



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 13, 2017 – 08:45 AM EDT

PDB ID : 5LP3
EMDB ID: : EMD-4094
Title : Three tetrameric rings of Isoaspartyl Dipeptidase fitted in an EM volume.
Authors : Garcia-Seisdedos, H.; Empereur-Mot, C.; Elad, N.; Levy, E.D.
Deposited on : unknown
Resolution : 10.50 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

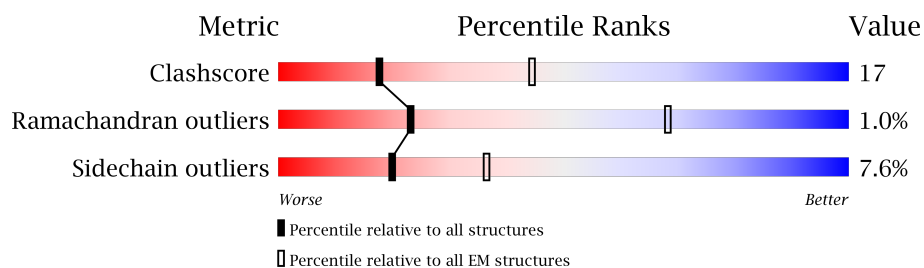
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.50 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	390	
1	B	390	
1	C	390	
1	D	390	
1	E	390	
1	F	390	
1	G	390	
1	H	390	
1	I	390	

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Mol	Chain	Length	Quality of chain
1	J	390	<div><div></div><div>61%</div><div>32%</div><div></div><div></div><div></div></div>
1	K	390	<div><div></div><div>62%</div><div>31%</div><div></div><div></div><div></div></div>
1	L	390	<div><div></div><div>62%</div><div>31%</div><div></div><div></div><div></div></div>

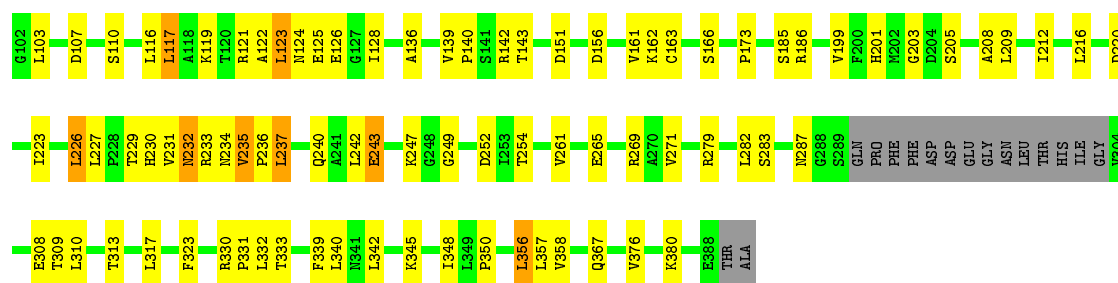
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 33200 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

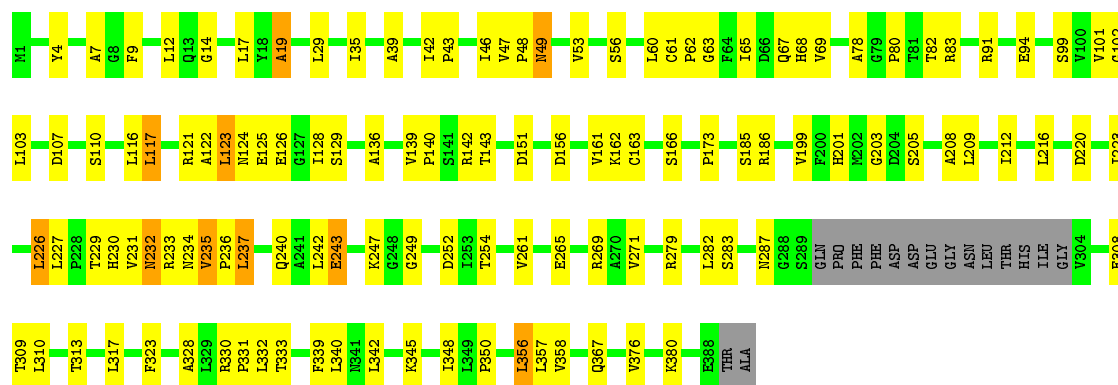
- Molecule 1 is a protein called Isoaspartyl dipeptidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	374	Total	C	N	O	S	0	0
			2756	1734	473	537	12		
1	C	374	Total	C	N	O	S	0	0
			2756	1734	473	537	12		
1	D	374	Total	C	N	O	S	0	0
			2756	1734	473	537	12		
1	E	374	Total	C	N	O	S	0	0
			2756	1734	473	537	12		
1	A	377	Total	C	N	O	S	0	0
			2778	1748	478	540	12		
1	F	377	Total	C	N	O	S	0	0
			2778	1748	478	540	12		
1	G	377	Total	C	N	O	S	0	0
			2778	1748	478	540	12		
1	H	377	Total	C	N	O	S	0	0
			2778	1748	478	540	12		
1	I	376	Total	C	N	O	S	0	0
			2766	1741	476	537	12		
1	J	376	Total	C	N	O	S	0	0
			2766	1741	476	537	12		
1	K	376	Total	C	N	O	S	0	0
			2766	1741	476	537	12		
1	L	376	Total	C	N	O	S	0	0
			2766	1741	476	537	12		



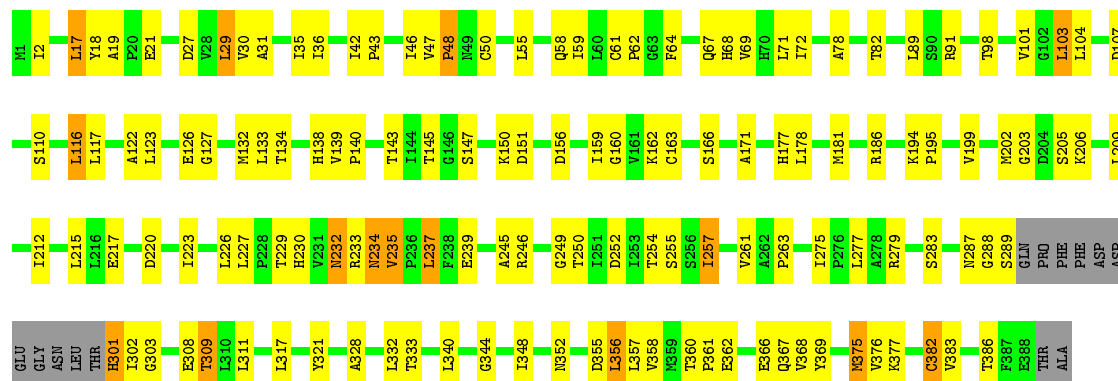
• Molecule 1: Isoaspartyl dipeptidase

Chain E: 65% 28%



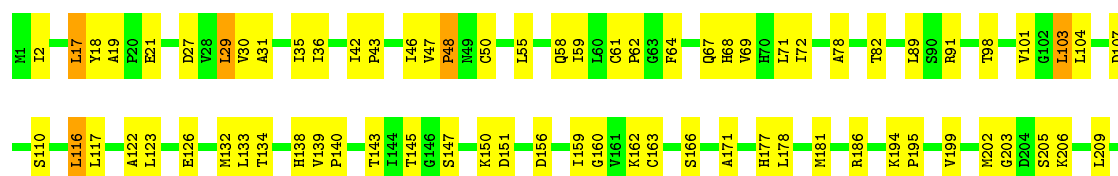
• Molecule 1: Isoaspartyl dipeptidase

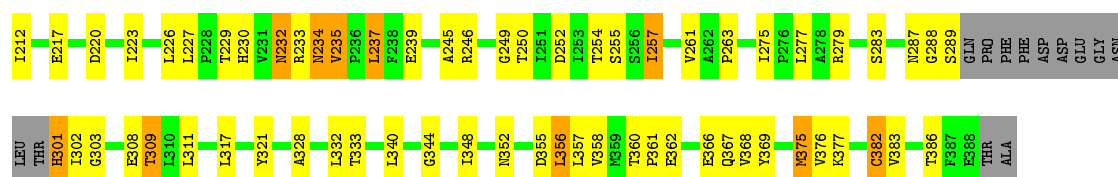
Chain A: 61% 32%



• Molecule 1: Isoaspartyl dipeptidase

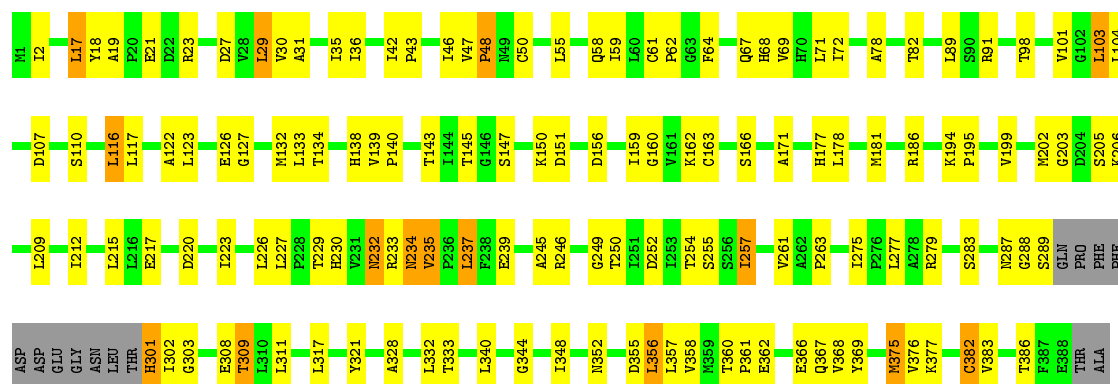
Chain F: 62% 31%





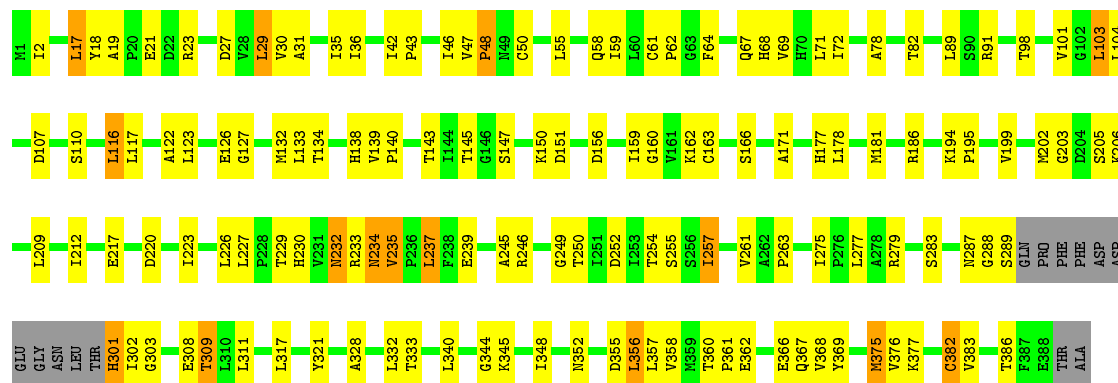
• Molecule 1: Isoaspartyl dipeptidase

Chain G: 61% 32%



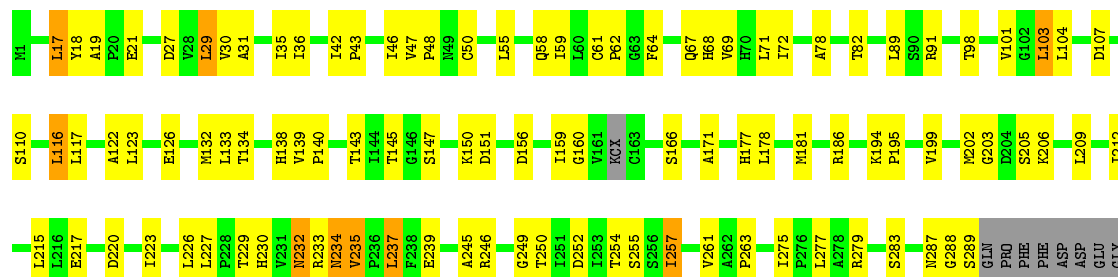
• Molecule 1: Isoaspartyl dipeptidase

Chain H: 61% 32%



• Molecule 1: Isoaspartyl dipeptidase

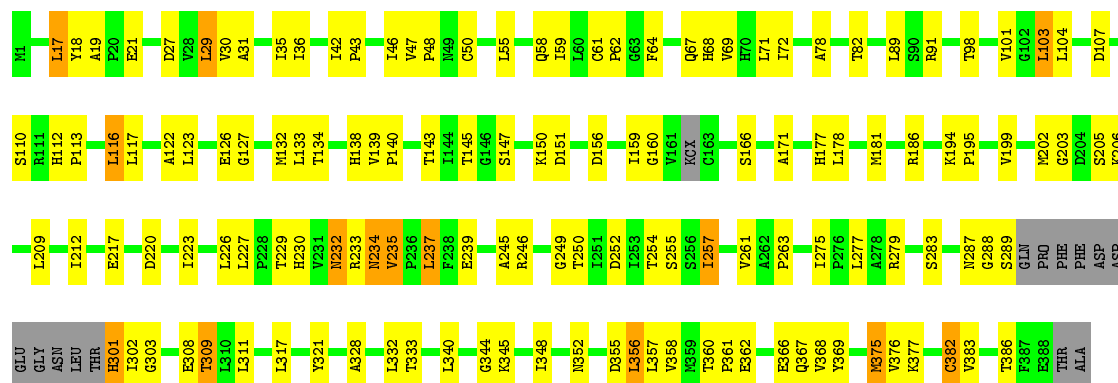
Chain I: 62% 31%





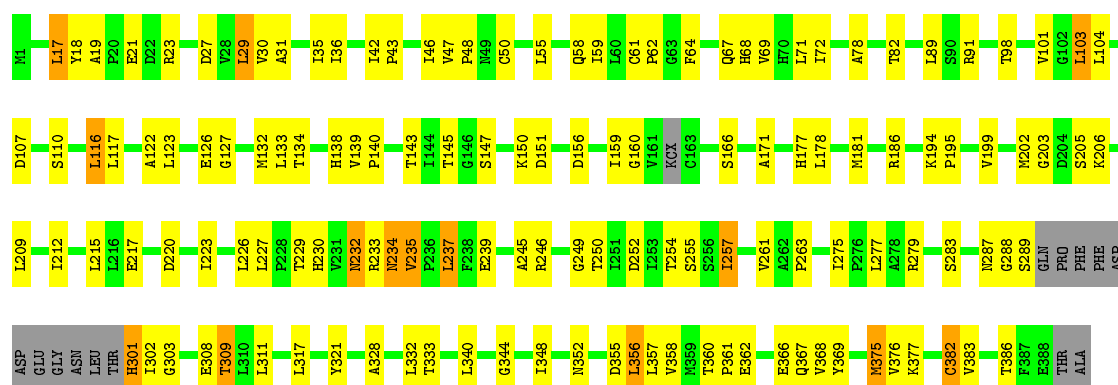
• Molecule 1: Isoaspartyl dipeptidase

Chain J: 61% 32%



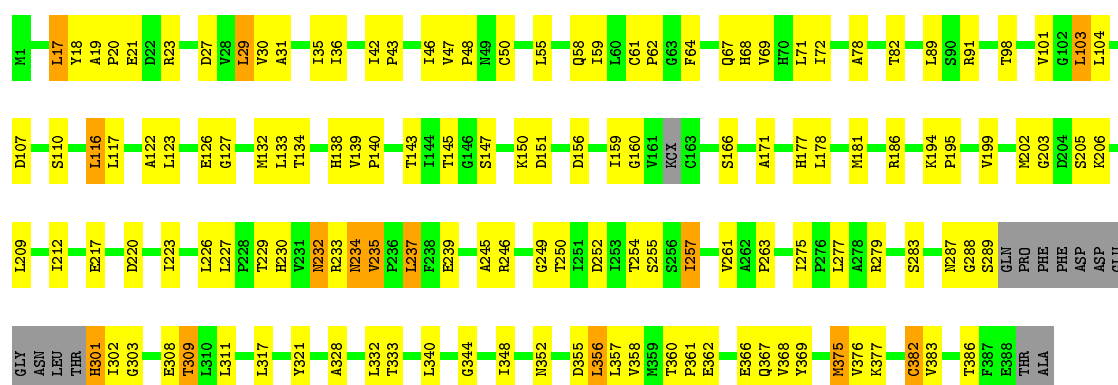
• Molecule 1: Isoaspartyl dipeptidase

Chain K: 62% 31%



• Molecule 1: Isoaspartyl dipeptidase

Chain L: 62% 31%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D4	Depositor
Number of particles used	17277	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI 20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32.0	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KCX

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.37	0/2811	0.71	1/3825 (0.0%)
1	B	0.36	0/2788	0.67	0/3794
1	C	0.36	0/2788	0.67	0/3794
1	D	0.36	0/2788	0.67	0/3794
1	E	0.36	0/2788	0.67	0/3794
1	F	0.37	0/2811	0.71	1/3825 (0.0%)
1	G	0.37	0/2811	0.71	2/3825 (0.1%)
1	H	0.37	0/2811	0.71	2/3825 (0.1%)
1	I	0.37	0/2811	0.71	1/3825 (0.0%)
1	J	0.37	0/2811	0.71	1/3825 (0.0%)
1	K	0.37	0/2811	0.71	2/3825 (0.1%)
1	L	0.37	0/2811	0.71	2/3825 (0.1%)
All	All	0.37	0/33640	0.70	12/45776 (0.0%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	321	TYR	N-CA-C	-5.76	95.44	111.00
1	F	321	TYR	N-CA-C	-5.75	95.47	111.00
1	G	321	TYR	N-CA-C	-5.75	95.48	111.00
1	L	321	TYR	N-CA-C	-5.73	95.52	111.00
1	A	321	TYR	N-CA-C	-5.73	95.53	111.00

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	2778	0	2800	104	0
1	B	2756	0	2779	93	0
1	C	2756	0	2779	87	0
1	D	2756	0	2779	91	0
1	E	2756	0	2779	95	0
1	F	2778	0	2800	101	0
1	G	2778	0	2800	99	0
1	H	2778	0	2800	101	0
1	I	2766	0	2789	97	0
1	J	2766	0	2789	101	0
1	K	2766	0	2789	98	0
1	L	2766	0	2789	97	0
All	All	33200	0	33472	1124	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 17.

The worst 5 of 1124 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:D:234:ASN:HD22	1:D:236:PRO:HD2	1.35	0.91
1:E:234:ASN:HD22	1:E:236:PRO:HD2	1.35	0.91
1:C:234:ASN:HD22	1:C:236:PRO:HD2	1.35	0.90
1:C:235:VAL:HG13	1:C:236:PRO:HD3	1.53	0.90
1:B:235:VAL:HG13	1:B:236:PRO:HD3	1.52	0.90

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 PDB entries followed by that with respect to all EM entries.

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	372/390 (95%)	342 (92%)	26 (7%)	4 (1%)	17	60
1	B	369/390 (95%)	337 (91%)	29 (8%)	3 (1%)	22	67
1	C	369/390 (95%)	337 (91%)	29 (8%)	3 (1%)	22	67
1	D	369/390 (95%)	337 (91%)	29 (8%)	3 (1%)	22	67
1	E	369/390 (95%)	337 (91%)	29 (8%)	3 (1%)	22	67
1	F	372/390 (95%)	342 (92%)	26 (7%)	4 (1%)	17	60
1	G	372/390 (95%)	342 (92%)	26 (7%)	4 (1%)	17	60
1	H	372/390 (95%)	342 (92%)	26 (7%)	4 (1%)	17	60
1	I	370/390 (95%)	340 (92%)	26 (7%)	4 (1%)	17	60
1	J	370/390 (95%)	340 (92%)	26 (7%)	4 (1%)	17	60
1	K	370/390 (95%)	340 (92%)	26 (7%)	4 (1%)	17	60
1	L	370/390 (95%)	340 (92%)	26 (7%)	4 (1%)	17	60
All	All	4444/4680 (95%)	4076 (92%)	324 (7%)	44 (1%)	23	61

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	48	PRO
1	C	48	PRO
1	D	48	PRO
1	E	48	PRO
1	A	48	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 PDB entries followed by that with respect to all EM entries.

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	299/312 (96%)	273 (91%)	26 (9%)	12	40
1	B	297/312 (95%)	281 (95%)	16 (5%)	26	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	297/312 (95%)	282 (95%)	15 (5%)	28	60
1	D	297/312 (95%)	281 (95%)	16 (5%)	26	58
1	E	297/312 (95%)	281 (95%)	16 (5%)	26	58
1	F	299/312 (96%)	273 (91%)	26 (9%)	12	40
1	G	299/312 (96%)	273 (91%)	26 (9%)	12	40
1	H	299/312 (96%)	273 (91%)	26 (9%)	12	40
1	I	299/312 (96%)	273 (91%)	26 (9%)	12	40
1	J	299/312 (96%)	273 (91%)	26 (9%)	12	40
1	K	299/312 (96%)	273 (91%)	26 (9%)	12	40
1	L	299/312 (96%)	273 (91%)	26 (9%)	12	40
All	All	3580/3744 (96%)	3309 (92%)	271 (8%)	20	47

5 of 271 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	116	LEU
1	H	186	ARG
1	L	98	THR
1	G	217	GLU
1	G	362	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	234	ASN
1	G	315	GLN
1	L	49	ASN
1	F	315	GLN
1	G	68	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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
1	KCX	A	162	1	8,11,12	0.78	0	6,12,14	1.06	0
1	KCX	B	162	1	8,11,12	0.87	1 (12%)	6,12,14	1.00	0
1	KCX	C	162	1	8,11,12	0.87	1 (12%)	6,12,14	1.00	0
1	KCX	D	162	1	8,11,12	0.86	1 (12%)	6,12,14	1.00	0
1	KCX	E	162	1	8,11,12	0.90	1 (12%)	6,12,14	1.01	0
1	KCX	F	162	1	8,11,12	0.76	0	6,12,14	1.03	0
1	KCX	G	162	1	8,11,12	0.77	0	6,12,14	1.04	0
1	KCX	H	162	1	8,11,12	0.77	0	6,12,14	1.04	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
1	KCX	A	162	1	-	0/6/10/12	0/0/0/0
1	KCX	B	162	1	-	0/6/10/12	0/0/0/0
1	KCX	C	162	1	-	0/6/10/12	0/0/0/0
1	KCX	D	162	1	-	0/6/10/12	0/0/0/0
1	KCX	E	162	1	-	0/6/10/12	0/0/0/0
1	KCX	F	162	1	-	0/6/10/12	0/0/0/0
1	KCX	G	162	1	-	0/6/10/12	0/0/0/0
1	KCX	H	162	1	-	0/6/10/12	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	162	KCX	CA-C	2.11	1.53	1.50
1	B	162	KCX	CA-C	2.13	1.53	1.50
1	C	162	KCX	CA-C	2.13	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	162	KCX	CA-C	2.23	1.53	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	162	KCX	2	0
1	B	162	KCX	2	0
1	C	162	KCX	2	0
1	D	162	KCX	2	0
1	E	162	KCX	2	0
1	F	162	KCX	2	0
1	G	162	KCX	2	0
1	H	162	KCX	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.