



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 24, 2023 – 12:59 AM EDT

PDB ID : 3AB4
Title : Crystal structure of feedback inhibition resistant mutant of aspartate kinase from *Corynebacterium glutamicum* in complex with lysine and threonine
Authors : Yoshida, A.; Tomita, T.; Kuzuyama, T.; Nishiyama, M.
Deposited on : 2009-11-30
Resolution : 2.47 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 2.36
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

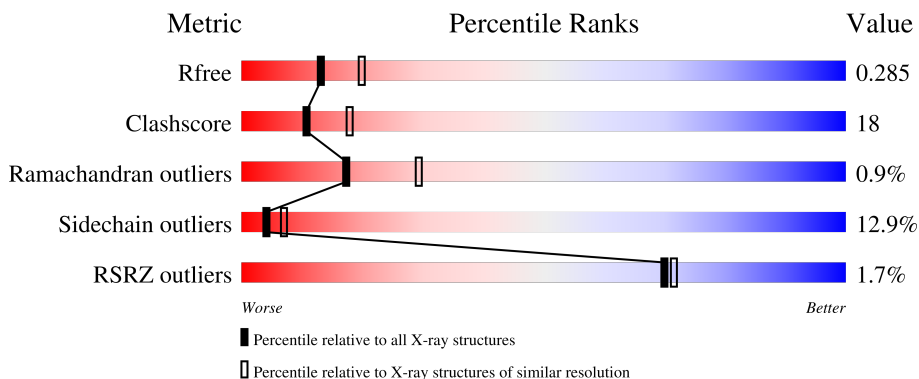
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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.



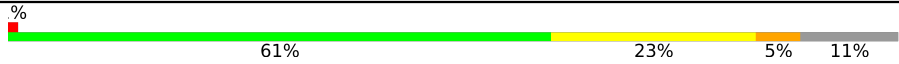

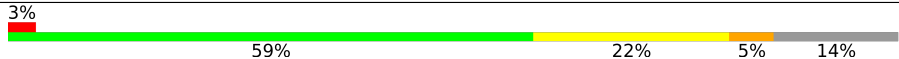
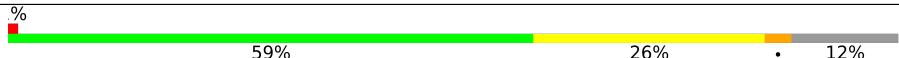
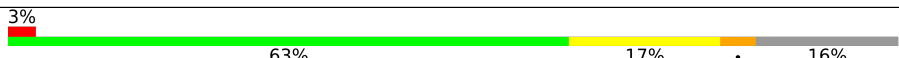
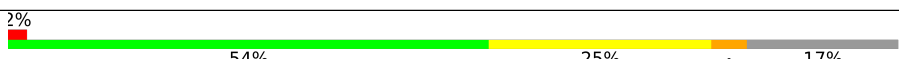
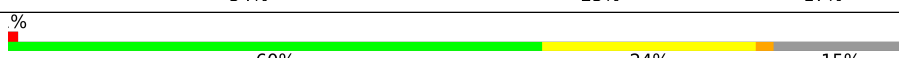
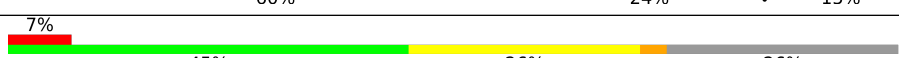
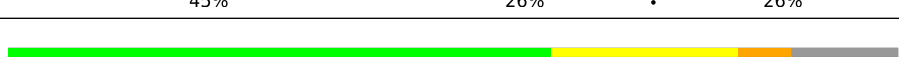


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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 $\leq 5\%$. 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	421	
1	C	421	
1	E	421	
1	G	421	
1	I	421	

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Mol	Chain	Length	Quality of chain
1	K	421	
1	M	421	
1	O	421	
2	B	178	
2	D	178	
2	F	178	
2	H	178	
2	J	178	
2	L	178	
2	N	178	
2	P	178	

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	B	201	-	-	X	-
3	THR	C	501	-	-	X	-
3	THR	D	201	-	-	X	-
3	THR	F	201	-	-	X	-
3	THR	G	501	-	-	X	-
3	THR	H	201	-	-	X	-
3	THR	I	501	-	-	X	-
3	THR	K	501	-	-	X	-
3	THR	O	501	-	-	X	-
4	LYS	K	601	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 30970 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
			Total	C	N	O	S			
1	A	370	2711	1687	463	547	14	0	0	0
1	C	367	2705	1686	463	542	14	0	0	0
1	E	368	2682	1669	462	537	14	0	0	0
1	G	357	2600	1620	443	523	14	0	0	0
1	I	360	2634	1645	445	530	14	0	0	0
1	K	373	2736	1704	469	549	14	0	0	0
1	M	377	2772	1725	479	554	14	0	0	0
1	O	364	2642	1637	457	534	14	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	301	PHE	SER	SEE REMARK 999	UNP P26512
C	301	PHE	SER	SEE REMARK 999	UNP P26512
E	301	PHE	SER	SEE REMARK 999	UNP P26512
G	301	PHE	SER	SEE REMARK 999	UNP P26512
I	301	PHE	SER	SEE REMARK 999	UNP P26512
K	301	PHE	SER	SEE REMARK 999	UNP P26512
M	301	PHE	SER	SEE REMARK 999	UNP P26512
O	301	PHE	SER	SEE REMARK 999	UNP P26512

- Molecule 2 is a protein called Aspartokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	157	1175	729	203	238	5	0	0	0
2	D	150	1133	706	198	224	5	0	0	0
2	F	148	1077	671	184	217	5	0	0	0
2	H	151	1108	691	188	224	5	0	0	0
2	J	132	974	608	167	195	4	0	0	0
2	L	156	1176	735	201	235	5	0	0	0
2	N	155	1153	716	199	233	5	0	0	0
2	P	149	1107	687	191	225	4	0	0	0

There are 64 discrepancies between the modelled and reference sequences:

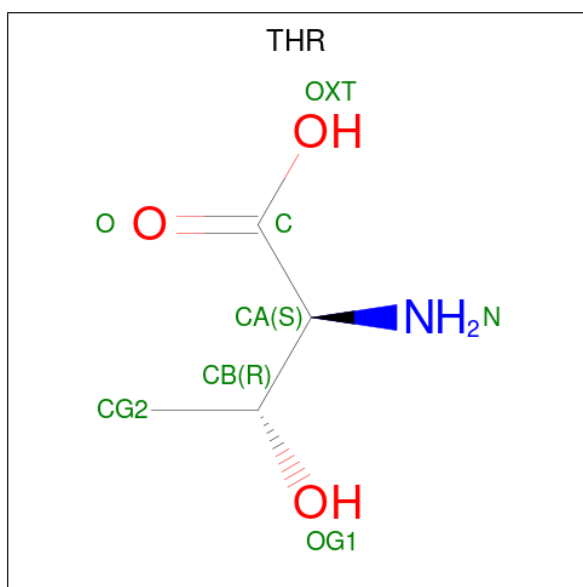
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P26512
B	52	PHE	SER	SEE REMARK 999	UNP P26512
B	173	HIS	-	expression tag	UNP P26512
B	174	HIS	-	expression tag	UNP P26512
B	175	HIS	-	expression tag	UNP P26512
B	176	HIS	-	expression tag	UNP P26512
B	177	HIS	-	expression tag	UNP P26512
B	178	HIS	-	expression tag	UNP P26512
D	1	MET	-	initiating methionine	UNP P26512
D	52	PHE	SER	SEE REMARK 999	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	52	PHE	SER	SEE REMARK 999	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

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Chain	Residue	Modelled	Actual	Comment	Reference
H	1	MET	-	initiating methionine	UNP P26512
H	52	PHE	SER	SEE REMARK 999	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	52	PHE	SER	SEE REMARK 999	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
J	178	HIS	-	expression tag	UNP P26512
L	1	MET	-	initiating methionine	UNP P26512
L	52	PHE	SER	SEE REMARK 999	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	52	PHE	SER	SEE REMARK 999	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	52	PHE	SER	SEE REMARK 999	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: C₄H₉NO₃).



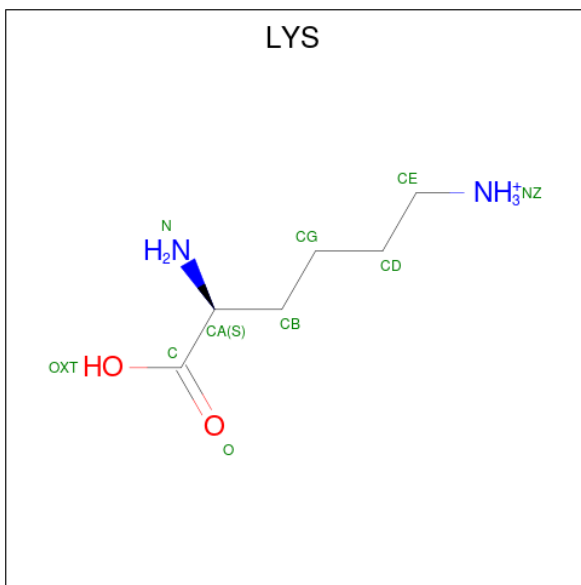
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	Total 8	4	1	3	0	0
3	B	1	Total 8	4	1	3	0	0
3	C	1	Total 8	4	1	3	0	0
3	D	1	Total 8	4	1	3	0	0
3	E	1	Total 8	4	1	3	0	0
3	F	1	Total 8	4	1	3	0	0
3	G	1	Total 8	4	1	3	0	0
3	H	1	Total 8	4	1	3	0	0
3	I	1	Total 8	4	1	3	0	0
3	J	1	Total 8	4	1	3	0	0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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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		

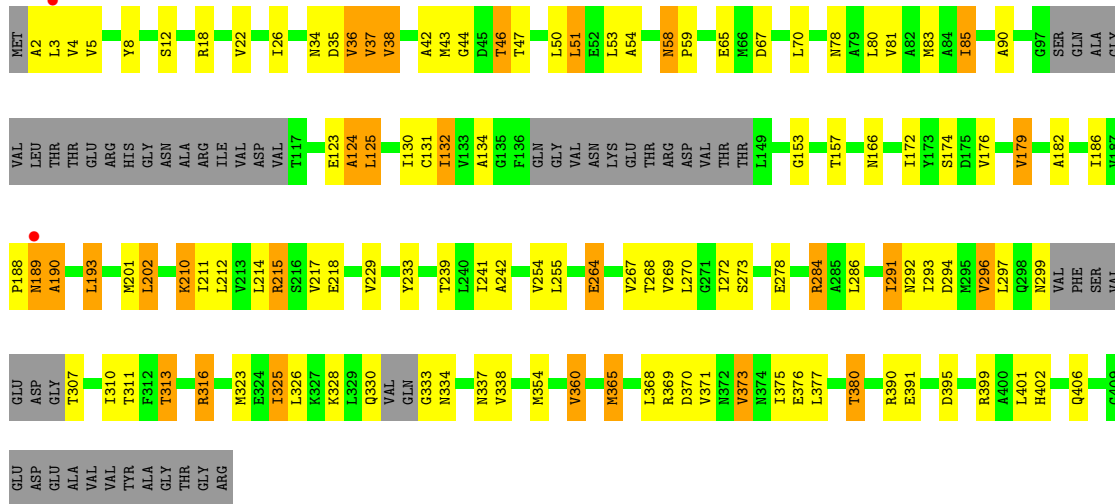
- Molecule 4 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



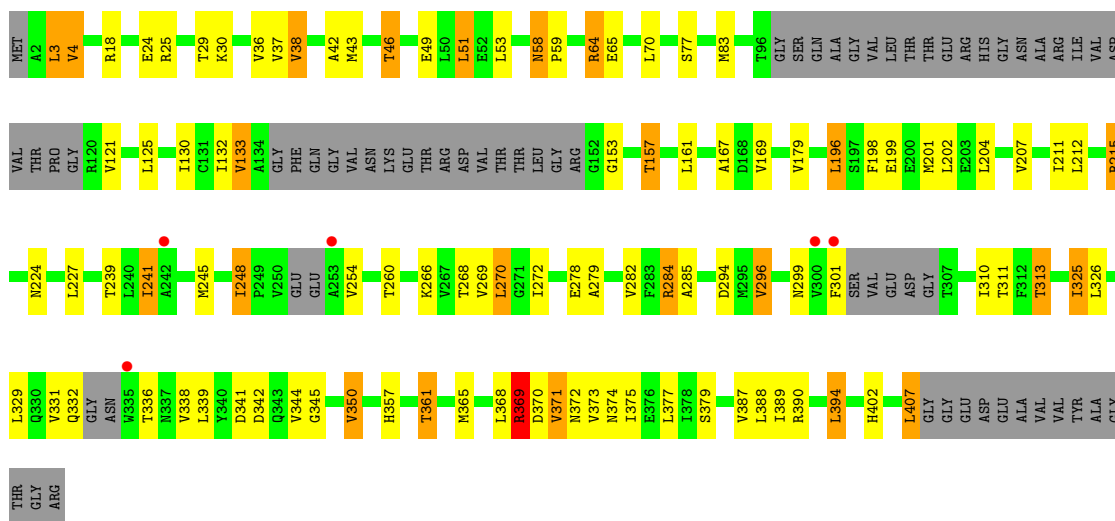
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	6	2	2		
4	C	1	Total	C	N	O	0	0
			10	6	2	2		
4	E	1	Total	C	N	O	0	0
			10	6	2	2		
4	G	1	Total	C	N	O	0	0
			10	6	2	2		
4	K	1	Total	C	N	O	0	0
			10	6	2	2		
4	M	1	Total	C	N	O	0	0
			10	6	2	2		
4	O	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 5 is water.

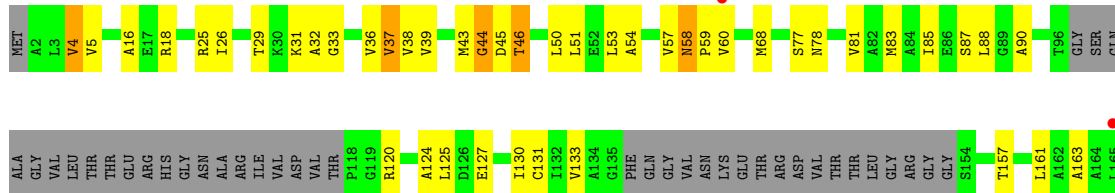
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	46	Total O 46 46	0	0
5	B	36	Total O 36 36	0	0
5	C	25	Total O 25 25	0	0
5	D	13	Total O 13 13	0	0
5	E	30	Total O 30 30	0	0
5	F	5	Total O 5 5	0	0
5	G	27	Total O 27 27	0	0
5	H	11	Total O 11 11	0	0
5	I	22	Total O 22 22	0	0
5	J	3	Total O 3 3	0	0
5	K	41	Total O 41 41	0	0
5	L	22	Total O 22 22	0	0
5	M	52	Total O 52 52	0	0
5	N	24	Total O 24 24	0	0
5	O	22	Total O 22 22	0	0
5	P	8	Total O 8 8	0	0

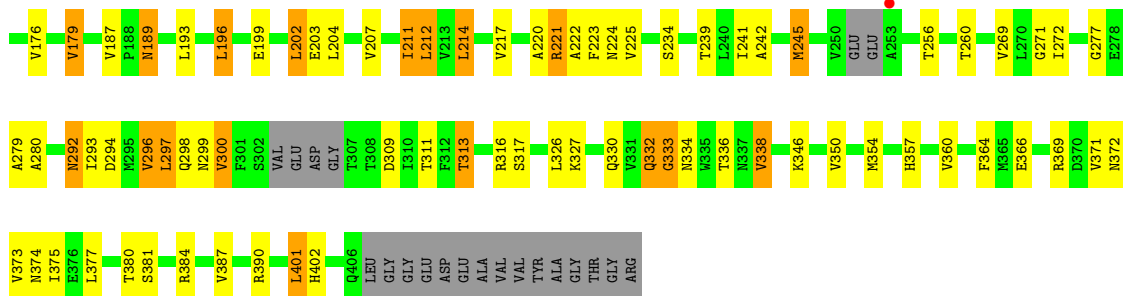


● Molecule 1: Aspartokinase

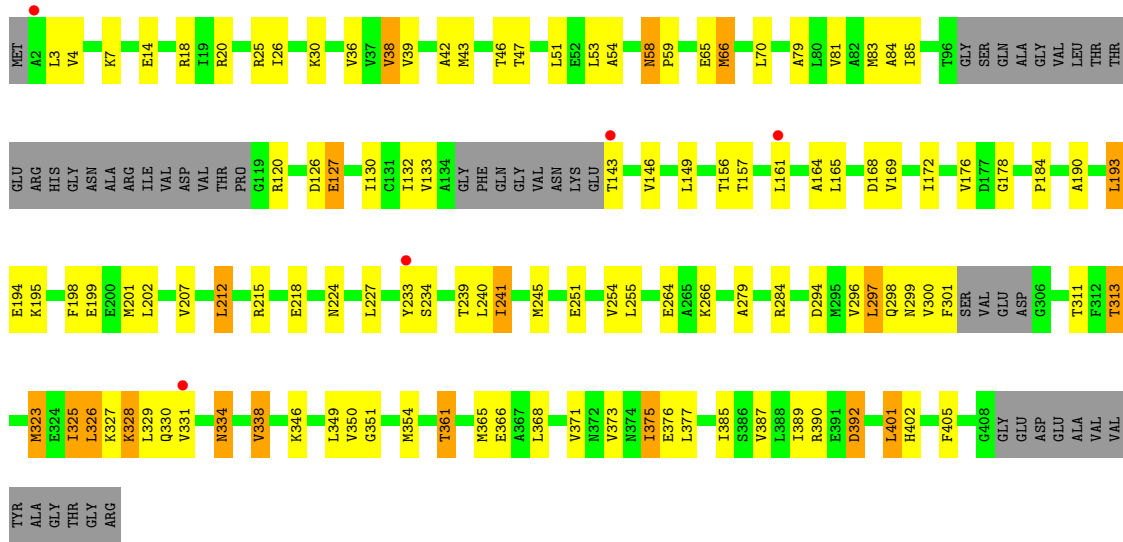


● Molecule 1: Aspartokinase

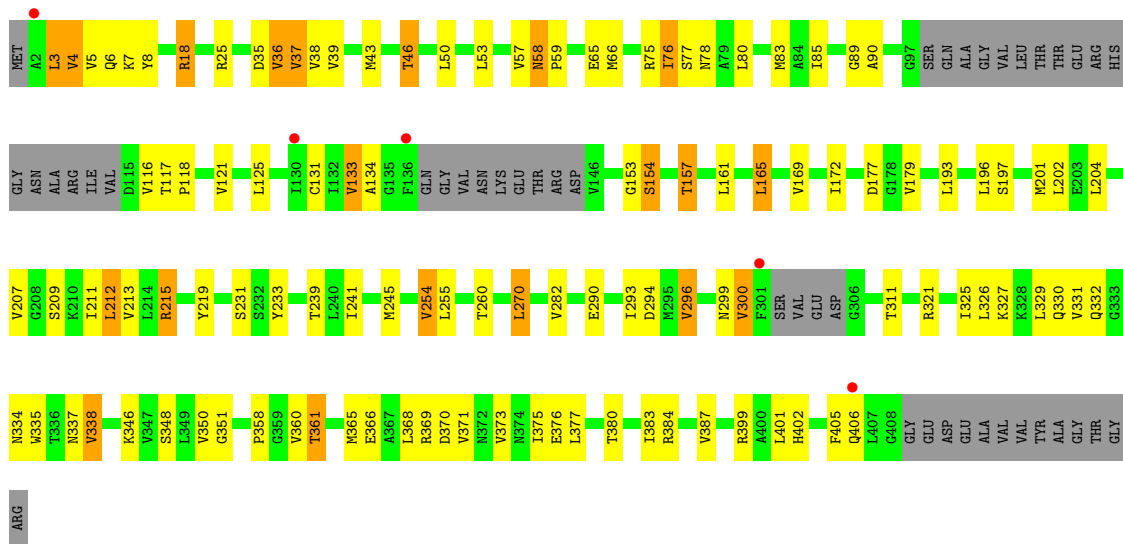




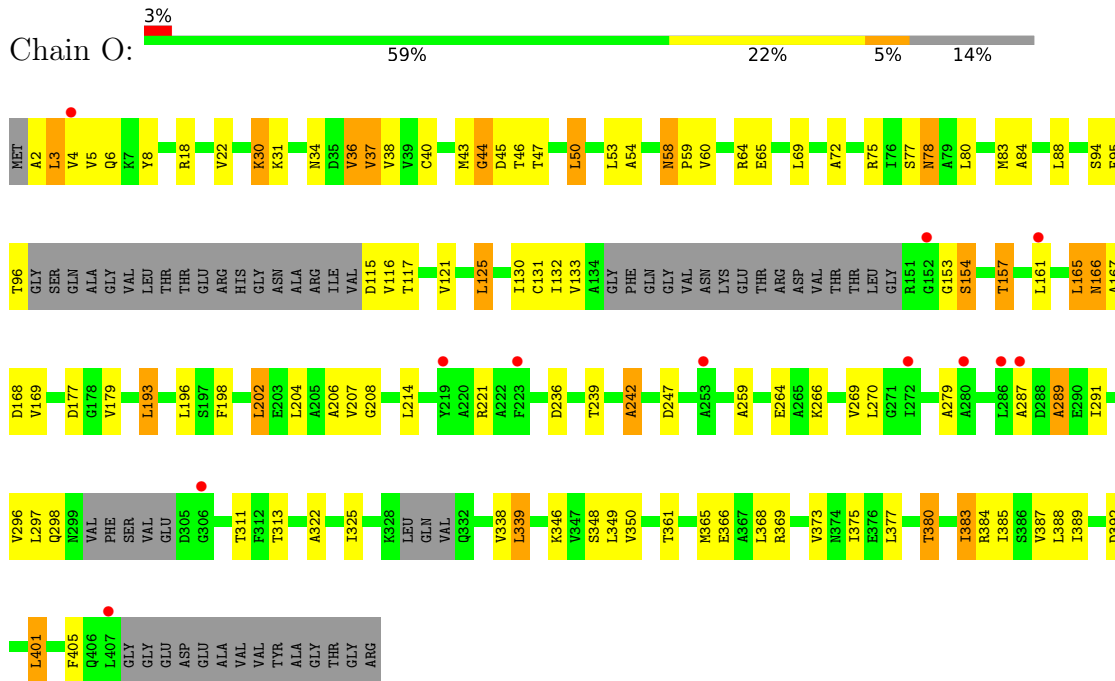
• Molecule 1: Aspartokinase



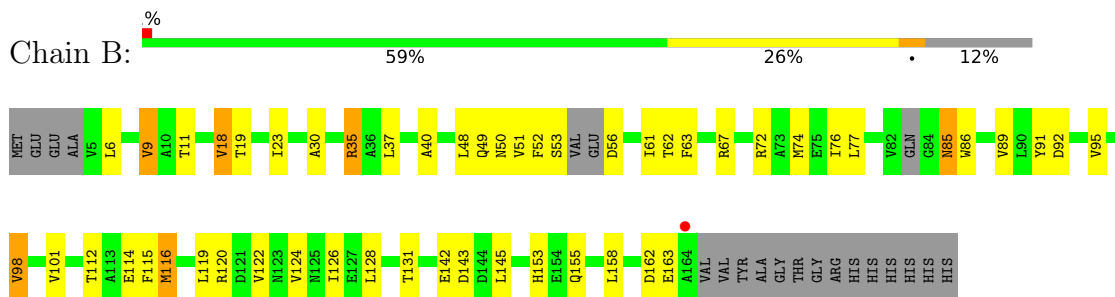
• Molecule 1: Aspartokinase



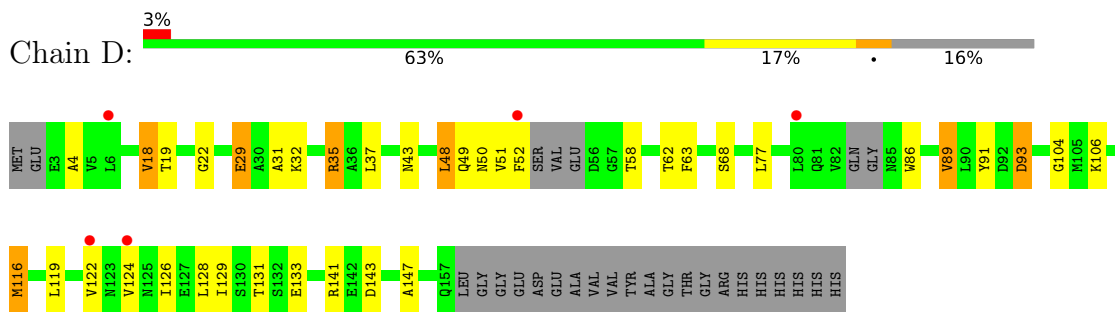
● Molecule 1: Aspartokinase



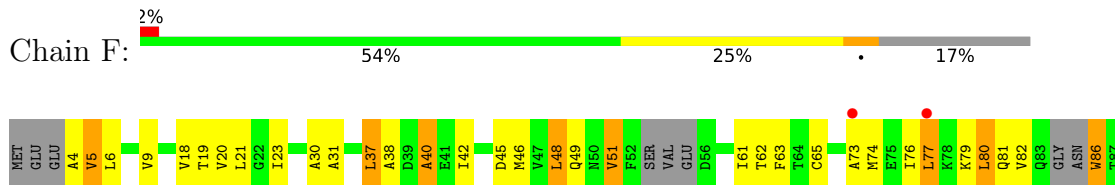
● Molecule 2: Aspartokinase



● Molecule 2: Aspartokinase

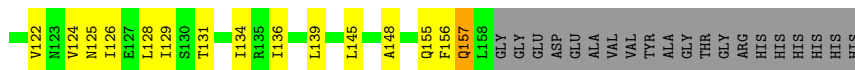


● Molecule 2: Aspartokinase

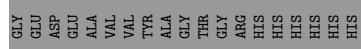
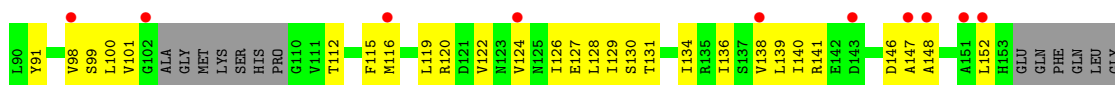
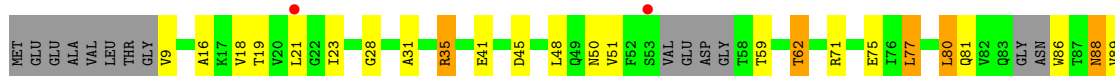
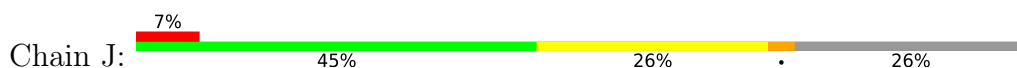




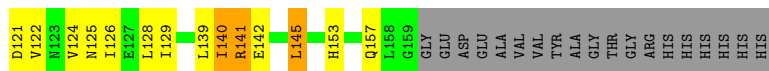
• Molecule 2: Aspartokinase



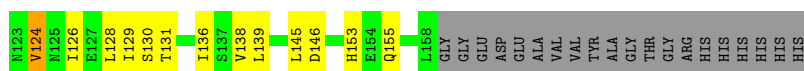
• Molecule 2: Aspartokinase



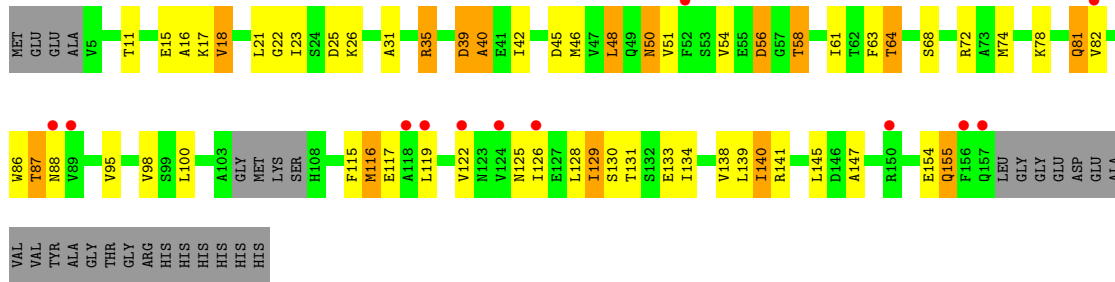
• Molecule 2: Aspartokinase



• Molecule 2: Aspartokinase



• Molecule 2: Aspartokinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	99.03Å 112.87Å 120.01Å 76.03° 71.07° 74.50°	Depositor
Resolution (Å)	39.74 – 2.47 44.03 – 2.47	Depositor EDS
% Data completeness (in resolution range)	95.7 (39.74-2.47) 95.7 (44.03-2.47)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.48Å)	Xtrriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.223 , 0.288 0.225 , 0.285	Depositor DCC
R_{free} test set	8052 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtrriage
Anisotropy	0.164	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	30970	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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

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	0.49	0/2736	0.64	1/3712 (0.0%)
1	C	0.44	0/2730	0.64	0/3702
1	E	0.46	0/2706	0.63	0/3670
1	G	0.45	0/2623	0.64	1/3564 (0.0%)
1	I	0.42	0/2659	0.61	0/3610
1	K	0.48	0/2760	0.67	1/3743 (0.0%)
1	M	0.52	0/2797	0.69	0/3794
1	O	0.42	0/2665	0.59	0/3619
2	B	0.51	0/1185	0.72	0/1602
2	D	0.42	0/1142	0.62	0/1543
2	F	0.38	0/1085	0.59	0/1473
2	H	0.42	0/1118	0.59	0/1516
2	J	0.38	0/980	0.59	0/1329
2	L	0.49	0/1187	0.67	0/1606
2	N	0.48	0/1164	0.65	0/1580
2	P	0.38	0/1115	0.59	0/1512
All	All	0.45	0/30652	0.64	3/41575 (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	A	0	1
1	M	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	369	ARG	NE-CZ-NH1	5.66	123.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	K	392	ASP	CB-CG-OD1	5.24	123.01	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	370	ASP	Peptide
1	M	380	THR	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	2711	0	2702	95	0
1	C	2705	0	2721	143	0
1	E	2682	0	2672	106	0
1	G	2600	0	2554	87	0
1	I	2634	0	2613	92	0
1	K	2736	0	2729	95	0
1	M	2772	0	2790	130	0
1	O	2642	0	2590	103	0
2	B	1175	0	1155	61	0
2	D	1133	0	1140	38	0
2	F	1077	0	1053	52	0
2	H	1108	0	1076	42	0
2	J	974	0	934	41	0
2	L	1176	0	1177	44	1
2	N	1153	0	1138	39	1
2	P	1107	0	1090	60	0
3	A	8	0	6	0	0
3	B	8	0	6	6	0
3	C	8	0	6	6	0
3	D	8	0	6	5	0
3	E	8	0	6	0	0
3	F	8	0	6	6	0
3	G	8	0	6	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	8	0	6	6	0
3	I	8	0	6	4	0
3	J	8	0	6	2	0
3	K	8	0	6	6	0
3	L	8	0	6	1	0
3	M	8	0	6	0	0
3	N	8	0	6	0	0
3	O	8	0	6	4	0
3	P	8	0	6	1	0
4	A	10	0	12	0	0
4	C	10	0	12	5	0
4	E	10	0	12	2	0
4	G	10	0	12	2	0
4	K	10	0	12	6	0
4	M	10	0	12	5	0
4	O	10	0	12	2	0
5	A	46	0	0	1	0
5	B	36	0	0	0	0
5	C	25	0	0	2	0
5	D	13	0	0	1	0
5	E	30	0	0	0	0
5	F	5	0	0	0	0
5	G	27	0	0	1	0
5	H	11	0	0	0	0
5	I	22	0	0	1	0
5	J	3	0	0	0	0
5	K	41	0	0	0	0
5	L	22	0	0	0	0
5	M	52	0	0	1	0
5	N	24	0	0	0	0
5	O	22	0	0	1	0
5	P	8	0	0	0	0
All	All	30970	0	30314	1116	1

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 18.

The worst 5 of 1116 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:E:43:MET:O	1:E:46:THR:HG22	1.34	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:286:LEU:CD2	1:E:291:ILE:HD11	1.69	1.21
2:H:20:VAL:HG12	2:H:23:ILE:HD11	1.19	1.17
1:C:297:LEU:HD22	1:C:377:LEU:HD21	1.26	1.16
2:N:116:MET:HE2	2:N:126:ILE:HD13	1.23	1.14

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:39:ASP:OD2	2:N:39:ASP:OD2[1_655]	2.12	0.08

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	362/421 (86%)	346 (96%)	15 (4%)	1 (0%)	41 59
1	C	359/421 (85%)	341 (95%)	15 (4%)	3 (1%)	19 33
1	E	358/421 (85%)	335 (94%)	16 (4%)	7 (2%)	7 11
1	G	345/421 (82%)	329 (95%)	15 (4%)	1 (0%)	41 59
1	I	350/421 (83%)	327 (93%)	15 (4%)	8 (2%)	6 9
1	K	365/421 (87%)	349 (96%)	14 (4%)	2 (0%)	29 46
1	M	369/421 (88%)	355 (96%)	13 (4%)	1 (0%)	41 59
1	O	354/421 (84%)	326 (92%)	23 (6%)	5 (1%)	11 18
2	B	151/178 (85%)	141 (93%)	8 (5%)	2 (1%)	12 19
2	D	144/178 (81%)	136 (94%)	8 (6%)	0	100 100
2	F	142/178 (80%)	133 (94%)	5 (4%)	4 (3%)	5 6
2	H	147/178 (83%)	140 (95%)	5 (3%)	2 (1%)	11 18
2	J	124/178 (70%)	115 (93%)	9 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	152/178 (85%)	145 (95%)	7 (5%)	0	100	100
2	N	153/178 (86%)	149 (97%)	4 (3%)	0	100	100
2	P	145/178 (82%)	136 (94%)	7 (5%)	2 (1%)	11	18
All	All	4020/4792 (84%)	3803 (95%)	179 (4%)	38 (1%)	17	29

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	295	MET
1	C	333	GLY
1	E	124	ALA
1	E	190	ALA
2	F	74	MET

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	286/336 (85%)	252 (88%)	34 (12%)	5	9
1	C	287/336 (85%)	253 (88%)	34 (12%)	5	9
1	E	280/336 (83%)	239 (85%)	41 (15%)	3	5
1	G	270/336 (80%)	227 (84%)	43 (16%)	2	4
1	I	277/336 (82%)	238 (86%)	39 (14%)	3	5
1	K	286/336 (85%)	250 (87%)	36 (13%)	4	7
1	M	294/336 (88%)	254 (86%)	40 (14%)	3	6
1	O	272/336 (81%)	236 (87%)	36 (13%)	4	6
2	B	125/146 (86%)	113 (90%)	12 (10%)	8	15
2	D	122/146 (84%)	109 (89%)	13 (11%)	6	11
2	F	112/146 (77%)	105 (94%)	7 (6%)	18	32
2	H	115/146 (79%)	109 (95%)	6 (5%)	23	41
2	J	99/146 (68%)	84 (85%)	15 (15%)	3	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	127/146 (87%)	113 (89%)	14 (11%)	6	10
2	N	123/146 (84%)	107 (87%)	16 (13%)	4	7
2	P	117/146 (80%)	99 (85%)	18 (15%)	2	4
All	All	3192/3856 (83%)	2788 (87%)	404 (13%)	4	7

5 of 404 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	35	ARG
2	L	67	ARG
2	P	117	GLU
2	J	80	LEU
1	K	224	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	374	ASN
1	M	404	GLN
2	L	43	ASN
1	M	58	ASN
1	O	34	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](#)

23 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	A	501	-	6,7,7	0.92	1 (16%)	7,9,9	1.12	1 (14%)
3	THR	M	501	-	6,7,7	1.00	1 (16%)	7,9,9	1.45	2 (28%)
3	THR	J	201	-	6,7,7	1.02	1 (16%)	7,9,9	1.43	1 (14%)
4	LYS	M	601	-	8,9,9	0.95	1 (12%)	9,10,10	1.56	2 (22%)
3	THR	F	201	-	6,7,7	1.09	1 (16%)	7,9,9	1.43	2 (28%)
4	LYS	E	601	-	8,9,9	0.82	1 (12%)	9,10,10	1.14	1 (11%)
4	LYS	C	601	-	8,9,9	0.83	1 (12%)	9,10,10	1.19	1 (11%)
3	THR	D	201	-	6,7,7	0.96	1 (16%)	7,9,9	1.24	1 (14%)
3	THR	O	501	-	6,7,7	0.98	1 (16%)	7,9,9	1.32	2 (28%)
4	LYS	O	601	-	8,9,9	0.86	1 (12%)	9,10,10	1.24	2 (22%)
3	THR	I	501	-	6,7,7	0.94	1 (16%)	7,9,9	1.17	1 (14%)
3	THR	C	501	-	6,7,7	0.85	0	7,9,9	1.26	2 (28%)
3	THR	P	201	-	6,7,7	1.10	1 (16%)	7,9,9	1.47	1 (14%)
4	LYS	A	601	-	8,9,9	0.74	0	9,10,10	0.97	0
3	THR	E	501	-	6,7,7	0.97	1 (16%)	7,9,9	1.42	2 (28%)
3	THR	K	501	-	6,7,7	0.96	0	7,9,9	1.41	1 (14%)
3	THR	L	201	-	6,7,7	0.94	1 (16%)	7,9,9	1.35	1 (14%)
3	THR	N	201	-	6,7,7	0.91	0	7,9,9	1.03	1 (14%)
3	THR	H	201	-	6,7,7	0.99	0	7,9,9	1.34	1 (14%)
3	THR	G	501	-	6,7,7	0.90	0	7,9,9	1.27	2 (28%)
3	THR	B	201	-	6,7,7	1.06	0	7,9,9	1.13	1 (14%)
4	LYS	G	601	-	8,9,9	0.76	0	9,10,10	1.36	2 (22%)
4	LYS	K	601	-	8,9,9	0.99	1 (12%)	9,10,10	1.41	2 (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
3	THR	A	501	-	-	0/8/8/8	-
3	THR	M	501	-	-	0/8/8/8	-
3	THR	J	201	-	-	0/8/8/8	-
4	LYS	M	601	-	-	2/9/9/9	-
3	THR	F	201	-	-	3/8/8/8	-
4	LYS	E	601	-	-	1/9/9/9	-
4	LYS	C	601	-	-	4/9/9/9	-
3	THR	D	201	-	-	0/8/8/8	-
3	THR	O	501	-	-	0/8/8/8	-
4	LYS	O	601	-	-	4/9/9/9	-
3	THR	I	501	-	-	2/8/8/8	-
3	THR	C	501	-	-	0/8/8/8	-
3	THR	P	201	-	-	0/8/8/8	-
4	LYS	A	601	-	-	2/9/9/9	-
3	THR	E	501	-	-	3/8/8/8	-
3	THR	K	501	-	-	4/8/8/8	-
3	THR	L	201	-	-	0/8/8/8	-
3	THR	N	201	-	-	0/8/8/8	-
3	THR	H	201	-	-	4/8/8/8	-
3	THR	G	501	-	-	4/8/8/8	-
3	THR	B	201	-	-	4/8/8/8	-
4	LYS	G	601	-	-	1/9/9/9	-
4	LYS	K	601	-	-	3/9/9/9	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	201	THR	OXT-C	-2.46	1.22	1.30
3	J	201	THR	OXT-C	-2.41	1.22	1.30
3	P	201	THR	OXT-C	-2.40	1.22	1.30
4	M	601	LYS	OXT-C	-2.39	1.22	1.30
4	K	601	LYS	OXT-C	-2.34	1.22	1.30

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	601	LYS	OXT-C-O	-3.71	115.67	124.09
3	P	201	THR	OXT-C-O	-3.37	116.44	124.09
3	J	201	THR	OXT-C-O	-3.15	116.94	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	201	THR	OXT-C-O	-3.07	117.12	124.09
3	K	501	THR	OXT-C-O	-3.04	117.19	124.09

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	201	THR	N-CA-CB-OG1
3	B	201	THR	C-CA-CB-OG1
3	B	201	THR	C-CA-CB-CG2
3	E	501	THR	O-C-CA-CB
3	E	501	THR	OXT-C-CA-CB

There are no ring outliers.

18 monomers are involved in 76 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	201	THR	2	0
4	M	601	LYS	5	0
3	F	201	THR	6	0
4	E	601	LYS	2	0
4	C	601	LYS	5	0
3	D	201	THR	5	0
3	O	501	THR	4	0
4	O	601	LYS	2	0
3	I	501	THR	4	0
3	C	501	THR	6	0
3	P	201	THR	1	0
3	K	501	THR	6	0
3	L	201	THR	1	0
3	H	201	THR	6	0
3	G	501	THR	7	0
3	B	201	THR	6	0
4	G	601	LYS	2	0
4	K	601	LYS	6	0

5.7 Other polymers [i](#)

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 [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	370/421 (87%)	-0.07	1 (0%) 94 94	29, 45, 72, 83	0
1	C	367/421 (87%)	0.07	2 (0%) 91 91	38, 56, 69, 80	0
1	E	368/421 (87%)	-0.01	2 (0%) 91 91	35, 53, 72, 84	0
1	G	357/421 (84%)	-0.03	5 (1%) 75 77	38, 54, 74, 99	0
1	I	360/421 (85%)	0.06	3 (0%) 86 87	39, 61, 78, 101	0
1	K	373/421 (88%)	-0.04	5 (1%) 77 78	29, 50, 73, 90	0
1	M	377/421 (89%)	-0.02	5 (1%) 77 78	30, 45, 64, 74	0
1	O	364/421 (86%)	0.15	12 (3%) 46 49	37, 65, 88, 100	0
2	B	157/178 (88%)	-0.14	1 (0%) 89 90	27, 42, 66, 82	0
2	D	150/178 (84%)	0.13	5 (3%) 46 49	41, 61, 82, 92	0
2	F	148/178 (83%)	0.23	3 (2%) 65 67	46, 69, 91, 98	0
2	H	151/178 (84%)	0.03	1 (0%) 87 89	39, 65, 85, 94	0
2	J	132/178 (74%)	0.42	12 (9%) 9 8	55, 75, 91, 96	0
2	L	156/178 (87%)	-0.23	0 100 100	27, 44, 61, 69	0
2	N	155/178 (87%)	-0.10	0 100 100	31, 45, 63, 69	0
2	P	149/178 (83%)	0.38	12 (8%) 12 11	45, 71, 106, 120	0
All	All	4134/4792 (86%)	0.03	69 (1%) 70 71	27, 54, 81, 120	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	148	ALA	5.4
2	F	73	ALA	5.3
2	P	122	VAL	5.2
1	O	253	ALA	4.4
2	B	164	ALA	4.4

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, 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
4	LYS	K	601	10/10	0.87	0.17	23,31,32,33	0
3	THR	H	201	8/8	0.92	0.22	36,36,37,38	0
3	THR	P	201	8/8	0.92	0.17	29,29,29,30	0
3	THR	G	501	8/8	0.92	0.26	9,9,10,11	0
3	THR	D	201	8/8	0.93	0.18	29,30,31,32	0
3	THR	I	501	8/8	0.93	0.29	43,43,43,44	0
4	LYS	O	601	10/10	0.93	0.13	31,32,32,32	0
3	THR	F	201	8/8	0.94	0.24	2,2,2,2	0
4	LYS	A	601	10/10	0.94	0.16	21,26,27,27	0
4	LYS	E	601	10/10	0.94	0.12	25,26,27,27	0
3	THR	C	501	8/8	0.94	0.20	42,42,42,42	0
4	LYS	M	601	10/10	0.94	0.16	16,17,18,18	0
3	THR	O	501	8/8	0.94	0.32	49,49,49,49	0
4	LYS	C	601	10/10	0.95	0.14	31,32,32,33	0
3	THR	E	501	8/8	0.95	0.29	41,42,42,43	0
4	LYS	G	601	10/10	0.95	0.11	25,26,26,26	0
3	THR	J	201	8/8	0.96	0.08	37,37,37,37	0
3	THR	K	501	8/8	0.96	0.16	33,34,34,34	0
3	THR	L	201	8/8	0.96	0.13	22,24,24,24	0
3	THR	B	201	8/8	0.96	0.17	28,29,29,31	0
3	THR	N	201	8/8	0.97	0.09	23,24,24,24	0
3	THR	A	501	8/8	0.97	0.13	25,26,26,27	0
3	THR	M	501	8/8	0.98	0.14	25,25,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.