WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 16, 2023 – 03:50 PM EDT

PDB ID : 1ZS3
Title : The crystal structure of the Lactococcus lactis MG1363 DpsB protein
Authors : Stillman, T.J.; Upadhyay, M.; Norte, V.A.; Sedelnikova, S.E.; Carradus, M.; Tzokov, S.; Bullough, P.A.; Shearman, C.A.; Gasson, M.J.; Williams, C.H.; Artymiuk, P.J.; Green, J.
Deposited on : 2005-05-23
Resolution : 2.70 Å(reported)

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

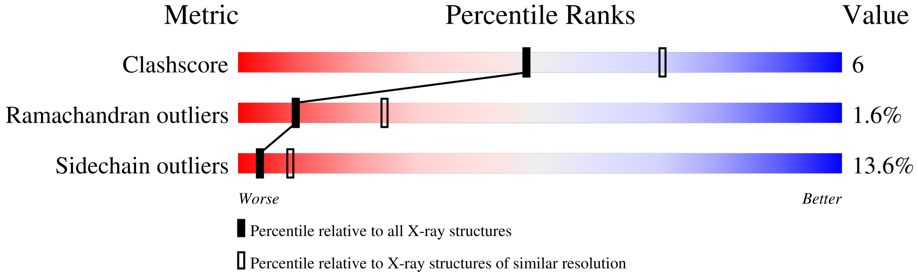
MolProbity : 4.02b-467
Xtriage (Phenix) : NOT EXECUTED
EDS : NOT EXECUTED
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

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 2.70 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	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	182	
1	B	182	
1	C	182	
1	D	182	
1	E	182	
1	F	182	
1	G	182	
1	H	182	

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Mol	Chain	Length	Quality of chain
1	I	182	
1	J	182	
1	K	182	
1	L	182	

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 16775 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 Lactococcus lactis MG1363 DpsA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	171	Total C N O S 1387 897 223 263 4	0	0	0
1	B	171	Total C N O S 1387 897 223 263 4	0	0	0
1	C	171	Total C N O S 1387 897 223 263 4	0	0	0
1	D	171	Total C N O S 1387 897 223 263 4	0	0	0
1	E	171	Total C N O S 1387 897 223 263 4	0	0	0
1	F	171	Total C N O S 1387 897 223 263 4	0	0	0
1	G	171	Total C N O S 1387 897 223 263 4	0	0	0
1	H	171	Total C N O S 1387 897 223 263 4	0	0	0
1	I	171	Total C N O S 1387 897 223 263 4	0	0	0
1	J	171	Total C N O S 1387 897 223 263 4	0	0	0
1	K	171	Total C N O S 1387 897 223 263 4	0	0	0
1	L	171	Total C N O S 1387 897 223 263 4	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	12	Total O 12 12	0	0
2	B	13	Total O 13 13	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	9	Total O 9 9	0	0
2	D	13	Total O 13 13	0	0
2	E	13	Total O 13 13	0	0
2	F	10	Total O 10 10	0	0
2	G	15	Total O 15 15	0	0
2	H	8	Total O 8 8	0	0
2	I	13	Total O 13 13	0	0
2	J	6	Total O 6 6	0	0
2	K	12	Total O 12 12	0	0
2	L	7	Total O 7 7	0	0

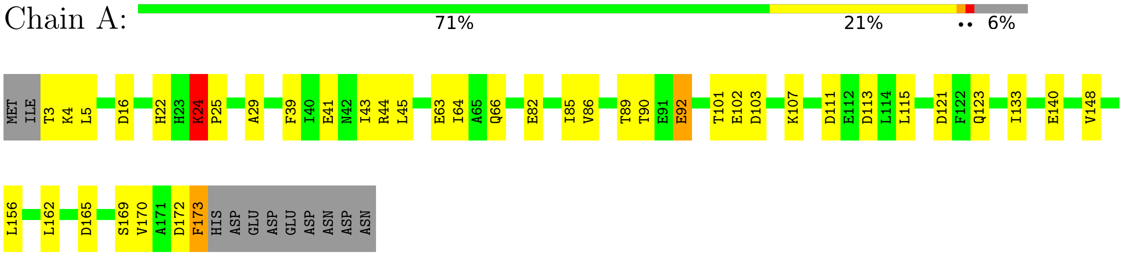
3 Residue-property plots ⓘ

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

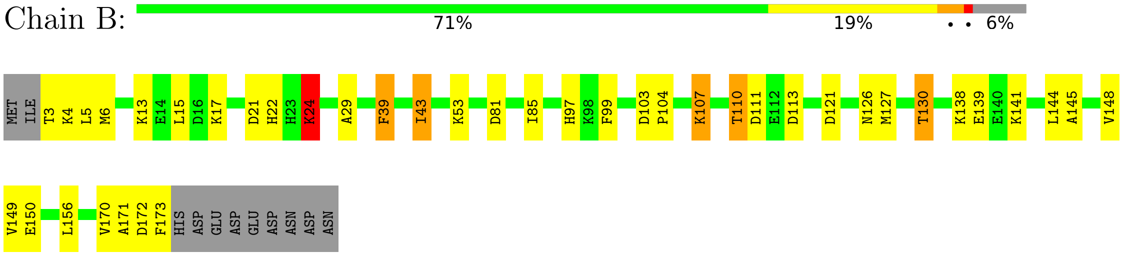
- Molecule 1: Lactococcus lactis MG1363 DpsA

Chain A:



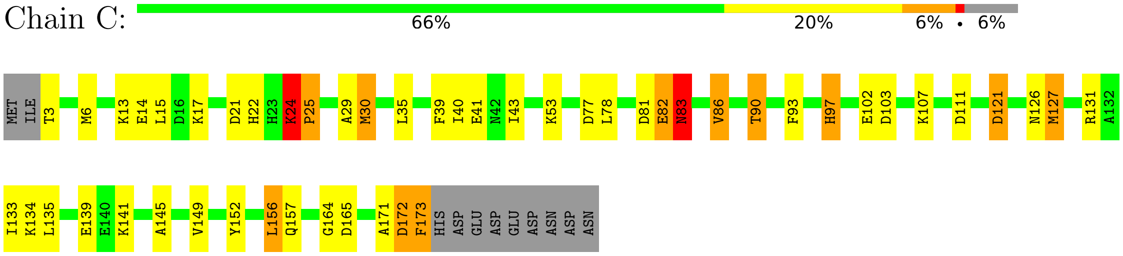
- Molecule 1: Lactococcus lactis MG1363 DpsA

Chain B:



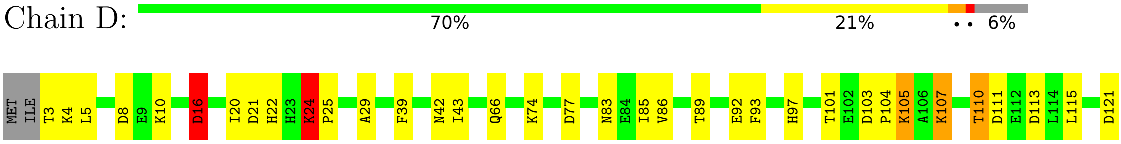
- Molecule 1: Lactococcus lactis MG1363 DpsA

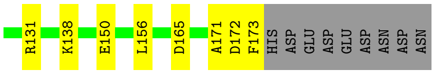
Chain C:



- Molecule 1: Lactococcus lactis MG1363 DpsA

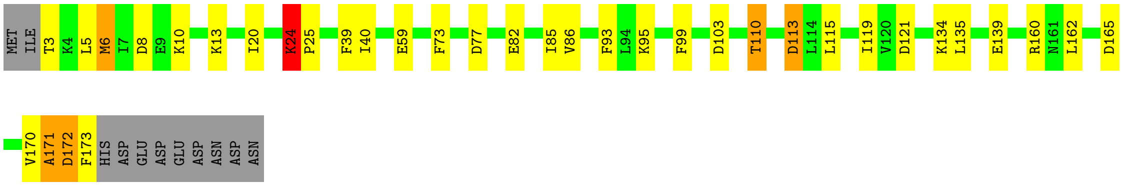
Chain D:





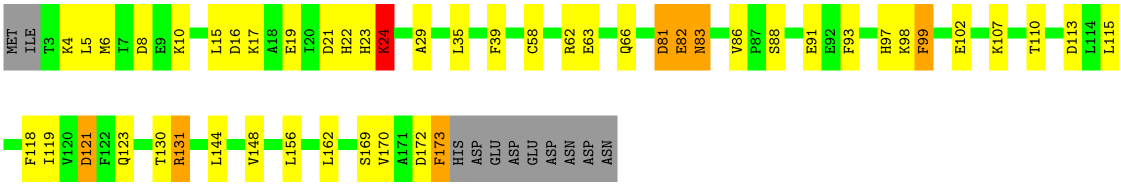
- Molecule 1: Lactococcus lactis MG1363 DpsA

Chain E:



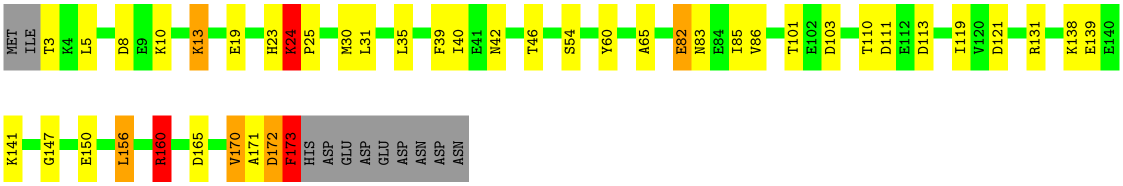
- Molecule 1: Lactococcus lactis MG1363 DpsA

Chain F:



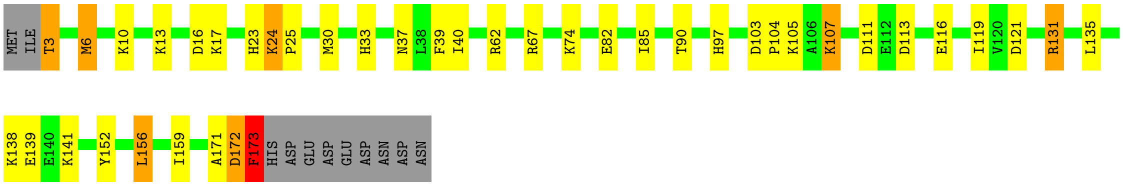
- Molecule 1: Lactococcus lactis MG1363 DpsA

Chain G:



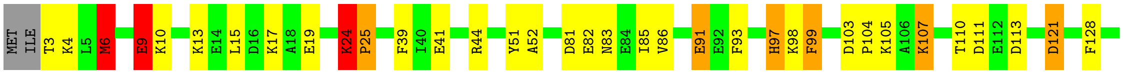
- Molecule 1: Lactococcus lactis MG1363 DpsA

Chain H:



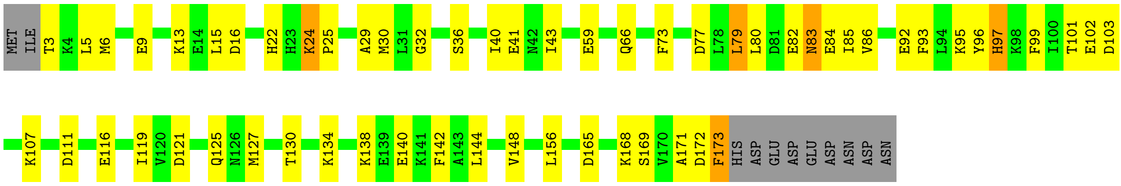
- Molecule 1: Lactococcus lactis MG1363 DpsA

Chain I:



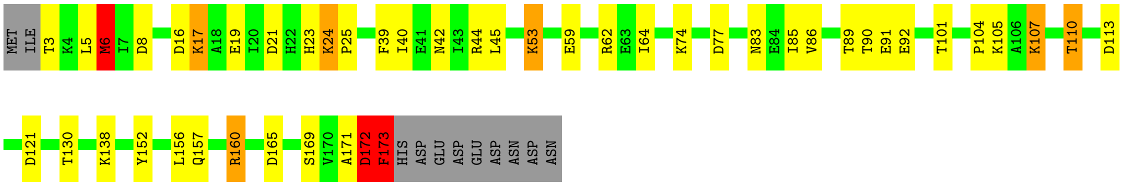
- Molecule 1: Lactococcus lactis MG1363 DpsA

Chain J:



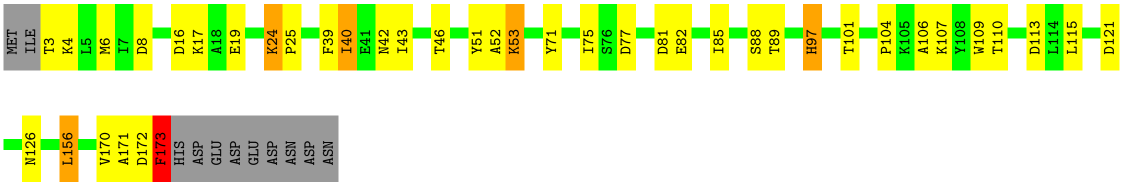
- Molecule 1: Lactococcus lactis MG1363 DpsA

Chain K:



- Molecule 1: Lactococcus lactis MG1363 DpsA

Chain L:



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	**Value**	**Source**
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	127.98Å 128.38Å 193.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70	Depositor
% Data completeness (in resolution range)	92.3 (15.00-2.70)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.207 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16775	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

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	0.86	0/1414	0.91	5/1907 (0.3%)
1	B	0.98	2/1414 (0.1%)	0.96	3/1907 (0.2%)
1	C	0.90	1/1414 (0.1%)	0.95	7/1907 (0.4%)
1	D	1.01	2/1414 (0.1%)	1.01	6/1907 (0.3%)
1	E	0.96	2/1414 (0.1%)	0.95	7/1907 (0.4%)
1	F	0.94	0/1414	1.00	6/1907 (0.3%)
1	G	1.00	4/1414 (0.3%)	1.03	7/1907 (0.4%)
1	H	0.95	2/1414 (0.1%)	0.98	7/1907 (0.4%)
1	I	1.72	6/1414 (0.4%)	1.04	9/1907 (0.5%)
1	J	0.91	1/1414 (0.1%)	0.96	6/1907 (0.3%)
1	K	1.04	5/1414 (0.4%)	1.13	13/1907 (0.7%)
1	L	0.87	0/1414	0.91	5/1907 (0.3%)
All	All	1.03	25/16968 (0.1%)	0.99	81/22884 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	2
1	L	0	1
All	All	0	13

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	9	GLU	CD-OE1	41.07	1.70	1.25
1	I	9	GLU	CD-OE2	29.05	1.57	1.25
1	K	173	PHE	N-CA	14.25	1.74	1.46
1	I	91	GLU	CD-OE2	10.75	1.37	1.25
1	I	6	MET	SD-CE	9.91	2.33	1.77

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	62	ARG	NE-CZ-NH2	16.21	128.41	120.30
1	K	172	ASP	CB-CG-OD2	11.62	128.76	118.30
1	I	9	GLU	OE1-CD-OE2	10.75	136.20	123.30
1	G	172	ASP	CB-CG-OD2	10.58	127.83	118.30
1	F	172	ASP	CB-CG-OD2	10.37	127.64	118.30

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	24	LYS	Peptide
1	B	24	LYS	Peptide
1	C	24	LYS	Peptide
1	D	24	LYS	Peptide
1	E	24	LYS	Peptide

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	1387	0	1386	14	0
1	B	1387	0	1386	19	0
1	C	1387	0	1386	22	0
1	D	1387	0	1386	13	0
1	E	1387	0	1386	18	0
1	F	1387	0	1386	24	0
1	G	1387	0	1386	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1387	0	1386	15	0
1	I	1387	0	1386	21	0
1	J	1387	0	1386	23	0
1	K	1387	0	1386	20	0
1	L	1387	0	1386	15	0
2	A	12	0	0	0	0
2	B	13	0	0	1	0
2	C	9	0	0	0	0
2	D	13	0	0	0	0
2	E	13	0	0	3	0
2	F	10	0	0	3	0
2	G	15	0	0	4	0
2	H	8	0	0	4	0
2	I	13	0	0	1	0
2	J	6	0	0	5	0
2	K	12	0	0	4	0
2	L	7	0	0	1	0
All	All	16775	0	16632	202	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 6.

The worst 5 of 202 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:G:13:LYS:CE	1:G:13:LYS:NZ	1.70	1.52
1:K:173:PHE:N	1:K:173:PHE:CA	1.74	1.47
1:E:6:MET:CE	1:E:6:MET:SD	2.03	1.46
1:B:127:MET:SD	1:B:127:MET:CE	2.05	1.44
1:K:6:MET:SD	1:K:6:MET:CE	2.05	1.43

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	169/182 (93%)	160 (95%)	5 (3%)	4 (2%)	6	15
1	B	169/182 (93%)	162 (96%)	6 (4%)	1 (1%)	25	50
1	C	169/182 (93%)	157 (93%)	9 (5%)	3 (2%)	8	21
1	D	169/182 (93%)	161 (95%)	6 (4%)	2 (1%)	13	32
1	E	169/182 (93%)	158 (94%)	7 (4%)	4 (2%)	6	15
1	F	169/182 (93%)	160 (95%)	7 (4%)	2 (1%)	13	32
1	G	169/182 (93%)	161 (95%)	6 (4%)	2 (1%)	13	32
1	H	169/182 (93%)	159 (94%)	9 (5%)	1 (1%)	25	50
1	I	169/182 (93%)	158 (94%)	7 (4%)	4 (2%)	6	15
1	J	169/182 (93%)	160 (95%)	4 (2%)	5 (3%)	4	10
1	K	169/182 (93%)	162 (96%)	5 (3%)	2 (1%)	13	32
1	L	169/182 (93%)	158 (94%)	9 (5%)	2 (1%)	13	32
All	All	2028/2184 (93%)	1916 (94%)	80 (4%)	32 (2%)	9	24

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	D	24	LYS
1	G	25	PRO
1	H	24	LYS
1	J	25	PRO

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	148/159 (93%)	131 (88%)	17 (12%)	5	13
1	B	148/159 (93%)	133 (90%)	15 (10%)	7	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	148/159 (93%)	127 (86%)	21 (14%)	3	8
1	D	148/159 (93%)	130 (88%)	18 (12%)	5	11
1	E	148/159 (93%)	133 (90%)	15 (10%)	7	17
1	F	148/159 (93%)	125 (84%)	23 (16%)	2	7
1	G	148/159 (93%)	127 (86%)	21 (14%)	3	8
1	H	148/159 (93%)	127 (86%)	21 (14%)	3	8
1	I	148/159 (93%)	127 (86%)	21 (14%)	3	8
1	J	148/159 (93%)	124 (84%)	24 (16%)	2	6
1	K	148/159 (93%)	122 (82%)	26 (18%)	2	4
1	L	148/159 (93%)	128 (86%)	20 (14%)	4	9
All	All	1776/1908 (93%)	1534 (86%)	242 (14%)	3	8

5 of 242 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	30	MET
1	K	173	PHE
1	H	97	HIS
1	K	165	ASP
1	L	97	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	83	ASN
1	H	123	GLN
1	L	161	ASN
1	H	83	ASN
1	I	42	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.