	7 (1%) 70 41	67, 105, 166, 195	1 (0%)
1	J	425/446 (95%)	-0.26	6 (1%) 75 49	58, 93, 154, 194	0
1	K	421/446 (94%)	-0.09	20 (4%) 30 11	54, 97, 191, 220	1 (0%)
1	L	421/446 (94%)	0.21	32 (7%) 13 4	61, 120, 203, 273	1 (0%)
All	All	5108/5352 (95%)	-0.28	74 (1%) 75 49	36, 82, 149, 273	6 (0%)

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	362	CYS	9.0
1	L	347	LEU	8.3
1	L	366	SER	7.0
1	L	363	ASN	6.6
1	L	308	ASN	5.4

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

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	LYS	G	507	10/10	0.29	0.78	56,64,67,68	10
3	LYS	H	508	10/10	0.57	0.56	70,72,76,81	10
3	LYS	C	503	10/10	0.58	0.60	71,73,73,73	10
2	ASP	A	451	9/9	0.60	0.50	55,59,60,61	9
2	ASP	G	457	9/9	0.68	0.44	53,55,58,58	9
3	LYS	A	501	10/10	0.69	0.46	59,62,65,66	10
2	ASP	H	458	9/9	0.75	0.41	64,66,71,74	9
2	ASP	L	462	9/9	0.75	0.42	74,78,86,87	9
3	LYS	B	502	10/10	0.75	0.38	56,58,59,60	10
2	ASP	I	459	8/9	0.76	0.39	63,64,69,73	8
3	LYS	D	504	10/10	0.76	0.40	59,61,62,62	10
2	ASP	D	454	9/9	0.76	0.35	61,69,78,81	9
2	ASP	E	455	9/9	0.80	0.36	62,63,64,66	9

6.5 Other polymers (i)

There are no such residues in this entry.